UNIVERSITEIT GENT

DIRECTIE **ONDERZOEKSAANGELEGENHEDEN**

Afdeling **Onderzoekscoördinatie**

Aan Prof. F. Du Prez
Vakgroep Organische Chemie
Krijgslaan 281 S4
9000-Gent

05/157481
07831
2

Prjdef: B/07831 Doctyp: Contract

uw kenmerk	**ons kenmerk**	**Datum : 18/12/2006**
	DOZA/IL/DDC/PB/06-120C51C7	
		tel. en fax
contactpersoon	**e-mail**	T +32 9 264 30 39
Pascale Blancquaert	Pascale.Blancquaert@UGent.be	F +32 9 264 35 83

Betreft: **Vervroegde openstelling van een kredietlijn voor een onderzoeksproject**

Waarde collega

Gebruikmakend van de bevoegdheidsdelegatie voor het vervroegd openstellen van kredietlijnen noodzakelijk voor dringende aanwervingen en het ter beschikking stellen van werkingsmiddelen mij *verleend door het bestuurscollege van 8 januari 2004, ga ik akkoord met een vervroegde openstelling* van een bijkomende kredietlijn ten bedrage van **€ 770** om het opstarten van het onderzoeksproject *"IUAP VI – KUL/51"* mogelijk te maken.

Ik heb acte genomen van de garantstelling via de financier.

Het bedrag zal ter beschikking worden gesteld via projectcode **120C51C7** (budgetplaats:– **B/07831/02-IV2**) en kan enkel als personeelsmiddelen worden besteed.

Ik geef hierbij opdracht aan de bevoegde directie om het nodige te doen.

Met collegiale groet

Prof. P. Van Cauwenberge
Rector

DIRECTIE ONDERZOEKSAANGELEGENHEDEN

UNIVERSITEIT GENT

Afdeling Onderzoekscoördinatie

Aan Prof. F. Du Prez
Vakgroep Organische Chemie
Krijgslaan 281 S4
9000-Gent

1 bP2
1078311o2
051155013.

01000108260001
Prjdef: B/07831 Doctyp: Contract

uw kenmerk	ons kenmerk	Datum : 01/12/2006
	DOZA/IL/DDC/PB/06-120C51C7	tel. en fax
contactpersoon	e-mail	T +32 9 264 30 39
Pascale Blancquaert	Pascale.Blancquaert@UGent.be	F +32 9 264 35 83

Betreft: **Vervroegde openstelling van een kredietlijn voor een onderzoeksproject**

Waarde collega

Gebruikmakend van de bevoegdheidsdelegatie voor het vervroegd openstellen van kredietlijnen noodzakelijk voor dringende aanwervingen en het ter beschikking stellen van werkingsmiddelen mij verleend door het bestuurscollege van 8 januari 2004, ga ik akkoord met een vervroegde openstelling van een kredietlijn ten bedrage van **€ 57.500** om het opstarten van het onderzoeksproject *"IUAP VI – KUL/51"* mogelijk te maken.

Ik heb acte genomen van de garantstelling via de financier.

Het bedrag zal ter beschikking worden gesteld via projectcode **120C51C7** (budgetplaats:– **B/07831/02-IV2**) en kan enkel als personeelsmiddelen worden besteed.

Ik geef hierbij opdracht aan de bevoegde directie om het nodige te doen.

Met collegiale groet

Prof. P. Van Cauwenberge
Rector

UNIVERSITEIT GENT

DIRECTIE **ONDERZOEKSAANGELEGENHEDEN**

Afdeling **Onderzoekscoördinatie**

Aan Prof. F. Du Prez
Vakgroep Organische Chemie
Krijgslaan 281 S4
9000-Gent

2pm.
B/07831/02
ES/176917

uw kenmerk	**ons kenmerk**	**Datum : 26/3/2007**
	DOZA/IL/DDC/PB/07-120C51C7	
		tel. en fax
contactpersoon	**e-mail**	T +32 9 264 30 39
Pascale Blancquaert	Pascale.Blancquaert@UGent.be	F +32 9 264 35 83

Betreft: **Vervroegde openstelling van een kredietlijn voor een onderzoeksproject**

Waarde collega

Gebruikmakend van de bevoegdheidsdelegatie voor het vervroegd openstellen van kredietlijnen noodzakelijk voor dringende aanwervingen en het ter beschikking stellen van werkingsmiddelen mij verleend door het bestuurscollege van 8 januari 2004, ga ik akkoord met een vervroegde openstelling van een bijkomende kredietlijn ten bedrage van **€ 15000** om het opstarten van het onderzoeksproject *"IUAP VI – KUL/51"* mogelijk te maken.

Ik heb acte genomen van de garantstelling via de financier.

Het bedrag zal ter beschikking worden gesteld via projectcode **120C51C7** (budgetplaats:– **B/07831/02-IV2**) en kan enkel als personeelsmiddelen worden besteed.

Ik geef hierbij opdracht aan de bevoegde directie om het nodige te doen.

Met collegiale groet

Prof. P. Van Cauwenberge
Rector

WO-Fiche

Pieter Van Mulders (09)264 95 06

Ingevoerd

WBS-Element:	B/07831/02	Fonds:	IV2	Gecreëerd/gewijzigd door:	Pascale BLANCQUAERT	09 264 30 39	
Kredietcode:	120C51C7	Begindatum:	01/01/2007		Datum:	27/03/2007	Vak Administratie
Kredietnaam:	IUAP VI - Du Prez	Einddatum:	31/12/2011		Financieringsbron:	4106	
Kredietgever:	POD-Wetenschapsbeleid				Vakgroepnummer:	WE07	
Contractnummer:	P6/KUL/51	Titel:					
Promotor:	Prof F Du Prez						
Copromotor 1:					Gekoppelde	Kredietcodes:	
Copromotor 2:		WO-Fiche:	bijkomend	bijk prefina	Gekoppelde	WBS-elementen:	
Copromotor 3:		Versie:	3		Promotor.		
Contractueel Overhead-regime:		procentueel	CTRL+N = nieuwe versie WO-fiche		CTRL+S = kopie extern budget naar SAP		

Budgetdrager	EXTERN			INTERN			Toe te kennen budget	SAP	
	Netto-Budget (Excl. Overhead)	OH (contract)	Bedrag OH	Netto-Budget (Excl. Overhead)	OH (intern)	Bedrag OH	Budget	Budget	WBS-element
Werking	0,00	0,00%	0,00	0,00	0.00%	0.00	0.00		
Recuperatie OH				0,00	0.00%	0.00			
2007	0,00			0,00				0,00	B/07831/02
2008	0,00			0,00				0,00	B/07831/02
2009	0,00			0,00				0,00	B/07831/02
2010	0,00			0,00				0,00	B/07831/02
2011	0,00			0,00				0,00	B/07831/02
	0,00			0,00				0,00	B/07831/02
Person	15.000,00	0,00%	0,00	15 000,00	0,00%	0,00	15.000,00		
2007	0,00			0,00				0,00	B/07831/02
2008	15.000,00		0,00	15 000,00		0,00	15.000,00	15.000,00	B/07831/02
2009	0,00			0,00				0.00	B/07831/02
2010	0,00			0,00				0,00	B/07831/02
2011	0,00			0,00				0,00	B/07831/02
0	0,00			0,00				0,00	B/07831/02
	0,00	0,00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0,00	B/07831/02
2008	0,00			0,00				0,00	B/07831/02
2009	0,00			0,00				0,00	B/07831/02
2010	0,00			0,00				0,00	B/07831/02
2011	0,00			0,00				0,00	B/07831/02
0	0,00			0,00				0,00	B/07831/02
	0,00	0,00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0,00	B/07831/02
2008	0,00			0,00				0,00	B/07831/02
2009	0,00			0,00				0,00	B/07831/02
2010	0,00			0,00				0,00	B/07831/02
2011	0,00			0,00				0,00	B/07831/02
0	0,00			0,00				0,00	B/07831/02
	0,00	0,00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0.00	B/07831/02
2008	0,00			0,00				0,00	B/07831/02
2009	0,00			0,00				0,00	B/07831/02
2010	0,00			0,00				0,00	B/07831/02
2011	0,00			0,00				0,00	B/07831/02
0	0,00			0,00				0,00	B/07831/02
Netto-inkomsten	15.000,00	0,000000%	0,00	15 000,00	0,000000%	0,00	15.000,00	Netto-inkomsten	Moeten de inkomsten ingegeven worden in SAP? NEE
Overhead financier	0,00			0.00			0,00	OH in SAP	
Bruto-inkomsten	15 000,00			15 000,00			15.000,00	Bruto-inkomsten	

05/176917

Gem. OH-% op te nemen in SAP	Omzetting vreemde munt	Brutobedrag	OH-Percentage	Nettobedrag	OH
0,00%		0,00	0.00%	0,0000	0,0000
	=	0,00	0,00%	0,0000	0,0000
		OH (vast bedrag)	Brutobedrag	Nettobedrag	OH-Percentage
	www tijd be/koersen/index.asp?page=wisselkoersen&view=	0,00	0.00	0,0000	
	Datum:	0.00	0.00	0,0000	0,0000%

Totaalbudget=400 000 EUR

UNIVERSITEIT GENT

DIRECTIE **ONDERZOEKSAANGELEGENHEDEN**

Afdeling **Onderzoekscoördinatie**

2P.
B/07831/02
05/13T946

Aan Prof. F. Du Prez
Vakgroep Organische Chemie
Krijgslaan 281 S4
9000-Gent

Prjdef: B/07831 Doctyp: Contract

uw kenmerk	**ons kenmerk**	**Datum : 24/05/2007**
	DOZA/IL/DDC/PB/07-120C51C7	
		tel. en fax
contactpersoon	**e-mail**	T +32 9 264 30 39
Pascale Blancquaert	Pascale.Blancquaert@UGent.be	F +32 9 264 35 83

Betreft: **Vervroegde openstelling van een kredietlijn voor een onderzoeksproject**

Waarde collega

Gebruikmakend van de bevoegdheidsdelegatie voor het vervroegd openstellen van kredietlijnen noodzakelijk voor dringende aanwervingen en het ter beschikking stellen van werkingsmiddelen mij verleend door het bestuurscollege van 8 januari 2004, ga ik akkoord met een vervroegde openstelling van een bijkomende kredietlijn ten bedrage van **€ 14.152** om het opstarten van het onderzoeksproject *"IUAP VI – KUL/51"* mogelijk te maken.

Ik heb acte genomen van de garantstelling via de financier.

Het bedrag zal ter beschikking worden gesteld via projectcode **120C51C7** (budgetplaats:– **B/07831/02-IV2**) en kan enkel als werkingsmiddelen worden besteed.

Ik geef hierbij opdracht aan de bevoegde directie om het nodige te doen.

Met collegiale groet
Voor de Rector afwezig,
Prof. Dr. L. MOENS
Vice-rector

Prof. P. Van Cauwenberge
Rector

29 MEI 2007

WO-Fiche

Pieter Van Mulders (09)264 95 06

WBS-Element:	B/07831/02	Fonds:	IV2	Gecreëerd/gewijzigd door.	Pascale BLANCQUAERT	09 264 30 39	
Kredietcode:	120C51C7	Begindatum.	01/01/2007		Datum.	29/05/2007	Vak Administratie
Kredietnaam:	IUAP VI - Du Prez	Einddatum:	31/12/2011		Financieringsbron.	4106	
Kredietgever:	POD-Wetenschapsbeleid				Vakgroepnummer:	WE07	
Contractnummer:	P6/KUL/51	Titel:					
Promotor:	Prof. F. Du Prez						
Copromotor 1:					Gekoppelde	Kredietcodes:	
Copromotor 2:		WO-Fiche:	bijkomend	bijk prefinancierng	Gekoppelde	WBS-elementen:	
Copromotor 3:		Versie:	4		Promotor:		

Contractueel Overhead-regime: procentueel

CTRL+N = nieuwe versie WO-fiche

CTRL+S = kopie extern budget naar SAP

Budgetdrager	EXTERN			INTERN			Toe te kennen budget	SAP	
	Netto-Budget (Excl. Overhead)	OH (contract)	Bedrag OH	Netto-Budget (Excl. Overhead)	OH (intern)	Bedrag OH	Budget	Budget	WBS-element
Werking	14.152,00	0,00%	0,00	14.152,00	0,00%	0,00	14.152,00		
Recuperatie OH				0,00	0,00%	0,00			
2007	14 152,00		0,00	14.152,00		0,00	14.152,00	14.152,00	B/07831/02
2008	0,00			0,00				0,00	B/07831/02
2009	0,00			0,00				0,00	B/07831/02
2010	0,00			0,00				0,00	B/07831/02
2011	0,00			0,00				0,00	B/07831/02
	0,00			0,00				0,00	B/07831/02
Person	0,00	0.00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0,00	B/07831/02
2008	0,00			0,00				0,00	B/07831/02
2009	0,00			0,00				0,00	B/07831/02
2010	0,00			0,00				0,00	B/07831/02
2011	0,00			0,00				0,00	B/07831/02
0	0,00			0,00				0,00	B/07831/02
	0,00	0,00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0,00	B/07831/02
2008	0,00			0,00				0,00	B/07831/02
2009	0,00			0,00				0,00	B/07831/02
2010	0,00			0,00				0,00	B/07831/02
2011	0,00			0,00				0,00	B/07831/02
0	0,00			0,00				0,00	B/07831/02
	0,00	0.00%	0,00	0,00	0,00%	0.00	0,00		
2007	0,00			0,00				0,00	B/07831/02
2008	0,00			0,00				0,00	B/07831/02
2009	0,00			0,00				0,00	B/07831/02
2010	0,00			0,00				0,00	B/07831/02
2011	0,00			0,00				0,00	B/07831/02
0	0,00			0,00				0,00	B/07831/02
	0,00	0.00%	0,00	0,00	0.00%	0,00	0,00		
2007	0,00			0,00				0,00	B/07831/02
2008	0,00			0,00				0,00	B/07831/02
2009	0,00			0,00				0,00	B/07831/02
2010	0,00			0,00				0,00	B/07831/02
2011	0,00			0,00				0,00	B/07831/02
0	0,00			0,00				0,00	B/07831/02
Netto-inkomsten	14.152,00	0,000000%	0,00	14.152,00	0,000000%	0,00	14.152,00	Netto-inkomsten	Moeten de inkomsten ingegeven worden in SAP?
Overhead financier	0,00			0,00			0,00	OH in SAP	NEE
Bruto-inkomsten	14.152,00			14.152,00			14.152,00	Bruto-inkomsten	

Gem. OH-% op te nemen in SAP

0,00%

Omzetting vreemde munt

=

www tijd.be/koersen/index.asp?page=wisselkoersen&view=

Datum.

Brutobedrag	OH-Percentage
0,00	0,00%
0,00	0,00%

Nettobedrag	OH
0,0000	0,0000
0,0000	0,0000

OH (vast bedrag)	Brutobedrag
0,00	0,00
0,00	0,00

Nettobedrag	OH-Percentage
0,0000	
0,0000	0,0000%

Totaalbudget=400.000 EUR

UNIVERSITEIT GENT

DIRECTIE **ONDERZOEKSAANGELEGENHEDEN**

Afdeling **Onderzoekscoördinatie**

29.
B/07831/03
05/185172

Aan Prof. M. Waroquier
Vakgroep Subatomaire en stralingsfysica
Proeftuinstraat 86
9000-Gent

uw kenmerk	**ons kenmerk**	**Datum : 16/05/2007**
	DOZA/IL/DDC/PB/07-120C51B7	
		tel. en fax
contactpersoon	**e-mail**	T +32 9 264 30 39
Pascale Blancquaert	Pascale.Blancquaert@UGent.be	F +32 9 264 35 83

Betreft: **Vervroegde openstelling van een kredietlijn voor een onderzoeksproject**

Waarde collega

Gebruikmakend van de bevoegdheidsdelegatie voor het vervroegd openstellen van kredietlijnen noodzakelijk voor dringende aanwervingen en het ter beschikking stellen van werkingsmiddelen mij verleend door het bestuurscollege van 8 januari 2004, ga ik akkoord met een vervroegde openstelling van een kredietlijn ten bedrage van **€ 6000** om het opstarten van het onderzoeksproject *"IUAP VI – KUL/51"* mogelijk te maken.

Ik heb acte genomen van de garantstelling via de financier.

Het bedrag zal ter beschikking worden gesteld via projectcode **120C51B7** (budgetplaats:– **B/07831/03-IV2**) en kan enkel als werkingsmiddelen worden besteed.

Ik geef hierbij opdracht aan de bevoegde directie om het nodige te doen.

Met collegiale groet

Prof. P. Van Cauwenberge
Rector

WO-Fiche

WBS-Element	B/07831/03	Fonds:	IV2	Gecreeerd/gewijzigd door:	Pascale BLANCQUAERT	09 264 30 39	
Kredietcode:	120C51B7	Begindatum:	01/01/2007		Datum:	16/05/2007	Vak Administratie
Kredietnaam:	IUAP VI - Waroquier	Einddatum	31/12/2011		Financieringsbron:	4106	
Kredietgever	POD-Wetenschapsbeleid				Vakgroepnummer:	WE05	
Contractnummer.	P6/KUL/51	Titel:					
Promotor:	Prof. M Waroquier						
Copromotor 1:					Gekoppelde	Kredietcodes:	120C51C7
Copromotor 2.		WO-Fiche:	origineel	prefinanciering	Gekoppelde	WBS-elementen:	B/07831/02
Copromotor 3:		Versie:	1		Promotor:		Prof. F. Du Prez

Contractueel Overhead-regime: procentueel

CTRL+N = nieuwe versie WO-fiche

CTRL+S = kopie extern budget naar SAP

Budgetdrager	EXTERN			INTERN			Toe te kennen budget	SAP	
	Netto-Budget (Excl. Overhead)	OH (contract)	Bedrag OH	Netto-Budget (Excl. Overhead)	OH (intern)	Bedrag OH	Budget	Budget	WBS-element
Werking	6.000,00	0,00%	0,00	6.000,00	0,00%	0,00	6.000,00		
Recuperatie OH				0,00	0,00%	0,00			
2007	6.000,00		0,00	6 000,00		0,00	6 000,00	6.000,00	B/07831/03
2008	0,00			0,00				0,00	
2009	0,00			0,00				0,00	
2010	0,00			0,00				0,00	
2011	0,00			0,00				0,00	
	0,00			0,00				0,00	
Person	0,00	0,00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0,00	B/07831/03
2008	0,00			0,00				0,00	0
2009	0,00			0,00				0,00	0
2010	0,00			0,00				0,00	0
2011	0,00			0,00				0,00	0
0	0,00			0,00				0,00	0
Investering	0,00	0,00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0,00	B/07831/04
2008	0,00			0,00				0,00	
2009	0,00			0,00				0,00	0
2010	0,00			0,00				0,00	0
2011	0,00			0,00				0,00	0
0	0,00			0,00				0,00	0
	0,00	0,00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0,00	
2008	0,00			0,00				0,00	0
2009	0,00			0,00				0,00	0
2010	0,00			0,00				0,00	0
2011	0,00			0,00				0,00	0
0	0,00			0,00				0,00	0
	0,00	0,00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0,00	0
2008	0,00			0,00				0,00	0
2009	0,00			0,00				0,00	0
2010	0,00			0,00				0,00	0
2011	0,00			0,00				0,00	0
0	0,00			0,00				0,00	0
Netto-inkomsten	6.000,00	0,000000%	0,00	6.000,00	0,000000%	0,00	6.000,00	Netto-inkomsten	Moeten de inkomsten ingegeven worden in SAP?
Overhead financier	0,00			0,00			0,00	OH in SAP	NEE
Bruto-inkomsten	6.000,00			6.000,00			6.000,00	Bruto-inkomsten	

Gem. OH-% op te nemen in SAP

0,00%

Omzetting vreemde munt

=

www.tijd.be/koersen/index.asp?page=wisselkoersen&view=

Datum:

Brutobedrag	OH-Percentage	Nettobedrag	OH
0,00	0,00%	0,0000	0,0000
0,00	0,00%	0,0000	0,0000
OH (vast bedrag)	**Brutobedrag**	**Nettobedrag**	**OH-Percentage**
0,00	0,00	0,0000	
0 00	0.00	0,0000	0,0000%

Totaalbudget=450.000 EUR

Els Vanhee

Van: Lieven De Vriendt [L.DeVriendt@UGent.be]
Verzonden: vrijdag 13 juli 2007 10:29
Aan: Els Vanhee
Onderwerp: Investerin op B/07841/05

Els,

Er moet op de B/07841/05 investerin, volgens contract 7000 euro staan.
Door de boekingen van gisteren staat er nu 4000 euro op.
Ik heb er dus nog 3000 euro bijgeboekt.

B/ 07841/05

Boekingsnummer:

05/193820

Mvg. 05/ 193 820 teruggeboekt

Lieven

Lieven De Vriendt
Afdeling Onderzoekscoördinatie
Directie Onderzoeksaangelegenheden
St. Pietersnieuwstraat 25
9000 Gent
Tel. (09)264 95 06
Fax:(09)264 35 83
L.Devriendt@UGent.be

or/194406
or/194407
or/194408
or/194409
or/194410.

or/194411
or/194412
or/194413
or/194414
or/194415

13/07831/01.

250 fr.

Service public fédéral de programmation
Politique scientifique

Programmatorische federale overheidsdienst
Wetenschapsbeleid

Pôles d'attraction interuniversitaires
Phase VI

Interuniversitaire attractiepolen
Fase VI

Contrat PAI n° P6/27

Contract IUAP nr. P6/27

Conformément à la décision du Conseil des Ministres du 3 février 2006 relative aux Pôles d'attraction interuniversitaires, il est convenu ce qui suit :

Overeenkomstig de beslissing van de Ministerraad van 3 februari 2006 betreffende de Interuniversitaire attractiepolen, is overeengekomen als volgt :

ENTRE

l'Etat belge,
représenté par le Ministre de la Politique scientifique,
ci-après dénommé "l'Etat",

d'une part,

TUSSEN

de Belgische Staat,
vertegenwoordigd door de Minister van Wetenschapsbeleid,
hierna te noemen "de Staat",

enerzijds,

ET

EN

- de Katholieke Universiteit Leuven vertegenwoordigd door haar rector de heer M. VERVENNE ;
- l'Université de Liège représentée par son recteur Monsieur B. RENTIER ;
- l'Université de Mons-Hainaut représentée par son recteur Monsieur B. LUX;
- de Universiteit Gent vertegenwoordigd door haar rector de heer P. VAN CAUWENBERGE ;
- l'Université Catholique de Louvain représentée par son recteur Monsieur B. COULIE;
- de Vrije Universiteit Brussel vertegenwoordigd door haar rector de heer B. VAN CAMP;
- l'Université Libre de Bruxelles représentée par son recteur Monsieur Ph. VINCKE;
- les Facultés Universitaires Notre-Dame de la Paix à Namur représentées par son recteur le Révérend-Père M. SCHEUER;
- de Universiteit Hasselt vertegenwoordigd door haar rector de heer I. DE SCHEPPER ;

ci-après dénommées "les Institutions",

hierna te noemen "de Instellingen",

d'autre part,

anderzijds,

Article 1 – Objet

En vue de développer des collaborations entre des équipes de recherche actives dans les mêmes domaines de recherche ou dans des domaines connexes, l'Etat accorde aux Institutions un financement pour la création d'un réseau interuniversitaire d'excellence en recherche fondamentale, également appelé pôle d'attraction interuniversitaire, dans le domaine suivant :

Artikel 1 – Voorwerp

Met het oog op de ontwikkeling van samenwerkingsverbanden tussen onderzoekploegen die op dezelfde of aanverwante gebieden werkzaam zijn, verleent de Staat aan de Instellingen een financiering voor de oprichting van een uitmuntend interuniversitair netwerk van fundamenteel onderzoek, ook interuniversitaire attractiepool genoemd, op het volgende gebied :

Functional supramolecular systems (FS2).

Les recherches effectuées dans ce cadre, ci-après dénommées le projet, sont précisées dans l'annexe I au présent contrat. Elles sont assurées par les promoteurs suivants :

Het in dit kader uit te voeren onderzoek, hierna te noemen het project, wordt nader omschreven in bijlage I bij dit contract. Het onderzoek wordt verricht door de volgende promotoren :

- Prof. Pierre Jacobs, KULeuven[1], coördinator
- Prof. Marc Van Der Auweraer, KULeuven[2]
- Prof. Christine Jérome, ULg
- Prof. Roberto Lazzaroni, UMH
- Prof. Guy Marin, UGent[1]
- Prof. Alain Jonas, UCL
- Prof. Filip Du Prez, UGent[2]
- Prof. Gino Baron, VUB
- Prof. Andrée De Mesmaeker, ULB
- Prof. Johan Wouters, FUNDP
- Prof. Dirk Vanderzande, UHasselt
- Prof. Jos Vanderleyden, KULeuven[3]
- Prof. Michel Waroquier, UGent[3]
- European Partner(s)

Article 2 – Durée du contrat

Le contrat entre en vigueur le 1er janvier 2007 et prend fin le 31 décembre 2011.

Artikel 2 - Duur van het contract

Het contract treedt in werking op 1 januari 2007 en eindigt op 31 december 2011.

Article 3 – Conditions générales

3.1. Les promoteurs, agissant dans le cadre de leur Institution respective, dirigent la conduite journalière du projet et en portent la responsabilité scientifique. Ils veillent

Artikel 3 – Algemene voorwaarden

3.1. De promotoren, die handelen in het kader van hun respectieve Instelling, zijn belast met de dagelijkse leiding van het project en dragen er de wetenschappelijke

à ce que les travaux soient menés avec diligence et continuité. Il leur incombe de veiller à ce que toute information et tout document inhérents à la réalisation du présent contrat soient soumis en due forme et en temps utile à l'Etat.

verantwoordelijkheid voor. Zij zien toe op de stipte uitvoering en op de continuïteit van de werkzaamheden. Het is aan hen ervoor te zorgen dat alle informatie en elk document over de uitvoering van dit contract volgens de vereiste vorm en te gelegener tijd aan de Staat worden voorgelegd.

3.2. Les Institutions mettent l'infrastructure, le matériel et le personnel compétent dont elles disposent au service des recherches telles que définies à l'article 1.

3.2. De Instellingen stellen de infrastructuur, het materiaal en het bevoegde personeel waarover zij beschikken ten dienste van het onderzoek zoals bepaald in artikel 1.

3.3. Le financement étant exclusivement accordé pour la réalisation des recherches telles que définies à l'article 1, les Institutions sont tenues de le consacrer à cette seule destination. Dès l'instant où son utilisation n'est plus conforme à cette obligation, le financement ou, suivant le cas, la partie du financement dont l'usage ne peut être dûment justifié par les bénéficiaires, doit être remboursé au Trésor.

3.3. Daar de financiering uitsluitend wordt verleend voor de verwezenlijking van het onderzoek zoals bepaald in artikel 1, zijn de Instellingen ertoe gehouden ze alleen hieraan te besteden. Zodra de aanwending ervan niet meer met die verplichting overeenkomt, moet de financiering of, al naargelang het geval, het gedeelte van de financiering waarvan de besteding niet degelijk kan worden gerechtvaardigd door de begunstigden, terugbetaald worden aan de Schatkist.

Article 4 – Organisation du réseau

4.1. Le projet est un ensemble cohérent de tâches réalisées par des équipes de recherche qui constituent un réseau thématique multidisciplinaire. La réalisation du projet exige une étroite collaboration entre les promoteurs mentionnés à l'article 1. Les promoteurs s'engagent à mettre tout en œuvre en vue d'atteindre les objectifs du réseau et du projet.

Artikel 4 – Organisatie van het netwerk

4.1. Het project is een coherent geheel van taken uitgevoerd door onderzoekploegen die een multidisciplinair thematisch netwerk vormen. Voor de uitvoering van het project is nauwe samenwerking vereist tussen de in artikel 1 vermelde promotoren. De promotoren verbinden er zich toe alles in het werk te stellen om de doelstellingen van het netwerk en van het project te bereiken.

4.2. Le coordinateur désigné à l'article 1 constitue le porte-parole vis-à-vis de l'Etat. Sans préjudice de l'ensemble des droits et devoirs liant les promoteurs à l'Etat, le coordinateur est chargé des tâches suivantes : 1) coordonner l'ensemble des travaux de recherche à réaliser dans le cadre du projet et assurer le bon fonctionnement du réseau ainsi que la bonne circulation de l'information entre les promoteurs ; 2) organiser au moins une fois par an une réunion rassemblant tous les partenaires du réseau ainsi que

4.2. De in artikel 1 aangewezen coördinator is de woordvoerder ten aanzien van de Staat. Onverminderd alle rechten en plichten die de promotoren aan de Staat binden, is de coördinator met de volgende taken belast: 1) coördineren van alle onderzoekwerkzaamheden uit te voeren in het kader van het project en zorgen voor de goede werking van het netwerk en voor de goede informatie-doorstroming tussen de promotoren; 2) beleggen van minstens één vergadering per jaar met alle partners van het

l'administrateur de programme ; 3) coordonner la rédaction des rapports scientifiques et administratifs et leur transmission à l'administrateur de programme ; 4) informer l'administrateur de programme des difficultés éventuelles qui font obstacle à une collaboration efficace et, le cas échéant, lui proposer des mesures pratiques de remèdes; 5) veiller à la création et à la mise à jour d'une page d'accueil du réseau.

netwerk en de programma-administrateur; 3) coördineren van het opstellen van de wetenschappelijke en administratieve verslagen en van het doorsturen ervan naar de programma-administrateur; 4) op de hoogte brengen van de programma-administrateur van eventuele problemen die een efficiënte samenwerking in de weg staan en, zo nodig, hem praktische remediërende maatregelen voorstellen; 5) erop toezien dat een homepage van het netwerk gecreëerd en bijgewerkt wordt.

4.3. Il incombe aux promoteurs du réseau de communiquer à leurs partenaires, de leur propre initiative ou à leur demande, toute information obtenue dans le cadre de l'exécution des tâches qui leur sont imparties, et ce dans la mesure où les promoteurs ou un des promoteurs du réseau en ont besoin pour la bonne marche des travaux de recherche.

4.3. Het is aan de promotoren van het netwerk om aan hun partners, uit eigen beweging of op hun verzoek, iedere informatie te verstrekken verkregen in het kader van de uitvoering van de taken waarmee ze belast zijn, en dit voor zover de promotoren of een van de promotoren van het netwerk die nodig hebben voor het goede verloop van de onderzoekwerkzaamheden.

4.4. Les modalités de collaboration avec le(s) partenaire(s) européen(s) sont décrites à l'annexe III du présent contrat. Le partenariat européen a pour but de renforcer la collaboration scientifique internationale et l'expertise belge. Chaque partenariat européen est géré par un promoteur désigné par le réseau. Celui-ci est l'intermédiaire entre le partenaire européen concerné et l'ensemble du réseau, il lui transmet toutes les informations relatives à la bonne exécution du projet et rend compte de l'état d'avancement de ses travaux auprès des autres partenaires du réseau. Une copie du contrat relatif au partenariat européen est transmise à l'administrateur de programme par le promoteur concerné.

4.4. De samenwerkingsregeling met de Europese partner(s) wordt beschreven in bijlage III van dit contract. Het Europese partnerschap heeft als doel de internationale wetenschappelijke samenwerking en de Belgische expertise te versterken. Elke Europese partnerschap wordt beheerd door een door het netwerk aangewezen promotor, die als tussenpersoon fungeert tussen de betrokken Europese partner en het ganse netwerk. Hij verschaft hem alle informatie voor de goede uitvoering van het project en brengt verslag uit bij de andere partners van het netwerk over de voortgang van zijn werkzaamheden. Een kopie van het contract betreffende het Europese partnerschap wordt door de betrokken promotor aan de programma-administrateur bezorgd.

Article 5 - Suivi du projet

5.1. Le Président du Service public fédéral de programation Politique scientifique, ci-après dénommé "le Service", désigne le(s) membre(s) du Service, ci-après dénommé(s) "l'administrateur de programme", chargé(s) de veiller à la bonne exécution du projet et du contrat.

Artikel 5 - Follow-up van het project

5.1. De Voorzitter van de Programmatorische federale overheidsdienst Wetenschapsbeleid, hierna te noemen "de Dienst", wijst het lid (de leden) van de Dienst aan, hierna te noemen "de programma-administrateur", die moet(en) toezien op de goede uitvoering van het project en het contract.

5.2. Sans préjudice des contrôles prévus par les règles relatives à la comptabilité de l'Etat, les Institutions acceptent les contrôles administratifs, techniques et scientifiques nécessaires pour vérifier la bonne exécution du projet, le bon fonctionnement du réseau et l'utilisation du financement accordé. Ces contrôles sont effectués à la diligence du Service.

5.3. Sans préjudice de la remise des rapports visés à l'article 9, les Institutions s'engagent à fournir à l'administrateur de programme, chaque fois que celui-ci le requiert, toute forme de document exposant le projet et le déroulement du travail en réseau. Les modalités de présentation et de remise de ces documents sont fixées par l'administrateur de programme.

5.4. Les Institutions sont tenues de présenter, chaque fois qu'elles en sont requises, un état des travaux en cours et des dépenses encourues ou prévues, des extraits de comptabilité portant sur toute opération en rapport avec le projet ainsi qu'un relevé détaillé des mesures prises pour la bonne exécution du projet, et notamment pour le bon fonctionnement du réseau.

5.5. L'administrateur de programme a accès aux locaux où s'effectuent les travaux. Il peut vérifier la mise au travail du personnel affecté à l'exécution du projet, la nature des occupations de ce personnel, le déroulement des travaux, l'organisation du réseau et l'utilisation des équipements acquis à charge du projet.

5.2. Onverminderd de controles waarin is voorzien in de regels betreffende de Rijkscomptabiliteit, aanvaarden de Instellingen de noodzakelijke administratieve, technische en wetenschappelijke controles om de goede uitvoering van het project, de goede werking van het netwerk en de aanwending van de toegekende financiële middelen na te gaan. Die controles worden uitgevoerd op verzoek van de Dienst.

5.3. Onverminderd het indienen van de in artikel 9 bedoelde verslagen, verbinden de Instellingen zich ertoe de programma-administrateur welk document ook voor te leggen waarin het project en de voortgang van de werkzaamheden in netwerkverband worden toegelicht, telkens wanneer daarom gevraagd wordt. De wijze waarop die documenten worden opgesteld en bezorgd, wordt vastgelegd door de programma-administrateur.

5.4. Bij elk verzoek moeten de Instellingen een overzicht voorleggen van de lopende werkzaamheden, de gedane of geplande uitgaven, de boekhoudkundige uittreksels met betrekking tot alle verrichtingen in het kader van het project, alsook een gedetailleerd overzicht van de maatregelen die genomen zijn voor de goede uitvoering van het project, inzonderheid voor de goede werking van het netwerk.

5.5. De programma-administrateur heeft toegang tot de lokalen waar de werkzaamheden worden uitgevoerd. Hij kan de tewerkstelling nagaan van het personeel dat is aangesteld voor de uitvoering van het project, de aard van de bezigheden van dat personeel, het verloop van de werkzaamheden, de organisatie van het netwerk en de aanwending van de voor het project aangekochte uitrusting.

5.6. Le Service peut faire procéder à un audit afin de vérifier la comptabilité présentée par les Institutions à l'appui de toute demande de remboursement de dépenses relatives à l'exécution du projet.

5.6. Bij elke aanvraag tot terugbetaling van de uitgaven met betrekking tot de uitvoering van het project, kan de Dienst overgaan tot een audit om de door de Instellingen voorgelegde boekhouding te verifiëren.

5.7. Le Service se réserve le droit de procéder à tout moment à une évaluation externe des résultats du projet et des modalités de collaboration en fonction des objectifs fixés à l'article 1. Les Institutions sont tenues de fournir à l'administrateur de programme toute information requise à cet effet. A cette fin d'évaluation, le Service est habilité à se faire assister par les experts de leur choix.

5.7. De Dienst behoudt zich het recht voor op elk ogenblik de resultaten van het project en de wijze van samenwerking extern te evalueren in het licht van de doelstellingen die zijn vastgelegd in artikel 1. De Instellingen dienen de programma-administrateur daartoe alle nodige informatie te verlenen. Voor die evaluatie is de Dienst gerechtigd zich te laten bijstaan door experts naar eigen keuze.

Article 6 – Budget

6.1. Le montant du financement accordé s'élève à

Artikel 6 – Begroting

6.1. Het bedrag van de toegekende financiering beloopt

8.869.633,00 EUR

6.2. Le montant figurant à l'article 6.1. se répartit comme suit entre les Institutions :

6.2. Het bedrag vermeld in artikel 6.1. wordt op de volgende wijze over de Instellingen verdeeld:

- KULeuven[1]	1.250.000,00 EUR
- KULeuven[2]	1.250.000,00 EUR
- ULg	800.000,00 EUR
- UMH	751.778,00 EUR
- UGent[1]	905.740,00 EUR
- UCL	900.000,00 EUR
- UGent[2]	400.000,00 EUR
- VUB	462.115,00 EUR
- ULB	400.000,00 EUR
- FUNDP	400.000,00 EUR
- UHasselt	400.000,00 EUR
- KULeuven[3]	400.000,00 EUR
- UGent[3]	450.000,00 EUR
- European Partner(s)	100.000,00 EUR

6.3. Les Institutions tiennent une comptabilité détaillée de l'emploi du financement. Cette comptabilité présente séparément les frais de personnel, les frais de

6.3. De Instellingen voeren een omstandige boekhouding van de aanwending van de financiering. Die boekhouding wordt over de volgende uitgavencategorieën verdeeld :

fonctionnement, les frais d'équipement, les frais de sous-traitance, les frais généraux ou "overhead" et les frais liés au partenariat européen. Les montants de chacune de ces catégories sont fixés en annexe I.

6.4. Les frais de personnel, qui doivent couvrir au minimum 60 % du montant total du financement, attribué à chaque promoteur, comprennent les rémunérations brutes indexées, les charges sociales patronales et d'assurances légales ainsi que toute autre indemnité ou allocation légalement due, accessoire au traitement ainsi que les allocations pour bourses doctorales et postdoctorales défiscalisées. Par bourse défiscalisée, il faut entendre une bourse faisant l'objet d'une exonération fiscale en application de la législation fiscale. Le montant afférent aux allocations de bourses doctorales et postdoctorales ne peut excéder 60% du montant total des frais de personnel. Les promoteurs auxquels le montant total du financement accordé est inférieur à 500.000 euros peuvent toutefois dépasser cette limite de 60 %.

6.5. Les frais de fonctionnement comprennent les frais de documentation, les frais de voyage et de mission, les indemnités aux chercheurs visiteurs, l'utilisation d'installations de calcul ou de logiciels, les frais de télécommunications, les frais d'entretien des appareils et plus généralement les biens consomptibles.

6.6. Les frais d'équipement couvrent l'achat d'appareils et d'instruments scientifiques et techniques, y compris le matériel informatique et bureautique.

6.7. Les frais de sous-traitance représentent les frais encourus par un tiers pour l'exécution de tâches ou la prestation de services réclamant des compétences scientifiques ou techniques spéciales sortant du cadre normal des unités de recherche dirigées par les promoteurs. Toute demande de sous-traitance doit être approuvée par

personeelskosten, werkingskosten, uitrustingskosten, onderaannemingskosten, algemene kosten of "overhead" en kosten verbonden met het Europese partnerschap. De bedragen van elk van die categorieën worden in bijlage I vastgelegd.

6.4. De personeelskosten, die minimaal 60 % moeten belopen van de totale financiering toegekend aan elke promotor, omvatten de geïndexeerde brutowedden, de werkgeversbijdragen en wettelijke verzekeringen alsmede elke andere wettelijk verschuldigde vergoeding of toelage, als toeslag op de wedde, alsook de vergoedingen voor de belastingvrije doctoraatsbeurzen en postdoctorale beurzen. Onder belastingvrije beurs wordt een beurs verstaan die overeenkomstig de belastingwetgeving van belasting vrijgesteld is. Het bedrag van de vergoedingen voor doctoraatsbeurzen en postdoctorale beurzen mag niet meer bedragen dan 60% van de totale personeelskosten. De promotoren aan wie een totale financiering lager dan 500.000 euro toegekend werd, mogen deze limiet van 60% overschrijden.

6.5. De werkingskosten omvatten de documentatiekosten, de reis- en zendingskosten, de vergoedingen voor gastonderzoekers, het gebruik van rekenapparatuur of software, de telecommunicatiekosten, de kosten voor het onderhoud van apparatuur en meer algemeen de consumptiegoederen.

6.6. De uitrustingskosten omvatten de aankoop van wetenschappelijke en technische apparatuur en toestellen, met inbegrip van het informatica- en bureauticamateriaal.

6.7. De onderaannemingskosten betreffen de door een derde gedane kosten voor de uitvoering van taken of het leveren van diensten waarvoor bijzondere wetenschappelijke of technische kundigheden vereist zijn die buiten de gewone activiteiten van de onderzoekeenheden van de promotoren liggen. Elke

l'administrateur de programme.

6.8. Les frais généraux des Institutions (overhead) couvrent forfaitairement les frais d'administration, de téléphone, de courrier, d'entretien, de chauffage, d'électricité, de loyer, d'amortissement de matériel ou d'assurance. Leur montant ne peut dépasser 5 % du total annuel des frais de personnel et de fonctionnement.

6.9. La collaboration avec le partenaire européen se fait sur la base d'un cofinancement. Le partenariat européen est financé pour 50% par le partenaire européen et pour 50% par l'Etat. Ce dernier financement est géré par l'Institution du promoteur mentionné à l'article 4.4. et est subordonné au respect des modalités de collaboration figurant à l'annexe III. La part prise en charge par l'Etat couvre exclusivement les dépenses de personnel et de fonctionnement du partenaire européen. Ni les frais généraux, ni l'équipement, ni la sous-traitance ne sont pris en compte comme dépenses.

6.10. Tout transfert de crédits d'une catégorie de dépenses à une autre est subordonné à l'autorisation écrite de l'administrateur de programme. Les reports annuels au sein d'une même catégorie de dépenses sont automatiques pour autant qu'ils ne dépassent pas 60 % des montants inscrits au tableau budgétaire repris dans l'annexe I – section II du présent contrat.

Article 7 – Liquidation du financement

7.1. Le financement fixé à l'article 6.1. du présent contrat est liquidé en six tranches annuelles (2007 à 2012) sur la base du tableau figurant à l'annexe II.

7.2. La tranche 2007 est liquidée au cours du premier semestre de l'année 2007.

aanvraag voor onderaanneming moet door de programma-administrateur worden goedgekeurd.

6.8. De algemene kosten van de Instellingen (overhead) omvatten forfaitair de kosten voor administratie, telefoon, post, onderhoud, verwarming, elektriciteit, huur, afschrijving van materiaal of verzekering. Die kosten mogen niet hoger liggen dan 5% van de totale jaarlijkse personeels- en werkingskosten.

6.9. De samenwerking met de Europese partner gebeurt op basis van een cofinanciering. Het Europese partnerschap wordt voor 50% gefinancierd door de Europese partner en voor 50% door de Staat. Deze laatste financiering wordt beheerd door de Instelling van de promotor vermeld in artikel 4.4 en is afhankelijk van de naleving van de samenwerkingsregeling die als bijlage III is opgenomen. Het gedeelte ten laste van de Staat dekt uitsluitend de personeels- en werkingsuitgaven van de Europese partner. Noch de algemene kosten, noch de uitrusting, noch de onderaanneming worden als uitgaven beschouwd.

6.10. Elke overdracht van kredieten van de ene uitgavencategorie naar een andere is onderworpen aan de schriftelijke toestemming van de programma-administrateur. De jaarlijkse overdrachten binnen eenzelfde uitgavencategorie vinden automatisch plaats voor zover de overdrachten niet meer bedragen dan 60% van de in de begrotingstabel ingeschreven bedragen die in bijlage I – Sectie II van dit contract is opgenomen.

Artikel 7 - Vereffening van de financiering

7.1. De in artikel 6.1. van dit contract vastgelegde financiering wordt in zes jaarlijkse schijven vereffend (2007 tot 2012) op basis van de als bijlage II opgenomen tabel.

7.2. De schijf 2007 wordt vereffend in het eerste semester van 2007.

7.3. Les tranches 2008 à 2011 sont liquidées au cours des années respectives après justification des dépenses de l'année précédente. La tranche 2011 peut être réduite à l'initiative de l'administrateur de programme si la différence entre le financement déjà perçu par l'institution et les justificatifs fournis pour les années 2007 à 2010 est supérieure à 60 % du montant de cette tranche.

7.3. De schijven 2008 tot 2011 worden vereffend in de loop van de respectieve jaren nadat de uitgaven van het voorgaande jaar zijn verantwoord. De schijf 2011 kan worden verminderd op initiatief van de programma-administrateur als het verschil tussen de door de Instelling al ontvangen financiering en de ingebrachte bewijsstukken van de jaren 2007 tot 2010 meer bedraagt dan 60% van die schijf.

7.4. La tranche 2012 est liquidée au cours de l'année 2012, après réception des rapports visés à l'article 9 et après justification des dépenses réelles encourues au titre du présent contrat pour autant que les justificatifs parviennent au Service le 30 juin 2012 au plus tard. Le montant des dépenses non justifiées fait retour au Trésor.

7.4. De schijf 2012 wordt vereffend in de loop van 2012 na ontvangst van de in artikel 9 bedoelde verslagen en nadat de gedane reële uitgaven in het kader van dit contract zijn verantwoord, voor zover de bewijsstukken uiterlijk 30 juni 2012 bij de Dienst toekomen. Het bedrag van de niet verantwoorde uitgaven gaat terug naar de Schatkist.

7.5. A l'état récapitulatif annuel des dépenses, fourni au Service, les Institutions annexent les pièces justificatives : factures, états des traitements et des salaires, etc. Ces pièces justificatives doivent avoir trait à des frais repris aux articles 6.4. à 6.8. du présent contrat. Les dépenses qui font l'objet des pièces justificatives ci-avant doivent avoir été supportées avant le 31 décembre 2011.

7.5. Bij het jaarlijkse overzicht van de uitgaven dat aan de Dienst wordt bezorgd, voegen de Instellingen de bewijsstukken, te weten facturen, loon- en weddestaten enz. Die bewijsstukken moeten betrekking hebben op de in artikel 6.4. tot 6.8. van dit contract vermelde kosten. De bewijsstukken moeten betrekking hebben op uitgaven vóór 31 december 2011.

7.6. Les payements sont suspendus si les Institutions ne respectent pas les obligations du présent contrat, et particulièrement si elles ne fournissent pas en temps requis les états récapitulatifs des dépenses semestrielles et les rapports visés aux articles 5.3., 5.4., 5.7. et 9.

7.6. De betalingen worden gestaakt als de Instellingen de verplichtingen van dit contract niet nakomen, en in het bijzonder als zij niet te gelegener tijd het overzicht van de semestriële uitgaven en de in artikel 5.3., 5.4., 5.7. en 9. bedoelde verslagen indienen.

Article 8 – Propriété et valorisation des résultats des recherches

8.1. Les résultats des recherches sont la propriété de(s) (l')Institution(s) ainsi que de(s) (l')équipe(s) de recherche qui les a(ont) obtenus.

Artikel 8 - Eigendom en valorisatie van de onderzoekresultaten

8.1. De onderzoekresultaten zijn eigendom van de Instelling(en) alsook van de onderzoekploeg(en) die ze heeft (hebben) verworven.

8.2. Le Service se réserve le droit d'utiliser les données scientifiques ainsi que celles relatives au fonctionnement du réseau, fournies par les Institutions en exécution du présent

8.2. De Dienst behoudt zich het recht voor om de wetenschappelijke gegevens, alsook de gegevens met betrekking tot de werking van het netwerk, verstrekt door de

contrat, dans le cadre d'actions d'information, de diffusion et de publication destinées à l'illustration et à la mise en valeur du programme PAI.

Article 9 – Rapports

Le coordinateur remet à l'administrateur de programme les rapports suivants, rédigés conformément aux dispositions pratiques qui seront indiquées dans les directives administratives :

9.1. Rapport initial

Le rapport initial est remis avant le 30 avril 2007. Ce rapport reprend, pour chaque promoteur du réseau, la liste des membres du personnel travaillant dans le cadre du projet PAI (à charge et non à charge du budget PAI) ainsi que la liste des équipements dont dispose l'unité de recherche du promoteur.

9.2. Rapports d'activités annuels

Dans les trois mois qui suivent la fin de chaque exercice, le coordinateur transmet à l'administrateur de programme un rapport d'activités de l'année écoulée. Ce rapport comporte d'une part, un rapport administratif qui présente la situation du personnel mis à disposition du projet et d'autre part, un rapport scientifique qui décrit l'état d'avancement et le fonctionnement du réseau. Ces informations se réfèrent explicitement aux tâches du projet défini à l'article 1. Ce rapport reprend également la liste des publications réalisées au cours de l'année écoulée.

9.3. Rapport destiné à l'évaluation

Au cours de l'année 2010, le coordinateur fait parvenir à l'administrateur de programme une description complète des activités de recherche des années 2007 à 2010, des résultats obtenus et les éventuelles applications. Ce rapport, rédigé en vue de l'évaluation ex-post du projet, remplacera la partie scientifique du rapport d'activités annuel 2010.

Instellingen in het kader van de uitvoering van dit contract, te gebruiken voor informatie, verspreiding en publicatie teneinde het IUAP-programma te valoriseren.

Artikel 9 – Verslagen

De coördinator bezorgt de volgende verslagen aan de programma-administrateur, die worden opgesteld conform de praktische bepalingen vervat in de administratieve richtlijnen :

9.1. Aanvangsverslag

Het aanvangsverslag wordt vóór 30 april 2007 ingediend. Dat verslag bevat, voor elke promotor van het netwerk, de lijst van het personeel dat aan het IUAP-project meewerkt (al dan niet ten laste van het IUAP-buget) alsook de lijst van de uitrusting waarover de onderzoekeenheid van de promotor beschikt.

9.2. Jaarlijkse activiteitenverslagen

Binnen drie maanden na afloop van ieder dienstjaar, bezorgt de coördinator de programma-administrateur een activiteitenverslag van het afgelopen jaar. Dat verslag omvat enerzijds een administratief verslag met een lijst van het personeel dat ter beschikking staat van het project en anderzijds een wetenschappelijk verslag waarin de vooruitgang van het onderzoek en de werking van het netwerk worden toegelicht. Die informatie verwijst uitdrukkelijk naar de taken van het in artikel 1 gedefinieerd project. Dat verslag omvat eveneens de lijst van de publicaties van het voorbije jaar.

9.3 Verslag bestemd voor de evaluatie

In de loop van het jaar 2010 bezorgt de coördinator aan de programma-administrateur een volledige beschrijving van de verrichte onderzoekwerkzaamheden van 2007 tot 2010, de resultaten en de eventuele toepassingen. Dit verslag dat opgesteld wordt voor de ex *post* evaluatie, vervangt het wetenschappelijk deel van het jaarlijkse activiteitenverslag 2010.

9.4. Rapport final

A la fin des recherches financées dans le cadre du présent contrat, et au plus tard le 31 mars 2012, le coordinateur fournit au Service un résumé global des activités de recherche couvrant les années 2007 à 2011.

Article 10 – Communications et publications

Les communications et les publications relatives aux recherches telles que définies à l'article 1 mentionnent les nom et qualité des chercheurs qui y sont associés et précisent que ces recherches s'inscrivent dans le cadre du programme *Pôles d'attraction interuniversitaires* pour le compte de l'Etat belge, *Service public fédéral de programmation Politique scientifique*.

Article 11 – Personnel

11.1. Les Institutions s'engagent à appliquer au personnel qu'elles recrutent pour l'exécution des activités de recherche telles que définies à l'article 1, des conditions de rémunération et de qualification identiques à celles qu'elles appliquent à leur personnel de cadre. Le recrutement se fait conformément à la législation relative aux contrats d'emploi et aux bourses doctorales et postdoctorales défiscalisées.

11.2. Le personnel rémunéré à charge du présent contrat est exclusivement affecté à l'exécution du projet durant la période pour laquelle il est payé par l'Etat. Le nombre d'équivalents temps plein (ETP) scientifiques, techniques et administratifs requis pour l'exécution du projet et dont l'engagement est prévu à charge des frais de personnel figure à l'annexe I du présent contrat.

11.3. Les Institutions ont seules qualité d'employeur à l'égard des membres du personnel qu'elles engagent. Elles gèrent ce personnel sous leur seule responsabilité.

9.4. Eindverslag

Na afloop van het in het kader van dit contract gefinancierde onderzoek en uiterlijk 31 maart 2012, dient de coördinator bij de Dienst een samenvatting in van de onderzoekwerkzaamheden van 2007 tot 2011.

Artikel 10 - Mededelingen en publicaties

De mededelingen en de publicaties betreffende het onderzoek zoals bepaald in artikel 1 vermelden de naam en de hoedanigheid van de onderzoekers die erbij betrokken zijn en vermelden dat dit onderzoek werd uitgevoerd in het kader van het programma *Interuniversitaire attractiepolen* gefinancierd door de Belgische staat, Programmatorische federale dienst Wetenschapsbeleid

Artikel 11 – Personeel

11.1. De Instellingen verbinden er zich toe aan het personeel dat zij aanwerven voor de uitvoering van de onderzoekactiviteiten zoals bepaald in artikel 1, dezelfde voorwaarden qua bezoldiging en kwalificaties toe te kennen als aan hun kaderpersoneel. De aanwerving vindt plaats conform de wetgeving betreffende de arbeidsovereenkomsten en de belastingvrije doctoraatsbeurzen en postdoctorale beurzen.

11.2. Het personeel bezoldigd ten laste van dit contract wordt exclusief ingezet voor de uitvoering van het project voor de periode tijdens welke het door de Staat betaald wordt. Het aantal wetenschappelijke, technische en administratieve fulltime equivalenten (FTE) nodig voor de uitvoering van het project en waarvan de aanwerving zal gebeuren ten laste van de personeelskosten, is als bijlage I bij dit contract opgenomen.

11.3. Alleen de Instellingen zijn werkgever ten opzichte van het personeel dat zij aanwerven. Zij beheren dat personeel onder hun eigen verantwoordelijkheid.

11.4. Les Institutions font parvenir au Service une copie des contrats d'emploi et de bourses (ainsi que de leurs avenants éventuels) concernant le personnel affecté aux recherches et rémunéré à charge du présent contrat. Les contrats d'emploi et de bourses doivent mentionner nommément le promoteur.

11.5. Les contrats d'emploi et de bourses auront une durée d'un an au minimum. Il sera toutefois fait exception pour les contrats conclus durant la dernière année.

11.6. Aucun coût salarial dû pour des prestations ou des délais de préavis dont la période de référence dépasse le terme du contrat n'est remboursé par l'Etat. Les Institutions veilleront dès lors à donner les préavis en temps utile.

11.7. Le non-respect de toutes les dispositions de l'article 11 conduit au refus de remboursement des coûts salariaux.

Article 12 – Equipement

12.1. Les promoteurs justifient le budget d'équipement par un plan d'acquisition de matériel qui figure à l'annexe I avec l'estimation du montant requis pour chaque acquisition.

12.2. Tout achat de matériel d'un coût supérieur à 25.000 EUR qui ne figure pas dans ce plan d'acquisition est soumis à l'autorisation de l'administrateur de programme.

12.3. Toute acquisition à charge du projet doit être effectuée conformément aux dispositions légales et réglementaires concernant les marchés publics.

12.4. Aucun équipement ne peut être acquis à charge du projet au-delà du 31 décembre 2010.

Article 13 - Responsabilité civile

L'exécution du présent contrat ne peut, en aucune façon, entraîner pour l'Etat une responsabilité quelconque dans les

11.4. De Instellingen bezorgen de Dienst een kopie van de arbeids- en beursovereenkomsten (alsook van alle eventuele aanhangsels) betreffende het personeel dat aan het onderzoek meewerkt en bezoldigd wordt ten laste van dit contract. De arbeids- en beursovereenkomsten dienen de naam van de promotor te vermelden.

11.5. De arbeids- en beursovereenkomsten lopen over minimum één jaar. Tijdens het laatste jaar kunnen evenwel afwijkingen worden toegestaan.

11.6. De Staat vergoedt geen loonkosten voor prestaties of opzegtermijnen die de datum van de beëindiging van de werkzaamheden overschrijden. De Instellingen moeten ervoor zorgen dat de opzeggingen te gelegener tijd worden gegeven.

11.7. Het niet respecteren van alle bepalingen van artikel 11 leidt tot het niet terugbetalen van de loonkosten.

Artikel 12 – Uitrusting

12.1. De promotoren verantwoorden het budget inzake uitrusting met een aankoopplan opgenomen als bijlage I dat een raming bevat van het voor elke aankoop nodige bedrag.

12.2. Voor elke aankoop van materiaal van meer dan 25.000 EUR die niet in het aankoopplan voorkomt, is de toestemming vereist van de programma-administrateur.

12.3. Elke aankoop ten laste van het project moet worden verricht conform de wettelijke en reglementaire bepalingen betreffende de overheidsopdrachten.

12.4. Er mag geen uitrusting ten laste van het project worden aangekocht na 31 december 2010.

Artikel 13 - Burgerlijke aansprakelijkheid

De uitvoering van dit contract kan voor de Staat in geen geval welke aansprakelijkheid ook meebrengen in de schade

dommages aux personnes et aux biens résultant directement ou indirectement des activités de recherche financées.

Article 14 – Confidentialité

14.1. Les Institutions et les promoteurs s'engagent à ne pas divulguer les informations individualisées ou d'ordre privé portant sur des personnes physiques ou morales qui leur sont fournies en application du contrat, sans l'autorisation desdites personnes. Ils s'engagent à respecter strictement, lors de l'exécution du contrat, la législation portant sur la protection de la vie privée et le traitement automatisé de données à caractère personnel.

14.2. Ils s'engagent à respecter strictement, lors de l'exécution du contrat, la législation actuelle portant sur la protection des animaux d'expérience.

Article 15 – Résiliation

15.1. Le contrat se termine de plein droit lorsque le réseau se trouve dans l'impossibilité de poursuivre ses activités pour des raisons indépendantes de sa volonté. Dans ce cas, le terme du contrat est fixé au dernier jour du mois qui suit celui durant lequel l'impossibilité a été signifiée au Service.
Lorsqu'un promoteur se trouve dans l'impossibilité de poursuivre ses activités et que les autres promoteurs estiment être en mesure de poursuivre le projet sans ce promoteur, il en informe l'Etat, par l'entremise du coordinateur ou par celle d'un autre promoteur. Pour autant que le Président du Service ait marqué son accord, les modifications font l'objet d'un avenant au présent contrat.

15.2. Dans les cas visés à l'article 15.1, l'Etat n'est tenu à aucun remboursement de dépenses effectuées postérieurement à la date où la résiliation du contrat prend effet, hormis les cas suivants:

aan personen of goederen die rechtstreeks of onrechtstreeks volgt uit de gefinancierde onderzoekwerkzaamheden.

Artikel 14 – Geheimhouding

14.1. De Instellingen en de promotoren verbinden er zich toe geen informatie te verspreiden van individuele of persoonlijke aard over natuurlijke of rechtspersonen die hun overeenkomstig het contract verstrekt worden, zonder de toestemming van genoemde personen. Zij verbinden er zich toe tijdens de uitvoering van het contract zich strikt te houden aan de wetgeving met betrekking tot de bescherming van de persoonlijke levenssfeer en de computerverwerking van persoonlijke gegevens.

14.2. Zij verbinden er zich toe tijdens de uitvoering van het contract strikt de huidige wetgeving met betrekking tot de bescherming van proefdieren na te leven.

Artikel 15 – Opzegging

15.1. Wanneer het voor het netwerk buiten zijn wil om onmogelijk geworden is zijn werkzaamheden voort te zetten, eindigt het contract van rechtswege. In dat geval loopt het contract af op de laatste dag van de maand die volgt op die van de mededeling van die onmogelijkheid aan de Dienst. Wanneer het voor een promotor van het netwerk onmogelijk is zijn werkzaamheden voort te zetten en wanneer de overige promotoren menen dat het project toch kan doorgaan zonder deze promotor, wordt de Staat hiervan op de hoogte gebracht via de coördinator of een andere promotor. Voor zover de Voorzitter van de Dienst zijn toestemming geeft wordt deze wijziging vastgelegd in een aanhangsel aan dit contract.

15.2. In deze gevallen, als bedoeld in artikel 15.1, is de Staat niet verplicht tot enige terugbetaling van uitgaven die dateren van na de datum waarop de opzegging van het contract in werking treedt, buiten de volgende gevallen:

15.2.1. Les dépenses exposées par les Institutions et qui correspondent à la rémunération du personnel engagé à charge du contrat:
- pour une durée indéterminée et pour lequel un préavis court pendant la période postérieure à la date à laquelle il a été mis fin au contrat;
- pour une durée déterminée et pour lequel une indemnité est due du fait de la dénonciation avant terme de son contrat d'emploi.

15.2.1. De uitgaven van de Instellingen, voor het uitbetalen van de bezoldiging van het personeel dat ten laste van het contract:
- voor onbepaalde duur in dienst is genomen en waarvoor een opzeggingstermijn loopt tijdens de periode die komt na de datum waarop een einde werd gemaakt aan het contract;
- voor bepaalde duur is in dienst genomen, waaraan een vergoeding is verschuldigd gelet op de voortijdige opzegging van zijn arbeidscontract.

15.2.1.1. Les Institutions ont droit à cette intervention dans la mesure où elles ont :
- notifié le préavis ou la dénonciation du contrat d'emploi sans délai après avoir elles-mêmes reçu notification de la résiliation du contrat de recherche;
- réduit la durée du préavis ou le montant de l'indemnité au minimum, compte tenu de la législation en vigueur.

15.2.1.1. De Instellingen hebben recht op die tegemoetkoming voor zover zij :
- de opzegging van het arbeidscontract hebben meegedeeld onmiddellijk nadat zij zelf op de hoogte werden gebracht van de opzegging van het contract;
- de duur van de opzeggingstermijn of het bedrag van de vergoeding tot het minimum hebben beperkt, met inachtneming van de geldende wetgeving.

15.2.1.2. Pour le personnel engagé pour une durée indéterminée, l'intervention de l'Etat ne peut dépasser l'équivalent d'un délai de préavis calculé en fonction de la durée pendant laquelle la personne en cause a été rémunérée à charge du budget du contrat de recherche.

15.2.1.2. Voor het personeel dat voor onbepaalde duur in dienst is genomen, mag de tegemoetkoming van de Staat het equivalent niet overschrijden van een opzeggingstermijn die berekend is op grond van de duur tijdens welke de betrokken persoon werd betaald ten laste van de begroting van het contract.

15.2.1.3. Pour le personnel engagé pour une durée déterminée, l'intervention de l'Etat ne peut dépasser l'équivalent d'une indemnité calculée en fonction de la durée du projet établie à l'article 2. du contrat.

15.2.1.3. Voor het personeel dat voor bepaalde duur in dienst is genomen, mag de tegemoetkoming van de Staat het equivalent niet overschrijden van een vergoeding die berekend is op grond van de duur van het project zoals vastgelegd in artikel 2 van het basiscontract.

15.2.2. Les autres dépenses qui, avant la date où la résiliation du contrat prend effet, ont été déjà engagées par les Institutions au titre du contrat ou autorisées par l'Etat dans le cadre du programme et dont l'engagement ne peut être annulé ou ne peut l'être qu'en donnant lieu à des dommages et intérêts. Si les dommages et intérêts sont inférieurs à l'engagement fait par l'Institution, seul le

15.2.2. Andere uitgaven die de Instellingen, voor de datum waarop de opzegging van het contract ingaat, in het kader van het contract hebben aangegaan of die door de Staat al werden toegestaan in het kader van het programma en waarvan de vastlegging niet kan worden geannuleerd of slechts kan worden geannuleerd met een schadevergoeding. Indien de schadevergoeding lager is dan de uitgaven, is

montant de ceux-ci est dû.

15.3. L'Etat peut résilier le contrat si le réseau ne respecte pas les dispositions de celui-ci. La décision de résiliation est prise par le Ministre de la Politique scientifique sur proposition du Président du Service et notifiée par ce dernier via le coordinateur au réseau. Cette notification est motivée et adressée par envoi recommandé. La résiliation prend effet à la date de la notification de la décision. Dans ce cas, l'Etat n'est tenu à aucun remboursement de dépenses engagées postérieurement à la date où la résiliation du contrat prend effet ni à aucun dédommagement pour la rupture elle-même. Lorsqu'une partie du réseau fait défaut, mais que le reste du réseau considère qu'il peut continuer le projet, l'Etat peut décider d'exclure la partie du réseau qui fait défaut, conformément à cette même procédure.

slechts de schadevergoeding verschuldigd.

15.3. De Staat kan het contract opzeggen indien het netwerk bepalingen ervan niet naleeft. De beslissing tot opzegging wordt genomen door de Minister van Wetenschapsbeleid op voorstel van de Voorzitter van de Dienst, die deze beslissing, via de coordinator, meedeelt aan het netwerk. De gemotiveerde kennisgeving wordt per aangetekende brief verstuurd. De opzegging treedt in werking op de dag van de kennisgeving van de beslissing. In dat geval is de Staat niet verplicht tot enige terugbetaling van uitgaven gedaan na de datum waarop de opzegging van het contract van kracht wordt, noch tot enige schadevergoeding voor de verbreking zelf.
Wanneer slechts een deel van het netwerk in gebreke blijft, maar wanneer het overige deel van het netwerk meent het project te kunnen voortzetten, kan de Staat beslissen het ingebreke gebleven deel van het netwerk uit het contract te sluiten volgens dezelfde procedure.

Article 16 - Dispositions particulières

16.1. Sans préjudice des dispositions prévues aux articles 6.10 et 7.3, les dispositions du présent contrat et de ses annexes ne peuvent être amendées, modifiées ou complétées d'une quelconque manière que par voie d'avenant, dûment signé par les représentants autorisés des parties contractantes.

16.2. En cas de litige, les tribunaux de Bruxelles sont seuls compétents.

16.3. Les annexes au présent contrat en font partie intégrante. Ces annexes sont les suivantes :
Annexe I : Spécifications techniques (section I, section II).
Annexe II : Echéancier du financement.
Annexe III : Partenariat européen

Artikel 16 - Bijzondere bepalingen

16.1. Onverminderd de bepalingen vastgelegd in artikelen 6.10 en 7.3, kunnen de bepalingen van dit contract en van de bijlagen ervan enkel worden verbeterd, gewijzigd of aangevuld door middel van een aanhangsel, naar behoren ondertekend door de bevoegde vertegenwoordigers van de contracterende partijen.

16.2. In geval van geschil zijn alleen de rechtbanken van Brussel bevoegd.

16.3. De bijlagen bij dit contract maken er wezenlijk deel van uit. Die bijlagen zijn de volgende :
Bijlage I : Technische specificaties (sectie I, sectie II).
Bijlage II : Schema van de financiering.
Bijlage III : Europees Partnerschap

Ainsi fait, en 11 exemplaires,

Le

Pour l'Etat,
Pour le Ministre de la Politique scientifique,

Le Président du Service public fédéral de la programmation
Politique scientifique

Philippe METTENS

Aldus opgemaakt in 11 exemplaren,

De

Voor de Staat,
Voor de Minister van Wetenschapsbeleid,

De Voorzitter van de Programmatorische federale
overheidsdienst Wetenschapsbeleid

De rector van de Katholieke Universiteit Leuven

M. VERVENNE

De rector van de Vrije Universiteit Brussel

B. VAN CAMP

Le recteur de l'Université de Liège

B. RENTIER

Le recteur de l'Université Libre de Bruxelles

Ph. VINCKE

Le recteur de l'Université de Mons-Hainaut

B. LUX

Le recteur des Facultés Universitaires Notre-Dame de la Paix à Namur

M. SCHEUER

De rector van de Universiteit Gent

P. VAN CAUWENBERGE

De rector van de Universiteit Hasselt

I. DE SCHEPPER

Le recteur de l'Université Catholique de Louvain

B. COULIE

Ainsi fait, en 11 exemplaires,

Le

Aldus opgemaakt in 11 exemplaren,

De

Pour l'Etat,

Pour le Ministre de la Politique scientifique,

Le Président du Service public fédéral de la programmation Politique scientifique

Voor de Staat,

Voor de Minister van Wetenschapsbeleid,

De Voorzitter van de Programmatorische federale overheidsdienst Wetenschapsbeleid

Philippe METTENS

De rector van de Katholieke Universiteit Leuven

M. VERVENNE

Prof. Marc Vervenne
Rector K.U.Leuven

De rector van de Vrije Universiteit Brussel

B. VAN CAMP

Le recteur de l'Université de Liège

p.o.

Albert CORHAY
Vice-Recteur
Université de Liège
7, Place du 20 août - 4000 LIEGE

B. RENTIER

Le recteur de l'Université Libre de Bruxelles

Ph. VINCKE

31-05-2007

Le recteur de l'Université de Mons-Hainaut

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Le recteur des Facultés Universitaires Notre-Dame de la Paix à Namur

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P. VAN CAUWENBERGE

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B. COULIE

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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION I

Information on the network

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the coordinator : JACOBS Pierre Institution : Katholieke Universiteit Leuven (K.U.Leuven)

I. 1. NETWORK COMPOSITION

BELGIAN PARTNERS *

Coordinator : Partner 1 (P1) Name : JACOBS Pierre Institution : Katholieke Universiteit Leuven Institution's abbreviation :K.U.Leuven	Partner 8 (P8) Name : BARON Gino Institution : Vrije Universiteit Brussel Institution's abbreviation : VUB
Partner 2 (P2) Name : VAN DER AUWERAER Mark Institution : Katholieke Universiteit Leuven Institution's abbreviation : K.U.Leuven	Partner 9 (P9) Name : DE MESMAEKER Andrée Institution : Université Libre de Bruxelles Institution's abbreviation : ULB
Partner 3 (P3) Name : JEROME Christine Institution :Université de Liège Institution's abbreviation :ULg	Partner 10 (P10) Name : WOUTERS Johan Institution :Facultés Universitaires de Notre-Dame de la Paix Institution's abbreviation :FUNDP
Partner 4 (P4) Name : LAZZARONI Roberto Institution :Université de Mons-Hainaut Institution's abbreviation :UMH	Partner 11 (P11) Name : VANDERZANDE Dirk Institution : Universiteit Hasselt Institution's abbreviation : UHasselt
Partner 5 (P5) Name : MARIN Guy Institution :Universiteit Gent Institution's abbreviation :UGent	Partner 12 (P12) Name : VANDERLEYDEN Jos Institution :Katholieke Universiteit Leuven Institution's abbreviation :K.U.Leuven
Partner 6 (P6) Name : JONAS Alain Institution : Université Catholique de Louvain Institution's abbreviation :UCL	Partner 13 (P13) Name : WAROQUIER Michel Institution : Universiteit Gent Institution's abbreviation :UGent
Partner 7 (P7) Name : DU PREZ Filip Institution : Universiteit Gent Institution's abbreviation : UGent	

* Mention only **one** name per partner. The person listed here should be the one in charge of the operational aspects of the project. Indicate the full name (family name + first name) of the partner.

EUROPEAN PARTNERS * (if applicable)

EU-Partner 1 (EU1) Name :MULLEN Klaus Institution : Max Planck Institute for Polymer Research Mainz Institution's abbreviation : MPI Mainz Country : Germany	EU-Partner 3 (EU3) Name : Institution : Institution's abbreviation : Country :
EU-Partner 2 (EU2) Name : FEIJEN Jan Institution : Universiteit Twente Institution's abbreviation : UTwente Country : The Netherlands	EU-Partner 4 (EU4) Name : Institution : Institution's abbreviation : Country :

* Mention only one name per partner. The person listed here should be the one in charge of the operational aspects of the project. Indicate the full name (family name + first name) of the partner.

I. 2. TITLE AND SUMMARY OF THE PROJECT

Indicate clearly and briefly the project's major objectives and provide a concise description of the project.

A. Title and summary in English (2 pages maximum)

This IAP-PAI network Supramolecular Functional Systems (acronym FS2) will evolve from the previous network, entitled Supramolecular Chemistry and Supramolecular Catalysis. Supramolecular chemistry describes the chemistry beyond the molecule and studies chemical species held together by non-covalent intermolecular interactions. The aim of the project is to develop novel systems, to understand driving forces that allow bi- and tridimensional organisation, to develop methods and tools to investigate, address, manipulate supramolecular structures and exploit their specific properties. In comparison with the previous project, selected new topics will be emphasized, while other promising areas will be further explored. A special emphasis will be placed on the functionality of four major supramolecular systems (cfr *infra*), and the specific research packages will be tackled at four different platform levels by several partners with complementary expertise and instrumental capabilities. The previous frame of the network, *an organic, polymeric, inorganic and bio-approach to supramolecular phenomena*, has been redesigned so as to maximize networking and intensify the degree of focus.

The **following functional supramolecular systems** will be studied:

1. Nanostructured systems: Typical nanostructured systems are zero-dimensional metal and semiconductor nanodots. They are studied as such, or in conjugated liquid crystals and polymers.

2. (Hierarchically) structured nanoporous materials: Via supramolecular templating, block copolymer templating and (repeated) nanocasting, nanoporous materials with pore size covering the whole micro-mesopore domain, different architecture and even multimodal distribution are accessible for use in separation, catalysis of large (bio)molecules. Among them are of particular interest mesoporous organogels, nanostructured carbon materials, (multi)porous oxides, metal-organic frameworks and (supported) nanoparticles.

3. (Hybrid) biomaterials: Artificial biomaterials are mimicking the natural components that function by a complexity of equilibria, intracellular and extracellular catalysis, and interface phenomena, the intra- and extracellular function being governed by supramolecular arrangements of various biopolymers, inorganic and organic molecules. Biomimetic material design requires tailored chemistry leading to characterized biomimetic surfaces and matrices, membranes, probes for cellular components, biomimetic catalysts, nanosized patterned surfaces, and hybrid systems.

4. Thin films (organic, inorganic and hybrid): Functional systems are most often organized in thin films; this applies, e.g., to conjugated polymers incorporated as the active element in semiconducting devices, functional polymer coatings or molecular layers on surfaces, and (bio)membranes.

To guarantee intensive networking, the partners for each of the system classes will contribute at the level of **four different platforms**:

PLATFORM 1: THEORY & MODELING

Multiscale modeling starts from simple structures (single molecules, molecular building blocks) and extends towards systems of growing complexity: polymer chains and supramolecular assemblies built by non-covalent interactions, molecular systems embedded in a solvent or polymer matrix, (macro)molecules adsorbed at surfaces or within pores, and finally interfaces in organic/inorganic, or organic/organic, or organic/bio hybrid systems.

The major goals of the activities of this platform will be:
(i) to determine the nature and intensity of the intermolecular interactions on the nanoscale;
(ii) to provide interpretation to the spectroscopic data and the photonic properties;
(iii) to understand the molecular dynamics in space and time, for (photo)physical and chemical processes.

Theoretical tools adapted to the scale of the problem will be implemented, from state-of-the-art quantum chemical methods to force-field-based molecular modeling techniques designed for accurate simulations of both organic and inorganic compounds, as well as biomolecules.

PLATFORM 2: SYNTHESIS & FABRICATION (MOLECULAR ENGINEERING)

2.1. Building block Synthesis: Supramolecular chemistry relies on the capability of designing/tailoring building blocks of various nature (organic/inorganic), size (molecules, oligomers, (co)polymers, particles...), shape (spherical, cylindrical, sponge-like, vesicular,...) and reactivity. A work-package will focus on efficient and selective processes for synthesis of these elementary (meccano or lego) pieces, with special emphasis on controlled/living polymerizations, sol-gel processes, and nanoparticle fabrication.

2.2. Self-assembly and nanomanipulation of building blocks (0D; 1D; 2D; 3D): Strategies are devised for (self)assembly of complementary building blocks, for their adsorption, grafting and manipulation at surfaces, their dispersion and nanostructuring within matrices (inorganic, polymeric) with the purpose to trigger novel behavior and specific properties in optoelectronics, catalysis, (bio)sensing, biomaterials, engineering polymers, etc.

2.3. Biomimetic chemical design: In active sites of enzymes and supramolecular systems alike, key issues are control over the access, steric and polarity factors, and targeted active site modification. Favored assembly methods are 'ship-in-a-bottle' synthesis of coordination compounds in the channels and cages of porous materials, and molecular imprinting of transition states or analytes. High-throughput design methods copy the genetic strategies of natural evolution.

2.4 Nanopatterning of adsorbed monolayers and their use as stamps and templates will be explored. (Chirally) ordered 2D-structures will serve as a template for 3D-nanostructures, using building blocks such as chiral conjugated molecules or conducting polymers. Patterning of the adsorbed molecules will also be investigated starting from a patterned substrate.

PLATFORM 3: STRUCTURE & FUNCTIONALITY

3.1. Interaction and Recognition between two building blocks is the elementary event for supra-molecular function. Chemical synthesis and theory aid in designing new interactions with increased specificity.

3.2. Adsorption, Motion, Diffusion: We will investigate the effect of the nature of the chemical adsorbate on the structures formed and on the kinetics of adsorption at model surfaces and at real surfaces. The adsorption and diffusion of small molecules in nanoporous materials will be simulated and the results related to experimental data. The translational and rotational motion of individual polymer chains and even of chain segments will be recorded using single molecule spectroscopy on probes dissolved in or covalently bound to a polymer. Fluorescent probes (small molecules, or labeled proteins) will also be used to image the motion (processivity) of enzymes, to follow transport of substrates and products to or from single enzymes and through membranes, and to follow formation of rafts in synthetic and natural bilayer membranes. The diffusion and drift of excitons and charge carriers will be monitored in nanostructured systems consisting of a conjugated polymer and nanodots or with a bulk heterojunction between a conjugated polymer and small molecules or between two types of small molecules.

3.3. Chemical stimulation: Upon reception of a chemical signal or reagent, the supramolecular response can vary from a subtle change of a weak bond, to complex breaking and formation of covalent bonds as in supramolecular catalytic processes. Focus will be on how supramolecular organization contributes to concerted or consecutive bond activation. Methodology concentrates on real-time imaging of chemical activation over large spatial ranges, with increasing spatial resolution.

3.4. Dynamics upon other stimulation: External stimuli such as *T*, *E*, pH, flow, static magnetic field, shear forces or hv will be used to induce changes of the supramolecular organisation. The reversibility, hysteresis, the time constants and the spatial homogeneity of the response will be studied with advanced physical techniques. Smart materials with memory behavior or reversible switching capability will be developed.

PLATFORM 4: DEVICES & RESPONSIVE SYSTEMS

Concepts will be designed and proven for specific applications such as drug delivery devices, sensors, opto-electronic devices and shape memory polymers.

B. Title and summary in Dutch (2 pages maximum)

Functionele Supramoleculaire Systemen

IAP-PAI fase VI netwerk, getiteld *Functionele Supramoleculaire Systemen* (***FSS***), vloeit voort uit fase V netwerk *Supramoleculaire Chemie en Supramoleculaire Katalyse*. De supramoleculaire chemie beschrijft chemische fenomenen op een niveau hoger dan van de individuele moleculen en bestudeert chemische "soorten" die interageren via niet-covalente intermoleculaire krachten. Het project wil nieuwe systemen ontwikkelen en krachten verstaan die drijfveer zijn tot bi- en tridimensionele organisatie. Het wil verder methoden en gereedschappen ontwikkelen om supramoleculaire structuren te onderzoeken, te activeren, te manipuleren, en hun specifieke eigenschappen te exploiteren. De nadruk ligt op geselecteerde nieuwe systemen, en veelbelovende domeinen waarin reeds gewerkt werd. Het vorige netwerk gebaseerd op een organische, polymeer-, inorganische en bio-benadering van supramoleculaire fenomenen werd hertekend om maximale netwerking en focus te verzekeren. **Negen werkpakketten** worden gedefinieerd, waarin een maximaal aantal partners met complementaire expertise en instrumentarium op niveau van vier onderscheiden platforms actief zijn. Alle partners hebben kernactiviteiten in het domein van het project. Volgende **FFS** worden onderzocht:

1. ***Nanogestructureerde Systemen*** zoals zero-dimensionele metalen en halfgeleider "nanodots", worden bestudeerd onder de vorm van geconjugeerde vloeibare kristallen en polymeren. Nanokooien worden gevormd door het inbrengen van bi-dimensionele organische lagen in inorganische kristallen.
2. ***(Hiërarchisch) Gestructureerde Nanoporeuze Materialen*** worden aangemaakt met supramoleculaire templaten en blok-co-polymeren of via "nano-casting", variërend in porie-afmeting, -architectuur en -distributie, zoals mesoporeuze organogelen, nano-gestructureerde koolstofmaterialen, (multi-)poreuze oxides en metaal-organische roosters.
3. ***(Hybriede) Biomaterialen*** omvatten proteïnes met auto-fluorescerende en foto-schakelende eigenschappen, DNA-complexen met geïntercaleerde metaalverbindingen en biofilmen. Materiaal/systeemontwerp omvat de ontwikkeling van biomimetische oppervlakken en katalysatoren, zowel als oppervlakken met nano-patronen.
4. ***(Organische, Inorganische en Hybriede) Dunne Filmen*** worden onderzocht zoals geconjugeerde polymeren als actief element ingebed in halfgeleider-gebaseerde instrumenten, functionele polymeercoatings, moleculaire lagen aan opervlakken, en (bio)membranen.

De betreffende onderzoeksactiviteiten zijn gestructureerd als **9 werkpakketten** (***WP***):

WP1, "Nanodots" en Fotonische Kristallen, gebruikt anorganische metaal of niet-metaal nanodeeltjes aangemaakt in gastroosters en bestudeerd met fluorescentietechnieken, als katalysator.

WP2, Organische Nanostructuren, gebruikt macro-moleculaire synthese-methodieken om multi-functionele co-polymeren en organische "nanodots" aan te maken. Organisatie op nanoschaal zal gevolgd worden met STED, NMR, scattering-technieken, reologie, *etc.*

WP3, Poreuze Roosters, bouwt hiërarchische inorganische en metaalorganische roosters. Adsorptieve en katalytische eigenschappen worden in kaart gebracht met ruimte- en tijdsgebaseerde hyperresolutie. De microschaal convergeert met de macro-schaal in kinetische modellen en "release" studies.

WP4, Hybriede Materialen, bereid nanogelen met intelligente respons in media zoals superkritische (sc) CO_2, koolstof-nanobuisjes gericht en gefunctionalizeerd via templaat-gebruik of electro-spinning, polymeer/inorganische hybrieden zoals klei/polyester nano-composieten.

WP5, (Bio-)Membranen, bestudeert de dynamica van lipide bi-lagen en van bacteriële oppervlakken. Ze dienen als platform voor weefselengineering of als half-doorlaatbare barrières voor nanofiltratie.

WP6, Biomoleculen en Biokatalyse, visualiseert DNA conformaties en cellulaire compartimentalisatie met hyperresolutie met behulp van GFP's, Ru-proben, *etc.* Enzymes, RNAs en biomimetische hybriede materialen worden gebruikt in de organische katalyse.

WP7, ***Functionele Deklagen,*** ontwerpt thermo- of pH-responsieve electro-coatings, katalytische gefluorineerde polymeer coatings compatibel met sc CO_2, protëine afstotende synthetische coatings tegen biofilm-vorming.

WP8, ***Supramoleculaire Geconjugeerde Systemen,*** manipuleren optische en transporteigenschappen, gebruik makend van fase-gescheiden donor/acceptor systemen, blok-co-polymeren of discotische vloeibare kristallen met focus op organische chirale geleiders.

WP9, ***Zelf-Organisatie aan Oppervlakken,*** steunt op scanning-probé technieken zoals electro-chemische STM, om chirale, conformationeel flexibele monolagen met nanopatronen te bestuderen, stimuleren en manipuleren en ze te gebruiken als templaat voor de organisatie van 3D architecturen.

Samenwerking op **4 verschillende platformniveaus** garandeert intensieve/gefocusseerde netwerking in de WP.

Platform 1: Theorie & Modellering. Multischaal modellering gebeurt voor eenvoudige moleculen en bouwstenen en voor complexe systemen zoals polymeerketens, supramoleculaire associaties door niet-covalente interacties, moleculaire systemen ingebed in solvent of polymeermatrix, macromoleculen geabsorbeerd aan oppervlakken of in poriën, organische, inorganische, bio- of hybriede interfazen. Aard en intensiteit van intermoleculaire interacties op nanoschaal worden bepaald, spectroscopische gegevens en fotonische eigenschappen geïnterpreteerd, moleculaire dynamica in tijd en ruimte voor chemische en foto-fysische processen verstaan. Theoretische methoden worden geïmplementeerd variërend van geavanceerde kwantumchemische methodes tot 'force-field' gebaseerde moleculaire modelleringstechnieken.

Platform 2: Synthese & Fabricatie (moleculaire engineering).

2.1. Synthese van elementaire bouwelementen van verschillende aard (organisch/inorganisch), afmetingen (moleculen, oligomeren, copolymeren), vorm (sferisch, cylindrisch, sponsachtig, vesiculair), en reactiviteit gebeurt via gecontroleerde levende polymerisatie, sol-gel processen en fabricage van nano-particles.

2.2. Zelforganisatie en nanomanipulatiestrategieën van elementaire bouwstenen (0D, 1D, 2D verlopen via absorptie, grafting en manipulatie aan oppervlakken, dispersie en nano-structuur-vorming in inorganische of polymere matrices, om nieuw gedrag uit te lokken en specifieke eigenschappen te genereren in optische electronica, katalyse, bio-sensing en engineering van polymeren.

2.3. Ontwerp van biomimetische sites in enzymen en supramoleculaire systemen is gebaseerd op controle van sterische en polaire factoren die modificatie van actieve sites beheersen. "Ship-in-a-bottle"-synthese van complexen in poreuze materialen, moleculaire imprinting zijn geschikte methodieken. Hoge-doorvoer-methodes kopiëren genetische strategieën gevolgd bij natuurlijke evolutie.

2.4. Nano-patroon vorming in geadsorbeerde monolagen, en hun gebruik als templaat voor multilagen wordt onderzocht, met gebruik van bouwstenen zoals chirale geconjugeerde moleculen of geleidende polymeren.

Platform 3: Structuur & Functionaliteit

3.1. Interactie tussen en herkenning van bouwstenen zijn elementaire stappen in de supramoleculaire chemie. Chemische synthese en theoretische benaderingen worden gecombineerd om specifieke interacties te genereren.

3.2. Kinetiek van absorptie, diffusie, beweging van het chemisch adsorbaat aan modeloppervlakken wordt experimenteel bestudeerd en gemodelleerd en vergeleken met reële oppervlakken en poriën. De translatie en rotatie bewegingen van (segmenten van) polymeerketens wordt gevolgd via "single-molecule" spectroscopie. Fluorescerende probe-moleculen of gemerkte proteïnen laten toe beweging van enzymen en transport van substraten en producten van en naar individuele enzymen en door membranen te volgen. Diffusie en drift van geëxciteerde specimen en ladingsdragers wordt gevolgd door nanogestructureerde systemen zoals geconjugeerde polymeren en nanodots en tussen geconjugeerde polymeren en kleine moleculen, of 2 types kleine moleculen.

3.3. Na Chemische stimulatie antwoordt een supramoleculair systeem door veranderingen in zwakke bindingen, vormen van covalente bindingen en ontbinding van complexen. Er wordt onderzocht hoe supramoleculaire organisatie geconcerteerde of consecutieve activatie van bindingen beïnvloed via methodes die chemische activatie in brede domeinen beschrijven met ruimtelijke hyperresolutie.

3.4. Dynamica onder invloed van stimuli zoals *T*, *E*, pH, debiet, statisch magnetisch veld, hν of scheerkrachten liggen aan de basis van veranderingen in supramoleculaire organisatie. Om intelligente materialen met geheugeneffect of omkeerbare schakelcapaciteiten te ontwikkelen, worden reversibiliteit, hysteresis, tijdsconstanten en homogene ruimtelijke respons nagetrokken..

Platform 4: Instrumenten & Responsieve Systemen

Specifieke concepten worden ontwikkeld voor toepassingen als sensoren, optisch-electronische instrumenten, intelligente polymeren en systemen voor toedienen van geneesmiddelen

C. Title and summary in French (2 pages maximum)

Systèmes Supramoléculaires Fonctionnels

Le réseau PAI "*Systèmes Supramoléculaires Fonctionnels*" (en abrégé FS2) résulte de l'évolution d'un réseau précédent intitulé "*Chimie Supramoléculaire et Catalyse Supramoléculaire*". La chimie supramoléculaire s'attache à la synthèse d'entités polymoléculaires maintenues ensemble par des interactions non-covalentes faibles. Le but du présent projet est de synthétiser des entités nouvelles de ce type, de comprendre les principes permettant de contrôler leur organisation bi- et tri-dimensionnelle, de développer les méthodes et outils permettant d'étudier, d'adresser, ou de manipuler de telles entités supramoléculaires, et d'exploiter certaines de leurs propriétés fonctionnelles. Par rapport à notre projet antérieur, des thèmes nouveaux seront abordés, et des domaines de recherche prometteurs seront explorés.

Le réseau précédent, centré autour de l'étude des phénomènes supramoléculaires dans les domaines organiques, inorganiques et biologiques, a été complètement réorganisé de façon à maximiser les interactions entre partenaires et à focaliser les thématiques de recherche. **Neuf sous-programmes de travail** seront menés à bien dans le cadre de **quatre plateformes différentes** par des partenaires aux compétences et aux expertises techniques complémentaires.

Les **quatre systèmes supramoléculaires** suivants seront étudiés:

1. Systèmes nano-structurés: il s'agira typiquement de nano-boîtes quantiques métalliques ou semi-conductrices de dimension zéro. Elles seront étudiées en tant que telles ou en interaction avec des polymères conjugués et des cristaux liquides électro-actifs.

2. Matériaux nano-poreux structurés (de manière hiérarchique): des matériaux poreux à porosité contrôlée en taille, architecture ou distribution, peuvent être obtenus par réplication supramoléculaire, par réplication de phases de copolymères à blocs, ou par "(nano)-casting". Il s'agira ici typiquement d'organo-gels méso-poreux, de matériaux carbonés nano-structurés, d'oxydes multi-poreux et de nano-structures organo-métalliques.

3. Biomatériaux (hybrides): les protéines auto-fluorescentes et photo-ajustables, les complexes d'ADN avec des composés métalliques intercalés, et les bio-films sont des exemples de biomolécules ou de biomatériaux d'intérêt supramoléculaire. Ceux-ci permettront entre autres de réaliser des surfaces et des catalyseurs bio-mimétiques, ainsi que des bio-surfaces porteuses de nano-dessins.

4. Films minces (organiques, inorganiques et hybrides): les systèmes fonctionnels sont fréquemment organisés en films minces. En ce qui nous concerne, cela sera le cas pour, par exemple, des polymères conjugués utilisés comme éléments actifs de dispositifs semi-conducteurs, des revêtements polymères fonctionnels, des couches mono-moléculaires chemi- ou physi-sorbées, et des (bio-)membranes.

Le programme de recherche est structuré en neuf sous-programmes (WP's):

WP1, Nano-boîtes et cristaux photoniques, se concentrera sur la synthèse de nano-particules inorganiques métalliques ou non-métalliques au sein de matrices hôtes; ces nano-particules seront ensuite étudiées par fluorescence, utilisées en catalyse, etc.

WP2, Nano-structures organiques, utilisera des méthodes de synthèse macromoléculaires innovantes pour préparer des copolymères multi-fonctionnels, des nano-boîtes organiques, etc. Leur nano-organisation sera étudiée par STED, NMR, méthodes de diffraction, rhéologie, etc.

WP3, Réseaux poreux, aura pour tâche de construire des réseaux hiérarchiques inorganiques ou organo-métalliques. Leurs propriétés (catalyse, adsorption) seront imagées avec une hyper-résolution spatiale et temporelle. Des modèles macroscopiques permettront d'intégrer à un échelon supérieur les observations cinétiques microscopiques.

WP4, Matériaux hybrides, préparera a) des nanogels intelligents stimulables dans des milieux respectueux de l'environnement (CO_2 supercritique), b) des nanotubes de carbon orientés et fonctionnalisés par réplication de porosité ou électro-filage, c) des matériaux polymères/inorganiques hybrides contenant par exemple des polyesters et des plaquettes d'argile exfoliée.

WP5, (Bio)membranes, étudiera la dynamique des microdomaines ("rafts") dans les couches lipidiques et les surfaces bactériennes contenant des acides lipoteichoïques. Des membranes synthétiques seront utilisées comme matériau de base pour l'ingénierie tissulaire, ou comme membranes semi-perméables pour la nano-filtration.

WP6, Biomolécules et Biocatalyse, visualisera avec une résolution élevée les conformations de l'ADN, et des (sous-)compartiments cellulaires, en utilisant des GFPs, des sondes Ru, etc. Des enzymes, des ARNs ou des matériaux hybrides bio-mimétiques seront utilisés en catalyse organique.

WP7, Revêtements fonctionnels, concevra a) des électro-revêtements hémo- ou pH-stimulables à partir de divers monomères, b) des revêtements polymères fluorés et catalytiques, compatible avec le CO_2 supercritique, c) des revêtements synthétiques anti-biofilms.

WP8, Systèmes conjugués supramoléculaires, contrôlera les propriétés optiques et de transport de systèmes donneur/accepteur séparés en deux phases, de copolymères à blocs et de cristaux liquides discotiques, avec un intérêt particulier porté aux conducteurs organiques chiraux.

WP9, Auto-assemblage interfacial, *utilisera les microscopies de champ proche (par exemple le STM* électrochimique) pour étudier, stimuler et manipuler des monocouches chirales et nano-patternées, et examinera l'utilisation de couches 'nano-patternées' comme patrons pour la construction d'architectures 3D.

Pour garantir un maximum d'interactions, les partenaires apporteront leurs contributions au niveau de **quatre plateformes différentes**:

PLATEFORME 1: THÉORIE ET MODÉLISATION

La modélisation multi-échelle part de structures simples (molécules isolées, sous-éléments moléculaires) pour aborder des systèmes de complexité croissante: chaînes de polymères et assemblages supramoléculaires construits sur base d'interactions non-covalentes, systèmes moléculaires inclus dans un solvant ou une matrice polymère, (macro)molécules adsorbées en surface ou dans des pores, et enfin interfaces dans des *systèmes hybrides organiques/inorganiques, organiques/organiques et organiques/biologiques. Nos buts* premiers seront:

(i) de déterminer la nature et l'intensité des interactions moléculaires à l'échelle nanométrique;

(ii) d'interpréter les données spectroscopiques et les propriétés photoniques;

(iii) de comprendre la dynamique moléculaire dans l'espace et le temps, pour des processus chimiques et (photo)physiques.

Des outils théoriques adaptés à l'échelle des problèmes seront implémentés, depuis les méthodes de chimie quantique jusqu'aux techniques de modélisation moléculaire basées sur des champs de force.

PLATEFORME 2: SYNTHÈSE & FABRICATION (INGÉNIERIE MOLÉCULAIRE)

2.1. Synthèse de blocs de base: La chimie supramoléculaire repose sur la possibilité de dessiner des blocs de base de nature (organique/inorganique), de taille (molécules, oligomères, (co)polymères, particules,...), de forme (sphérique, cylindrique, en éponge, vésiculaire,...) et de réactivité variées. Il y a un grand besoin de méthodes efficaces et sélectives de synthèse de ces pièces élémentaires (lego). Une attention particulière sera donc portée aux polymérisations vivantes et contrôlées, aux procédés sol-gel, et à la fabrication de nanoparticules.

2.2. Auto-assemblage et nano-manipulation des blocs de base (0D; 1D; 2D; 3D): Des stratégies seront développées pour permettre l'(auto-)assemblage de blocs de base complémentaires, leur adsorption, leur greffage et leur manipulation en surface, leur dispersion et leur nano-organisation dans des matrices (inorganiques, polymères), en vue de générer de nouveaux comportements et d'obtenir des propriétés spécifiques dans les domaines de l'opto-électronique, de la catalyse, de la (bio-)détection, des bio-matériaux, des polymères d'ingénierie, etc.

2.3. Design chimique bio-mimétique: En ce qui concerne les sites actifs des enzymes et, de manière analogue, des systèmes supramoléculaires, un point clé est d'arriver à contrôler par des modifications ciblées l'accès au site actif, sa polarité et son encombrement stérique. Les méthodes qui seront privilégiées sont la synthèse de composés de coordination à l'intérieur même de matériaux poreux (à la manière d'un 'bateau dans une bouteille'), ainsi que l'impression moléculaire. En outre, des méthodes de design à haut rendement copieront les stratégies génétiques de l'évolution naturelle.

2.4 Des *'nanopatterns'* *de monocouches adsorbées, et leur utilisation comme cachet ou patron pour la* croissance de multi-couches, seront explorés en présence de blocs de base comme des molécules conjuguées chirales ou des polymères conducteurs.

PLATEFORME 3: STRUCTURE & FONCTIONNALITÉ

3.1. L'interaction et la reconnaissance entre deux blocs de base est l'événement élémentaire du fonctionnement de systèmes supramoléculaires. La synthèse chimique et la théorie procureront une aide au design de nouvelles interactions de spécificité accrue.

3.2. Adsorption, mouvement, diffusion: Nous étudierons expérimentalement et modéliserons l'effet de la nature des adsorbats chimiques sur les structures obtenues, ainsi que la cinétique d'adsorption et de diffusion sur des surfaces modèles, sur des surfaces réelles et dans des pores. Le mouvement de translation et de rotation de chaînes individuelles de polymère, et même de segments de chaînes, sera enregistré par spectroscopie de molécule unique. Des sondes fluorescentes (petites molécules, ou protéines marquées) seront également utilisées pour imager le mouvement (processivité) d'enzymes, pour suivre le transport des substrats et produits vers ou à partir d'enzymes ou encore à travers des membranes, et pour suivre la formation de micro-domaines ("rafts") dans des membranes bi-couches naturelles et artificielles. La diffusion et la dérive d'excitons et de porteurs de charge sera suivie dans des systèmes nano-structurés fabriqués à partir de polymères conjugués et de nano-boîtes quantiques, ou dans une hétéro-jonction entre un polymère conjugué et de petites molécules, ou entre deux types de petites molécules.

3.3. Stimulation chimique: A la réception d'un signal chimique ou d'un réactif, la réponse d'un système supramoléculaire ira du changement subtil d'une liaison faible, à une rupture complexe avec formation de

nouvelles liaisons covalentes comme lors d'un processus catalytique. Notre attention portera sur la façon dont l'organisation supramoléculaire peut résulter en une activation concertée ou consécutive des liaisons. Sur le plan méthodologique, nous nous concentrerons sur l'imagerie en temps réel de l'activation chimique sur de large domaines, avec une hyper-résolution spatiale.

3.4. Dynamique consécutive à d'autre stimuli: Des stimuli tels que *T*, *E*, pH, un flux, un champ magnétique statique, des forces de cisaillement ou des photons peuvent provoquer des changements d'organisation supramoléculaire. Nous en étudierons la réversibilité, l'hystérèse, les constantes de temps et l'homogénéité spatiale. Des matériaux intelligents à mémoire ou à réponse réversible seront développés.

PLATEFORME 4: DISPOSITIFS & SYSTÈMES RÉPONDANTS

Certains des concepts développés ci-dessus seront utilisés pour développer des applications spécifiques comme la délivrance contrôlée de médicaments, des capteurs, des dispositifs opto-électroniques ou des polymères à mémoire de forme

I. 3. OBJECTIVES, MOTIVATION AND STATE OF THE ART (5 pages maximum)

Describe the project's objectives and research goals.
Define the problems being addressed by positioning them in relation to the current state of knowledge.

Supramolecular chemistry describes the chemistry beyond the molecule and studies chemical species held together by non-covalent intermolecular interactions. The aim of the project is to develop novel systems, to understand driving forces that allow bi- and tri-dimensional organization, to develop methods and tools to investigate, address, manipulate supramolecular structures and to determine and exploit their specific properties.

Special emphasis will be placed on the functionality of four major supramolecular systems:
- **Nanostructured systems**
- **(Hierarchically) structured nanoporous materials**
- **(Hybrid) biomaterials**
- **Thin films (organic, inorganic and hybrid)**

Within this framework, nine specific research packages have been defined; they will be tackled at four different platform levels by several partners with complementary expertise and instrumental capabilities:
- **Theory and modeling**
- **Synthesis and fabrication (molecular engineering)**
- **Structure and functionality**
- **Devices and responsive systems**

In this project, **Nanostructured systems** are intended as zero-dimensional metal, oxide, or organic nanoparticles. The research activities will be focused on two themes: Nanodots and photonic crystals, and Organic nanostructures, forming workpackages (WP) 1 and 2 (it must be emphasized that strong interconnections between workpackages, and the research groups working on those workpackages, will be actively promoted throughout the project, as shown in table 1 and figure 1 of form D).
(Stabilized) metallic nanoparticles and clusters are known to act as catalysts and luminescent centers. The research here will be aimed at *stabilizing noble metal nanoparticles and increase their luminescence by coating them with oligopeptides*, which at the same time will act as attachment for lipids and enzymes. This will yield novel bright and stable probes to study membrane organization and enzyme kinetics. In the field of catalysis, *the catalytic properties of (novel) non-equilibrium clusters* will be explored. By the simultaneous characterization of the optical, morphological and catalytic properties of single metal clusters, structure/activity relationships will be obtained.
The catalytic properties of the oxides and nitrides of transition metals, prepared by wet methods and magnetron sputtering, are known. The ability of the consortium *to control the morphology of these transition metal oxide and nitrides nanoparticles and to probe the properties of adsorbed molecules in bulk samples as well the catalytic activity of single particles* will be used to elucidate the relation between morphology, preparation method, and catalytic properties. For the determination of single particle properties, the ability of the consortium to prepare patterned surfaces will be essential.
Recent studies show that incorporation of semiconductor (often II-VI) nanoparticles in conjugated polymers can lead to increased efficiency in electroluminescence and solar energy conversion. However, a global description of the optoelectronic properties of those systems is still out of reach. Combining the expertise of the partners in: (i) the preparation of tailor-made semiconductor nanoparticles, (ii) the controlled dispersion of inorganic particles in polymer matrices, (iii) the dynamic studies of the photophysical response of complex, multi-component systems, and (iv) the modeling of the electronic, optical, and interfacial properties of semiconducting materials, is expected to generate *detailed fundamental understanding of the 'chemical structure-morphology-optoelectronic properties' relationships in those organic/inorganic hybrid semiconducting devices*.
Organic nanoparticles that display remarkable stability can be obtained by micellar aggregation of amphiphilic block copolymers in a solvent selective for one block. The size and shape of those micelles can be controlled via the copolymer molecular parameters, and via the conditions used for their preparation (e.g., polymer concentration, temperature, pH,...). It is the goal of the consortium *to extend the approach relying on the micellar aggregation of block copolymers into a new domain, in order to produce organic nanodots with electronic properties similar to those of their 'classical' inorganic (metallic or semiconducting) counterparts*.

This will imply the design and synthesis of amphiphilic block or graft copolymers containing conjugated and/or semiconducting segment(s) likely to form the micelle core under selected aggregation conditions.
Along the same line, well-defined polymer nanostructures can be prepared based on recent developments of fully controlled synthetic mechanisms and strategies leading to macromolecular architectures (e.g., block and graft copolymers, either linked covalently or via supramolecular interactions) with perfectly defined molecular parameters such as chain length and chain length distribution, grafting density, molar ratio of the components. The major objective of the consortium here will be *to produce (multi-)stimuli-responsive systems able to act in solution (e.g., upon a change in the temperature, mechanical stress and/or pH) or in the solid state (as shape-memory polymers)* through a proper combination of amphiphilic and/or soft and hard segments. In the latter case, new synthetic concepts will be developed to design a new generation of shape-memory polymers based on multi-block copolymers with fast and quantitative response that can act within a broader temperature range than the existing materials.

(Hierarchically) structured nanoporous materials are systems with pore size covering the whole micro-mesopore domain, *different architecture and even multimodal distribution. A specific workpackage (*Porous frameworks, WP3) will be dedicated to this class of systems.
There is a strong need to tailor porous materials towards specific applications in adsorption, separation, catalysis and controlled release. Such progress is only possible if (i) materials can be assembled in a controlled way, and (ii) detailed information is available on the relations between structure and functionality. For the assembly of porous materials, e.g., siliceous solids in liquid crystalline media, this project will focus on *exploiting the liquid crystalline properties during assembly of zeolite building blocks or nanoslabs*, using a combination of rheology, Raman and diffraction techniques. Opportunities are also exploited in the *assembly of 2D or 3D metal-organic frameworks (MOFs) from cations and multicipital ligands*. Regarding structure-function relationships, a major lacuna in the current state-of-the-art is that most (*in situ*) characterization techniques only yield data for ensembles; the contributions of the individual crystal faces or edges, channels, pore mouths, and the outer surface to sorption and catalysis can hardly be disentangled. This consortium will *seek to advance knowledge of MOFs, zeolites or layered materials via highly spatially and/or temporally resolved studies of dynamic processes* (sorption, acid / base / redox catalysis) *combined with a range of modeling techniques*.

(Hybrid) biomaterials are mimicking the natural components that function by a complexity of equilibria, intracellular and extracellular catalysis, and interface phenomena, the intra- and extracellular functions being governed by supramolecular arrangements of various biopolymers, inorganic and organic molecules. The research activities on those systems will be organized under three workpackages: Hybrid Materials, (Bio)membranes, and Biomolecules and Biocatalysis (WP4, WP5, and WP6)
Hybrid nanomaterials that can exhibit synergistic effects are particularly in the scope of the present project. In this field, protein/polymer nanohybrids are potentially attractive systems that could trigger the delivery of a drug by the use of a biochemical stimulus. Pioneering work was recently reported on the synthesis of nanogels. However, the elaboration of doubly cross-linked nanogels would still constitute a major advance. From the synthetic point of view, the consortium will direct efforts to *the development of processes for the preparation of hybrid nanogels, especially in supercritical carbon dioxide*. The properties of these novel doubly cross-linked nanomaterials will be studied in detail to elaborate new concepts for drug release triggered by biochemical stimuli.
Carbon-based hybrid systems with a well-defined structure at the nanoscale are another promising class of materials, with a particular emphasis on the electrical and mechanical properties and their interactions with biomolecules. In this context, new synthetic methods, based on controlled radical polymerization, will be tested for *the preparation of polyacrylonitrile-containing block copolymers*. Their self-assembly in bulk or in solution followed by graphitization will be studied in order *to generate novel well-controlled carbon nanostructures and carbon/metal nanohybrids*. The physico-chemical properties of these novel materials will be compared with those of carbon nanotubes and fullerenes. Nanocomposites incorporating these nanofillers within a polymer matrix will also be investigated as potential new biomaterials. Strong anchoring of a ligand to the filler, which is expected to compatibilize the filler-matrix system, will be explored in detail. Novel synthetic approaches such as layer-by-layer deposition will also be developed for the preparation of those nanocomposites.
Over the past decade, evidence has accumulated for the existence of lipid rafts in cell membranes, i.e., localized membrane micro- and nanodomains that are enriched in saturated phospholipids, sphingolipids, and cholesterol. These constituents form liquid-ordered (Lo) domains that exhibit less fluidity than the surrounding liquid disordered (Ld) state of the plasma membrane. Despite the key roles lipid rafts may play in many diverse biological functions, experimental data demonstrating their existence are scarce. The consortium *will develop a platform of complementary molecular probing techniques, i.e., submicron fluorescence microscopy, space and time resolved spectroscopy, and atomic force microscopy, to visualize rafts in synthetic bilayers and cell*

membranes, particularly oligodendrocyte membranes. These tools will allow one to characterize the nanoscale structure, physical properties and stability of the membrane domains over a broad of time and space range and to study their response to relevant (bio)chemical stimuli.
The role of different proteins responsible for assembly and disassembly of bacterial biofilms has been determined on a scale involving always a large number of molecules. The consortium will investigate this role at the level of single protein molecules using both atomic force spectroscopy and single molecule fluorescence in order *to observe the expression, transport and interaction of the proteins responsible for assembly and disassembly of bacterial biofilms*. The membranes of lactic acid bacteria are known to be immunostimulatory counterparts to Gram-negative lipopolysaccharides. Combining the single molecule techniques mentioned above, the consortium will *elucidate the local inflammatory and anti-inflammatory responses to those bacteria and relate them with the amount and type of lipoteichoic acids present*.
It is well known that collagen networks, possibly coated by other relevant bio- or biomimetic molecules, can be used as scaffolds for growing different types of cells in view of tissue engineering applications. To offer new routes to the control of the process of cell growth and/or differentiation, the consortium will *prepare novel (block)copolymers that can be cast as membranes or electrospun to form nanofibers before being coated by proteins*. Fundamental studies based on surfaces patterned with proteins will also be conducted. Transferring the knowledge obtained on 2D systems to 3D scaffolds is expected to bring substantial progress to the field. Again the broad range of available techniques will allow a detailed characterization of both the scaffolds and the self-assembly process of biomolecules.
Besides exploring the biochemical and biological aspects of membranes, the consortium will also *use the existing expertise in polymer synthesis and characterization to develop and characterize novel synthetic membranes*. As alternative for solvent resistant nanofiltration membranes (SNRF) prepared by solidification of emulsified polymer via phase inversion (SEPPI), *novel nanofiltration membranes will be prepared based on segmental polymer networks, polyelectrolyte complexes and incorporation of metal organic frameworks (MOFs) in organic polymers*. The structure-activity relations will be determined by combining the exploration of their filtration and chromatography properties for a broad range of products (ranging from catalysts to metal and (bio)organic nanoparticles or macromolecules) with a broad range of optical and scanning probe characterization methods.
While fluorescence microscopy has long been a workhorse for cellular biology, major scientific advances can be expected if: (i) the resolution can be taken beyond the diffraction limit, and (ii) new, advanced and specific probes are available for studying DNA, enzymatic catalysts, and other proteins. The consortium will direct efforts to *improving the resolution beyond the diffraction limit, via stimulated emission depletion (STED) microscopy*, using pairs of synchronized laser pulses. More generally, saturable optical molecular transitions can be used for achieving resolution beyond the diffraction limit. *Novel optical probes will be considered*, with particular attention dedicated to Dronpa. Dronpa is the first reversibly photoswitchable fluorescent protein from the GFP family, and is a suitable candidate for superresolved microscopic experiments, especially when it is expressed in a fusion protein with another protein of interest. Such techniques will be applied to membranes and cellular subcompartments of, e.g., oligodendrocytes and gastro-intestinal tract cells. *New Ruthenium complex-based probes will be applied in structural and dynamic DNA studies*, concerning, e.g., plasmid DNA, vectorization with cationic polymers, telomeric sequences. Designing the right probes is also essential for studying enzyme kinetics at the single molecule level, e.g., regarding enantioselectivity of populations of biocatalysts. *Insights in biocatalysis at the single molecule level will be extended to macroscopic biocatalytic work, including the design of new biocatalytic proteins and RNAs via molecular biological techniques*. In a parallel approach, biomimetic catalysts will be designed, based on inorganic support materials.

Thin films (be they organic, inorganic, or hybrid) are ubiquitous in functional systems, e.g., as the active element in semiconducting devices, as functional polymer coatings or as molecular layers on surfaces, and (bio)membranes. Three workpackages will be focused on that class of systems: Functional coatings, Supramolecular conjugated systems, and Self-assembly at surfaces (WP7, WP8, and WP9)
In the field of functional coatings, the major pending question is the adhesion of the coating to the underlying substrate. A number of approaches exist, which generate strongly adhering films; however, this is often achieved at the expense of the outer surface functionality. It is the aim of the consortium to design and elaborate new, strongly adhering coatings with a broad variety of possible functionalities. For that purpose, various original methods such as *the electrografting of new acrylic derivatives or the synthesis of bioinspired copolymers prone to adhesion to metals will be developed*. The systems that are targeted by the grafting of these functional coatings are: (i) surfaces efficient in preventing biofouling, (ii) responsive coatings for the elaboration of biosensors, and (iii) superhydrophobic surfaces for anti-corrosion properties. Another major activity will be *to develop novel fluorinated coatings incorporating ligands for catalytic processes in supercritical CO_2*.

The performances of thin films of conjugated materials in semiconducting devices (OLEDs or solar cells) depend simultaneously on their solid-state optical properties and their charge transport capabilities, which in turn are deeply affected by the supramolecular organization of the polymer/oligomer molecules. The consortium activities will focus on *the design, the synthesis, and the characterization of supramolecular conjugated systems with optimal optical and transport properties, combined with controlled supramolecular organization and microscopic morphology*. While intense research is dedicated worldwide to the optimization of organic materials for electronic devices, the approach proposed by the consortium, which combines synthetic groups with relevant synthetic expertise with groups able to characterize the morphology and opto-electronic properties, will provide important advances, both in terms of fundamental understanding of structure-properties relationships and in terms of device performance. In particular, *control over the lateral length scale of phase separation in donor-acceptor systems* will be sought either by the spontaneous micro-domain structuration of block copolymers or liquid-crystalline materials, or by the generation on the substrate surface of nanopatterns with different affinities for the active polymers/molecules.
In terms of self-assembly at surfaces, the well-established methodology consists in determining the two-dimensional assembly of physisorbed functional molecules with scanning tunneling microscopy (STM). The consortium intends *to extend that STM-based approach to complex supramolecular systems able to undergo reversible structural changes by an external stimulus* (e.g., conformational changes in functional macrocycles upon ion complexation). Along the same line, *the generation of chiral functional monolayers* via the physisorption of chiral functional molecules will be investigated at the organic liquid/solid interface with a combination of STM and molecular modeling techniques. Another major goal of this activity will be *to understand the formation of 3-D structures from the ordered monolayers.*
Electrochemical scanning tunneling microscopy (EC-STM) will be implemented for *the formation and investigation of physisorbed monolayer-thick coatings at the interface between aqueous electrolytes and electrified metal surfaces*. For this project, an important advance expected from EC-STM operation is the possibility to influence the supramolecular ordering and dynamics of compounds at the aqueous electrolyte/solid interface by control of the applied potential. *Chemical reactivity within the monolayers will be induced in a controlled way and investigated on the molecular scale* via a twofold approach: on the one hand, UV irradiation or the electric field in the STM junction will be used to initiate polymerization processes *to produce single molecular wires and/or 2D polymers*. On the other hand, molecular adsorption on metal surfaces (with copper and gold as prototype systems) under potential control, studied via EC-STM, is expected to open many possibilities *to explore redox-sensitive switching or templated growth of metallic nanoparticles and wires*.
Over the last few years, considerable efforts have been made within the IAP partnership to develop original state-of-the-art methodologies to obtain a large variety of nano-patterned surfaces, by combining nanolithography methods such as e-beam lithography or nano-imprint lithography with chemical assembly methods. On that basis, several possibilities will be explored to control the spatial localization of selected functional systems developed in the project. In particular, this general approach will be used to: (i) *generate structured and nanopatterned thin film samples of dye molecules* by local grafting of chromophores or nano-imprinting of dye-loaded polymers; (ii) *control the local deposition of bio-macromolecules*, in order to prepare bio-active surfaces able to direct / control cell growth; (iii) *generate assemblies of conjugated oligomers and polymers* into well-defined semiconducting nanostructures; (iv) *realize nano-structured catalytic surfaces* for the case of heterogeneous catalysis, or by grafting locally homogeneous catalysts; and (v) *investigate the behaviour of small islands of responsive macromolecules* (temperature- or photo-sensitive systems) when confined into islands of size close to the intrinsic dimensions of the chains.

Besides the specific interactions between workpackages, which are described in Form D, integration of the research activities throughout the whole network will take place at the level of the four platforms:
The **Theory and modeling** platform will encompass systems of growing complexity, from simple structures (single molecules, molecular building blocks) to polymer chains and supramolecular assemblies built by non-covalent interactions, molecular systems embedded in a solvent or polymer matrix, (macro)molecules adsorbed at surfaces or within pores, and finally interfaces in organic/inorganic, or organic/organic, or organic/bio hybrid nanosystems. The modeling methods developed and implemented within this platform will be applied throughout the workpackages, for instance to understand (macro)molecule/substrate interactions or to unravel the electronic excitation dynamics in multi-component (organic/organic or organic/bio) systems.
Synthesis and fabrication (including molecular engineering) will be ubiquitous in the project. Fully controlled polymerization protocols and procedures for preparing, assembling and characterizing building blocks (e.g., nanodots or micelles) will be developed and 'exported' to activities related to different workpackages. Nanopatterning of adsorbed layers (e.g., starting from a patterned substrate) and their use as stamps and templates will be explored. (Chirally) ordered 2D-structures will serve as templates for 3D-nanostructures.

This network has built a very strong expertise in the use of single-molecule methods to probe the **Structure and functionality** of the supramolecular systems under study. Further developments of those approaches, including high-resolution microscopy techniques (stimulated emission depletion -STED, fluorescence recovery after photobleaching-FRAP), are planned in this project, which will spur the research activities in a number of workpackages. For instance, fluorescent probes (small molecules, or labeled proteins) will be used to image the motion (processivity) of enzymes, to follow transport of substrates and products to or from single enzymes and through membranes, and to follow formation of rafts in synthetic and natural bilayer membranes.
Finally, the activities of the Devices and responsive systems platform will rely on concepts discovered and/or demonstrated in the various research tasks. The application fields of those concepts are expected to be related to drug delivery devices, sensors, optoelectronic devices, and shape memory polymers. Several aspects of the design and fabrication of such devices will be very similar (e.g., for sensors and optoelectronic systems) and will then be used transversally between different workpackages.

I. 4. DETAILED DESCRIPTION OF THE PROJECT (15 pages minimum, 25 pages maximum)

- Submit a general description of the project as well as a description detailing each workpackage and indicate the partners involved in each workpackage.
- Illustrate by means of a table or scheme the interaction between the partners within a workpackage and the interaction between the workpackages.
- Describe and justify the methods and proposed approaches in relation to the state of the art.
- Describe and justify how the contribution of the different partners will be integrated.

1. GENERAL DESCRIPTION OF THE PROJECT

Supramolecular chemistry describes the chemistry beyond the molecule and studies chemical species held together by non-covalent intermolecular interactions. As described in Form B, the aim of the project is to develop novel systems, to understand driving forces that allow bi- and tridimensional organisation, to develop methods and tools to investigate, address, manipulate supramolecular structures and exploit their specific properties.

The **following functional supramolecular systems** will be studied:

1. Nanostructured systems: Typical nanostructured systems are zero-dimensional metal and semiconductor nanodots. They are studied as such, or in conjugated liquid crystals and polymers.

2. (Hierarchically) structured nanoporous materials: Via supramolecular templating, block copolymer templating and (repeated) nanocasting, nanoporous materials with pore size covering the whole micro-mesopore domain, different architecture and even multimodal distribution are accessible for use in separation, catalysis of large (bio)molecules. Among them are of particular interest mesoporous organogels, nanostructured carbon materials, (multi)porous oxides, metal-organic frameworks and (supported) nanoparticles.

3. (Hybrid) biomaterials: Artificial biomaterials are mimicking the natural components that function by a complexity of equilibria, intracellular and extracellular catalysis, and interface phenomena, the intra- and extracellular function being governed by supramolecular arrangements of various biopolymers, inorganic and organic molecules. Biomimetic material design requires tailored chemistry leading to characterized biomimetic surfaces and matrices, membranes, probes for cellular components, biomimetic catalysts, nanosized patterned surfaces, and hybrid systems.

4. Thin films (organic, inorganic and hybrid): Functional systems are most often organized in thin films; this applies, e.g., to conjugated polymers incorporated as the active element in semiconducting devices, functional polymer coatings or molecular layers on surfaces, and (bio)membranes.

To guarantee intensive networking, the partners for each of the system classes will contribute at the level of **four different platforms**:

PLATFORM 1: THEORY & MODELING

Multiscale modeling starts from simple structures (single molecules, molecular building blocks) and extends towards systems of growing complexity: polymer chains and supramolecular assemblies built by non-covalent interactions, molecular systems embedded in a solvent or polymer matrix, (macro)molecules adsorbed at surfaces or within pores, and finally interfaces in organic/inorganic, or organic/organic, or organic/bio hybrid systems.

The major goals of the activities of this platform will be:
(i) to determine the nature and intensity of the intermolecular interactions on the nanoscale;
(ii) to provide interpretation to the spectroscopic data and the photonic properties;
(iii) to understand the molecular dynamics in space and time, for (photo)physical and chemical processes.
Theoretical tools adapted to the scale of the problem will be implemented, from state-of-the-art quantum chemical methods to force-field-based molecular modeling techniques designed for accurate simulations of both organic and inorganic compounds, as well as biomolecules.

PLATFORM 2: SYNTHESIS & FABRICATION (MOLECULAR ENGINEERING)

2.1. Building block Synthesis: Supramolecular chemistry relies on the capability of designing/tailoring building blocks of various nature (organic/inorganic), size (molecules, oligomers, (co)polymers, particles...), shape (spherical, cylindrical, sponge-like, vesicular,...) and reactivity. A work-package will focus on efficient and selective processes for synthesis of these elementary (meccano or lego) pieces, with special emphasis on controlled/living polymerizations, sol-gel processes, and nanoparticle fabrication.

2.2. Self-assembly and nanomanipulation of building blocks (0D; 1D; 2D; 3D): Strategies are devised for (self)assembly of complementary building blocks, for their adsorption, grafting and manipulation at surfaces, their dispersion and nanostructuring within matrices (inorganic, polymeric) with the purpose to trigger novel behavior and specific properties in optoelectronics, catalysis, (bio)sensing, biomaterials, engineering polymers, etc.

2.3. Biomimetic chemical design: In active sites of enzymes and supramolecular systems alike, key issues are control over the access, steric and polarity factors, and targeted active site modification. Favored assembly methods are 'ship-in-a-bottle' synthesis of coordination compounds in the channels and cages of porous materials, and molecular imprinting of transition states or analytes. High-throughput design methods copy the genetic strategies of natural evolution.

2.4 Nanopatterning of adsorbed monolayers and their use as stamps and templates will be explored. (Chirally) ordered 2D-structures will serve as a template for 3D-nanostructures, using building blocks such as chiral conjugated molecules or conducting polymers. Patterning of the adsorbed molecules will also be investigated starting from a patterned substrate.

PLATFORM 3: STRUCTURE & FUNCTIONALITY

3.1. Interaction and Recognition between two building blocks is the elementary event for supra-molecular function. Chemical synthesis and theory aid in designing new interactions with increased specificity.

3.2. Adsorption, Motion, Diffusion: We will investigate the effect of the nature of the chemical adsorbate on the structures formed and on the kinetics of adsorption at model surfaces and at real surfaces. The adsorption and diffusion of small molecules in nanoporous materials will be simulated and the results related to experimental data. The translational and rotational motion of individual polymer chains and even of chain segments will be recorded using single molecule spectroscopy on probes dissolved in or covalently bound to a polymer. Fluorescent probes (small molecules, or labeled proteins) will also be used to image the motion (processivity) of enzymes, to follow transport of substrates and products to or from single enzymes and through membranes, and to follow formation of rafts in synthetic and natural bilayer membranes. The diffusion and drift of excitons and charge carriers will be monitored in nanostructured systems consisting of a conjugated polymer and nanodots or with a bulk heterojunction between a conjugated polymer and small molecules or between two types of small molecules.

3.3. Chemical stimulation: Upon reception of a chemical signal or reagent, the supramolecular response can vary from a subtle change of a weak bond, to complex breaking and formation of covalent bonds as in supramolecular catalytic processes. Focus will be on how supramolecular organization contributes to concerted or consecutive bond activation. Methodology concentrates on real-time imaging of chemical activation over large spatial ranges, with increasing spatial resolution.

3.4. Dynamics upon other stimulation: External stimuli such as *T*, *E*, pH, flow, static magnetic field, shear or hv will be used to induce changes of the supramolecular organisation. The reversibility, hysteresis, the time constants and the spatial homogeneity of the response will be studied with advanced physical techniques. Smart materials with memory behavior or reversible switching capability will be developed.

PLATFORM 4: DEVICES & RESPONSIVE SYSTEMS

Concepts will be designed and proven for specific applications such as drug delivery devices, sensors, opto-electronic devices and shape memory polymers.

2. DETAILED DESCRIPTION OF THE WORK PACKAGES

Work package 1: Nanodots and photonic crystals

For zero-dimensional structures of metals, semiconductors, oxides, carbides and nitrides, various applications exist, such as building blocks of photonic crystals, catalysts or diagnostics. This requires, however, reliable and flexible ways to prepare those entities as well as different methodologies to characterize them. The latter will allow to determine structure-properties relationships and to understand their behaviour. To rationalize these objectives, in parallel to the characterization a modeling approach using molecular mechanics as well as semi-empirical and *ab initio* methods will be used, to simulate the properties and get a deeper insight in their functioning.

Task 1.1: Photonic crystals (2, 6, 8, 10, EU1)
Through other collaborations inside K.U.Leuven partner 2 has access to photonic crystals prepared by convection-driven self-assembly of nanospheres of silica and/or polymer particles. Alternating layers of particles of different size or refractive index is expected to lead to self-assembled photonic heterostructures, optical pn-junctions, nanocavities and photonic atoms. On the level of platform 2 partner 6 will prepare templates, incorporation of patterned layers will be attempted in order to get a more "complete" stop band (p 2 and 6) for the deposition of patterned layers (stripes or chess board), and design, in collaboration with partner 2, methods to transfer the patterned layers to the photonic crystal. It will also be attempted to incorporate metal or semiconducting nanoparticles in the photonic crystals, either as a full layer or as random or patterned doping of a layer (p 2 and p 6). The metal and semiconductor particles will be obtained from EU1 (cfr infra), commercial sources or from other collaborations outside the IAP project.
On the level of platform 3, the influence of the stop and pass band on the emission spectra and decay times of the incorporated dye molecules will be investigated at the bulk and single molecule level by partner 2. Additionally, nanocavity effects on the fluorescence properties of an ensemble of dyes in a photonic crystal resonator will be explored at the bulk level (p 2) using femtosecond transient absorption or Z-scan methods, and at the single molecule level (p 2) using confocal or widefield fluorescence microscopy. The coupling of embedded semiconductor and metal nanoparticles with photon modes will be investigated with luminescence and absorption spectroscopy for bulk samples as well as single molecules (p 2).
In order to understand the properties (spectral characteristics, fluorescence decay time, fluorescence polarization) of dye molecules incorporated in these structures partner 10 will, on the level of platform 1, perform theoretical modeling based on electrostatic interaction schemes
At the device level (platform 4), it will be investigated how to create highly ordered nano- and micro-sphere packings or negative replicas thereof in the microfluidic chromatographic separation devices that are currently being developed by partner 8. Such highly ordered structures could yield a dramatic improvement of the chromatographic separation efficiency of biomolecules as compared with the current state-of-the-art.

Task 1.2: Catalytic metal nanoparticles (1, 2, 3, 4, 5, 6, 13, EU 1)
Catalytic metal nanoparticles will be prepared by partner 5 by sputtering onto non-porous supports (platform 2) and by CVD (chemical vapor deposition) on porous supports. The former approach has the important advantage that non-equilibrium clusters, e.g. gold-iron clusters can be made, for which the catalytic action is unexplored yet. Partner 6 will prepare nano-patterned catalytic surfaces by chemical nanolithography of silicon wafers, starting from nano-features of mercaptopropylsilanes onto which noble metal clusters will be selectively adsorbed or grown. For e.g. gold and silver, the clusters can be characterized optically by fluorescence spectroscopy and scanning probe microscopy (p 2). In case the distance between neighboring clusters is large enough (low coverage) the application of single molecule spectroscopy will be possible (p 2). In parallel the clusters deposited on a suitable "transparent" substrate will be characterized by TEM (p 5). Partner 1 will study the catalytic properties of the clusters (platform 3). Target reactions are selective hydrogenations of polyfunctional molecules, e.g. enones, unsaturated nitriles, substituted aromatics etc. These reactions will be studied at the macroscopic level, but also at the single molecule level using dedicated fluorescent reagents or products. This will allow to establish relationships between reaction selectivity and metal particle size or structure. Partner 2 will explore the use of surface enhanced Raman spectroscopy, which allows one to detect adsorbed molecules with single molecule sensitivity. Model clusters will be investigated theoretically by partners 4 and 13 to determine their electronic structure, with the aim of establishing relationships with the catalytic properties (Platform 1). The catalytic properties of nano-patterned catalytic surfaces will be investigated with respect to efficiency and selectivity by partner 6 in collaboration with partners 1 and 2, using scanning probe microscopy and confocal fluorescence microscopy (for reactions involving fluorescent products). Partner 5 will develop models for the kinetics of the reactions catalyzed by the clusters

considering reaction, adsorption and transport processes. This will also be performed for the nano-patterned surfaces prepared by partner 6, for which optimal designs will be suggested from simulation results.
As an alternative to the clusters prepared by vacuum techniques and deposited directly on a support, noble metal clusters will be prepared by "wet" methods and stabilized by adsorption or grafting of suitable polymers (p 1, 3 and EU1). Partner 2 and partner 5 will characterize those clusters using respectively optical or scanning probe methods and TEM. Catalysis by those clusters will be explored by partner 1 (vide supra).

Task 1.3: Peptide-stabilized fluorescent silver/gold atomic clusters as probes for single molecule spectroscopy (1, 2, 3, 4, 5, 10, 11, 12)
It has been shown recently that highly fluorescing silver, gold and palladium clusters can be prepared by reduction of the corresponding salts. Fluorescing silver and gold nanoclusters prepared by partner 2 will be stabilized in the presence of a library of oligopeptide fragments (FLiTrx) expressed in membrane proteins of *E. Coli*. by partner 12. Using fluorescence activated cell sorting (FACS) it will be possible to separate highly luminescent bacteria and to correlate the luminance of the particles to their size (p 12). By depositing the nanoclusters on a grid, their size can be checked by TEM (p 3 and 5). By growing colonies of the highly fluorescent bacteria and analyzing their genome, one can find out which peptide sequences stabilize metal clusters with a specific size, with a potential use as fluorescent label. Using molecular mechanics and semi-empirical calculations it will be attempted to rationalize why certain peptides stabilize clusters of a certain size (p 4 and 10). As soon as the optimal peptide length and sequence are determined, the stability and photophysical properties of the fluorescing nanoclusters will be determined by both bulk and single molecule optical experiments (p 2). Linking the peptide fragments to lipids or enzymes it will be possible to use the gold nanoparticles to study "rafts" in lipid membranes in collaboration with partner 11 (see also WP 5) . The link will probably change the partition coefficient of the lipids between the liquid ordered (L_o) and disordered (L_d) phases. This, however, is not problematic as long as the mobility and/or affinity of the lipid-linked gold particles remain sufficiently different in the L_d and L_o-phases. When the peptide fragments are coupled to enzymes, they can be used as labels in the study of single enzyme kinetics in collaboration with partner 1 (WP 6). Partner 1 will also evaluate the catalytic properties of nanoscale Au or Ag clusters, e.g. in olefin reduction or alcohol/aldehyde oxidation.

Task 1.4: Nonmetallic inorganic nanodots as catalysts, and as diagnostic or therapeutic agents (1, 2, 3, 4, 5, 6, 13, EU1)
Partner 5 will prepare nanometer-sized particles of ZrO_2 coated by consecutive layers of SiO_2 and transition metal oxides, nitrides or carbides. These layers should have a thickness varying between 1 and 100 nm (platform 2). Alternatively, partner 5 will prepare nanometer-sized particles of transition metal oxides and nitrides embedded in an amorphous tissue material, i.e. an amorphous phase joining the nanoparticles with "ordered" structure. Partner 5 will also explore the combination of particle growth and needle growth (platform 2). The properties of particles prepared by sputtering will be compared to those prepared by precipitation of precursor salts in the presence of random copolymers and block copolymers (p 3, 4, EU1). The latter approach allows one to obtain hydrophobic particles of oxides and sulfides, like some of the wide bandgap semiconductors. By designing suitable, surface-modifying copolymers, the interaction with a polymeric matrix can be optimized. Partners 3 and 4 will also explore the coating of inorganic nanoparticles with a polymer layer to ensure optimal stability against aggregation.
Partner 1 will explore the catalytic behavior of these inorganic nanoparticles (platform 3), e.g. in base-catalyzed condensation reactions or in redox processes. Partners 4 and 13 will model the electronic structure of the interface and the interfacial interactions with adsorbates (platform 1). It will be attempted to relate those interactions to the catalytic properties determined by partner 1. Partner 5 will develop the kinetics of the reactions catalyzed by the clusters considering ab initio models for the reactions and accounting for transport processes. Partner 6 will prepare patterned catalytic surfaces as described in task 1.2, with the size of adsorbing regions close to the size of the catalytic nanoparticles, while the distance between adsorbing regions will be in the micrometer range. These regular arrays of isolated catalytic nanodots will allow us to study catalysis at the single nano-particle level by fluorescence microscopy, using reactions involving fluorescent products or reagents. Such reactions may consist of the transformation of a non-fluorescent substrate into a fluorescent product, of the scission of a reagent bearing two complementary chromophores, or of the coupling of two reagents bearing complementary chromophoric groups. By following the fluorescence intensity and wavelength, and taking advantage of energy transfer from chromophores in close proximity (FRET), partners 1, 2 and 6 will quantify the functioning of these catalytic nano-islands. As a specific example of a patterned catalytic surface, one may think of surfaces decorated with e.g. basic oxide particles, catalyzing the in situ formation of dyes such as coumarins . In a later stage, one may expand the approach to preparation of bifunctional catalytic surfaces for consecutive transformations of organics.

Partner 3 will prepare magnetic iron oxide nanoparticles coated by functional polymers, suitable for NMR imaging or hyperthermia. For example, drug containing thermosensitive polymer coatings will be prepared with the purpose to release the drug where hyperthermia has been triggered by the action of a magnetic field. Moreover, specific tissues will be targeted by appropriate molecules grafted to the particles' surface, in order to minimize side effects. In addition to this therapeutic application, diagnostics will also be studied by NMR imaging.

Task 1.5: Semiconductor and metal clusters in OLEDS and solar cells (2, 4, 11, EU1)
Charge carrier recombination in organic materials leads to a ratio of 1:3 for singlet and triplet states. A possibility to recuperate the latter for luminescence is the incorporation of highly luminescent semiconductor nanoparticles which can either trap the triplet states, and convert them into luminescent electron-hole pairs, or which directly act as recombination center. Such particles have furthermore an extremely high photostability. In the present project polycarbazoles, poly(p-phenylene vinylene) or copolymers with oligofluorenes and naphthothiadiazole (available through partners 2, 11 or EU1) will be doped with semiconductor CdS or CdSe nanoparticles (2 to 6 nm). These nanoparticles are available to partner 2 through international collaboration (Platform 2) or are prepared by EU1 by precipitation of metal salts in the presence of a suitable, if possible partly conjugated copolymer and block copolymer. Modulation of hydrophilicity of such materials will be pursued via appropriate substitution of the side chains, e.g. with alcohol or carboxylic acid functional groups. The electron and hole mobility will be determined by the TOF (time-of-flight) method in the presence and absence of the nanoparticles, in order to determine hole or electron trapping by the particles (Platform 3). Furthermore determination of the time-resolved luminescence of the particles will yield information on the possible trapping of triplet excitons generated in the matrix, and hence also on the mobility of the triplet excitons (p 2). These layers will be incorporated into OLED devices by partner 11, who will also characterize the OLED devices (Platform 4). Using a higher loading of semiconductor particles, with formation of a bulk heterojunction with the polymer, and changing the energy levels of the polymer to allow for efficient photoinduced charge separation (p 2, 11 or EU1), the same approach can be used to build photovoltaic cells (p 11). In this context the range of matrix materials will be extended to incorporate poly(3-alkylthiophene) derivatives and copolymers, which will lead to a red shift of the absorption characteristics of the polymer component. Parallelly, this will result in a shift of the charge carrier mobility to higher values. As a reference system fullerene derivatives will also be studied as acceptor component (see also WP 8). By the use of theoretical modeling an integrated model to understand electronic characteristics and possible interactions between semiconductor materials will be built (p 4). The charge transport and charge separation in those devices will be investigated by partner 2.

Work package 2: Organic nanostructures

Task 2.1: Multifunctional Copolymers: structuring, dynamics, conformations (2, 3, 4, 5, 6, 7, 10, 11, 13, EU1, EU2)
The preparation of well-defined polymer nanostructures first relies on the development of fully controlled synthetic mechanisms and strategies leading to macromolecular architectures (e.g., block and graft copolymers, either linked covalently or via supramolecular interactions) with perfectly defined molecular parameters such as chain length and chain length distribution, grafting density, molar ratio of the components, etc. The major aim in this task will be to produce (multi-)stimuli-responsive systems able to act in solution (e.g., upon a change in the temperature, mechanical stress and/or pH) or in the solid state (as shape-memory polymers) through a proper combination of amphiphilic and/or soft and hard segments. In the latter case, new synthetic concepts will be developed to design a new generation of shape-memory polymers based on multi-block copolymers with fast and quantitative response that can act over a broader temperature range than the existing materials (p 7).
On the level of platform 2 new amphiphilic macromolecular architectures (mikto-arm, macroring, copolymers) including at least one stimuli-responsive segment (pH responsive such as poly-2-vinylpyridine, temperature responsive such as poly-N-isopropylacrylamide (p 6, EU2) will be designed by combining various synthetic methods (e.g. ring-opening, anionic and controlled radical polymerizations) (p 3, 4, 6, 7 and EU2). Their self-assembly in water (association and micellization) and their response towards external stimuli will be studied by light scattering (p 6 and EU2), NMR (p 11) or using fluorescent probes (p 2 and EU2). As further examples of amphiphilic copolymers, those which combine hydrophobic blocks with stimuli responsive hydrophilic ones are of particular interest (poly(aminated) (meth)acrylate, backbones bearing pendant carboxylic acid functions, poly(ethylene glycol), etc.) (p 4). As an alternative, multifunctional copolymers derived from glycopolymers and combining hydrophilic and hydrophobic sequences within copolymer chains will also be investigated for their potential to segregate both in solution and in the solid state providing well-defined nanostructures (p 4).

Similarly polyelectrolyte complexes made of oppositely charged homo- and block copolymers open the way to nanostructured architectures either in solution or in bulk, the physical properties of which can be tuned by various external stimuli as temperature, pH, salt concentration, etc (p 4). New amphiphilic macromolecular architectures will also be prepared on the basis of branched block-copolymers and block-copolymers containing different enantiomeric polymeric chains. Stereo-complexation in water will be used as a tool for forming well defined nanostructures (EU2). At the level of platform 1 the development of new synthetic routes will be efficiently guided by QM/MM molecular modelling (p 13). Multiscale modeling of the chemical processes involved in the polymerization will be used to optimize the polymers and copolymers produced (p 5 and 13); in this context, atom transfer radical polymerization (ATRP) of specific methacrylic monomers will be investigated as a model process (p 4, 5 and 7). Simulations of the EPR signatures of nitroxides will be carried out in order to elucidate initiation step reactions of the radical polymerization of styrene (p 3 and 10). EU1will contribute block copolymers made by combination of polycondensation and ATRP or NMP (nitroxide-mediated polymerization). End-functionalized conjugated polymers will be synthesized; these can be used as macroinitiator for ATRP to create amphiphilic structures for the self-assembly on surfaces and in bulk.

The formation of well-defined nanostructures in the solid state will be investigated with a combination of scattering and microscopic techniques (small-angle X-ray scattering, transmission electron microscopy, atomic force microscopy (p 2, 3, 4, 5, 6 and 7). On the level of platform 3, the dynamics of the systems will be analyzed for all stimuli-responsive systems, both in solution and in the solid state (shape memory polymers). State-of-the art NMR analysis (p 11) will be carried out to determine the time constants and speed of the stimuli-responsive processes, with the aim of developing fast responsive smart materials. Theoretical studies of the polymer chain structure and conformation, along with calculations of the chemical shifts and coupling constants (p 10), will allow for optimal interpretation of the NMR data with emphasis on the characterization of structural defects including unsaturations and branches (p 5, 10 and 11). Conformational sampling techniques combining ab initio with MM methods will be explored by partner 13.

Fundamental studies will be dedicated to understanding polymer chain dynamics on the local scale, based on spectroscopic (p 2) methods, with the assistance of environment-dependent modeling of the molecular optical properties (platform 1, p 4). That approach, which has recently been applied to bulk homopolymer materials, will be extended to more complex systems such as blends and nanophase-separated copolymers. Through the selection of fluorescent probes specific for a given polymer phase, it will be possible to address the polymer chain dynamics in each phase, for instance as a function of temperature during the phase separation process, or as a function of the size of the polymer nanodomains, thereby probing the effect of chain confinement on the dynamics. The feasibility to make such probes consisting of a chromophore (carbocyanine) coupled to one or two oligomers has recently been proven by partner 2. As an alternative for probes selective for a specific polymer phase, the behaviour of dyes linked covalently to a specific polymer segment will be used. Using a probe with unit quantum yield (e.g. indoleninetricarbocyanine, perylene imides or diimides, EU1) fluctuations in the fluorescence decay time of a single probe reflect fluctuations of the coupling with the electromagnetic field and fluctuations of the free volume around the probe. From the decay of autocorrelation of the fluctuations of the fluorescence decay time, it will hence be possible to determine the mechanical relaxation time of a polymer chain around a single probe. Comparing signals coming from different probes allows one to establish to what extent local fluctuations of the relaxation processes occur. Matching the relaxation of the fluctuations to theoretical models for phase transitions will give insight in this process. Using probes where the fluorescence decay is governed by local polarity (donor-acceptor compounds as triphenylamino-decorated perylene diimides, (EU1) or aminosubstituted Bodipy's (partner 2) can give insight in the size and relaxation rate of temporal and spatial fluctuations of solvation, a parameter relevant for charge transport in amorphous materials. To observe the spatial fluctuations with a higher resolution the use of STED (stimulated emission depletion) will be explored.

Task 2.2: Organic nanodots (2, 4, 6, 10, 11, EU1)
(in close relation to WP 8: supramolecular conjugated systems, and WP 1: Nanodots)
Organic nanoparticles that display remarkable stability can be obtained by micellar aggregation of amphiphilic block copolymers in a solvent selective for one block. The size and shape of those micelles can be controlled via the copolymer molecular parameters, and via the conditions used for their preparation (e.g., polymer concentration, temperature, pH,...). It is the goal of this task to extend that approach into a new domain, in order to produce organic nanodots with electronic properties similar to those of their 'classical' inorganic (metallic or semiconducting) counterparts. This will imply the design and synthesis of amphiphilic block or graft copolymers containing conjugated semiconducting segment(s) likely to form the micelle core under selected aggregation conditions (p 11 and EU1). The morphology of those micelles, either dispersed in solution or as thin solid deposits, will be probed by light-scattering techniques (p 6), atomic force microscopy (p 4) and NMR relaxometry (p 11). The electronic and optical properties of the semiconducting core will be investigated by spectroscopic methods at the bulk and single-particle level (p 2) and by Scanning Tunnelling Spectroscopy

(STS) (p 6). The excited state dynamics will be interpreted in terms of polymer chain conformation and aggregation, with the help of quantum-chemical calculations (p 4 and p 10). At the single molecule level the temporal evolution of the fluorescence maximum, decay time, polarisation and intensity of a single chain will yield information on the intrachain exciton mobility and the possible nature of trapping sites. In solution more information on the micellar size and micellar dynamics can be obtained by fluorescence quenching with a quencher solubilized preferentially at the micellar surface or by fluorescence correlation spectroscopy (FCS) (p 2).
In a further step, doping will be applied to the pre-formed micelles, in order to generate metallic organic nanodots. This will be carried out either by a chemical process (for micelles in solution) or by an electrochemical process (for thin micellar layers adsorbed on electrodes). When luminescent semiconducting particles are targeted, the conjugated segment will be composed of, e.g., polyphenylene vinylene or polyfluorene. To generate metallic nanodots, conjugated polymers which are more readily dopable, such as polypyrrole, polythiophene, or polyaniline are among the best candidates.
Using the same approach, the generation of micelles of conjugated polymers/oligomers with different shapes (cylinders or vesicles of controlled size and thickness) will also be explored. Those activities will be carried out in close connection to the synthesis of conjugated nanowires and nanotubes based on (electro)chemical polymerization in porous polymer matrices, which is being developed by partner 6.

Work package 3: Porous frameworks

Task 3.1: Self-assembly of porous materials and pore-directed particle growth (1, 2, 13)
In the preparation of new porous frameworks, e.g. zeolites, a supramolecular bottom-up approach will be followed. Low dimensional porous bodies with 36-436 Si atoms are isolated from the templating solution; such zeosil precursor units and nanoslabs are assembled into porous, hierarchical structures (p 1). The interaction between nanoslabs or other precursors leading to more complex structures can be understood on an atomistic level by force field methods (p 13). Liquid crystal characteristics during assembly are crucial for aggregation into bodies of higher dimensionality, and the colloidal and thermal properties of these suspensions will be studied by partner 1. An essential tool in this study is the new integrated Raman – X-ray diffraction setup of partner 1.
Pore-directed particle growth will be pursued for the preparation of size-controlled clusters, e.g. of Ag, in the pores and channels of suitable zeolites (platform 2; p 1 and 2). This objective is closely related to task 1.2 in WP 1.

Task 3.2: Metal-organic frameworks as adsorbents and catalysts (1, 2, 5, 8, 13)
Metal-organic frameworks (MOFs) can be assembled from a variety of metal cations and bi- or tricipital ligands. For complex syntheses of such ligands, e.g. based on dendrimers, expertise from partner 2 will be invoked. The structural flexibility of MOF design is exploited by partner 1 to prepare materials with either known or previously unknown structures (platform 2). Structural characterization and identification are based on diffraction and physisorption techniques. Combinatorial strategies can be followed to prepare materials that contain either a single metal ion or mixtures of ions, in combination with one or more ligands.
In view of the expectations raised by MOFs in selective separation of small molecules, host-guest interactions between adsorbates and the framework will be studied by partners 1 and 8, either in batch, in column mode (zero-length column, breakthrough), or with MOFs embedded in membranes (see task 5.5). Gravimetric and volumetric techniques will be used. Challenging sorption problems that will be tackled are *e.g.* separation of small alkanes, of alkenes and alkynes, aromatics, CO_2 abatement or storage of H_2 and methane. For effective separations, experiments will be conducted to distinguish between enthalpic and entropic effects and to determine mass transfer effects in the pores of these materials (partner 8). Potential mechanisms for host acceptance or rejection are shape selectivity, interactions of π-systems with exposed cations in the structure, stacking of the molecules in pores and cages etc. The joint experimental work of partners 1 and 8 (platform 3) will allow to advance models for the active sorption sites. The mechanisms underlying selective sorption will be verified by modeling by partners 4 and 13 (platform 1).
On the level of platform 3, catalytic properties of MOFs will be studied by partner 1, with special attention for structures with exposed metal cations. Expertise of partners 5 and 13 will be brought into this study, in order to understand the interplay of diffusion and reaction kinetics, and to develop guidelines for the design of new materials. Partner 13 will extend the modeling aspect by also investigating the role of specific metal-organic combinations on possible reaction mechanisms for certain catalytic applications, e.g. in Lewis-acid catalyzed transformations, leading to a microscopic understanding or even new predictions on the kinetic consequences of the chosen functionalization.

Task 3.3: Mapping and modelling of diffusion and catalytic activity in zeolites and mesoporous molecular sieves (1, 2, 3, 5, 8, 11, 13, EU1)

Understanding sorption and reaction in microporous solids such as zeolites requires tools that allow to follow the dynamics of these processes with the best spatial and temporal resolution possible. Building on the joint expertise of partners 1 and 2 in visualisation of catalysis by fluorescence microscopy, we will tackle new challenges in this domain. Exposure of zeolites to small fluorogenic precursors results in *in situ* conversion to fluorophores inside the pore system (platform 3). These fluorogenic precursors can be synthesized by partner 2 if not commercially available. In this way the location of catalytic activity will be determined in a variety of zeolites. At the synthetic level (platform 2), this might require the preparation of large zeolite crystals of varying composition, size and habitus (p 1). For instance in ZSM-5 or Boralite zeolites with MFI topology, this will allow to discriminate between zones with different catalytic activity. In intergrown zeolites, this also allows to relate pore orientation and pore accessibility to crystal habitus (p 1). Other zeolites under study will be ZSM-22, MCM-22, Ferrierite, mordenite etc. Active acid sites at the outer surface of the zeolite crystal will be imaged (p 2) using dedicated probes, e.g. of the perylene imide or diimide type, as supplied by EU1(platform 2). Amine substituents on such probes are able to quench the fluorescence by photoinduced electron transfer to the reporter chromophore. When the amines bind to acidic sites, the electron transfer will be blocked and the fluorescence restored. Additional perspectives for improvement of spatial resolution are offered by the advent of STED (stimulated emission depletion) in the lab of partner 2 (see task 6.1).

On the modelling level (p 13) attempts will be made to model the acid site(s) in a variety of zeolites (both alumino-silicates and silico-alumino-phosphates) on which experimental information is available, allowing experimental validation at every step to the point where the entire cage is reproduced. Additionally for dynamical and temperature dependent properties model development of a QM/MM molecular dynamics code is required. A new methodology of developing force fields on basis of ab initio data is also envisaged. The final aim is to model selectivity differences between different framework structures and to tentatively predict the characteristics of improved catalytic materials.

The verification of the new insights in sorption, diffusion and catalysis on the macroscopic scale is a joint effort of partners 1, 5 and 8. Besides conventional macroscale instrumentation, the Temporal-Analysis-of-Products setup (p 5) will be used to provide high accuracy data on diffusion and reaction rates. The single event microkinetic modelling using material descriptors (p 5) will link physicochemical properties to functionality. Quantum chemical methods will be applied for the selection and implementation of descriptors.

The expertise of partner 13 will be exploited to develop an efficient many-body technique to account correctly for the internal motions (torsional motions, skeletal vibrations, anharmonicities) of the guest molecule captured in the pores. In (large) supramolecular systems, where QM/MM methods are the only viable modeling techniques at high level, a suitable method will be developed to determine the normal frequencies appropriate for describing the chemical active site of the system and to predict accurately chemical kinetics.

In a device-oriented extension of this approach, structured meso- and microporous materials will be used as release vehicles for drugs or biomacromolecules (platform 4; partners 1 and 8). Preferred host matrices are micro-or mesoporous siliceous materials, possibly with a structural hierarchy (platform 2). The recognition between the guest drug molecule and the host will be manipulated through decoration of the host with cations, coordination compounds etc, and will be monitored by optical methods (e.g. FRET) by partners 2 or 11 (platform 3). Partner 1 has ample experience in assembly of coordination compounds in zeolite cages and channels, e.g. via the ship-in-the-bottle approach. Effects of acidity, solvent polarity, pore size and topology on loading and desorption (e.g. via configurational diffusion) of the drug molecule will be measured and modelled, either as single component molecular transport, or as counter diffusion in mixtures. Synergisms are expected between this inorganic-excipient based approach and the organic approach (WP4, p 3).

Task 3.4: Layered porous materials (1, 2, 5, 6, EU1)

This task focuses on cationic and anionic clays, such as the Layered Double Hydroxides (LDHs), and layered materials, e.g. oxides, derived from these materials by post-treatments such as calcination. The porosity in such materials will be modulated by intercalation of guest pillars of different sizes in the interlayer galleries. Additionally, the new class of two-dimensional metal-organic frameworks will be included, in which covalent or ionic layers are held together by weaker interactions, such as Van der Waals or hydrogen bonds. Such materials, prepared by partner 1, either have intrinsic catalytic acid-base or sorptive properties or they acquire redox activity upon decoration, e.g. via the sputtering techniques of partner 5. Fluorescent or fluorogenous reporter molecules of varying sizes, as supplied by partner 2 and EU1(platform 2) will again be the tools to map the distribution of the active sites over the intracrystalline volume or at the external surface. Target reactions for the joint spectroscopy-catalysis studies of partners 1 and 2 are base-catalyzed condensations, e.g. the Knoevenagel condensation leading to fluorescent coumarines, or the related aldol condensation. Particular attention is devoted to imaging of redox catalysis on structural or exchanged metal ions, such as Fe^{n+}, Mn^{n+}. On-off switching of the fluorescence by a proximate fluorescent label is the strategy that we

advance for determining the time that a metal ion stays in either the lowest or the highest oxidation state, for instance during a H_2O_2 mediated oxidation reaction. Fluorophores sensitive to the presence of metal cations will be provided by partner 6 and EU1 if required.

Work package 4: Hybrid materials

Task 4.1: (Multi-)responsive nanogels (2, 3, 6, 7, 8, EU2)

Nanomaterials are playing an increasingly important role as injectable carriers for advanced drug delivery systems. Design of smart nanomaterials, from which drug release is triggered by an external stimulus, such as a specific biomolecule, is highly desirable. Although many smart materials are able to respond to physical or chemical external stimuli (temperature, ionic strength, pH), only few examples of materials sensitive to biomolecules have been reported. Moreover, preparation of nanometric vehicles (nanohydrogels) with the assistance of supercritical CO_2, i.e. a benign apolar solvent, is a very attractive method for making nanomaterials available for biomedical purposes and "in vivo" injections. At the time being, macromolecular engineering has the capacity of tuning the properties of polymeric materials, such as responsiveness to a variety of stimuli, including specific biomolecules. For example, very promising glucose-responsive materials have been reported recently, that rely on reversible supramolecular self-assembly as result of interactions of carbohydrates with specific ligands (lectins). Indeed, glucose containing glycopolymers form self-assemblies when mixed with concanavalin A (ConA), i.e., a tetravalent lectin selectively recognized by glucose. Formation of these supramolecular assemblies is reversible, because the polymer-bound glucose / concanavalin A complex is dissociated by addition of free glucose. Based on this concept, glucose-responsive hydrogels have been prepared, that deliver a suitable amount of insulin in response to an increase in the glucose concentration (*S. Lee et al., J. Mol. Recogn., 1996, 9, 549)*. Indeed, the cross-linking density decreases substantially, which allows the originally entrapped insulin to be released. Preliminary studies (*L. You et al., Macromolecules, 2003, 36, 1)* have reported on the development of "smart micelles" that dissociate in the presence of glucose. These micelles were however not loaded with drugs.

In this task, effort will be made to develop smart nanoparticles able to immobilize a drug and to release it under a chemical external stimulus (such as, for example, an excess of free glucose). For this purpose, nano-sized hydrogels will be prepared, the swelling of which is substantially increased by addition of the triggering molecule (e.g. glucose). Actually, hydrophilic nanoparticles will be cross-linked by two independent methods. First, they will loosely be cross-linked by permanent chemical bonds in order to preserve the nanometric shape of the hydrogel. Then, a reversible cross-linking will be promoted by complexation with a multifunctional biomolecule, such as glucose-lectin complexes. These complexes are unstable in the presence of a glucose excess, which explains the cross-linking reversibility. These sub-micronic objects, with a size well suited for intravenous administration, must be permeable to a hydrophilic drug after the first (irreversible) cross-linking step, and impermeable to this drug after the (reversible) cross-linking by the complexation reaction.

The nanosized hydrogels will be prepared (p 3) by chemical cross-linking of preformed reactive hydrophilic or thermoresponsive polymers (p 3 and 7) within water pools dispersed in supercritical CO_2 (platform 2). These nanogel particles will be further cross-linked by complexation with a biomolecule (p 3). Nanogels will also be prepared by cross-linking of preformed reactive hydrophilic or thermoresponsive polymers, which have been incorporated in biodegradable non-reactive polymer based vesicles. The vesicle will be used as a reactor for crosslinking of the polymer system inside the vesicle. After formation of the hydrogel, the wall of the vesicle will be degraded and the nanogel can be further derivatized and characterized by the other partners (p 3, 6, 7, ·; and EU2). The size / swelling upon various stimuli (T, pH, mechanical stress or addition of bioreceptors) will be monitored by DLS (p 6), and by hr-MAS NMR (high-resolution Magic Angle Spinning) (platform 3). Fluorescent probes (labeled proteins) will be used to image the motion of incorporated enzymes within the porous hybrid material (wide field microscopy by p 2), and to monitor the supramolecular response upon reception of a chemical signal by confocal fluorescence microscopy. Adsorption, diffusion and release properties of the nanohybrids will be investigated by Zero-Length-Chromatography and high-throughput frontal analysis methods (p 8), with the purpose to develop and optimize new triggered drug delivery systems (platform 4).

Task 4.2: Nanotubes: preparation, functionalization and devices therefrom (3, 4, 5, 6, 7, 8, 10)

Carbon based nanomaterials, particularly carbon nanotubes, retain a very special attention because of high potential in optical devices, fuel cells, nanoelectronics, catalysis, and in chemical and biochemical sensors. Although carbon nanotubes are among the most promising nanomaterials, their production techniques (laser ablation, arc discharge, chemical vapor deposition) are far from being very selective, so that formation of well-defined carbon nanotubes without any purification remains a challenge. Moreover, for numerous applications, the carbon nanoobjects have to be oriented (2D or 3D) and ordered in the final material. Due to their sizes, their manipulation is very difficult and requires the use of special techniques such as nanolithography (electron

beam, dip-pen,...) and microscopies, e.g., AFM, STM,... . Up to now, the efficient and selective preparation of well-defined carbon nanoobjects, and their 3D orientation remains very challenging.
Novel chemical strategies for the production of well-defined organic/inorganic nanohybrids, particularly carbon and metal based nanoobjects with 2 nanodimensions, will be developed (platform 2) with the ultimate goal of tuning the structure and surface functionality of the nanohybrids in order to control finely their properties and capacity to self-assemble into desirable functional systems. Two strategies are envisaged in this task: (i) the use of nanoporous membranes as templates (these membranes are track-etched nanoporous membranes in polycarbonate, PET, ...) (p 6), (ii) the electrospinning of block copolymers containing one type of block which is the precursor to metal or carbon by pyrolysis, and a second, sacrificial block (p 3).
The template method is a common and versatile technique for producing nanotubes and nanowires with monodisperse diameters and lengths and is one of the simplest ways to synthesize rod-shaped multilayer nanostructures. Various segmented metal-electroactive (macro)molecule (for instance, conjugated polymers) nanowires presenting different in-wire organic junction length will be grown within the pores of membranes by an all-electrochemical process. Using this method, the length of each segment as well as the total length of the wires will be easily varied and adjusted at the desired length. Depending on the desired application, the obtained nanostructures will be either kept inside the pores, or will be liberated from the template membrane and collected as an ensemble of free particles. Alternatively, ensembles of nanostructures that protrude from the surface like the bristles of a brush will also be prepared by using supported nanoporous thin films as template.
The implementation of the electrospinning strategy requires that well-defined block copolymers are made available, which consist of a first block that is transformed to either a metal (a macroligand of metallic ions) or carbon (polyacrylonitrile) upon thermolysis. The second block will be selected for making the self-assembly of the copolymers quite easy under non-demanding experimental conditions. Strategies will be designed and developed for the controlled synthesis of polyacrylonitrile containing diblocks, and of a polyaminated block containing diblocks. Their composition will be optimized for the non-sacrificial block to form cylinders (tubes) by self-assembly, particularly under specific conditions of electrospinning. Last but not least graphitization of the polyacrylonitrile nanodomains and conversion of the metal ion containing nanophases into metal will be carefully investigated. In this respect, the modelling expertise of partner 5 in pyrolysis chemistry will be instrumental.
All these novel nanoobjects and the intermediate precursors will be characterized by HRTEM (p 6, 7) and AFM (p 4, 6) in terms of size, morphology, mechanical (nano-mechanics by AFM) and functional properties (chemical force microscopy). Their (nano)porosity, particularly important for catalysis and storage purposes, will be characterized by partner 8. Raman spectroscopy will also contribute to unravel the structural and electronic properties of these materials by addressing the effects of conformation, size, and chemical doping. Whenever necessary, the spectra will be modelled by partner 10 (platform 1) in order to elucidate the underlying structural information.
Finally, the surface functionalization of these novel nanoobjects, e.g. by biomolecules, will be considered in order to incorporate them into devices. The surface functionalization will be assessed by hr-MAS NMR. Ultimately, the potential applications of these hybrid nano-objects in biosensing devices, such as nanojunctions, nanostorage systems or transistors will be explored (platform 4).

Task 4.3: Nanostructured hybrid materials (1, 2, 3, 4, 13)
The aim of this task will be to produce inorganic/polymer hybrid systems with a well-defined structure on the nanoscale. The dimensionality of the inorganic component can either be zero (nanoparticles), one (nanoneedles, nanorods or nanotubes), or two (nanoplatelets). The tubular materials elaborated in task 4.2 will also be considered here as nanofillers in addition to more conventional fillers such as carbon nanotubes, clays, ... :

- grafting polymer chains on carbon nanotubes or other nanoparticles allows for better dispersion, thereby reinforcing the polymer matrix with improved interfacial adhesion and providing it with electrical conductivity. The preparation of the polymers and their grafting to the nanotubes will be done by partners 3 and 4. Whatever the process, nanoparticle-surface coating or grafting, catalyzed polymerization reactions will be investigated with initiator and/or catalytic species anchored onto the nanofiller surface. As an example, carbon nanotubes coated by a sleeve of HDPE can be obtained by metallocene-catalyzed polymerization of ethylene initiated at the surface of the nanofiller. This improves the dispersion of the tubes in the HDPE matrix, and also improves several other properties including electrical conductivity at very small nanoparticles content. Surface-copolymerization reactions will be studied as well, e.g., between ethylene and functionalized norbornene, yielding in a straightforward way functionalized (and reactive) polymer coatings around individually dispersed nanoparticles;
- self-assembly and Langmuir-Blodgett techniques will be applied to generate hybrid nanofilms, consisting of monolayers of elementary clay mineral platelets, alternating with monolayers of amphiphilic cations (p 1 and

2). By choosing the right cation, and by controlling the organisation of these cations in the monolayer, hybrid nanofilms are produced with nonlinear optical and with sensing properties.

- nanocomposite polymer materials with superior mechanical flame retardant and barrier properties will be generated by grafting polymer chains compatible with the matrix onto clay nanoplatelets, which is expected to lead to excellent dispersion of the inorganic component (p 3 and 4). As a typical example, poly(caprolactone), a polymer which is miscible with a number of commodity polymers, can be chemically grafted on montmorillonite-type clay nanoplatelets, strongly improving their affinity for the polymer matrix. Extrapolation to other highly anisotropic nanoparticles will be investigated, including needle-like magnesosilicate (sepiolite), carbon nanofibers and crystalline cellulose nanofibers.

Molecular modelling of such hybrid systems will be carried out in parallel to the synthesis and characterization, in order to shed light on the structure and dynamics of the inorganic/polymer interfaces (p 4), and on the parameters which control the organisation of molecules and clay-type nanoplatelets (p 1 and 13) (platform 1). Grafted polymers will be characterized by high resolution Magic Angle Spinning NMR (hr-MAS NMR) (p 4).

Novel synthetic approaches will be explored, aimed at imparting an amphiphilic character to the nanoparticles. This means that their surface should possess regions with different properties (e.g., hydrophobic-hydrophilic). For instance, needle-like clay will be surface-modified (platform 2) by various functionalized agents, either by alkyl ammonium cation exchange reactions or by reaction with selected alkoxy- (or halogeno-)silanes (p 4). The amphiphilic character imparted to the nanoparticle surface will be tuned by the chemical nature of the (functional) ammonium cations and silanes as well as their relative content. Along the same line, 'multiblock copolymers' made of alternating inorganic moieties and polymers chains will also be considered (p 4). For that purpose, functionalized polyhedral silsesquioxanes (POSS) will be studied as multifunctional macro-initiator in controlled lactone ring-opening polymerization, or in (meth)acrylate radical polymerization leading to α,ω-functional telechelic prepolymers. A final coupling reaction between the resulting functional end groups will be carried out via condensation or "click" reactions yielding the expected 'multiblock copolymers' embedding along the chains the inorganic POSS cages.

Work package 5: (Bio)membranes

While lipid bilayers and cell walls are formed in living organisms by self-assembly of resp. lipids and biopolymers, synthetic molecules can self-assemble to biomimetic membranes. The latter can be used to *model specific functions of cell membranes as substrates for organized cell growth. Due to the expected* synergy within the project, the research on synthetic membranes will be interconnected with research on bio- *and biomimetic membranes The research of work package has obvious connections with WP3, on porous* frameworks, and with WP6, on biomolecules and biocatalysis. Five tasks are planned.

Task 5.1: Organization of lipid membranes: characterization of structure and dynamics of "rafts" (2, 4, 6, 10, 11, EU1)

This task aims at the acquisition of more insight in the lateral membrane organization of synthetic membranes *and membranes of living cells such as oligodendrocytes (the myelin forming cells within the central nervous* system) and at the development of dedicated biosensors for membranes. On the level of platform 2, probes will be synthesized which either bind specifically to the L_d (liquid disordered) or (less obvious) liquid ordered (L_o) phase of lipid bilayers and oligodendrocyte membranes, or which show different photophysics in both phases. Starting from a carboxylic acid substituted perylene imide, for which preliminary results were obtained, new probes will be prepared, which display bathochromic absorption and emission spectra (terrylene), specific binding to L_d (and if possible L_o)-phases, or better solubility in the gel phase. The synthesis will be performed in collaboration with European partner 1 (EU1). Partner 2 will develop new probes based on dipyrromethenes (Bodipy); it will be investigated whether the presence of phenol moieties with different substitution patterns can lead to highly fluorescing and stable probes that show a different behavior (spectrum and/or decay time) in L_o-L_d- and gel phases. While for the rylene probes the transition dipole is perpendicular to the membrane, it is parallel for the dipyrromethenes. For cellular imaging it is important to have both types of orientation. To determine local mobility, also stable probes for rotational diffusion will be developed. Again, both types of probe molecules can be used, for probing wobbling around a normal to the plane and rotation in the plane of the membrane, respectively. In case exchange of the probe between two phases during the singlet decay time would be important, partners 2 and 11 will investigate the identifiability of the kinetic parameters of molecules undergoing rotational diffusion coupled to an exchange within the excited state. Partners 4 and 10 will model (platform 1) the interactions of the probes with the different membrane phases to explain the difference in photophysics and to provide guidelines for the development of more efficient probes (larger stability, larger

difference in decay rate in both phases). Partner 2 will visualize the L_d- and L_o-phase (rafts) using FLIM (fluorescence lifetime imaging). Dynamic data on the stability of the L_o-domains will be obtained by partner 2 with single particle tracking and fluorescence correlation microscopy (platform 3). Partner 11 will do complementary experiments using FRAP (Fluorescence recovery after photobleaching), FRET (Förster resonance energy transfer) and RICS (raster image correlation spectroscopy) with confocal laser scanning microscopy. To the extent they are sufficiently persistent partner 6 will try to visualize the rafts (L_o-phases) in membranes of living cells such as oligodendrocytes deposited on mica using high-resolution AFM. It will also be explored (using both optical and scanning probe techniques) how (bio)chemical stimuli (cholera toxin, macrolides, ω-3-carboxylic acids and poly-unsaturated acids) will influence the structuration of the lipid membranes. As one of the confocal microscopes of partner 2 is equipped with an AFM tip, the AFM-experiments will be combined with FRET: a donor- or acceptor will be linked to the AFM-tip and FRET to a partner in the membrane will be investigated (platform 3). The FRET-partner suitable for binding to AFM tips will be synthesized by partner 2 or EU1 (depending upon the type of chromophore) in collaboration with partner 6.

Task 5.2: Dynamics of bacterial biofilms and structure function analysis of bacterial surfaces containing lipoteichoic acids (1, 2, 6, 11, 12, EU1)

In order to study the dynamics of bacterial biofilms and, more specifically, the role of different proteins on their assembly and disassembly, partner 12 will fuse genes expected to be relevant for these processes with genes encoding autofluorescent proteins (Platform 2). Partners 2 and : :will use microfluorimetric methods (confocal and wide field, FLIM, FRAP, FRET, RICS) to follow expression, transport and association of those proteins on a single molecule level (platform 3). The combination of wide field microscopy with FRAP and RICS will allow us to follow transport and diffusion over an extended time range. In this task photoswitchable proteins which partner 2 is developing through international collaboration will play an important role (see task 6.1). The interaction of proteins expected to be responsible for the association of the cells will be investigated by atomic force spectroscopy using tips to which a protein molecule is attached (p 6).

In the structure-function analysis of bacterial surfaces aimed at the elucidation of inflammatory and anti-inflammatory responses to lactic acid bacteria, partner 2 will, in collaboration with EU1, develop highly fluorescent probes for bacterial cell membranes containing lipoteichoic acids (platform 2). The lactic acid bacteria and mutants thereof with different amounts and different types of lipoteichoic acids will be available through partner 12. Those membranes are expected to be immunostimulatory counterparts to Gram-negative lipopolysaccharides. While the morphology of the cell surfaces will be characterized by partners 2 and 6 using AFM, wide field and confocal microscopy on the fluorescent probes will be used by partner 2 to study molecular mobility on a local scale. FRET will be used by partner 11 to study association with labeled target molecules (platform 3). Using modified AFM tips partner 6 will probe the same interactions in a complementary way using force spectroscopy and recording force maps. Partner 2 will try to map the presence of fluorescence by FRET involving dyes linked to an AFM tip (see task 5.1). In this way the inflammatory and anti-inflammatory response will be observed directly and on a local scale (platform 3). After incorporation of catalytic centers (p 1) in the cell membranes it will be possible to monitor their catalytic activity using fluorescence microscopy (p 2). Upon sufficient dilution even single catalytic events will be observed from single catalytic centers. This aspect of task 5.2 is strongly linked to the developments in WP 3 and 6.

On the level of platform 4 the use of lactic acid bacteria as vectors for enzyme delivery in the gastrointestinal tract (GIT) will be explored while partner 12 will develop enzymes labeled with autofluorescent or photoswitchable proteins, partner 2 and 11 will use fluorescence microscopy techniques to investigate their transfer from lactic acid bacteria to cells of the GIT. Finally, partner 6 will design AFM tips functionalized with relevant biomolecules (antibodies, ligands, membrane proteins) in order to detect and map the distribution of specific receptors on the surface of living cells, e.g. GIT cells, or bacteria, e.g. lactic acid bacteria.

Task 5.3: Spectroscopic study of natural imidazolenine chromophores in membranes (2, 4, 10, 12)

On the level of platform 2, the chromophore of GFP, which is available in several variants through site-directed mutagenesis of the autofluorescent protein, will be attached by adsorption or covalent binding to synthetic and natural bilayer membranes (p 12). Synthetic imidazolenine chromophores (p 2) will also be attached to or incorporated in the membranes.

On platform 3, the linear optical properties and $\mathrm{Im}\chi_3$ of these membranes will be investigated by partner 2. Through other collaborations P 2 will also characterize the χ_2 of these molecules.

These parameters will be correlated to morphological properties of the films determined by scanning probe microscopy (SPM) by partner 2. At the level of platform 1, the influence of the surroundings on the linear and non-linear optical properties will be rationalized. These simulations (p 4 and 10) will address, for both the protonated and unprotonated forms of the chromophores, the effects of hydrogen bonding and conformational

constraints on, first, the energy levels and oscillator strengths, and then, on the non-linear response properties.

Task 5.4: Biomimetic polymer membranes (2, 3, 5, 6, 11, 12, EU1, EU2)
Partner 3 will prepare novel biocompatible copolymers consisting of functionalized polyesters and poly(vinylalcohol). They will be cast as membrane or electrospun as nanofibers. Both the membranes and networks of nanofibers will be coated with proteins (p 3) and tested as substrates for the growth of endothelial and cartilage cells (p 6, EU2). The surface of the fibers will be modified by bioactive molecules (p 3) in order to direct and control cell differentiation and growth (e.g. differentiation of stem cells into endothelial cells) (EU2, cross-link with WP 6 and WP 7) (platform 2). Solid substrates will be patterned by lithography or soft lithography (p 6); this will enable selective deposition of suitable amphiphilic block copolymers consisting of hydrophilic poly(ethylene oxide) and hydrophobic polyesters, polystyrene or poly(vinyl acetate) (p 3). This leads to patterns with specific properties, such as protein binding and protein repellency. After adsorption of proteins, those substrates will be tested as scaffolds for tissue engineering (p 6, EU2). If the pattern size is in one dimension smaller than the size of the protein, anisotropic adsorption can occur for e.g. collagen. This is a possible strategy to control the orientation of growing cells, in case they are anisotropic. In a next step it will be attempted to transfer the knowledge obtained on 2D systems to 3D scaffolds.

On the level of platform 3 the protein-covered polymer membranes as well as the network of nanofibers of synthetic polymers prepared by electrospinning will be characterized using XPS, optical and SPM techniques (p 2 and 6). The structures will be compared with layers of adsorbed biomacromolecules such as albumin, fibrinogen, collagen, or fibronectin) (p 6) or S-layers (p 12). Because the formation of biomolecular self-assemblies at interfaces could be governed by the lateral diffusion of the biomolecules, diffusion in layers prepared by partner 6 will be investigated by partners 2 and 11 using single particle tracking and FRAP. For this aim, proteins fused with GFP (green fluorescent protein) and related molecules could be used (p 12). Self-assembly of biomacromolecules in membranes will be determined using TEM (p 5), dynamic light scattering (p 6) and FRET (p 11). Changes in supramolecular organization will be monitored with optical techniques (p 2 and 11) using suitable fluorescence probes developed by EU1 (rylene derivatives) and partner 2 (DPP, Bodipy's, cyanine dyes) as well as AFM (p 6).

Task 5.5: Functional nanoporous membranes (1, 2, 3, 5, 6, 7, 8, 10, EU1)
Functional membranes with applications in nanofiltration (molecular weight cut-off smaller than 1000 Dalton) will be prepared (platform 2) based on segmented polymer networks or polyelectrolyte complexes (p 7). Both types of membranes are stabilized by cross-linking. While the former approach allows one to tune polarity by selection of bismacromonomers and monomers, the latter approach grants a high rejection of charged compounds in polar systems. These membranes will provide a cross-link to WP 4 and WP 3. They will enable challenging filtrations in polar, aprotic solvents such as THF, NMP, DMA, etc.. MOFs or zeolites (see WP3) will be incorporated in organic polymers to prepare highly selective composite membranes for liquid and gas separations (p 1).
The membranes will be characterized by atomic force microscopy (p 2, p 6), in membrane filtration (p 1, *cfr. infra*) and TEM (p 3, 5 and 6). Partners 1 and 2 will follow the transport of fluorescently labeled molecules or particles (available through partner 2 or EU1) through the pores using wide field microscopy and single particle tracking. As an alternative, partner 2 can use confocal microscopy where e.g. the fluorescence polarization of a single molecule (which is a measure of its rotational mobility) can be followed as a function of time. Partner 10 will try to assess the microstructure of the membrane forming polymers by means of NMR, combining experimental recording and a mixture of *ab initio* and molecular mechanics calculations (platform 1).
The possibility to use those membranes for different separation processes in solvent-resistant nanofiltration (SNRF) will be investigated (platform 3). Partner 2 will prepare homogeneous catalysts with a molecular weight sufficient to be separated by the nanofiltration membranes. Partner 1 will assess the separation of these homogeneous catalysts from a reaction mixture, while partner 3 will check the separation of metal catalysts from synthesized polymers. Partner 8 will explore to which extent the membranes in which nanostructured polymers are arranged in a thin layer of nano-obstacles on a planar substrate can be used as a sieving matrix to perform size-dependent separations of nano-particles, proteins and polymer strands. In addition to size-dependent separations, it will also be investigated whether the transport through extremely narrow gaps (order < 40 nm) allows to differentiate between different degrees of polymer branching (platform 3). A number of simplified nano-separation and sorting structures (nano-steps arranged in a linear flow channel) will also be investigated on the device level (platform 4). The functionalized membranes (p 7) will be tested for possible use in affinity chromatography (p 1 and 8) and controlled release of drugs and growth factors (p 1, 3 and 8). Similarly, thin films deposited in high capacity microporous materials would allow use in larger scale chromatography or adsorptive separation operations. However, very little information is available on mass transfer and overall physisorption properties in such multilevel structured porous systems, and such

information needs to be gathered for rational design and operation (p 1 and 8). This aspect of task 5.5 is strongly linked to the developments in WP 3 and 4.
In another approach novel block copolymer structures in which one of the blocks can be selectively removed via an efficient thermolysis process (p 7), will be organized in thin films (20-50 nm). By appropriate selection of the film thickness and microscopic morphology (e.g. a cylindrical morphology) such process will lead to well-defined nanoporous templates (in collaboration with partner 6). In relation with WP 3, the surface structure can also be addressed by *ab initio* modelling of the vibrational signatures (p 10). In a closely related approach, virgin or gold-coated track-etched nanoporous polymer membranes will be prepared and used as starting nanoporous templates. By making use of functionalized polymer segments, the pores will be functionalized (e.g. with acid groups) for chemical interaction with other (bio)macromolecules (p 6). Furthermore the pores will be coated with polymer chains, the coiling of which is temperature, pH or ionic strength dependent (p 6 and p 7). This will allow us to tune the permeability of those membranes with external stimuli.
The use of self-assembly to obtain nanopatterned membranes will be explored by partner 6 using molecules prepared by partners 3, 6 and 7. Depending on the required size and the molecules that have to be incorporated, both top down (nanolithographic) or bottom-up (self-assembly) techniques will be used.

Work package 6: Biomolecules and Biocatalysis

Task 6.1: Autofluorescent and photoswitchable proteins and use as probes (2, 4, 10, 11, 12, EU1)
In this work package the newest developments in fluorescent protein (FP) design will be combined with advances in high resolution microscopy. One way of overcoming the diffraction barrier in an all optical way is using Stimulated Emission Depletion microscopy or STED-microscopy which will be set up by partner 2 (platform 3). STED relies on pairs of synchronized laser pulses used in sequence. The first pulse, the excitation pulse, is focused into the sample, producing an ordinary diffraction limited spot of excited molecules. The excitation pulse is immediately followed by a depletion pulse, referred to as 'STED-pulse' (or dump-pulse). The wavelength of the STED pulse is towards the red edge of the emission spectrum of the dye and hence quenches excited dye molecules to the ground state by stimulated emission. The net effect of the STED pulse is that the affected excited molecules cannot fluoresce because their energy is dumped and lost in the STED pulse. By spatially arranging the STED pulse for example in a doughnut mode, only the molecules at the periphery of the exciting spot are quenched. In the center of the doughnut, where the STED pulse is vanishing, fluorescence ideally remains unaffected. By increasing the STED pulse intensity, the depletion becomes complete at the spot's periphery and increasingly more ineffective towards the middle. STED microscopy is just a first example in which the concept of overcoming the diffraction barrier by means of saturation of a reversible molecular transition with an intensity distribution having a strong spatial gradient is exploited. The chromophores that will be used for STED will be synthesized by partner 2 and EU1. (platform 2). As the competition between induced emission and $S_1 \rightarrow S_n$-absorption is very important, partner 2 will also characterize the photophysics of those photoswitchable proteins using time resolved absorption and fluorescence (platform 3).
The concept developed above is much broader than just stimulated emission: any photo-induced transition between two different states A and B of a molecule (different conformations, protonated/deprotonated froms of the molecule...) can be used in principle to obtain superresolution, as long as the transition from A to B is a saturable optical transition and the spontaneous back reaction is sufficiently slow. In this context partner 2 proposes the use of Dronpa, the first reversible photoswitchable fluorescent protein from the family of GFP's (green fluorescent proteins). Dronpa and its mutants, available to partner 2 through an international collaboration, can be switched fast and reliably between a highly fluorescent form and a non-fluorescent form by applying 488 nm and 405 nm light. In order to use the full potential of Dronpa photoswitching, the following scheme is proposed. A three-pulse sequence (reset, erase, detection) is necessary to realize Dronpa-photoswitching high resolution microscopy (platform 3). The reset beam (400 nm) converts all Dronpa to the 'on'-state. Next, the erase beam is applied. The erase beam is a 488 nm doughnut mode beam with zero intensity at the center. This beam will switch Dronpa molecules to the 'off'-state except for the molecules in the intensity node. Finally, the detection beam is applied and the fluorescence from the Dronpa molecules in the node is detected. Partner 2 will also characterize the photophysics of those photoswitchable proteins using time-resolved absorption and fluorescence (platform 3). On the level of platform 1 intense collaboration with partner 4 and partner 10 is expected to rationalize the photophysics of the photoswitchable probes and to relate it to the protein environment surrounding the chromophores (H-bonding, protonation and deprotonation). In this way partner 4 will try to rationalize the effect of the different mutations of the apoprotein on the properties of Dronpa.
After delivering a proof of principle, Dronpa will be used to mark and image with unprecedented resolution cell membranes and cellular subcompartiments of interest of oligodendrocytes (task 5.1, available through partner

11) and cellular subcompartiments of epithelial cells of the gastro-intestinal tract (task 5.2 available through partner 12). This approach will require the expression of fusion proteins of Dronpa (partner 12).
An alternative to this approach is breaking the diffraction limit with analysis of dynamic saturation. The concept is that in dynamic saturation the fast decay component is most prominent at the center of the excitation area, and the plot of the contribution of the fast component enables us to extract an image with superresolution. The photoswitching of Dronpa can be saturated. Partner 2 simulated the resolution improvement of photo-switching imaging with Dronpa, and the resolution is expected to be ~100nm. The theoretical results will now be evaluated experimentally.

Task 6.2: DNA and oligonucleotides probed by metal complexes, and use for construction of bio-inorganic materials (2, 4, 8, 9, EU2)
Luminescent and DNA-photoreactive metal complexes, particularly those of Ru (II), are useful tools to study the structures and dynamics of DNA. Therefore at the synthetic level (platform 2), new mono-, di-, or even polynuclear Ru(II) complexes with polyazaaromatic ligands and bridging ligands such as for example the tetrapyrido-acridine (TPAC) will be prepared (partner 9). Some of the metal compounds designed previously present a puzzling behavior in emission. In order to determine the mechanism at the origin of these luminescence properties, modeling and calculations (platform 1) will be needed (partner 4). Various polycationic macromolecular architectures based on protonated aminated poly(meth)acrylates will be synthesized by controlled polymerization reactions (partner 4) and their interactions with the photoactive metal complexes and DNA will be investigated by partner 9. At the level of applications (platform 4) this investigation ultimately aims at vectorization of DNA into cells. Model systems for the vectorization of DNA into cells are available via EU2. Different well defined cationic polymer systems based on PEI-PEO block-copolymers, polymers prepared by Michael addition of amines and bis-acrylates and polymers containing reducible disulfide linkages will be prepared by EU2. Their interaction with photoactive metal complexes and DNA will be studied (p 9).
Telomeric sequences constitute a particularly interesting target: they could be damaged to inhibit the telomerase function in order to restore normal cell apoptosis in cancerous cells. Special attention will thus be focused on the interaction and photoreaction of designed dinuclear Ru(II) compounds with telomeric DNA sequences. This will be achieved by a combination of photophysical, photochemical and biological methods with theoretical approaches (partners 4 and 9).
The different forms of plasmid DNA and the relaxation dynamics of their conformations due to photocleavage or photocrosslinking induced by the interaction with Ru(II) complexes under illumination, will be monitored (platform 3) using AFM and optical microscopy as prime tools (partners 2 and 9). The effects of photocrosslinking between a long DNA template and a short Ru-derivatized complementary strand, on the activity of the enzyme DNA polymerase, marked by a luminophore, will be monitored in real time by single molecule spectroscopy. Thus the rate of nucleotide incorporation before and after illumination of the Ru(II) complex (after photocrosslinking) will be followed (partners 2 and 9).
The above set of measurements will be complemented by a real-time visualization study of the transport and binding kinetics of fluorescently labeled individual DNA strands through open and nano-structured flow channels (partner 8). The focus will be on the observation and description of the fundamental transport and binding parameters such as restricted Brownian motion, flow-dependent molecular binding kinetics, shape and size selective transport of randomly coiled polymer strands through structures that are either larger or smaller than the radius of gyration etc.
On the other hand, novel bio-inorganic materials (platform 2) will be obtained by the self-assembly of metal ions such as Cu^{2+} or Ru^{2+} with polyazaaromatic ligands derivatized with complementary oligonucleotides (partner 9); the structure of these materials after deposition on a substrate (see WP9; platform 3) can be studied by AFM or STM (partner 2).

Task 6.3: Biocatalysis with proteins and RNAs (1, 2, 5, 12, 13, EU1)
As biocatalysis is more and more considered a technology that is complementary to classical homogeneous and heterogeneous catalysis, synergisms can be expected from the interaction between groups with catalytic expertise (partners 1 and 5) and groups specialized in DNA and protein technology (partner 12). Specifically, existing collaborations will be deepened around the design of biocatalysts with improved activity and enantioselectivity (platforms 2 and 3). A potential group of target reactions are carboligase-mediated transformations, catalyzed by (phenyl, indole-)pyruvate decarboxylases. Starting from a keto-acid donor and an aldehyde acceptor, these enzymes catalyze the formation of hydroxyketones (acyloins), often with high selectivity. Apart from activity and enantioselectivity, an additional goal is to broaden the scope of acceptor aldehydes. Random mutagenesis by error-prone PCR is one of the available techniques to create libraries of

mutant enzymes (partner 12). Screening and detailed study of the catalytic activity are performed by partner 1.
The screening may be efficiently guided by performing molecular modelling based on QM/MM techniques (with incorporation of solvent effects) of some key target reactions (partner 13). Joint expertise in the domains of bio- and chemocatalysis (partners 1 and 12) will also be valorized for one-pot reactions using both chemical and biocatalysis. *This combo-catalysis is especially valuable for dynamic kinetic resolutions, in which two* enantiomers are kinetically differentiated by an enantioresolving enzyme, while the undesired enantiomer is racemized by a chemocatalyst. While benzylic alcohols and amines can more or less successfully racemized, there is still an urgent need for catalysts that can racemize *aliphatic* alcohols and amines, in conditions that are sufficiently mild to be compatible with an enzyme-catalyzed resolution (e.g., $T < 353K$) (partner 1). In a one-pot process containing two catalysts (bio- and chemo), at least two reactants and possibly more than one liquid phase, transport phenomena may play a crucial role in determining overall rates, and therefore the engineering expertise of partner 5 will be invoked to identify slow steps and to design more performant systems.
Fundamental insight in the working mechanisms of enzymes can be gathered by single molecule spectroscopy on individual working enzymes, using confocal fluorescence spectroscopy (partners 1. 2 and 12). For instance, in enantioselective catalysis by a population of enzymes, insufficient enantioselectivity can be due to a similar error frequency in all enzymes of the population; alternatively, a few individual enzymes might display a substantially lower enantiodiscrimination than the rest of the population, e.g. because of a different conformation. Therefore, we will use confocal (single molecule) spectroscopy to count turnovers of individual immobilized enzymes in the conversion of enantiopure fluorogenic substrates. An enantioselective enzyme is expected to be highly active with one enantiomer and almost silent with the other. At the synthetic level (platform 2), this requires preparation of enantiopure (ester or amide) derivatives of fluorophores (partner 2 *and* EU1).
A new area within biocatalysis is the potential use of catalytic RNAs (ribozymes). Even if ribozymes are quite rare in cells, synthetic RNAs can be produced that display distinct catalytic activity, in the absence or presence of metal ions. Activities will be started jointly by partners 1 and 12. A target reaction is the decarboxylative Claisen condensation.

Task 6.4: Biomimetic Catalysis (1, 3, 5, 8)
The basic strategy to prepare biomimetic catalysts is to decorate a matrix (emulating the protein) with a catalytic centre (e.g. a metal ion), and to provide locally the optimal physicochemical conditions for maximizing *turnover frequency and selectivity. Partner 1 will continue research to design solid matrices (platform 2) with* optimal acid-base and polarity properties to elicit this activity optimum. Examples of supports, mimicking the apoenzyme, are zeolites, amorphous or ordered hybrid SiO_2 materials with pendant organic functional groups, and layered materials such as the Layered Double Hydroxides (see also WP 3.4). Target reactions within the next few years are selective hydrogenation, (oxidative) incorporation of nitrogen into hydrocarbons, C-C coupling reactions, conversion of renewables etc. For the best catalysts, adsorption and kinetic properties will be studied in detail by partners 5 and 8. In order to make fair comparisons between organic and inorganic support materials, functionalized polymers will be designed by partner 3 and used as supports for catalytic reactions. A new focal point of attention will be the design of organocatalysts.

Task 6.5: Design of molecules interfering with bacterial communication (partners 1, 6, 12)
As explained in task 5.2, bacterial biofilms will be studied with i.a. FLIM, FRAP and FRET using fluorescent proteins as markers. In order to control film growth, interference at the molecular level with the bacterial cell-cell communication is a necessity. Therefore, at the level of platform 2, we will design new agonists or antagonists for quorum sensing. These molecules are related to the acylated homoserine lactones, to 1,2-hydroxy-3,4-pentanedione (AI-2, DPD) or to the halofuranones. Partner 1 is designing new catalytic synthesis pathways, e.g. for the assembly of the furanone rings, or for the enantioselective biocatalytic coupling of acyl chains to the homoserine lactone core. These molecules are then tested in bioscreens by partner 12, e.g. on *Vibrio harveyi or Salmonella typhimurium. Using force spectroscopy and AFM-tips covered with the agonists* and antagonists, partner 6 will be able to check the strength of the interaction of those molecules with receptors on the cell surface. By force mapping it will be possible to visualize the distribution of those receptors over the cell surface. Combining force maps with height images will allow to see whether those receptors are located in L_o-phases or liquid phases of the cell membrane.

Work package 7: Functional coatings

Task 7.1: Functional electrocoatings on carbon, metals and semi-conductors (3, 6, 7)
Under cathodic polarization, metals, semi-conductors and carbon can be electrografted by poly(meth)acrylate chains. The growing chains initiated at the cathode surface are effectively chemisorbed, which is a unique solution for the lack of adhesion between inorganic surfaces and organic coatings. The cathodic polymerization of (meth)acrylates containing functional groups (protected or not) is a direct extension of this strategy, and makes the electrocoating functional. The approach will therefore be extended to novel monomers such as cationic quaternary ammonium salts containing acrylates (p 3). These monomers are suitable candidates to create an anchoring layer for a subsequent coating via the layer-by-layer deposition process (p 6).
The very low thickness of the electrografted films, and the restriction to poly(meth)acrylates are two remaining limitations, and these problems will also be addressed in this task. Indeed, macromonomers of various architectures will be synthesized by controlled/living radical or ionic polymerization; the polymerizable end group(s) will be of the (meth)acrylate type, and thus prone to electrografting. Macromonomers of polyesters (e.g. polylactides), polyethers (e.g. polyoxirane) and poly(vinyl ethers) (e.g., polymethylvinyl ether) will be synthesized (p 3 and 7) (platform 2) and cathodically (co)polymerized. The surface will be analyzed by dedicated techniques (XPS, ellipsometry,...) in order to establish the experimental conditions for successful synthesis and control over thickness, homogeneity, and adherence, in relation to the molecular weight and the functionality of the macromonomers (one or more polymerizable end-groups). Particular attention will be devoted to the elaboration of stimuli-responsive coatings. Beside the macromonomer strategy, which can easily afford thermoresponsive films by using poly(methylvinylether) macromonomers, the electrografting of N-succinimidyl acrylate (NSA) is also a nice platform for simple derivatization. Indeed, hydrolysis provides pH-responsive poly(acrylic acid) and reaction with isopropylamine gives the well-known thermoresponsive poly(N-isopropylacrylamide). The activated ester of NSA can also be reacted with a wide variety of amino-derivatives such as aptamers, enzymes, or DNA for more specific recognition and sensing. Changes in the coating organisation induced by an external stimulus (e.g. T, pH, analyte addition, and so on) will be studied (platform 3) by a combination of techniques, such as cryo-XPS, temperature-dependent AFM in liquid cells, wetting in dynamic conditions, in situ ellipsometry, etc.
Recently, poly(meth)acrylate chains have been successfully electrografted onto AFM-tips, which proved to be a very promising surface modification for manipulating single molecules and assessing the chemisorption of the cathodically polymerized chains. This tool will be exploited by partners 3 and 6 in order to study in situ the growth mechanism of the polymer chains, and the behavior of electrografted coatings under stimulation. From these experiments, principles governing smart coatings with reversible switching capabilities will be extracted. Concepts for building responsive (bio)sensors will then be developed (platform 4).

Task 7.2. Supported fluorinated ligands for catalysis in supercritical carbon dioxide (1, 3, 4, 5, 6)
In order to cope with cost and toxicity of organic solvents, attention is paid nowadays to chemical reactions conducted either under solvent-free conditions or in cheap and benign solvents, such as supercritical carbon dioxide (sc CO_2). Because of insolubility, organometallic catalysts cannot be used in sc CO_2, except when they are bonded to soluble chains, typically fluorinated polymers. Therefore aminated ligands will be attached to fluoropolymers, mainly by copolymerization of fluorinated acrylates with either ligands containing acrylates, or with acrylates to which ligands can easily be grafted after copolymerization (p 3) (platform 2). These soluble macroligands will ultimately be attached to the surface of inorganic particles (silica, porous carbon) and used to support metal compounds for catalysis in sc CO_2 (p 1 and 3). Surface modification of the inorganic supports will be analyzed in terms of thickness and homogeneity by ellipsometry, X-ray Reflectometry, and AFM (p 4 and 6). The grafting/coating efficiency will be studied in order to determine the density of metallic species available for catalysis. Catalytic activity, possible recycling and turn-over will be investigated in model reactions in sc CO_2, including controlled radical polymerization (particularly Atom Transfer Radical Polymerization, ATRP), selective hydrogenation or hydrogenolysis, selective oxidation, formation of carbamates and urethanes, etc (platform 3). Efficiency of soluble catalysts and supported catalysts will be compared (p 1 and 3). The new high throughput supercritical screening reactor of partner 1 will be a highly valuable instrument for this purpose. Modeling of the ATRP polymerization in sc CO_2 will be carried out by partner 5 (platform 1).

Task 7.3: Biomimetic and protein repellent coatings (3, 4, 6, 7, 12, EU2)
In vivo, cells are in contact with highly structured matrices of biomolecules, which regulate cell functions. The design of biomimetic surfaces consisting of layers of biomolecules organized at the supramolecular level is expected to bring advances in controlling cell-material interactions. Therefore, bio-inspired copolymers will be designed in order to anchor strongly polyelectrolyte chains onto metallic surfaces (p 3). Appropriate

polyelectrolytes and/or charged bio-macromolecules will be deposited layer-by-layer with the purpose of providing the coating with specific properties, such as super-hydrophobicity, anti-corrosion, etc. (p 6)
Coatings of biomaterials with protein repellent properties will be synthesized by plasma polymerization and by grafting chains to surfaces onto which the initiator was previously attached (p 3 and 7) (Platform 2). In addition to the characterization of the coatings by AFM, X-ray reflectometry and XPS (p 4 and 6), special attention will be paid to protein adsorption to modified surfaces compared to the pristine surface (p 6 and 7, EU2) (platform 3).
Biofouling is a typical example of a nanoscale adhesion process occurring at the interface between fouling organisms and all man-made surfaces in both marine and freshwater environments. Thus, creating an external surface with nanoscale features to prevent adhesion of organisms will enhance the surface engineering of silicone coatings which are already known for their low-adhesion properties. This will be achieved by fine dispersion of nanofillers (carbon nanotubes, acicular clays and nanoclays) that will significantly increase the surface nano-rugosity without compromising the low surface energy of this inorganic polymeric matrix. Alternatively, specific surface localization of amphiphilic block copolymers made of silicone and quaternized or protonable poly(aminated acrylates) will be investigated due to the repellent effect they might have against the adhesion of marine organisms (p 4). Performances of modified surfaces will be evaluated by using mutant bacteria strains that are particularly efficient in biofilm formation (p 12).

Work package 8: Supramolecular conjugated systems

Task 8.1: Joint control of the optical, transport, and morphological properties (2, 4, 5, 6, 9, 10, 11, EU1)
The performances of conjugated materials in semiconducting devices (OLEDs or solar cells) depend simultaneously on their solid-state optical properties and their charge transport capabilities, which in turn are deeply affected by the supramolecular organization of the polymer/oligomer molecules. It is therefore the aim of this task to design, synthesize, and characterize supramolecular conjugated systems with optimal optical and transport properties, combined with controlled supramolecular organization and microscopic morphology.
The first major activity in this task will be dedicated to donor-acceptor mixed systems for photovoltaic operation. Phase separation on the appropriate lateral scale will be generated by depositing mixed solutions onto nanopatterned substrates (fabricated by partner 6), which are expected to direct the adsorption of the two components and the growth of separated domains. It will be attempted to find out if spatially resolved fluorescence microscopy (especially considering the increased optical resolution obtained by STED) will be able to observe separately the fluorescence of the donor phases and to show in this way their morphology (p 2). This approach will first be applied to well-established systems, i.e., blends of electron-acceptor molecules (e.g., C_{60} derivatives, perylene imids) into an electron-donor polymer matrix (e.g., polythiophenes). As alternative for low molecular weight derivatives of C_{60}, C_{60} molecules grafted to a polymer will be used to stabilize the percolating structures. Studies of the optical, photophysical and transport properties (time of flight) will be paralleled with modelling of the light absorption, charge generation, (picosecond fluorescence, femtosecond transient absorption), separation (polarized femtosecond transient absorption), migration (time of flight), and recombination (nanosecond transient absorption) processes involving quantum-chemical and Monte-Carlo methods (p 2, 4 and 10). The opto-electronic experiments of partner 11 will yield complementary information on the efficiency of the interconversion of light into electric energy (and vice versa) and the device properties (current voltage plots) (platform 4). This approach will then be extended to the development of novel small-bandgap conjugated polymers designed to maximize light absorption (p 4 and 11).
Another approach to generate a well-defined phase morphology on the nanoscale will be through phase-separated block copolymers. This will imply the design and the controlled synthesis of copolymers with conjugated donor and acceptor blocks, e.g., polythiophenes or polyphenylene vinylenes as the donors combined with perylene imide or diimide polymers as the acceptors and light harvesting units (p 4, 11 and EU1). Also a copolymer of TPD and polyfluorene (p 2 and EU1) or a polymer of indolocarbazole (p 2) acting as donor will be combined with monomer and polymer perylene imides. Kinetic and mechanistic studies of the polymerization reaction will provide relations between synthesis conditions and product properties (p 2, p 5, 11 and EU1). This approach will be extended toward side chain grafted structures in which a donor type backbone is combined with an acceptor type graft or vice versa. In this context also new acceptor systems will be studied based on polymers in which substructure elements of C_{60}, e.g. fluoranthene, are incorporated. The phase behaviour, micro-morphology and crystallisation behaviour of these materials both in the pure state, as well as in solutions and blends, are crucial for an optimal performance in devices. A concerted research action will provide more fundamental insights in the essential "(synthesis)-structure-processing-property" relationships of mixtures of conjugated polymers (p 11). These results will be compared with morphological data obtained from fluorescence, electron and scanning probe microscopies, solid state NMR and molecular modelling (p 2, 4, 5, 6, 10, 11). These fundamental studies of the phase-separated morphologies, e.g., as a

function of the block ratio, film thickness or specific interactions with the substrate will allow us to link the structural properties with the photophysical (*cfr. supra*) and optoelectronic properties (p 2 and 11).
Generating thin organic layers with outstanding transport properties can also be done using discotic liquid crystalline compounds (prepared by partner 9 and EU1), made of a π-electron-rich core surrounded by a corona of flexible side groups. As pure compounds, these systems are of particular interest to transport charges within organic field-effect transistors, since one-dimensional assemblies (columns) of such discotic molecules can be considered as molecular wires. This project will focus on blends of electron-donor (e.g., indolocarbazoles (p 2), phthalocyanines (p 2, 9)), hexabenzocoronene (p 9, EU1), or liquid crystalline OPV's (available thorough collaboration with TU Eindhoven)) and electron-acceptor (e.g., perylene imids and diimids (EU1), fluorosubsituted phthalocyanines (p 2 and 9)) liquid crystals for photovoltaic application. In addition to blends of donor and acceptor discotic liquid crystals, more sophisticated molecules will be synthesized such as donor disk-like molecules coupled with acceptor molecules that are either disk-like or spherical (C_{60}). The intrinsic optical and photophysical properties of the components and mixtures thereof, the orientation of the columns with respect to the electrodes, the phase behavior of the blends and the charge separation efficiency, charge carrier mobility and recombination rate are all aspects that will be investigated (p 2, 4, 6, 9, and EU1). Methods to align locally such molecules, using either chemically nano-patterned surfaces, or by nano-molding using nano-imprint lithography, will be explored by partner 6 in order to obtain isolated organic nanowires and to measure their electrical properties (as described in WP 9). Other schemes will also be explored, based on rod-shaped molecules forming smectic liquid crystalline phases.

Work package 9: Self-assembly at surfaces

Task 9.1: Molecular-scale studies of the structure, dynamics, and electronic properties in adsorbed monolayers (2, 4, 6, 9, 10, EU1)
This task will strongly rely on the use of scanning probe techniques to study the structure, the dynamics, the reactivity and the electronic properties of molecular layers adsorbed on conductive surfaces. The well-established methodology consisting in determining the two-dimensional assembly of physisorbed functional molecules with scanning tunneling microscopy will be extended to complex supramolecular systems able to undergo reversible structural changes by an external stimulus (e.g., conformational changes in functional macrocycles upon ion complexation). Along the same line, the generation of chiral functional monolayers via the physisorption of chiral functional molecules (e.g., tetrathiafulvalenes, oligothiophenes or oligoparaphenylenevinylenes with chiral side groups) will be investigated at the organic liquid/solid interface with a combination of scanning tunneling microscopy (STM) and molecular modeling techniques (p 2 and 4).
In addition, electrochemical scanning tunneling microscopy (EC-STM) will be implemented for the formation and investigation of physisorbed monolayer thick coatings at the interface between aqueous electrolyte and electrified metal surfaces (p 2). An important benefit of EC-STM is the possibility to influence the supramolecular ordering and dynamics of compounds at the aqueous electrolyte/solid interface by control of the applied potential. The implementation of EC-STM for the study of water-soluble compounds is straightforward. In addition, EC-STM also allows the investigation of water-insoluble compounds under potential control. The latter approach will be extremely useful for the stabilization of these monolayer-thick coatings by exploiting the hydrophobic effect.
The water-insoluble layer modifies the substrate and therefore, it is itself a template layer. We aim at the formation of chiral templates. Given that an enantiopure chiral insoluble isophthalic acid derivative is physisorbed on the metallic substrate, automatically, a chiral surface is created. Partner 2 will explore the possibility to physisorb water-soluble molecules on top of the insoluble chiral template layer. The effect of the chiral template layer on the structure and chirality of the host layer will be explored. Given that the template layer is chiral, enantioselective adsorption and interactions are anticipated.
Besides structural investigations, this task will also be dedicated to the elucidation of the electronic properties of the adsorbates through a combination of bias-dependent STM imaging and scanning tunneling spectroscopy (p 2). For this purpose, sets of aromatic/conjugated compounds decorated with different substituents (e.g., electron-donors or –acceptors) will be designed and synthesized (p 9 and EU1). The measurements will be rationalized with the help of calculations modeling charge transport through molecular junctions (p 4, p 10).
Self-assemblies of dendrimers or polymers at surfaces, formed exclusively by metallic ions (Ru(II) or Cu(I)) and bridging polyazaaromatic ligands (platform 2) (p 9) will be examined by STM (p 2) with the geometry of adsorption investigated with molecular modeling and ab initio theoretical approaches (p 4) (see WP6).
Chemical reactivity within the monolayers will be induced in a controlled way and investigated on the molecular scale via a twofold approach: on the one hand, UV irradiation or the electric field in the STM junction will be used to initiate polymerization processes (e.g., in diacetylene or functionalized hexabenzocoronene

assemblies) to produce single molecular wires (p 2 and EU1) and/or 2D polymers. On the other hand, molecular adsorption on metal surfaces (with copper and gold as prototype systems) under potential control, studied via EC-STM, opens many possibilities to explore redox-sensitive switching (e.g., in metal-centered porphyrins prepared by EU1. tetrathiafulvalenes) or template growth of metallic nanoparticles and wires. In the latter approach, the water-insoluble molecular two-dimensional crystal acts as template: the non-exposed areas of the surface are accessible for the electrochemically induced formation of metallic nanostructures. Adsorbed films formed with Cu(I) and special bridging polyazaaromatic ligands (p 9), will also be examined by EC-STM (p 2): when oxidized into Cu(II), they should become non-luminescent and should change geometry around the Cu centre.
Another major aspect of this task will be to explore the formation of 3-D structures from the ordered monolayers. This is of particular interest for thin films of dendrimers, prepared by EU1or partner 2, or organic semiconductors, in which both optimal interaction with the electrode surfaces and high ordering in the organic layer are required. This type of investigation will be based on the combination of STM and AFM measurements, applied for instance to differently substituted discotic compounds such as phthalocyanines or benzocoronenes, in pure or mixed layers (p 2, 4, 9 and EU1; in connection with WP 8).
Also related to this task are studies of the dynamics and mechanical response of single polymer chains adsorbed at surfaces. These properties can be probed by force measurements carried out with a scanning force microscope, a methodology which requires that the AFM tips be functionalized with a coating specific for the polymer and intermolecular interaction/chemical reaction under study (see task 7.1). Similarly the behaviour of (block co)polymers at liquid/liquid or gas/liquid interfaces will be investigated both in the static and dynamic mode using interfacial rheometry (p 6)

Task 9.2: Controlling the spatial localization of functional systems at surfaces (1, 2, 3, 4, 6, 7, 9, 10, 11, 12, EU1)
Over the last few years, considerable efforts have been made by partner 6 to develop methodologies to obtain a large variety of nano-patterned surfaces, by combining nanolithography methods such as e-beam lithography or nano-imprint lithography with chemical assembly methods. On that basis, several possibilities will be explored to control the spatial localization of selected functional systems developed in the project, in collaboration with the partners of the project. In particular, this general approach will be used to:

- generate structured and nanopatterned thin film samples of dye molecules by local grafting of chromophores or nano-imprinting of dye-loaded polymers. These structures will then be used as bench marks for the development of high-resolution microscopy techniques (STED, DOSM) (p 2 and 6);
- generate structured hybrid thin films of elementary clay mineral platelets and bio-macromolecules by self assembling and Langmuir-Blodgett techniques (p 1 and 2) for biosensing and biocatalysis;
- control the local deposition of bio-macromolecules, in order to prepare bio-active surfaces able to direct / control cell growth (p 3, and 6, and partner 12). These systems will also be used to study the lateral diffusion of bio-macromolecules at interfaces by fluorescence techniques (p 2, 6 and 11), which will complement studies proposed in WP 5;
- generate assemblies of conjugated oligomers and polymers into well-defined semiconducting nanostructures. This will be carried out by templated adsorption of electro-active block copolymers, controlled dewetting of electro-active liquid crystals or polymers on patterned surfaces, polymerization from patterns (grafting from or onto), or nano-imprinting to orient molecular nano-crystals (p 2, 3, 4, 6, 9, 11, and EU1). This will be performed in close interaction with WP 8);
- control the adsorption of complex fluoroionophores with cation-detecting capabilities, which will be studied by a joint spectroscopic and theoretical approach in solution and after grafting (p 2, 6, and 10);
- arrange polymer micelles into well-defined arrays through spatially-controlled adsorption and characterize the micelles by scanning probe microscopy (p 2 and 6);
- realize nano-structured catalytic surfaces as described in WP 1 for the case of heterogeneous catalysis (p 1, 2 and 6), or by grafting locally homogeneous catalysts;
- investigate the behaviour of small islands of responsive macromolecules (temperature- or photo-sensitive systems) when confined into islands of size close to the intrinsic dimensions of the chains. These nano-islands will be obtained by combining the grafting methods developed in WP 7 (p 3, 4, and 7) with the nano-patterning methods of partner 6. The collective behaviour of collections of such nano-ensembles of responsive molecules will be studied by wettability measurements in dynamic conditions, atomic force microscopy in solution and as a function of temperature, in-situ ellipsometry and cryo-XPS (p 6).

I. 5. PARTICIPATION OF THE PARTNERS IN THE DIFFERENT WORKPACKAGES

Tick off in the table the participation of the different partners in the different workpackages (delete not used rows and columns in the table). Mention for each partner his/her name and the institution's *abbreviation*.

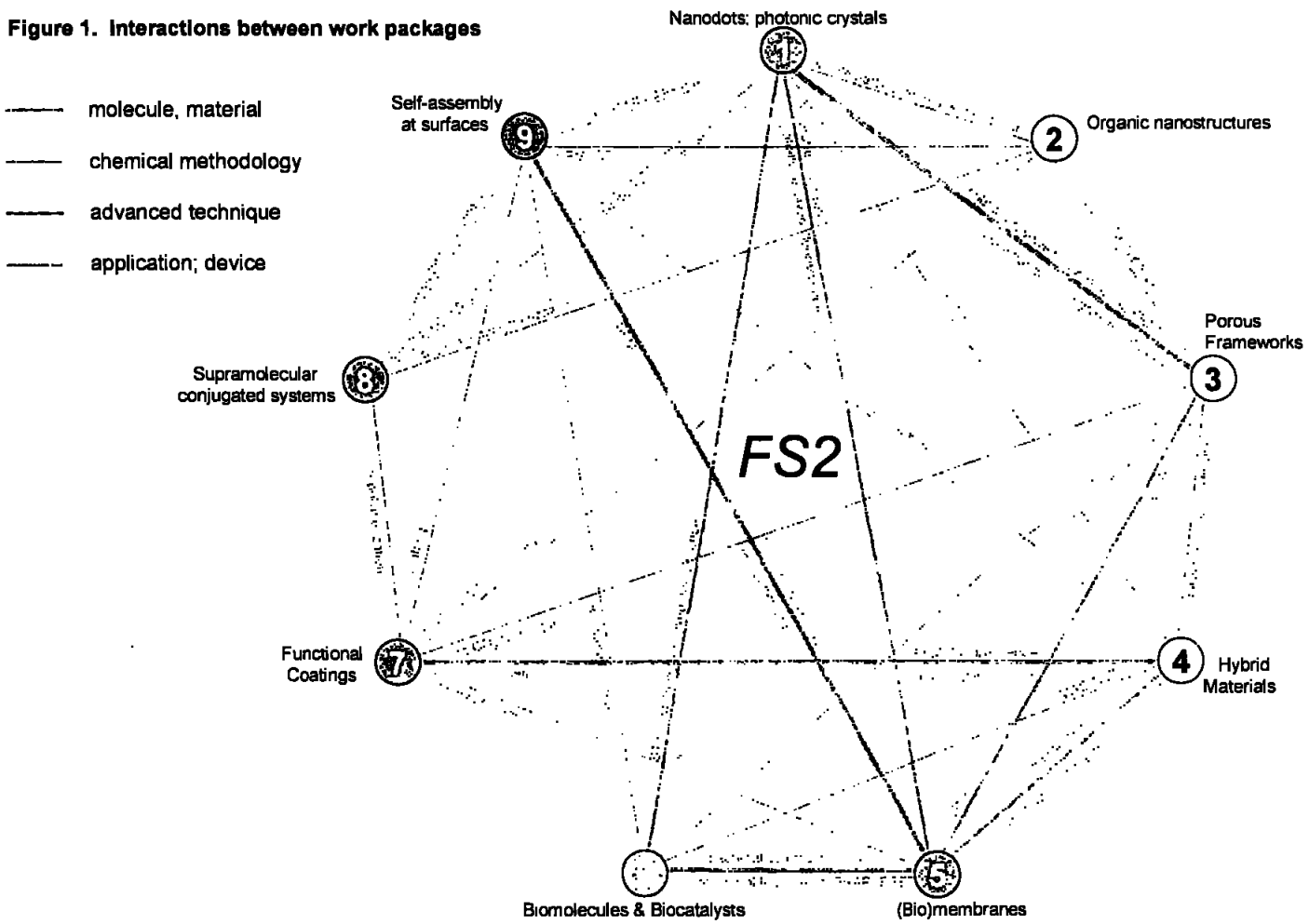
	PARTNER	WP1	WP2	WP3	WP4	WP5	WP6	WP7	WP8	WP9
P1	Name : JACOBS Pierre Institution : K.U.Leuven	2,3,4		1,2, 3,4	3	2,5	3,4,5	2		2
P2	Name : VAN DER AUWERAER Mark Institution : K.U.Leuven	1,2,3 ,4,5	1,2	1,2, 3,4	1,3	1,2,3 4,5	1,2,3		1,2	1,2
P3	Name : JEROME Christine Institution : ULg	2,3,4	1	3	1,2, 3	4,5	4	1,2,3		2
P4	Name : LAZZARONI Roberto Institution : UMH	2,3,4 ,5	1,2		2,3	1,3	1,2	2,3	1,2	1,2
P5	Name : MARIN Guy Institution : UGent	2,3,4	1	2,3, 4	2	4,5	3,4	2	1	
P6	Name : JONAS Alain Institution : UCL	1,2,4	1,2	4	1,2	1,2,4 5	5	1,2,3	1	1,2
P7	Name : DU PREZ Filip Institution : UGent		1		1,2	5		1,3		2
P8	Name : BARON Gino Institution : VUB	1		2,3	1,2	5	2,4			
P9	Name : DE MESMAEKER Andrée Institution : ULB						2		1	1,2
P10	Name : WOUTERS Johan Institution : FUNDP	1,3	1,2		2	1,3,5	1		1,2	1,2
P11	Name : VANDERZANDE Dirk Institution : UHasselt	3,5	1,2	3		1,2,4	1		1	2
P12	Name : VANDERLEYDEN Jos Institution : K.U.Leuven	3				2,3,4	1,3,5	3		2
P13	Name : WAROQUIER Michel Institution : UGent	2,4	1	1,2, 3	3		3			
EU1	Name : MULLEN Klaus Institution : MPI Mainz	1,2,4 5	1,2	3,4		1,2,4 ,5	1,3		1	1,2
EU2	Name : FEIJEN Jan Institution : UTwente		1		1	4	2	3		1

The figures refer to the respective tasks in each work package

The numbers in the cells refer to the partners (1 to 16, EP1, EP2), participating in the various WPs / Tasks at the respective platform levels.

Platform	task	1 Theory & Modelling	2.1 Building blocks	2.2 Self-assembly	2.3 Biomimetic design	2.4 Nano-patterning	3.1 Interaction Recognition	3.2 Adsorption Motion Diffusion	3.3 Chemical stimuli, Catalysis	3.4 Other stimuli (hv, *T*, *E*, ..)	4 Devices
WP1: Nanodots, Photonic Crystals	1	10	2, EU1	2		6				2	8
	2	4, 5, 13	1, 3, EU1			6			1, 2, 6	2	
	3	4, 10	2, 3, 5, 12	11			12		1	2	
	4	4, 5, 13	3, 4, 5, EU1			1, 6		1	1, 2, 6	2	3
	5	4	2, 11, EU1	2, 11, EU1						2, 11	11
	1	4, 5, 10, 13	2,3,4,6, 7, EU1	2, 6, 11				2,6, 11	3, 4	2,3,4,6,7,10,EU1	
	2	4, 10	6, 11, EU1	2,4, 6, 11, EU1				2, 11		2, 6	
WP3: Porous frameworks	1	13	1, 2	1			1				
	2	5, 13	2	1				1, 8	1, 5		
	3	5, 10, 13	1, 2, EU1		1		1, 2, 11	1, 2, 8	1, 2, 5	2	1, 3, 8
	4		1, 2, 5, 6, EU1	1			1, 2, 6, EU1	1	1, 2	2	
WP4: Hybrid materials	1		3, 7	3	3		3	8	3, 6	2, 3, 6, 7	3, 8
	2	5, 10	3, 5, 6, 7	3, 6, 7	.			8		4, 6, 7	3
	3	4, 13	3, 4	1, 2, 3, 4						4	
	1	4, 10	2, EU1	2, 11	2, 11			2, 11		2, 6, 11	
	2		2, 12		1		2, 6, 11	2, 6, 11	1	2, 11	12
	3	4, 10	2, 12		2, 12					2	
	4		2, 3, EU1	2, 3, 5, 6, 11	3, 6, EU2, 12	6	2, 3, 12, EU2	2, 11		2, 6	
	5	10	1, 2, 3, 5, 6, 7	6, 7		3, 6, 7		1, 2, 8	1, 3, 6, 7	2	1, 3, 8
WP5: Biomolecules & Biocatalysis	1	4, 10	2, 11, 12, EU1					2, 11		2, 11	
	2	4	9	2, 9	9			2, 8	9	2	9
	3	5, 13	1, 2, 12					1, 2	1, 2, 12	1, 2, 12	
	4		1, 3	1	1, 3			1, 5, 8	1, 3		
	5		1, 12			6			1, 6, 12	6	
WP7: Functional coatings	1		3, 7	3, 6			3	6	3, 6	3, 6	3
	2	5	3	3, 4, 6				4, 6	1, 3		
	3		3, 4, 6, 7		3, 6		3, 12, EU2	6, 7, EU2			
WP8: Conjugated systems	1	4, 5, 10	2, 9, 11, EU1	4, 11		2, 6	4	2		2, 4, 6, 9, EU1	11
WP9: Self-assembly at surfaces	1	4, 10	2, 9, EU1	2, 4, 6, 9				6	2	2, 4, 6	
	2	10	3, 4, 7, EU1	1, 2, 9, 11	3, 6, 12	2, 6	2, 6, 10	2, 6, 11	1, 2, 6	2, 6	

Figure 1. Interactions between work packages



I. 6. MAIN SKILLS OF THE PARTNERS

Describe the main skills of each of the partners in relation to the project (15 lines maximum per partner).
Delete not used lines.

P1 - Name : JACOBS Pierre
Institution : K.U.Leuven
Main Skills : tailor-made design of super-selective, (supramolecular) catalysts for fine chemicals, biomimicking and (chiral) membrane preparation; in-situ characterization of solids interacting with gases and liquids; catalytic characterization; including membrane and high-throughput reactors; single molecule catalysis; operando spectroscopy.

P2 - Name : VAN DER AUWERAER Mark
Institution : K.U.Leuven
Main Skills : Time-resolved and stationary absorption and fluorescence spectroscopy; photoconduction; energy and electron transfer; Langmuir Blodgett; fluorescence microscopy; STED; single molecule spectroscopy; single particle catalysis; heterocyclic chemistry; dendrimers; porphyrins; (electrochemical)scanning tunnelling microscopy; atomic force microscopy.

P3 - Name : JEROME Christine
Institution : ULg
Main Skills : Macromolecular engineering; polymeric (nano)materials; biomaterials

P4 - Name : LAZZARONI Roberto
Institution : UMH
Main Skills : supramolecular organisation in polymer materials; design and synthesis of multifunctional polymer and composite materials; epitaxial/oriented growth, thin film instability, confinement of molecules, surface patterning; electronic, optical and charge transport properties of organic materials; microscopic morphology of polymer materials.

P5 - Name : MARIN Guy
Institution : UGent
Main Skills : Contribute to the understanding of the effects of the synthesis conditions on the structure and function of block copolymers, engineering polymers, nanostructured carbon materials, (multi) porous oxides and (supported) nanoparticles by multiscale modelling and experimentation.

P6 - Name : JONAS Alain
Institution : UCL
Main Skills : synthesis, (self-)assembly, and characterisation of functional and/or responsive macromolecules and nano-systems, such as block copolymers and catalytic supra-molecules, nano-rods and nano-wires, nano-patterned surfaces, and organic nano-structures made therefrom.

P7 - Name : DU PREZ Filip
Institution : UGent
Main Skills : Synthesis and characterization of tailor-made complex polymer structures for novel supramolecular systems.

P8 - Name : BARON Gino
Institution : VUB

Main Skills : Measurement and modelling of adsorption and diffusion in microporous materials, chromatography, nanotechnology, lab-on-a-chip.

P9 - Name : DE MESMAEKER Andrée
Institution : ULB
Main Skills : Photochemistry of bio-inorganic supramolecular systems and synthesis of discotic compounds for liquid crystals.

P10 - Name : WOUTERS Johan
Institution : FUNDP
Main Skills : a) theoretical aspects including the elaboration and applications of theoretical chemistry tools to predict and interpret structural, electronic, optical, and vibrational properties of molecules, polymers, and solids, including the nonlinear optical properties, the electronic absorption and emission spectra, various vibrational signatures as well as to establish structure-function relationships; b) structural biology aspects encompassing the use of small molecules and protein crystallography in order to understand mechanisms of inhibition of potential drug targets including enzymes involved in the biosynthesis of isoprenoïds.

P11 - Name : VANDERZANDE Dirk
Institution : UHasselt
Main Skills : Organic and polymer synthesis of conjugated systems; advanced NMR spectroscopic techniques; microfluorimetric techniques in biological systems.

P12 - Name : VANDERLEYDEN Jos
Institution : K.U.LEUVEN
Main Skills : Biochemistry and cell biology of signalling and metabolic pathways in homogenous and mixed microbial communities.

P13 - Name : WAROQUIER Michel
Institution : UGent
Main Skills : molecular modelling – heterogeneous and homogeneous catalysts – solvent effects – QM/MM.

EU1 - Name : MULLEN Klaus
Institution : Max Planck Institute for Polymer Research Mainz
Main Skills : new polymer-forming reactions including methods of organometallic chemistry; dye cheimstry, multi-dimensional polymers with, e.g., ribbon-type, sheet-type or shape-persistent three-dimensional structures; chemistry with single molecules; charge-transport properties of polymers and related oligomers including doping mechanisms and charge-storage capacity; supramolecular chemistry, molecular materials with liquid crystalline properties

EU2 - Name : FEIJEN Jan
Institution : Universiteit Twente
Main Skills : biodegradable polymers, amphiphilic polymers, hydrogels, drug delivery systems and nano-systems, interaction between cells and surfaces, tissue engineering, protein adsorption, and vectorization of DNA into cells

I. 7. NETWORK ORGANISATION AND MANAGEMENT (4 pages maximum)

Describe the network's organisation and the practical terms governing collaboration and interaction between the partners (meetings, newsletters, doctoral school, ...).

Coordination Committee and Coordinator

The general scientific and administrative management of the network will be performed by the Coordination Committee (**CC**), consisting of Pierre Jacobs (P1), Dirk De Vos (P1), Mark Van Der Auweraer (P2), Christine Jérome (P3), Roberto Lazzaroni (P4), Frans De Schryver (Prof. Em.), and Robert Jérome (Prof. Em. from 2007). All individuals have been active in the two previous IAP phases (IV& V), belonging to major partners and were exerting major tasks when setting up the present IAP Phase VI proposal. The CC will take on a unanimous basis all major scientific and administrative decisions. They will meet at least every six months.
The Coordinator (**C**) (P. Jacobs) will preside the CC meetings and will also function as official spokesman and contact person of the network.
The names of the individuals associated with the different partners (P1 - P13; EU1, EU2) are administratively and scientifically responsible for the performance of the different institutions involved, viz. scientific activity in the different WP, reporting and administrative follow-up.

International Advisory Board

For renowned scientists that have been active in different areas belonging to the core activity of the network have been invited to become member of the International Advisory Board (**IAB**) for the network, *viz.* Prof. Em. Jan Verhoeven (U Amsterdam, photophysics), Prof. Em. Jean-Pierre Vairon (U Paris VI, polymer scientist), Prof. Eric Derouane (U Algarve, catalysis), Prof. B.J.J. Lugtenberg (U Leiden, microbial manipulation for bio-control), Prof. H. Masuhara (U Osaka, photophysics, laser abalation, fluorescence microscopy, NSOM, nano crystals). The IAB will have access to all scientific data generated. The IAB will meet annually with CC at the occasion of the annual meeting of the network scientists (see below). They will discuss scientific progress in relation to the defined tasks of the project.

Work Package Coordinators

The network activity consists of 9 work packages, each covering the study of relevant functional supramolecular systems at the following 4 different platforms: 1., Theory and Modeling, 2., Synthesis and Fabrication, 3., Structure and Functionality, and 4., Devices and Responsive Systems. The CC proposed individuals as Work Package Coordinator (**WPC**) from different partners according to their main expertise. Each WPC is responsible for the scientific activity in each WP according to the goals defined in the proposal. The WPC will organize regular meetings with all concerned scientists of the partners involved at least on a six-monthly basis and be responsible for the in-time collection of all data required for reporting. The WPC are the following for the respective WP: WP1, Mark Van Der Auweraer (P2); WP2, Guy Marin (P5); WP3, Dirk De Vos (P1); WP4, Filip Du Prez (P7); WP5, Marcel Ameloot (P11); WP6, Jos Vanderleyden (P12); WP7, Christine Jérome (P3); WP8, Roberto Lazzaroni (P4); WP9, Alain Jonas (P6).
Specific items covering activities by several partners at the level of the 4 different platforms are grouped as tasks. Each WP consists of a set of related tasks.
WPCs should assure that postdoc and Ph.D. scientists involved in common WP or task(s) interact intensively via informal meetings, short exchange stays at each others premises, and sharing of specific equipment.
WPCs are also responsible that accepted co-publications involving several partners appear ASAP on the confidential part of the website. They should assure that in each scientific publication the proper acknowledgments are made, *viz.* to DWTC.

WP Review Meetings and Reports

WP review meetings will be informal scientific meetings open to all interested scientists belonging to the network. Such meetings aim at defining specific goals and deliverables for the next working period for/by scientists in the WP concerned. Specific longer term milestones and decision making points for each WP will be defined as well. Items concerning the exchange of scientists, the use of each others facilities will be discussed at this level. Each contributor will report on its activity and a short (electronic) *WP review meeting report* will be made by the respective WPCs. WP review meeting reports will be made available to each partner (via the confidential part of the website (see below)). Such meetings will be organized at least twice a year.
Work package review reports by the responsible WPC will critically examine the progress made in every WP or task, formulate suggestions for further work and input from other WPs or tasks, judge on achievements in

terms of milestones or deliverables, and on scientific output in general. The work package review reports will be part of the annual report.
Although all defined tasks in the WPs are of a fundamental scientific nature and mainly concerned with generation of generic scientific knowledge, partners at the occasion of WP review meetings, should define whether IP is possibly generated in the past period. If so, all measures should be taken to protect it. Unless otherwise defined at the level of the general contract between DWTC and the respective partners, the generated IP will be shared among the partners who contributed to the WP/Task concerned. The names of the scientists involved should figure as inventors on patents taken to protect this IP.

Annual Scientific Meeting
Annually, a general two-day scientific meeting will be organized, chaired by C, in presence of the members of IAB. This *annual meeting of all scientists belonging to the network* aims to report on the progress made by the individual scientists working in the general frame of the network. An international expert in the area of interest to the network will be invited to deliver a plenary lecture on a timely topic. Among the network scientists, oral and poster presentations will be solicited. Representatives of DWTC, members of the Research Councils of the participating Institutions as well as representatives of potentially interested companies will also be invited to attend.
At this occasion, the international board will meet with the CC, the partner's representative and the WPCs to discuss the scientific achievements in the frame of the network research, confront them with the proposed milestones and propose changes in topics and approach. Interactions between the board members, the participating groups and representatives of DWTC will be encouraged. Reporting on protected IP will be done explicitly.
C and CC will be responsible to make major achievements available to a broader public in a suitable form, *viz.* a newspaper publication.

Annual Report
The annual report, both in electronic and hard copy-form, will give an overview of scientific achievements, the scientific activities/output of the individual members and the relevant administrative information required by DWTC. Emphasis will be on achievements obtained via networking. At this occasion, major scientific achievements will be highlighted for a larger (non-scientific) audience..

This strict management scheme does not refrain the individual scientist from informal contacts and discussions with colleagues. Communications among partners and scientists in the frame of activities in a WP will occur via electronic mail, with copy to WPC.

Doctoral School
In the context of the network the existing Doctoral School on Supramolecular Chemistry and Supramolecular Catalysis (IAP-V-03) will be further extended. Basically, invitations to attend lectures organized by visiting scientists at the location of one of the network partners or registration for workshops or symposia organized by a network partner will be extended to all scientists of the network. The doctorate school will be linked to an already existing EU network of excellence (NoE) in Supramolecular Catalysis (IDECAT) and to an international school organized by the MPG on Polymer Chemistry. Further on, it will be attempted to establish an agreement between this network (P6/27) and the one proposed on Advanced Complex Inorganic Materials (P6/) in order to open sessions of the graduate school and to invite all researchers to each other's activities.

Website
The network will have its **website**, partly accessible to the public, and partly confidential. The latter part will contain information for network scientists, members of the board and DWTC and will be accessible by password. The website will be accessible via the URL of C. The secretarial staff of C will be responsible for updating the website.
The public part of the site will contain general information on the project, the list of partners and will highlight main achievements and contain a list of co-publications. Links to websites of the partners will be set up.
The part of the site with restricted access will contain both the WP Review Meeting reports.

In view of already established interactions and methodologies during IAP phases IV and V, it is possible to start the tasks at several levels at once. The interrelation of the different tasks can be visualized in the following scheme.
Interactions among different Tasks / WPs will occur at one of the following levels: 1., exchange of materials; 2., sharing of procedures, *viz.* for materials synthesis; 3., sharing of experimental techniques; 4., joint work on

concepts. Interrelated tasks will be geared to allow the study of the respective materials as soon as available by in parallel and /or previously developed methodologies.

I. 8. RE-ORGANISATION OF THE PROJECT (maximum 3 pages)

To be completed only if the initial proposal has to be adapted as a result of the selection outcome. If this implies changes in the composition of the network and/or the budget, it may be that it is not longer possible to pursue (achieve) the originally proposed objectives.

In this case, describe and clarify the re-organisation of the project compared to the initial proposal.

As a result of the selection procedures, three partners were removed. The work packages were changed accordingly.
These changes involve contributions to the work packages where these partners were involved. Technically, it comes to the elimination of actions where the specific equipment of these partners was involved. This is related to the use of typical rheological equipment and instrumentation for determining NLO (non-linear optical) properties of some materials. Only Task 8.2 has been removed explicitly, as it involved the preparation and characterization of specific materials which belongs to the specific expertise of one of the eliminated partners.

I. 9. **BUDGET** (global distribution per partner for the 5 years)

(in EURO, without decimals)

The detailed distribution per partner is given in Section II

	Name Partner	Institution	Budget
P1	JACOBS Pierre	K.U.Leuven	1 250 000
P2	VAN DER AUWERAER Mark	K.U.Leuven	1 250 000
P3	JEROME Christine	ULg	800 000
P4	LAZZARONI Roberto	UMH	751 778
P5	MARIN Guy	UGent	905 740
P6	JONAS Alain	UCL	900 000
P7	DU PREZ Filip	UGent	400 000
P8	BARON Gino	VUB	462 115
P9	DE MESMAEKER Andrée	ULB	400 000
P10	WOUTERS Johan	FUNDP	400 000
P11	VANDERZANDE Dirk	UHasselt	400 000
P12	VANDERLEYDEN Jos	K.U.Leuven	400 000
P13	WAROQUIER Michel	UGent	450 000
EU1*	MULLEN Klaus	MPI Mainz	50 000
EU2*	FEIJEN Jan	U Twente	50 000
TOTAL BUDGET			8 869 633

* The budget for the EU-partner is the budget attributed by the IAP-programme only (without the 50% contribution of the EU-partner)

* The budget for the EU-partner is the budget attributed by the IAP-programme only (without the 50% contribution of the EU-partner and with a maximum of 150.000 EUR per proposal).

I. 10. PREVIOUS IAP-PHASES

To be completed only if the present network was funded during earlier phases of the IAP programme.

Mention the earlier phases of the IAP programme (I, II, III, IV, or V) and the titles of projects in which the partners of the present network has participated.

Phase	Period	Network title	Partner *
I	1987-1991	"Catalysis"	P1, P5
I	1987-1991	"Polymer Materials"	P2 , P3, P7
II	1990-1996	P2/16 "Supramolecular Chemistry and Catalysis"	P1, P2, P4, P7, P8, P11
III	1992-1996	P3/39 "Catalysis"	P1, P5
III	1992-1996	P3/40 "Polymer Materials"	P2, P3, P7
IV	1997-2001	P4/19 "Supramolecular Chemistry and Supramolecular Catalysis"	P1, P2, P3, P4, P5, P6, P7, P8, P9, P11
V	2002-2006	P5/03 "Supramolecular Chemistry and Catalysis"	P1, P2, P3, P4, P5, P6, P7, P8, P9, P10, P11, P12, EU1

*notation of partners from the present proposal; the research group remained unchanged; the academic responsible may have changed.

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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION II

Information on the partners

to be completed by each network partner including the EU-partner(s)

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the partner : Jacobs Pierre (P1) *Institution : Katholieke Universiteit Leuven*

II. 1. PARTNER CONTACT DETAILS

PARTNER N° 1 (consult the list in Section I of Annex I)* : P1

- Family Name : Jacobs
- First Name : Pierre
- Title (Prof., Dr., ...) : Prof. Dr. Ir.
- Institution : Katholieke Universiteit Leuven
- Institution's abbreviation : K.U.Leuven
- Faculty/Department :Faculteit Bio-Ingenieurswetenschappen/ Departement Microbiële en Moleculaire Systemen
- Research Unit : Centrum voor Oppervlaktechemie en Katalyse (COK)
- Road/Street, n° : Kasteelpark Arenberg 23
- Post Code : 3001
- Town/City : Heverlee
- Country : België
- Tel : 0032 16 32 15 95
- Tel secretariat : 0032 16 32 16 10
- Fax : 0032 16 32 19 98
- E-mail : Pierre.Jacobs@biw.kuleuven.be

Website : http://www.biw.kuleuven.be/ifc/cok/home.htm

* For Belgian partners : P1 to P13
For EU-partners : EU1 to EU4

II. 2. STAFF MEMBERS WORKING ON THE PROJECT (paid and not paid by the IAP-budget)

Staff	Number
Professor	8
Senior scientist	/
Post-doc	11
PhD student	40
Researcher without phD	/
Technician	9
Secretary	4
Other	/
TOTAL	72

II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, phD student, researcher without phD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name : JACOBS Pierre
   Profile : professor
   Skills : Supramolecular and heterogeneous catalysis.

2. Name : DE VOS Dirk
   Profile : professor
   Skills : Biomimetic and bio-catalysis; organic synthesis (dendrimers and ionic liquids); metallo-organic frameworks.

3. Name : SELS Bert
   Profile : professor
   Skills : Biomimetic catalysis with renewables.

4. Name : KIRSCHHOCK Christine
   Profile : professor
   Skills : Assembly of inorganic/organic entities via supramolecular forces; electron diffraction methodologies.

5. Name : VANKELECOM Ivo
   Profile : professor
   Skills : Membranes: organic, inorganic and hybrid.

6. Name : MARTENS Johan
   Profile : professor
   Skills : Synthesis solids via supramolecular forces; drug release.

7. Name : SCHOONHEYDT Robert
   Profile : professor
   Skills : Operando spectroscopy.

8. Name : DE WINNE Hendrik
   Profile : ph D student
   Skills : Design of biomimetic catalysts via high throughput methodologies.

9. Name : MOENS Bart
   Profile : ph D student
   Skills : Design of hybrid catalysts.

10. Name : VAN BERLO Boris
    Profile : ph D student
    Skills : Design of metathesis hybrid catalysts.

11. Name : TIELEN Maria
    Profile : technician
    Skills : Synthesis and testing of porous hybrid materials.

12. Name : LAERMANS Chris
    Profile : secretary
    Skills : Administrative project management.

13. Name : ALAERTS Luc
    Profile : ph D student (FWO)
    Skills : Synthesis and characterization of metallo-organic framework.

14. Name : HERMANS Ive
    Profile : post doc (FWO)
    Skills : Theoretical modelling of catalyzed reactions via transition state characterization.

15. Name : HOUTHOOFD Kristof
    Profile : ph D student
    Skills : MAS NMR of hybrid catalysts.

16. Name : LIN Kaifeng
    Profile : post doc
    Skills : Tailor-made synthesis of biomimetic catalysts.

17. Name : PARVULESCU Andrei
    Profile : ph D student
    Skills : Combination of chemo- with biocatalysts

18. Name : PESCARMONA Paolo
    Profile : post doc FWO
    Skills : Preparation and testing via high throughput methodology of biomimetic catalysts.

19. Name : VAN ERP Titus
    Profile : post doc
    Skills : Theoretician = development of advanced computational methods for catalyzed reactions.

20. Name : VARSZEGI Csaba
    Profile : ph D student
    Skills : Organic synthesis with bio-catalysts.

21. Name : VERMANDEL Walter
    Profile : technician
    Skills : Design of reactors; synthesis of hybrid catalysts.

22. Name : WAHLEN Joos
    Profile : post doc FWO
    Skills : Preparation and characterization of hybrid materials.

II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

Hybrid Langmuir Blodgett Monolayers Containing Clay Minerals: Effect of Clay Concentration and Layer Charge Density on the Film Formation.
Ras R., Nemeth J., Johnston C.T., DiMasi E., Dekany I., and Schoonheydt R.A.
Phys. Chem. Chem. Phys., 6, 4174-4184, 2004.

Bromide-assisted Oxidation of Substituted Phenols with Hydrogen Peroxide to the Corresponding p-Quinol abd p-Quinol Ethers over WO_4^{2-} exchanged Layered Double Hydroxides.
Sels B., De Vos D.E., and Jacobs P.A.
Angew. Chem. (Int. Edit.), 44, 310-313, 2005.

Acid zeolites as alcohol racemization catalysts: Screening and application in a biphasic dynamic kinetic resolution.
Wuyts S., De Temmerman K., De Vos D.E., and Jacobs P.A.
Chem. Eur. J., 11, 386-397, 2005.

Benzimidazole-functionalized Dendrons as Molybdenum Supports for Selective Epoxidation Catalysis.
Chavan S., Maes W., Wahlen J., Jacobs P.A., De Vos D.E., and Dehaen W.
Catalysis Communications, 6, 241-246, 2005.

Design and Synthesis of Hierarchical Materials from Ordered Zeolitic Building Units.
Martens J.A., Kirschhock C., Kremer S.P.B., Vermant J., Van Tendeloo G., and Jacobs P.A.
Chem. Eur. J., 11, 4306-4313, 2005.

In situ Space and Time Resolved Sorption Kinetics of Anionic Dyes on Individual LDH Crystals.
Roeffaers M., Sels B., Loos D., Kohl C., Müllen K., Jacobs P.A., Hofkens J., and De Vos D.E.
Chem. Phys. Chem., 6, 2295-2299, 2005.

Template-Aluminosilicate Structures at the Early Stages of Zeolite ZSM-5 Formation. A Combined Preparative, Solid-State NMR and Computational Study.
Magusin P., Zorin V.E., Aerts A., Houssin C.J.Y., Yakovlev A.L., Kirschhock C., Martens J.A., and Van Santen R.A.
J. Phys. Chem. B., 109, 22767-22774, 2005.

Gold Nanoclusters as Colloidal Catalysts for Oxidation of Long Chain Aliphatic 1,2-diols in Alcohol Solvents.
Mertens P., Vankelecom I.F.J., Jacobs P.A., and De Vos D.E.
Gold Bulletin, 38, 157-162, 2005.

Spatially Resolved Observation of Single Turnover Events on Individual Catalytic Crystals by Fluorescence Microscopy.
Roeffaers M., Sels B., Loos D., Uji-i H., Müllen K., De Schryver F., Jacobs P.A., De Vos D.E., and Hofkens J.
Nature, 439, 572-575, 2006.

Porphyrin-Functionalized Dendrimers: Synthesis and Applications as Recyclable Photocatalysts in a Nanofiltration Membrane Reactor.
Chavan S., Maes W., Gevers L., Wahlen J., Vankelecom I.F.J., Jacobs P.A., Dehaen W., and De Vos D.E.
Chem. Eur. J., 11, 6754-6762, 2005.

II. 5. INTERNATIONAL CONTACTS IN THE PROJECT'S RESEARCH DOMAIN

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

International contacts:

Prof. David Gammon, University of Cape Town, Department of Chemistry, Rondebosch, SA-7701 Rondebosch, South-Africa (Prof. D. De Vos and B. Sels)

Prof. Vasile Parvulescu, University of Bucharest, Department of Chemical Technology and Catalysis, B-dul Regina Elisabeta 4-12, R-70346 Bucharest, Romania (Prof. D. De Vos and P. Jacobs)

Prof. Yeung Ho Park, Hanyang University, Department of Chemical Engineering, 1271 Sa 1-dong, Sangnok-gu, Ansan-si, Gyeonggi-do, 425-791, Korea (Prof. P. Jacobs)

Prof. Imre Dékány, University of Szeged, Department of Colloid Chemistry and Nanostructured Materials Research Group of Hung. Acad. Sci., Aradi vt. T. 1, H-6720 Szeged, Hungary (Prof. R. Schoonheydt)

Prof. Jean-Marie Basset, UMR 9986 CNRS - ESCPE Lyon, Laboratoire de Chimie Organométallique de Surface, 43, rue du 11 Novembre 1918, F-69626 Villeurbanne Cédex, France (Prof. P. Jacobs, D. De Vos and B. Sels)

Prof. Johannes Lercher, Technische Universität München, Lehrstuhl II für Technische Chemie (TC2), Lichtenbergstrasse 4, D-85747 Garching, Germany (Prof. P. Jacobs, D. De Vos and B. Sels)

International networks:

EU NoE IDECAT (Integrated Design of Catalytic Nanomaterials for a Sustainable Production) 2006-2010; 16 EU-partners (Prof. P. Jacobs, D. De Vos, B. Sels, C. Kirschhock)

II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,...).

G.O.A./2005/13
J. Martens (promoter)
D. De Vos, P. Jacobs, A. Maes, R. Schoonheydt, I. Vankelecom, M. Groothaert, C. Kirschhock, B. Sels (Co-promotors)
High-throughput and combinatorial approach to the design and understanding of the active site in catalysis.
Period : 01/10/2004 – 30/09/2009

E.U. – FP6 - Network of Excellence (NoE) IDECAT
P. Jacobs, D. De Vos, B. Sels, C. Kirschhock
Integrated Design of Catalytic Nanomaterials for a Sustainable Production.
Period : 01/04/2005 – 31/03/2010

Centre of Excellence 2005 (EF/05/009) (K.U.Leuven)
J. Martens (spokesman)
Co-promotors: D. De Vos, P. Jacobs, C. Kirschhock, R. Schoonheydt, B. Sels, I. Vankelecom, J. Hofkens
Centre of Excellence in Catalytic Science (CECAT)
Period : 01/11/2005 – 31/10/2010

F.W.O.- Vlaanderen No. G.0363.06
J. Martens (promotor)
Co-promotors : P. Jacobs, C. Kirschhock, K. Maex
Study of the formation process of hierarchical silica materials and carbon nanotubes with an integrated Raman spectroscopy-X-ray diffraction combination.
Period : 01/01/2006 – 31/12/2009

E.U. – FP6 – CARBonCHIP STREP
NMP4 – CT – 2006 – 016475
Carbon Nanotubes technology on Si IC's.
Period : 01.04.2006 – 31.03.2009

I.U.A.P. – netwerk fase V (N°: P5/01/03)
P. Jacobs
Supramolecular chemistry and supramolecular catalysis [sc]2
Period: 01.01.2002 – 31.12.2006

E.C. COST Action no. D24 - COST Chemistry Working Group Proposal (D24/0007/02)
P. Jacobs, D. De Vos
Synthesis and application of new ligands for asymmetric heterogeneous catalysis
Period: 01.05.2002 – 30.04.2006

IWT – SBO "BIPOM" nr 030202 - K.U.Leuven Research & Development (040372)
P. Jacobs
BIPOM: Design of bimodal porous materials for catalysis and sorption
Period: 01.11.2003 – 31.10.2007

F.W.O.-Vlaanderen nr G.0375.04
J. Martens, promotor

Synthese en karakterisering van een nieuwe familie hiërarchische materialen: stapeling en koppeling van zeolitische nanoblokjes tot driedimensionele mozaïekstructuren
Period: 01.01.2004 – 31.12.2007

F.W.O. nr G.0323.04
Dirk De Vos, promotor
Intensifiëring van karakterisatie en screening van katalysatoren voor vloeistoffase C-C koppeling en oxidatiereacties
Period: 01.01.2004 – 31.12.2007

ZISCOAT (Spin-off)
K.U.Leuven Research & Development
P. Jacobs, J. Martens
The Third Generation Prothesis
Period: June 2004 – summer 2007

F.W.O.-Vlaanderen Nr. WO.014.05 N - Wetenschappelijke Onderzoeksgemeenschap (WOG)
R. Schoonheydt
De actieve plaats: van katalysator tot reactor
Period: 01.01.2005 – 31.12.2009

F.W.O.-Vlaanderen nr. G.0314.05
I. Vankelecom (promotor); Filip Du Prez, RUG (hoofdpromotor en woordvoerder)
Gesegmenteerde polymeernetwerken en polyioncomplexen: aanmaak, karakterisatie en gebruik in membraanprocessen
Period: 01.01.2005 - 31.12.2008

Vlaanderen – Hongarije, BIL 04/32 (Prof. Imre Dekany, partner)
R. Schoonheydt
Hybrid nanofilms based on silica or clay minerals and bio polymers.
Period: 01.01.2005 - 30.06.2007

Vlaanderen – Roemenië, BIL 04/42
D. De Vos, P. Jacobs
Composite catalysts for the transformation of natural compounds via combinatorial approaches.
Period: 01.01.2005 – 31.12.2006

Vlaanderen – Zuid-Afrika, BIL 04/53
P. Jacobs (promoter); D. DeVos (co-promotor), B. Sels (co-promotor)
Heterogeneous Lewis acids for the promotion of cycloadditions and other c-c bond forming reactions on anhydrosugars
Period: 01.01.2005 – 31.12.2006

Impulsfinanciering – zware apparatuur – ZWAP/05/12 - VIRKAT
K.U.Leuven P. Jacobs (woordvoerder, promotor) and J. Martens (co-promotor); VUB G. Baron (co-promotor); UGent G. Marin (co-promotor);
VIRKAT – A Interuniversity Platform for High Throughput Experimentation for the Development and Design of Heterogeneous Catalysts.
Period: 01.04.2005 – 31.03.2009

1. F.W.O.-Vlaanderen GP.038.05N – J. Hajek - Junior postdoctoral fellowship

2. Onderzoeksfonds – junior postdoctoral fellowship – J. Hajek
P. Jacobs (promoter); D. De Vos (woordvoerder)
High throughput, combinatoriële benadering van de heterogene katalyse.
Period: 1. 01.05.2005 - 30.04.2006
Period: 2. 01.05.2006 – 30.04.2007

IWT – FLAMAC - K.U.Leuven Research & Development
P. Jacobs
Formulation, application and screening of high-viscous solutions, dispersion and pastes (SDP).
Period: 27/01/2005 – 26/01/2008

ESA /ESTEC Contract n° 19136/05/NL/UJ - Topical Teams: "Zeolite Crystallization"
J. Martens, C. Kirschhock
Self-assembly of hierarchical catalysts and adsorbent materials from ordered liquid phases (OLPs)
Period: 01.03.2005 – 28.02.2007

F.W.O.-Vlaanderen nr. G.0363.06
J. Martens (promotor, verantwoordelijk woordvoerder); P. Jacobs, C. Kirschhock, K. Maex (IMEC) (co-promotoren)
Studie van het vorminsproces van hiërarchische silica materialen en koolstof nanotubes met een geïntegreerde Raman spectroscopie-X-stralendiffractie combinatie.
Period: 01.01.2006 – 31.12.2009

EU. – COST ACTION n° 036
R. Schoonheydt
Moleculair Structure – Performance Relationships at the Surface of Functional Materials"
Period: starting from 24/02/2006

Bilaterale samenwerking Vlaanderen – Polen (BIL 05/19)
F. Du Prez, UGent (promotor); I. Vankelecom (co-promotor)
Segmented polymer networks and polyelectrolyte complexes: design and their use in membrane processes
Period: 01.01.2006 – 31.12.2007

ESA/ESTEC contract n° C90229 - "PRODEX"
C. Kirschhock, J. Martens
Self-assembly of hierarchical catalysts and adsorbent materials from ordered Liquid Pases (OLPs)
Period: 01.01.2006 – 31.12.2008

IOF – Hefboomproject
I. Vankelecom
Nanofiltratiemembranen met lag 'MWCO' in apnotische, aromatische en gehalogeneerde solventen.
Period: 01.06.2006 – 31.05.2007

II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: WP1, Nanodots and photonic crystals (tasks 2, 3, 4)
2. Workpackage number and title: WP3, Porous framework (tasks 1, 2, 3, 4)
3. Workpackage number and title: WP4, Hybrid materials (task 3)
4. Workpackage number and title: WP5, (Bio)membranes (tasks 2, 5)
5. Workpackage number and title: WP6, Biomolecules and biocatalysis (tasks 3, 4, 5)
6. Workpackage number and title: WP7, Functional coatings (task 2)
7. Workpackage number and title: WP9: Self-assembly at surfaces (task 2)

II. 8. BUDGET (distribution per year) *

(in EURO)

	2007	2008	2009	2010	2011	Total
Personnel	153.145,00	156.250,00	160.020,00	166.405,00	175.530,00	**811.350,00**
Operating costs	75.426,43	72.321,43	68.551,43	62.166,43	62.565,24	**341.030,96**
Equipment	10.000,00	10.000,00	10.000,00	10.000,00	Not allowed	**40.000,00**
Overheads	11.428,57	11.428,57	11.428,57	11.428,57	11.904,76	**57.619,04**
Subcontracting	0,00	0,00	0,00	0,00	0,00	**0,00**
Subtotal	***250.000,00***	***250.000,00***	***250.000,00***	***250.000,00***	***250.000,00***	***1.250.000,00***
EU 1 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 2 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 3 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 4 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
Total	***250.000,00***	***250.000,00***	***250.000,00***	***250.000,00***	***250.000,00***	***1.250.000,00***

* This table should not be completed by the European partner as his/her budget is mentioned in the budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership

- Personnel: indexed gross remunerations; employer's social contributions; statutory insurance costs as well as any other compensation or allocation legally due in addition to the salary; the reimbursements for PhD and postdoctoral grant holders (exempt from tax and benefiting from social security). Personnel costs must account for minimum 60% of the total budget attributed to each partner of the network. The costs for the tax-free PhD grants and postdoctoral grants may not account for more than 60% of the total personnel costs.

- Operating costs: documentation; travel and accommodation; hosting of visiting foreign researchers use of computing facilities; software; telecommunications; maintenance and operation of equipment and, more generally, consumables;.

- Equipment: acquisition and installation of scientific and technical appliances and instruments, including IT equipment placed at the project's disposal. Equipment cannot be asked for during the last year of the programme.

- Overheads: general expenses of the institutions covering, on an inclusive basis, administrative, telephone, postal, maintenance, heating, electricity, rental, material depreciation and insurance costs. The total amount for this heading may not exceed 5% of total personnel and operating costs.

- Subcontracting: costs incurred by a third party in order to perform tasks or provide services necessitating specific scientific or technical skills outside the normal framework of the institution's activities. Each request for subcontracting needs a approval from the programme administrator.

II. 9. EQUIPMENT

Indicate the equipment (with an estimation of the cost) that will be purchased from the IAP-budget for the coming from four years (2007-2010) and justify.

A minimum annual amount of office equipment (PC's, labtops, printers) (10.000 euro) is foreseen. This will be used as support for researchers (data, treatment and managing) and partly for secretarial duties (P1 is network coordinator).

II. 10. SUBCONTRACTING

To be completed only if subcontracting is foreseen.

Describe and justify the tasks and/or services that will be provided by a third party.

No subcontracting is foreseen.

BELGIAN SCIENCE POLICY
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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION II

Information on the partners

to be completed by each network partner including the EU-partner(s)

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the partner : Mark Van Der Auweraer (P2) Institution : K.U.Leuven

II. 1. PARTNER CONTACT DETAILS

PARTNER N° (consult the list in Section I of Annex I) * : P2

- Family Name : Van Der Auweraer
- First Name : Mark
- Title (Prof., Dr., ...) : Prof
- *Institution : Katholieke Universiteit Leuven*
- Institution's abbreviation : K.U.Leuven
- Faculty/Department :Chemistry
- Research Unit : Laboratory for Photochemistry and Spectroscopy
- Road/Street, n° : Celestijnenlaan 200F bus 2404
- Post Code : 3001
- Town/City : Leuven
- Country : Belgium
- Tel : 0032 16 32 74 96
- *Tel secretariat : 0032 16 32 74 18*
- Fax : 0032 16 32 79 90
- E-mail : mark.vanderauweraer@chem.kuleuven.be
- Website : http://www.chem.kuleuven.ac.be/research/mds/mds_en.html

* For Belgian partners : P1 to P13
For EU-partners : EU1 to EU4

II. 2. STAFF MEMBERS WORKING ON THE PROJECT (paid and not paid by the IAP-budget)

Staff	Number
Professor	5
Senior scientist	3
Post-doc	13
PhD student	23
Researcher without phD	4
Technician	3.5
Secretary	0.5
Other	
TOTAL	52

II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, phD student, researcher without phD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name : Mark Van Der Auweraer
   Profile : Professor
   Skills : Time-resolved and stationary absorption and fluorescence spectroscopy, photoconduction, energy and electron transfer, Langmuir Blodgett, diffusion supervision

2. Name : Johan Hofkens
   Profile : Professor
   Skills : fluorescence microscopy, STED, fluorescence correlation spectroscopy, single molecule spectroscopy, enzymes, single particle catalysis, supervision

3. Name : Wim Dehaen
   Profile : Professor
   Skills : heterocyclic chemistry, oligo(indolo)carbazoles, dendrimers, porphyrins, supervision

4. Name : Steven De Feyter
   Profile : Professor
   Skills : (electrochemical)scanning tunnelling microscopy, atomic force microscopy, chirality, self-assembly, templating, supervision

5. Name : Noel Boens
   Profile : Professor
   Skills : synthesis of pyrromethenes and fluorescent ion-probes, supervision

6. Name : Gerd Schweitzer
   Profile : senior scientist
   Skills : transient absorption spectroscopy

7. Name : Mario Smets
   Profile : senior scientist
   Skills : synthesis of dendrimers and hyperbranched polymers

8. Name : Hiroshi Ujii
   Profile : senior scientist
   Skills : *fluorescence microscopy, polymer dynamics, scanning tunnelling spectroscopy,* defocused wide field microscopy

9. Name : Tom Vosch
   Profile : senior postdoc
   Skills : fluorescence of metal nanoparticles, single molecule spectroscopy, photophysics

10. Name : Renaud Vallee
    Profile : senior postdoc
    Skills : polymer dynamics, analysis of single molecule data, simulations

11. *Name : Junichi Hotta*

Profile : senior postdoc
Skills : STED, fluorescence microscopy

tics

12. Name : Wouter Maes
Profile : postdoc
Skills : synthesis, porphyrins/macrocycles

13. Name : John Clifford
Profile : postdoc
Skills : preparation, characterization and photophysics of conjugated polymers doped with metal and semiconductor nanoparticles, solar cells

14. Name : Christina Flors
Profile : postdoc
Skills : *autofluorescent proteins (GFP and analogues), photoswitchable proteins, single* molecule spectroscopy

15. Name : Philippe Marsal
Profile : postdoc
Skills : theory of molecular solvation, analysis of single molecule fluorescence trajectories

16. Name : Shuhei Furukawa
Profile : postdoc
Skills : scaning probe microscopy

17. Guojie Wang
Profile : postdoc
Skills : STM, Templating

18. Name : Mikhail Parchin
Profile : postdoc
Skills : photoconduction, electroluminescence

19. *Dominique Wöll*
Profile : postdoc
Skills : Single molecule spectroscopy

20. Virginia Lopez
Profile : postdoc
Skills : Single molecule spectroscopy

21. Name : Anja Deres
Profile : doctoral student
Skills : cell membrane dynamics, fluorescence microscopy

22. Name : Ellen Gielen
Profile : doctoral student
Skills : cell membrane dynamics, fluorescence microscopy

23. Name : Hong Xu
Profile : doctoral student
Skills : scaning probe microscopy

24. Name : Anca Margineanu
Profile : postdoc
Skills : membrane dynamics, FLIM, single molecule spectroscopy

25. Name : Els Braeken
Profile : doctoral student
Skills : single molecule spectroscopy, polymer dynamics

26. Name : Eduard Fron
Profile : doctoral student
Skills : femtosecond transient absorption spectroscopy

27. Name : Peter De Decker
Profile : doctoral student
Skills : STED, single molecule spectroscopy

28. Name : Jeroen Ollevier
Profile : doctoral student
Skills : photoconduction, laser induced opto-accoustic spectroscopy, electroluminescence

29. Name : Kris Metten
Profile : doctoral student
Skills : synthesis: Hyperbranched polymers

30. Name : Annelies Vandendriessche
Profile : doctoral student
Skills : synthesis: Hyperbranched polymers

31. Name : Joice Thomas
Profile : doctoral student
Skills : synthesis: Hyperbranched polymers

32. Name : Gu Rong
Profile : doctoral student
Skills : synthesis: indolocarbazoles

33. Name : Thein Ngo Huynh
Profile : doctoral student
Skills : synthesis: corroles/ porphyrin dendrimers

34. Name : Lingam Kishore
Profile : doctoral student
Skills : synthesis: pyrimidine macrocycles

35. Name : Maarten Costermans
Profile : doctoral student
Skills : synthesis: pyrrole anion sensors

36. Name : Taoufik Rohand
Profile : doctoral student
Skills : synthesis: Bodipy

37. Name : Wienand Nulens
    Profile : doctoral student
    Skills : synthesis: helicenes

38. Name : Lesley Pandey
    Profile : doctoral student
    Skills : electroluminescence, photoconduction

39. Name : Inge Decat
    Profile : doctoral student
    Skills : scanning probe microscopy

40. Name . Susanna Roccha
    Profile : doctoral student
    Skills : single molecule spectroscopy

41. Willem Vanderlinden
    Profile : doctoral student
    Skills : atomic force microscopy, DNA manipulation

42. Jess Lycoops
    Profile : undergraduate student
    Skills : fluorescence, synthesis

43. Han Jin Adisojosoe
    Profile : undergraduate student
    Skills : STM

44. Robrecht Vergauwe
    Profile : undergraduate student, plans to start PhD in October
    Skills : fluorescence, microscopy, biomiolecules

45. Jihong Lu
    Profile : undergraduate student, plans to start PhD in October
    Skills : STM, templating

46. Name : Wim Van Rossom
    Profile : doctoral student
    Skills : synthesis: pyrimidine macrocycles

47. Name : Volker Leen
    Profile : doctoral student
    Skills : synthesis: fluorescing pyrrole anion sensors

48. Name : Marino Fumarola
    Profile : technician
    Skills : IP, laser maintenance,electronics

49. Name : Carine Jackers
    Profile : technician
    Skills : chemistry, scanning probe, administration

50. Name : Karel Duerinckx
    Profile : technician

Skills : NMR

51. Name : Bert Demarsin
Profile : technician
Skills : mass spectroscopy

52. Name : Dirk Henot
Profile : technician
Skills : HPLC

53. Name : Ann Petré
Profile : secretary
Skills : secretary

II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

R. Gronheid, Johan Hofkens, Fabian Köhn, T. Weil, E. Reuther, K. Müllen, Frans C. De Schryver,
Intramolecular Förster Transfer in a Dendritic Sysytem at the Single Molecule Level,
J. Am. Chem. Soc., 124, 2418-2419 (2002).

M. Lor, S. Jordens, G. De Belder, G. Schweitzer, M. Cotlet, J. Thielemans, J. Hofkens, T. Weil, K Müllen, J.W. Verhoeven, L. Viaene, M. Van der Auweraer and F.C. De Schryver,
Electron transfer in Rigid Aminecore Dendrimers
J. Am. Chem.Soc., 124, 9918-9925 (2002).

M. Lor, R. De, S. Jordens, G. De Belder, G. Schweitzer, J. Hofkens, T. Weil, A. Herrmann, U.K. Wiesler, K. Müllen, M. Van Der Auweraer, F. C. De Schryver
Generation Dependent Energy Dissipation in Rigid Dendrimers studied by Femto- to Nanosecond Time Resolved Fluorescence Spectroscopy,
J. Phys. Chem. A, 106, 2083-2090 (2002).

A. Miura, Z. Chen, H. Uji-i, S. De Feyter, M. Zdanowska, P. Jonkheijm, A.P.H.J. Schenning, E.W. Meijer, F. Würthner, F C. De Schryver
Bias-dependent Visualization of Electron Donor (D) and Electron Acceptor (A) Moieties in a Chiral DAD Triad Molecule
J. Am. Chem Soc., 125, 14968-14969 (2003).

P. Jonkheijm, A. Miura, M. Zdanowska, F.J.M. Hoeben, S. De Feyter, A.P.H.J. Schenning, F.C. De Schryver, E.W. Meijer
π-conjugated Oligo-(*p*-phenylenevinylene) Rosettes and their tubular Self Assembly
Angew.Chem.Int.Ed., 43, 74-78 (2004), Angew.Chem. 116, 76-80 (2004).

M. Cotlet, S. Masuo, G. Luo, J. Hofkens, M. Van der Auweraer, J. Verhoeven, K. Müllen, X. S. Xie, F. De Schryver
Probing conformational dynamics in single donor-acceptor synthetic molecules by means of photoinduced reversible electron transfer
Proceedings National Academy of Sciences USA, 101, 14343-14348 (2004).

S. A. Chavan, W. Maes, L. E. M. Gevers, J. Wahlen, I. F. J. Vankelecom, P. A. Jacobs, W. Dehaen, D. E. Devos,
Porphyrin-functionalized dendrimers : synthesis and application as recycable photocatalysts in a nanofiltration membrane reactor,
Chem. Eur. J., 11, 6754-6762 (2005).

M. Baruah, W. Qin, R.A.L. Vallée, D. Beljonne, T. Rohand, W. Dehaen, N. Boens,
A highly potassium-selective ratiometric fluorescent indicator based on BODIPY azacrown ether and excitable with visible light,
Org. Lett. 7, 4377-80 (2005).

O. Flomenbom, K. Velonia, D. Loos, S. Masuo, M. Cotlet, Y. Engelborghs, J. Hofkens, A.E. Rowan, R.J.M. Nolte, M. Van der Auweraer, F.C. De Schryver J. Klafter,
Stretched exponential decay and correlations in the catalytic activity of fluctuating single lipase molecules
Proceedings National Academy of Sciences USA 102, 2368-2372 (2005).

M.B.J. Roeffaers, B.F.Sels, H. Uji-i, F.C. De Schryver, P.A. Jacobs, D. De Vos, J. Hofkens,
Spatially resolved observation of crystal-face-dependent catalysis by single turnover counting
Nature 439 , 572-575 (2006)

II. 5. INTERNATIONAL CONTACTS IN THE PROJECT'S RESEARCH DOMAIN

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

1) Collaboration (De Feyter, Hofkens, Van der Auweraer) with K. Müllen (MPI für Polymerforschung Mainz)

- Synthesis of oligomers and polymers with interesting opto-electronic properties, synthesis of dendrimers, synthesis of probes based on perylene (di)imid,

Inter-universitary attraction pool IAP V/03: Supramolecular Chemistry and Katalysis.

- Common papers, other common papers in preparation

2) Collaboration (De Feyter, Hofkens, Van der Auweraer) with B. Meijer, A.P.H.J. Schenning (T.U. Eindhoven)

- Synthesis of dendrimers with conjugated oligophenylenevinylene branches
- Common papers, other common papers in preparation

3) Collaboration (De Feyter, Hofkens, Van der Auweraer) with J. Verhoeven (University Amsterdam)

- *Intramolecular photo-induced electron transfer in supramolecular systems.*
- Common papers, other common papers in preparation

4) Collaboration (De Feyter, Hofkens) with A. Rowan, R. Nolte (K.U. Nijmegen)

- Synthesis of polychromoforic molecules for femtosecond spectroscopy, confocal microscopy and scanning microscopies
- *STREP project (EU): Bioscope:"Self-reporting biological nanosystems to study and control bio-molecular mechanisms on the single molecule level"*
- *Visiting professor at K.U.Leuven*
- Common papers, other common papers in preparation

5) Collaboration (Hofkens) with prof. M. Sauer (University Bielefeld)

- Single molecule spectroscopy, biomolecules, coincidence experiment
- Common papers, other common papers in preparation

6) Collaboration (Hofkens) with J. Enderlein (Forschungszentrum Jülich, Institute for Biological Information Processing)

- Picosecond Fluorescence Lifetime Imaging
- Common paper, other common paper in preparation

7) Collaboration (Hofkens) with Nanocenter Kopenhagen

- *Single molecule kinetics, wild-type mutants of lipase of CALB*

- Fluorescence enhancement by silver coated AFM tip
- *STREP project (EU): Bioscope "Self-reporting biological nanosystems to study and control bio-molecular mechanisms on the single molecule level"*
- *Common paper, other common papers in preparation*

8) Collaboration (Hofkens, Van der Auweraer) with H. Masuhara (Osaka University)

- Transient "attenuated total reflection" and transient diffuse reflection, optical trapping, confocal microscopy, laser ablation.
- *Exchange of postdocs*
- Common papers, other common papers in preparation

9) Collaboration (Hofkens) with S. Xie (Harvard Medical School)

- Analysis of trajectories of fluorescence intensity and fluorescence decay times of single mollecules
- Common papers

10) Collaboration (Hofkens, Van der Auweraer) with M. Orrit (Leiden University)

- Modeling of interaction between single molecules and the radiation filed and of fluctuations thereof
- Common papers

11) Collaboration (Hofkens) with A. Visser (Landbouwhogeschool Wageningen)

- Collaboration related to mutants of the "Green Fluoresent Proteine" (GFP) and reference compounds for single photon timing
- *Visiting professor at K.ULeuven*
- *Masters thesis Wouter Schroeyens, K.U.Leuven 199*
- Common papers, other common papers in preparation

12) Collaboration (De Feyter) with K. Wandelt, D. Broekmann (Bonn University)

- Electrochemical STM

Patterning and reactivity at the nanoscale, research project 2005-2008

- Common papers in preparation

13) Collaboration (De Feyter) with B. Feringa and J. van Esch (University Groningen)

- Scanning tunneling microscopy" (STM)
- Common papers, other common papers in preparation

14) Collaboration (De Feyter) with S. Höger (Bonn University)

- Scanning tunneling microscopy, synthesis of macrocycles
- Common paper, other common papers in preparation

15) Collaboration (De Feyter) with V. Percec (Pennsylvania)

- Synthesis of molecules for scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS)
- Common paper, other common papers in preparation

16) Collaboration (De Feyter, Hofkens, Van der Auweraer) with F. Würthner (Würtzburg)

- Synthesis of molecules for STM and STS
- Common paper, other common papers in preparation

17) Collaboration (Van der Auweraer) with A. Vitukhnovsky (Lebedev Institute, Moskou)

Photophysics of J-aggregates, Organic light emitting diodes with semiconductor nanoparticles, preparation of semiconductor nanoparticles

Bilaterale Collaboration Rusland "Novel Semiconducting Organic and Hybrid Materials Based on Branched Polyphenylenes for Electroluminescence Applications" (euro 701000)

- Common papers

18) Collaboration (De Feyter) with Tobe (Osaka University)

- STM-imaging of macrocyclic compounds and annulenes, co-adsorption and solvent effects
- Common papers in preparation

19) Collaboration (Van der Auweraer) with J. Salbeck (University Kassel), Sensient, Merck, Philips, K. Leo (IAP Dresden), R. Cingolani (University Lecce)

- Synthesis of interesting opto-electronic molecules (matrices and dopants)
- Vapor deposition of amorphous organic layers

Integrated project OLLA (High brightness OLED's for ICT & Next Generation Lighting Applications)

Research project 2004-2008, 533.542 euro (wherein 61 man months for Laboratory Photochemistry and Spectroscopy

20) Collaboration (Van der Auweraer) with L. Peteanu (Carnegie Mellon University)

- Electro-absorption experiments on donor-acceptor compounds
- Common paper

21) Collaboration (Dehaen) with A. Dworak (Gliwice, Poland)

- synthesis of hyperbranched polymers, synthesis of amphiphiles

Bilateral collaboration Flanders - Poland

- Common papers in preparation

22) Collaboration (Dehaen) with X. Zhang (Jilin University, China)

- synthesis of hyperbranched polymers, biomimetic catalysis, micelle stabilisation, (dendron)thiols on gold nanoparticles or surfaces

Bilateral collaboration Flanders - China

- Common papers

23) Collaboration (Dehaen) with J. Costamagna (Santiago De Chile, Chile)

- synthesis of porphyrins, polyazahmacrocycles, bipyridines

Bilateral collaboration Flanders - Chili

- Common paper, other common papers in preparation

24) Collaboration (Dehaen) with S. Campagna (Messina, Italy)

- photophysics of dendrimers and oligocarbazoles
- Common paper, other common papers in preparation

25) Collaboration (Dehaen) with Phil Gale (University of Southampton, UK), Markus Albrecht (Aachen, Germany), Jerzy Radecki (PAN Olsztyn, Poland), Janez Plavec (Ljubljana, Slovenia), Pavel Lhotak (Prague, Czech Republic)

Working Group "Novel and Specific Anion Receptors for use in Sensor Technology" *(WG D31/0021/05) of COST D31 (Organizing Non-Covalent Chemical structures with Selected Functions*

- Common paper, other common papers in preparation

II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,...).

K.U.Leuven or Research Fund K.U.Leuven
Probing (Bio)molecular Dynamics
Geconcerteerde onderzoeksactie 2006/2
Onderzoeksproject 2006-2010
(Van der Auweraer coordinator, De Feyter and Hofkens promotor)

Spin-related phenomena in photonics of organized media
Geconcerteerde onderzoeksactie 2006/3
Onderzoeksproject 2006-2010
(K. Clays coordinator, Dehaen, Smet promotor)

Time- and space resolved linear and non-linear spectroscopy
Impulsactie Vlaamse Gemeenschap i.v.m Zware Apparatuur (ZWAP 04/007)
Onderzoeksproject 2004-2008
(Van der Auweraer coordinator)

Partner in Center of Excellence Nanoscale Physics and Chemistry: (INPAC) (defiscalizatie)
Onderzoeksproject 2005-2010
(Van der Auweraer, group leader)

Partner in Center of Excellence in Catalytic Science (CECAT) (defiscalizatie)
Onderzoeksproject 2005-2010
(Hofkens partner)

Novel Semiconducting Organic and Hybrid Materials Based on Branched Polyphenylenes for Electroluminescence Applications
Bilateral Cooperation with Russia, partner prof. A. Vitukhnovsky
Research Project 2006-2007
(Van der Auweraer, promotor)

Bilateral Cooperation with Poland, partner prof. A. Dworak
Research Project 2005-2007
(Dehaen, promoter, Smet copromotor)
Nanotechnological applications of synthetic nucleic acids.
IDO
Research Project 2003-2007
(De Feyter promotor, P. Herdewijn (pharmacy), promotor)

Flemish Community
Combination of Scanning Probe and Optical Microscopy of Nano-objects
F.W.O.- G. G.0421.03
Research Project 2003-2006
302.500 euro (Van der Auweraer coordinator, De Feyter and Hofkens promotor)

An Improved Optical Resolution by Stimulated Emission Depletion (Sted) Microscopy
FWO G.036606
Research project 2006-2009
(Hofkens coordinator, Van der Auweraer promotor)

Role of a bacterial cationic peptide in cellular de-differentiation,
FWO project
Resaerch Project 2004-2007
(promotor Hofkens, Jan Michiels coordinator)

French Community
Spectroscopie de fluorescence et Raman de molécules isolées (Single molecule fluorescence and Raman spectroscopy),
FNRS project
Research project 2004-2006
(Hofkens, coordinator)

Federal Government
Supramolecular Chemistry and Catalysis
IAP/5-03 Van der Auweraer part of partner 1.

European Union
High brightness OLED's for ICT & Next Generation Lighting Applications,
IP project OLLA IST 2002 -004607:
Research project 2004-2008,
(Van der Auweraer partner)

Self-reporting biological nanosystems to study and control bio-molecular mechanisms on the single molecule level "Bioscope"
STREP project (EU):
Research project (Hofkens, partner)

Chiral expression and transfer at the nanoscale (Chextan)
Marie Curie Network 2004-2008 (De Feyter partner)

Novel and Specific Anion Receptors for use in Sensor Technology
WG D31/0021/05 of COST D31 (Organizing Non-Covalent Chemical structures with Selected Functions
COST Network 2005-2008
(Dehaen, Partner) with Phil Gale (University of Southampton, UK), Markus Albrecht (Aachen, Germany), Jerzy Radecki (PAN Olsztyn, Poland), Janez Plavec (Ljubljana, Slovenia), Pavel Lhotak (Prague, Czech Republic)

II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: WP1, Nanodots and photonic crystals (tasks 1, 2, 3, 4, 5)
2. Workpackage number and title: WP2, Organic nanostructures (tasks 1, 2)
3. Workpackage number and title: WP3, Porous frameworks (tasks 1, 2, 3, 4)
4. Workpackage number and title: WP4, Hybrid Materials (tasks 1, 3)
5. Workpackage number and title: WP5, (Bio)membranes (tasks 1, 2, 3, 4, 5)
6. Workpackage number and title: WP6, Biomolecules and Biocatalysis (tasks 1, 2, 3)
7. Workpackage number and title: WP8, Supramolecular conjugated systems (tasks 1)
8. Workpackage number and title: WP9, Self-assembly at surfaces (tasks 1, 2)
9. Workpackage number and title:
10. Workpackage number and title:
11. Workpackage number and title:
12. Workpackage number and title:
13. Workpackage number and title:
14. Workpackage number and title:
15. Workpackage number and title:

II. 8. BUDGET (distribution per year) *

(in EURO) Deleted: , without decimals

	2007	2008	2009	2010	2011	Total
Personnel	142.685,00	146.252,00	149.908,00	153.657,00	157.498,00	750.000,00
Operating costs	95.530,00	91.960,00	88.310,00	84.560,00	80.116,19	440.476,19
Equipment	0,00	0,00	0,00	0,00	'Not allowed	0,00
Overheads	11.910,75	11.910,60	11.910,90	11.910,85	11.880,71	59.523,81
Subcontracting	0,00	0,00	0,00	0,00	0,00	0,00
Subtotal	250.125,75	250.122,60	250.128,90	250.127,85	249.494,90	1.250.000,00
Mullen	10.000,00	10.000,00	10.000,00	10.000,00	10.000,00	50.000,00
EU 2 (name)	0,00	0,00	0,00	0,00	0,00	0,00
EU 3 (name)	0,00	0,00	0,00	0,00	0,00	0,00
EU 4 (name)	0,00	0,00	0,00	0,00	0,00	0,00
Total	260.125,75	260.122,60	260.128,90	260.127,85	259.494,90	1.300.000,00

* This table should not be completed by the European partner as his/her budget is mentioned in the budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership

- Personnel: indexed gross remunerations; employer's social contnbutions; statutory insurance costs as well as any other compensation or allocation legally due in addition to the salary; the reimbursements for PhD and postdoctoral grant holders (exempt from tax and benefiting from social security). Personnel costs must account for minimum 60% of the total budget attributed to each partner of the network. The costs for the tax-free PhD grants and postdoctoral grants may not account for more than 60% of the total personnel costs.

- Operating costs: documentation; travel and accommodation; hosting of visiting foreign researchers use of computing facilities; software; telecommunications; maintenance and operation of equipment and, more generally, consumables;.

- Equipment: acquisition and installation of scientific and technical appliances and instruments, including IT equipment placed at the project's disposal. Equipment cannot be asked for during the last year of the programme.

- Overheads: general expenses of the institutions covering, on an inclusive basis, administrative, telephone, postal, maintenance, heating, electricity, rental, material depreciation and insurance costs. The total amount for this heading may not exceed 5% of total personnel and operating costs.

- Subcontracting: costs incurred by a third party in order to perform tasks or provide services necessitating specific scientific or technical skills outside the normal framework of the institution's activities. Each request for subcontracting needs a approval from the programme administrator.

II. 9. EQUIPMENT

Indicate the equipment (with an estimation of the cost) that will be purchased from the IAP-budget for the coming from four years (2007-2010) and justify.

No equipment will be purchased

II. 10. SUBCONTRACTING

To be completed only if subcontracting is foreseen.

Describe and justify the tasks and/or services that will be provided by a third party.

No subcontracting is foreseen

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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION II

Information on the partners

to be completed by each network partner including the EU-partner(s)

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the partner : Jérôme Christine (P3) Institution : University of Liège

II. 1. PARTNER CONTACT DETAILS

PARTNER N° (consult the list in Section I of Annex I) * : P3

- Family Name : Jérôme
- First Name : Christine
- Title (Prof., Dr., ...) : Prof.
- Institution : University of Liège
- *Institution's abbreviation* : *ULg*
- Faculty/Department :Faculty of Sciences/Department of Chemistry
- Research Unit : Center for Education and Research on Macromolecules (CERM)
- Road/Street, n° : Institute of Chemistry, Allée du 6 août, Bldg B6a, Sart Tilman
- Post Code : 4000
- Town/City : Liège
- Country : Belgium
- Tel : 0032 4 366 34 91
- *Tel secretariat* : 0032 4 366 34 92
- Fax : 0032 4 366 34 97
- E-mail : c.jerome@ulg.ac.be
- Website : http://www.ulg.ac.be/cerm

* For Belgian partners : P1 to P13
For EU-partners : EU1 to EU4

II. 2. STAFF MEMBERS WORKING ON THE PROJECT (paid and not paid by the IAP-budget)

Staff	Number
Professor	2
Senior scientist	2
Post-doc	7
PhD student	20
Researcher without phD	5
Technician	6
Secretary	1
Other	-
TOTAL	**43**

II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, phD student, researcher without phD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name : ALAIMO David
   Profile : phD student
   Skills : Biomaterials

2. Name : AQIL Abdelhafid
   Profile : phD student
   Skills : Nanomaterials

3. Name : BOZUKOVA Dimitrya
   Profile : phD student
   Skills : Surface chemistry

4. Name : BRYASKOVA Rainy
   Profile : post-doctoral
   Skills : Supramolecular chemistry

5. Name : CAES Sébastien
   Profile : master student
   Skills : Synthesis/Polymerization

6. Name : CAJOT Sébastien
   Profile : master student
   Skills : Biomaterials

7. Name : CARTIGNY Grégory
   Profile : technician
   Skills : Synthesis

8. Name : CECIUS Michaël
   Profile : phD student
   Skills : Electrochemistry

9. Name : COLLARD Valérie
   Profile : technician
   Skills : Polymer characterization

10. Name : CROISIER Florence
    Profile : master student
    Skills : Synthesis/polymerization

11. Name : DANNEMARK Charlotte
    Profile : technician
    Skills : Polymer synthesis and characterization

12. Name : DEBUIGNE Antoine
    Profile : post-doctoral
    Skills : Synthesis/Polymerization

13. Name : DEJENEFFE Martine
    Profile : technician
    Skills : Electron microscopy

14. Name : DETREMBLEUR Christophe
    Profile : senior scientist
    Skills : Synthesis/Polymerization

15. Name : ESSERS Raphaël
    Profile : technician
    Skills : Synthesis

16. Name : FREICHELS Hélène
    Profile : phD student
    Skills : Biomaterials

17. Name : GABRIEL Sabine
    Profile : phD student
    Skills : Electrochemistry

18. Name : GRIGNARD Bruno
    Profile : phD student
    Skills : Supported catalysis

19. Name : GROGNA Mathurin
    Profile : phD student
    Skills : Nanomaterials

20. Name : HALUSIAK Emilie
    Profile : phD student
    Skills : Biosensors

21. Name : HERWATS Stéphane
    Profile : phD student
    Skills : Nanomaterials

22. Name : HUBENS Christophe
    Profile : technician
    Skills : Synthesis

23. Name : HURTGEN Marie
    Profile : master student
    Skills : Synthesis/Polymerization

24. Name : JEROME Christine
    Profile : "Chargé de cours"
    Skills : Surface chemistry/Biomaterials

25. Name : JEROME Robert
    Profile : Full professor

Skills : *Macromolecular chemistry*

26. Name : LECOMTE Philippe
Profile : senior scientist
Skills : Synthesis/Polymerization

27. Name : MITU Alina
Profile : post-doctoral
Skills : Biomaterials

28. Name : NAVEAU Elodie
Profile : phD student
Skills : Nanocomposites

29. Name : NEDELCHEVA Anna
Profile : phD student
Skills : Nanomaterials

30. Name : PIETTE Yasmine
Profile : phD student
Skills : Nanomaterials

31. Name : RIEGER Jutta
Profile : post-doctoral
Skills : Biomaterials

32. Name : RIVA Raphaël
Profile : phD student
Skills : Synthesis/Polymerization

33. Name : SCHMEITS Stéphanie
Profile : phD student
Skills : Synthesis/Polymerization

34. Name : SERWAS Harry
Profile : phD student
Skills : Catalysis

35. Name : SIBRET Pierre
Profile : phD student
Skills : Biomaterials

36. Name : SORLIER Pierre
Profile : post-doctoral
Skills : Nanomaterials

37. Name : SWIERKOWICZ Krystyna
Profile : secretary
Skills : accountancy

38. Name : THOMASSIN Jean-Michel
Profile : post-doctoral
Skills : Membranes

39. Name : TUDOSE Adriana
    Profile : *post-doctoral*
    Skills : Synthesis/polymerization

40. Name : URBANCZYK Laëtitia
    Profile : phD student
    Skills : Nanocomposites

41. Name : VAN BUTSELE Kathy
    Profile : phD student
    Skills : Biomaterials

42. Name : WARNANT Jérôme
    Profile : master student
    Skills : Nanomaterials

43. Name : WILLET Nicolas
    Profile : phD student
    Skills : Supramolecular chemistry

II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

Combination of Electrografting and Ring-Opening Metathesis Polymerization: An Efficient Way to Prepare Polynorbornene Brushes on Conducting Substrates.
C. Detrembleur, C. Jérôme, M. Claes, P. Louette, R. Jérôme
Angew. Chem. Int. Ed., 113, 1308-1311 (2001)

Full-electrochemical preparation of conducting/insulating binary polymer films
C. Jérôme, V. Geskin, R. Lazzaroni, J.L. Brédas, A. Thibaut, C. Calberg, I. Bodart, M. Mertens, L. Martinot, D. Rodrigue, J. Riga and R. Jérôme
Chem. Mater. 13, 1656-1664 (2001).

Controlled free radical polymerization of styrene initiated from alkoxyamine attached to polyacrylate chemisorbed onto conducting surfaces
S. Voccia, C. Jérôme, C. Detrembleur, Ph. Leclère, R. Gouttebaron, M. Hecq, B. Gilbert, R. Lazzaroni, R. Jérôme
Chem. Mater. 15, 923-927 (2003)

PLA-coated gold nanoparticles for the labeling of PLA biocarriers
H. Qiu, J. Rieger, B. Gilbert, R. Jérôme, C. Jérôme
Chem. Mater., 16, 850-856 (2004)

Electrografting of Poly(ethylene glycol) Acrylate : A One-Step Strategy for the Synthesis of Protein-Repellent Surfaces
S. Gabriel, P. Dubruel, E. Schacht, A.M. Jonas, B. Gilbert, R. Jérôme, C. Jérôme
Angew. Chem. Int. Ed., 44, 5352-5361 (2005)

Combination of ring-opening polymerization and "click" chemistry towards functionalization of aliphatic polyesters
Riva Raphaël, Schmeits Stephanie, Stoffelbach François, Jérôme Christine, Jérôme Robert, Lecomte Philippe
Chemical Communications, 42, 5334-53363 (2005)

Synthesis of amphiphilic copolymers of poly(ethylene oxide) and poly(ε-caprolactone) with different architectures and their role in the preparation of stealthy nanoparticles
Rieger Jutta, Passirani Catherine, Benoit Jean-Pierre, Van Butsele Kathy, Jérôme Robert, Jérôme Christine
Advanced functional materials, 16(11), 1506-1514 (2006)

New Nanostructured Materials Based on Fullerene and Biodegradable Polyesters.
Stoilova Olya, Jérôme Christine, Detrembleur Christophe, Mouithys-Mickalad Ange, Manolova Nevena, Rashkov Iliya, Jérôme Robert.
Chemistry of Materials, 18(20), 4917-4923 (2006)

Mechanochemistry: targeted delivery of single molecules.
Duwez Anne-Sophie, Cuenot Stéphane, Jérôme Christine, Gabriel Sabine, Jérôme Robert, Rapino Stefania, Zerbetto Francesco.
Nature Nanotechnology, 1(2), 122-125 (2006)

Thermoresponsive Coatings Strongly Adhering to (Semi)conducting Surfaces.

Gabriel Sabine Duwez Anne-Sophie, Jérôme Robert, Jérôme Christine.
Langmuir 2007, 23(1), 159-161.

II. 5. INTERNATIONAL CONTACTS IN THE PROJECT'S RESEARCH DOMAIN

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

FAME ("*Functionalized Advanced Materials Engineering of Hybrids and Ceramics*)
Network of Excellence (NOE)

RWTH-Aachen,
"Biointerface - Detektion und steuerung grenzflächeninduzierter biomolekularer und zellularer funktionen"

University of Angers, France, CGRI - INSERM
«*Synthèse de macromolécules originales pour l'élaboration de vecteurs furtifs*»

SURFOLIO, DGTRE Convention First Europe Objectif 3
"Surfaces fonctionnelles pour lentille intraoculaire"

University Claude-Bernard, Lyon 1, CGRI - Programme Tournesol
«*Cristallisation des polyesters aliphatiques en couche mince sur un support solide: influence de l'organisation moléculaire et de l'épaisseur*»

CGRI – bilateral collaboration Bulgaria/Walloon Region (Académie Bulgare des Sciences; Prof. Rashkov)
"Nouveaux matériaux nanostructurés (polymères en étoile, gels, et nanoparticules) à base de fullerènes et polyesters biodégradables"

SELF-CLEANING GLASS - European research programme
"Technologies associated with the production, transformation and processsing of knowledge-based multifunctional materials, and biomaterials"

SC-TEC-07 - 4ème commission mixte permanente Wallonie-Bruxelles et Québec (Univ. Montréal)
"Synthèse et auto-assemblage de copolymères séquencés à des fins de matériaux thermo- et photosensibles

SONS-EUROCORES, European Science Foundation (Dresden, Toulouse, Liège)
"Nanoscale electronic devices via templating supramolecular polyelectrolytes"

ERASMUS-SOCRATES Programme (University of Chemical Technology and Metallurgy; Prof. R. Mateva)

Belgian Science Policy Fellowships :

- Bulgarian Academy of Sciences (Dr. O. Stoilova)
- Charles University, Prague, Czech Republic (Dr. J. Zednik)
- University of Chemical Technology and Metallurgy (Dr. R. Bryaskova)
- Slovak Academy of Sciences, Slovak Republic (Dr. M. Stach and Dr. J. Kollar)

II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,...).

Région Wallonne, "Nanotechnologies" (2002-2006), "Procédé novateur de blindage électromagnétique par recours à des nanotubes de carbone" (ENABLE)

Région Wallonne, "Nanotechnologies" (2002-2007), "Nanoparticules pour détection optique et magnétique" (NOMADE)

Région Wallonne, "Réseaux" (2004-2008), "Mise au point d'un biosenseur pour le diagnostic des maladies virales" (SENSOTEM)

Région Wallonne, "Réseaux" (2004-2008), "Développement d'un dispositif contraceptif local, sûr et n'induisant pas de métrorragies" (IMPUT)

Région Wallonne, "Réseaux" (2004-2008), "Surfaces micro- et nano-structurées auto-nettoyanges anti-corrosion" (CORRONET)

Région Wallonne, "Winnomat" (2004-2009), "Développement d'un procédé continu du moussage de nanocomposites par CO2 supercritique" (PROCOMO)

Région Wallonne, "Winnomat" (2004-2008), "Nouveaux nanovecteurs biodégradables pour la vaccination par voie orale par ciblage des cellules M" (VACCINOR)

Région Wallonne, "Waleo2" (2006-2009), "Pansement acellulaire bioactivé pour la régénérescence cutanée" (GOCELL)

Région Wallonne, "Waleo2" (2006-2009), "Mise au point d'un nouveau traitement sous forme d'implant péritonéal contre l'endométriose" (IMPEIOSE)

Région Wallonne, "Piles à Combustible" (2005-2007), "Innovation dans les membranes pour pile à combustible de type PEM" (INNOPILE)

Région Wallonne, "Objectif Europe" (2005-2006), "Surfaces fonctionnelles pour lentilles intraoculaires" (SURFOLIO)

Convention Européenne, 6ème Programme Cadre (2004-2006), "Technologies associated with the production, transformation and processsing of knowledge-based multifunctional materials, and biomaterials (Self-Cleaning Glass)

FRFC 2.4522.03, Projet EUROCORES/SONS (2004-2005), "Synthèse des échantillons de poly(2-vinylpyridine) de masse moléculaire (jusqu'à plusieurs centaines de mille) et celle des copolymères séquencés P2VP/PS, linéaires et en étoile (de différentes masses moléculaires et compositions)"

CGRI/Région Wallonne/Bulgarie (2004-2005), "Nouveaux matériaux nanostructurés (polymères en étoile, gels et nanoparticules) à base de fullerènes et polyesters biodégradables

Convention Région Wallonne – WALEO2 (2006-2010), "Pansement acellulaire bioactivé pour le traitement des ulcères cutanés"

Convention Région Wallone - First-Spin-Off (2005-2007),"Production de nanocharges de spécialité" (FINECLAY)

RWTH Aachen (2004-2006), "Bionterface – Detektion und Steuerung grezflächeninduzierter biomolekularer un zellulärer Funktionen"

TOTAL S.A (2005), "Etude sur l'incorporation de structures rigides dites"Rod coil" dans des matrices polymériques obtenues par le procédé""

Centre TUDOR Luxembourg (2005), "Etude et développement des Nanocomposites à matrice polymère"

SOLVIN (2006-2008), "Chlorure de vinyle – polymérisation radicalaire contrôlée"

II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: WP1, Nanodots and photonic crystals (tasks: 2, 3, 4)
2. Workpackage number and title: WP2, Organic nanostructures (task 1)
3. Workpackage number and title: WP3,Porous frameworks (task 3)
4. Workpackage number and title: WP4, Hybrid Materials (tasks 1, 2, 3)
5. Workpackage number and title: WP5, (Bio)membranes (tasks 4 ,5)
6. Workpackage number and title: WP6, Biomolecules and Biocatalysis (task 4)
7. Workpackage number and title: WP7, Functional coatings (tasks 1, 2, 3)
8. Workpackage number and title: WP9, Self-assembly at surfaces (task 2)
9. Workpackage number and title:
10. Workpackage number and title:
11. Workpackage number and title:
12. Workpackage number and title:
13. Workpackage number and title:
14. Workpackage number and title:
15. Workpackage number and title:

II. 8. BUDGET (distribution per year) *

(in EURO)

	2007	2008	2009	2010	2011	Total
Personnel	89.813,00	92.313,00	94.813,00	99.813,00	104.813,00	**481.565,00**
Operating costs	62.567,95	60.067,95	57.567,95	52.567,95	47.567,95	**280.339,75**
Equipment	0,00	0,00	0,00	0,00	Not allowed	**0,00**
Overheads	7.619,05	7.619,05	7.619,05	7.619,05	7.619,05	**38.095,25**
Subcontracting	0,00	0,00	0,00	0,00	0,00	**0,00**
Subtotal	**160.000,00**	**160.000,00**	**160.000,00**	**160.000,00**	**160.000,00**	**800.000,00**
EU 1 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 2 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 3 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 4 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
Total	**160.000,00**	**160.000,00**	**160.000,00**	**160.000,00**	**160.000,00**	**800.000,00**

* This table should not be completed by the European partner as his/her budget is mentioned in the budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership

- Personnel: indexed gross remunerations; employer's social contributions; statutory insurance costs as well as any other compensation or allocation legally due in addition to the salary; the reimbursements for PhD and postdoctoral grant holders (exempt from tax and benefiting from social security). Personnel costs must account for minimum 60% of the total budget attributed to each partner of the network. The costs for the tax-free PhD grants and postdoctoral grants may not account for more than 60% of the total personnel costs.

- Operating costs: documentation; travel and accommodation; hosting of visiting foreign researchers use of computing facilities; software; telecommunications; maintenance and operation of equipment and, more generally, consumables;.

- Equipment: acquisition and installation of scientific and technical appliances and instruments, including IT equipment placed at the project's disposal. Equipment cannot be asked for during the last year of the programme.

- Overheads: general expenses of the institutions covering, on an inclusive basis, administrative, telephone, postal, maintenance, heating, electricity, rental, material depreciation and insurance costs. The total amount for this heading may not exceed 5% of total personnel and operating costs.

- Subcontracting: costs incurred by a third party in order to perform tasks or provide services necessitating specific scientific or technical skills outside the normal framework of the institution's activities. Each request for subcontracting needs a approval from the programme administrator.

II. 9. EQUIPMENT

Indicate the equipment (with an estimation of the cost) that will be purchased from the IAP-budget for the coming from four years (2007-2010) and justify.

No equipment will be purchased

II. 10. SUBCONTRACTING

To be completed only if subcontracting is foreseen.

Describe and justify the tasks and/or services that will be provided by a third party.

No subcontracting is foreseen

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B-1000 BRUSSELS
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www.belspo.be

Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION II

Information on the partners

to be completed by each network partner including the EU-partner(s)

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the partner : Lazzaroni Roberto (P4) Institution : University of Mons-Hainaut

II. 1. PARTNER CONTACT DETAILS

PARTNER N° (consult the list in Section I of Annex I)* : P4

- Family Name : Lazzaroni
- First Name : Roberto
- Title (Prof., Dr., ...) : Prof.
- Institution : University of Mons-Hainaut
- Institution's abbreviation : UMH
- Faculty/Department :Department of Chemistry
- Research Unit : Service de Chimie des Matériaux Nouveaux
- Road/Street, n° : Place du Parc 20
- Post Code : 7000
- Town/City : Mons
- Country : Belgium
- Tel : 0032 65 37 38 60
- Tel secretariat : 0032 65 37 38 62
- Fax : 0032 65 37 38 61
- E-mail : Roberto@averell.umh.ac.be
- Website : http://morris.umh.ac.be/

* For Belgian partners : P1 to P13
For EU-partners : EU1 to EU4

II. 2. STAFF MEMBERS WORKING ON THE PROJECT (paid and not paid by the IAP-budget)

Staff	Number
Professor	3
Senior scientist	9
Post-doc	20
PhD student	24
Researcher without phD	2
Technician	9
Secretary	2
Other	
TOTAL	69

II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, phD student, researcher without phD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name : Roberto Lazzaroni
   Profile : prof
   Skills : supramolecular organisation in polymer materials

2. Name : Philippe Dubois
   Profile : prof
   Skills : design and synthesis of multifunctional polymer and composite materials

3. Name : Michael Alexandre
   Profile : senior scientist
   Skills : polymer blends, polymer (nano)composites, interfacial polymerization reactions

4. Name : David Beljonne
   Profile : senior scientist
   Skills : electronic and optical properties of organic materials

5. Name : Jérôme Cornil
   Profile : senior scientist
   Skills : Electronic and optical properties of organic materials

6. Name : Philippe Leclère
   Profile : senior scientist
   Skills : microscopic morphology of polymer materials

7. Name : Victor Geskin
   Profile : senior scientist
   Skills : electronic and transport properties of organic thin films

8. Name : Philippe Degée
   Profile : senior scientist
   Skills : macromolecular engineering, controlled polymer syntheses and catatysis in polymerization reactions

9. Name : Philippe Marsal
   Profile : post-doc
   Skills : electronic and optical properties of organic materials

10. Name : Vincent Lemaur
    Profile : post-doc
    Skills : electronic and optical properties of organic materials

11. Name : Patrick Brocorens
    Profile : post-doc
    Skills : supramolecular organisation in polymer materials

12. Name : Stéphane Bredeau

Profile : post-doc
Skills : metallocene catalysis, interfacial polymerization, nanohybrid materials, catalyzed olefin polymerization

13. Name : Olivier Coulembier
Profile : post-doc
Skills : Controlled ring opening polymerization of lactones, biodegradable polyesters, metal-free catalysis in polymer syntheses

14. Name : Mathieu Surin
Profile : Post-doc
Skills : supramolecular organisation in thin (bio)organic films

15. Name : Laetitia Mespouille
Profile : PhD student
Skills : tailored synthesis of amphiphilic gels, controlled radical polymerization, living ring-opening polymerization, stimuli-sensitive biodegradable and biocompatible polymeric systems

16. Name : Céline Labruyère
Profile : PhD student
Skills : polymer clay nanocomposites, synthesis of amphiphilic block and graft copolymers, controlled radical polymerization

17. Name : Andrea Minoia
Profile : PhD student
Skills : supramolecular organisation in thin organic films

18. Name : Bernard Van Averbeke
Profile : PhD student
Skills : electronic and optical properties of organic materials

19. Name : Sébastien Moins
Profile : technician
Skills : controlled polymer synthesis techniques (ATRP, NMP, ROP,...), polymer characterization (GPC, NMR, viscometry,...), chemical modification of polymeric materials

20. Name : Cécile Delcourt
Profile : technician
Skills : controlled polymer synthesis techniques (ATRP, NMP, ROP,...), polymer characterization (GPC, NMR, viscometry,...), chemical modification of polymeric materials

II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

Polymer-layered silicate nanocomposites: preparation, properties and uses of a new class of materials
M. Alexandre, Ph. Dubois; Materials Science and Engineering Report, 28 (2000) 1-63.

Supramolecular Organization in Block Copolymers Containing a Conjugated Segment: A Joint AFM/Molecular Modeling Study
Ph. Leclère, E. Hennebicq, A. Calderone, P. Brocorens, A.C. Grimsdale, K. Müllen, J.L. Brédas, and R. Lazzaroni; Progress in Polymer Science, 28 (2003) 55-81.

Controlled polymer grafting onto single clay nanoplatelets
P. Viville, R. Lazzaroni, E. Pollet, M. Alexandre, Ph. Dubois; Journal of the American Chemical Society, 126 (2004) 9007-9012.

Charge-Transfer and Energy-Transfer Processes in pi-Conjugated Oligomers and Polymers
JL Brédas, D. Beljonne, V. Coropceanu, J. Cornil; Chemical Reviews, 104 (2004) 4971.

Charge Transport Properties in Discotic Liquid Crystals: A Quantum-Chemical Insight into Structure-Property Relationships
V. Lemaur, D.A. Da Silva Filho, V. Coropceanu, M. Lehmann, Y. Geerts, J. Piris, M.G. Debije, A.M. Van De Craats, K. Senthilkumar, L.D.A. Siebbeles, J.M. Warman, J.L. Brédas, J. Cornil; Journal of the American Chemical Society, 126 (2004)3271-3279.

Photophysical Properties of Ruthenium(II) Polyazaaromatic Compounds: A Theoretical Insight
G. Pourtois, D. Beljonne, R. Lazzaroni, J.L. Brédas, C. Moucheron, S. Schumm, A. Kirsch-De Mesmaeker; Journal of the American Chemical Society, 126 (2004) 683-692.

Polystyrene-supported organotin dichloride as recyclable catalyst in lactone ring-opening polymerisation. Assessment by high resolution Magic Angle Spinning (hr-MAS) NMR
G. Deshayes, K. Poelmans, I. Verbruggen, C. Camacho-Camacho, Ph. Degee, V. Pinoie, J.C. Martins, M. Piotto, M. Biesemans, R. Willem, Ph. Dubois; Chem. Eur. J., 11 (2005) 4550-4559.

Latent, thermally activated organic catalysts for the on-demand living polymerization of lactide
O. Coulembier, A.P. Dove, R.C. Pratt, A.C. Sentman, D.A. Culkin, L. Mespouille, Ph. Dubois, R.M. Waymouth, J.L. Hedrick; Angew. Chem. Intern. Ed., 44 (2005) 4964-4968.

Nanorubbing of Polythiophene surfaces
G. Derue, S. Coppée, S. Gabriele, M. Surin, V. Geskin, F. Monteverde, P. Leclère, R. Lazzaroni, P. Damman; Journal of the American Chemical Society, 127 (2005) 8019-8020.

Single Molecule Spectroscopy as a Probe for Dye-Polymer Interactions
R.A.L. Vallée, Ph. Marsal, E. Braeken, S. Habuchi, F.C. De Schryver, M. Van Der Auweraer, D. Beljonne, J. Hofkens; Journal of the American Chemical Society, 127 (2005)1 2011-12020.

II. 5. INTERNATIONAL CONTACTS IN THE PROJECT'S RESEARCH DOMAIN

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

Prof. J.L. Brédas; Center for Organic Photonics and Electronics, Georgia Institute of Technology (USA)

Prof. Z. Shuai; Chemistry Department of the Chinese Academy of Sciences, Beijing (China)

Prof. W.R. Salaneck; Departement of Physics, Linköping University (Sweden)

Prof. E.W. Meijer and Prof. R.A.J. Janssen; Eindhoven University of Technology (The Netherlands)

Prof. J. Veciana, Prof. C. Rovira and Dr. D. Amabilino; Institute of Materials Science, Barcelona (Spain)

Prof. A-C. Albertsson; Royal Institute of Technology, Stockholm (Sweden)

Prof. G. Camino; Politecnico di Torino (Italy)

Prof. J.L. Hedrick; IBM Almaden Research Center, San Jose (USA)

Prof. R. Narayan; Michigan State University, Lansing (USA)

Prof. A. Müller; Universidad Simon Bolivar, Caracas (Venezuela)

II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,...).

EU Integrated project on 'Self-Organizing Multifunctional Organic Materials - NAIMO', 2004-2008

EU Integrated project on ' Advanced nanostructured surfaces for the control of biofouling- AMBIO', 2005-2008

EU Marie Curie RTN on 'Chirality Expression and Transfer at the Nanoscale – CHEXTAN', 2005-2008

EU Marie Curie RTN on ' Threaded Molecular Wires as Supramolecularly Engineered Multifunctional Materials – Threadmill – THREADMILL', 2006-2009

EU STReP project on ' Environmentally friendly multifunctional fire retardant polymer hybrids and nanocomposites – NANOFIRE', 2004-2007

EU STReP project on ' Designed nanostructured hybrid polymers : polymerization catalysis and tecton assembly – NANOHYBRID', 2005-2008

Région Wallonne PIMENT project on 'Conception et élaboration de cellules solaires plastiques – SOLPLAST', 2003-2006, coordinated by R. Lazzaroni

Région Wallonne INTERREG III project on ' Production of lactic acid-based biodegradable composite materials – MABIOLAC', 2004-2007, coordinated by Ph. Dubois

Région Wallonne WINNOMAT project on ' Development of a continuous process for nanocomposite foaming via supercritical CO_2 – PROCOMO', 2004-2008

Région Wallonne Network project on 'Elaboration et mise en œuvre de molécules électroactives pour la réalisation de transistors organiques - ETIQUEL', 2005-2008

II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: WP1, Nanodots and photonic crystals (tasks 2, 3, 4, 5)
2. Workpackage number and title: WP2, Organic nanostructures (tasks 1, 2)
3. Workpackage number and title: WP4, Hybrid materials (tasks 2, 3)
4. Workpackage number and title: WP5, (Bio)membranes (tasks 1, 3)
5. Workpackage number and title: WP6, Biomaterials (tasks 1, 2)
6. Workpackage number and title: WP7, Functional coatings (tasks 2, 3)
7. Workpackage number and title: WP8, Supramolecular conjugated systems (tasks 1)
8. Workpackage number and title: WP9, Self-assembly at surfaces (tasks 1, 2)
9. Workpackage number and title:
10. Workpackage number and title:
11. Workpackage number and title:
12. Workpackage number and title:
13. Workpackage number and title:
14. Workpackage number and title:
15. Workpackage number and title:

II. 8. BUDGET (distribution per year) *

(in EURO)

	2007	2008	2009	2010	2011	Total
Personnel	123.000,00	127.000,00	131.000,00	135.000,00	139.000,00	**655.000,00**
Operating costs	12.000,00	12.000,00	12.000,00	12.000,00	12.979,05	**60.979,05**
Equipment	0,00	0,00	0,00	0,00	Not allowed	**0,00**
Overheads	6.750,00	6.950,00	7.150,00	7.350,00	7.598,95	**35.798,95**
Subcontracting	0,00	0,00	0,00	0,00	0,00	**0,00**
Subtotal	**141.750,00**	**145.950,00**	**150.150,00**	**154.350,00**	**159.578,00**	**751.778,00**
EU 1 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 2 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 3 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 4 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
Total	**141.750,00**	**145.950,00**	**150.150,00**	**154.350,00**	**159.578,00**	**751.778,00**

* This table should not be completed by the European partner as his/her budget is mentioned in the budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership

- Personnel: indexed gross remunerations; employer's social contributions; statutory insurance costs as well as any other compensation or allocation legally due in addition to the salary; the reimbursements for PhD and postdoctoral grant holders (exempt from tax and benefiting from social security). Personnel costs must account for minimum 60% of the total budget attributed to each partner of the network. The costs for the tax-free PhD grants and postdoctoral grants may not account for more than 60% of the total personnel costs.

- Operating costs: documentation; travel and accommodation; hosting of visiting foreign researchers use of computing facilities; software; telecommunications; maintenance and operation of equipment and, more generally, consumables;.

- Equipment: acquisition and installation of scientific and technical appliances and instruments, including IT equipment placed at the project's disposal. Equipment cannot be asked for during the last year of the programme.

- Overheads: general expenses of the institutions covering, on an inclusive basis, administrative, telephone, postal, maintenance, heating, electricity, rental, material depreciation and insurance costs. The total amount for this heading may not exceed 5% of total personnel and operating costs.

- Subcontracting: costs incurred by a third party in order to perform tasks or provide services necessitating specific scientific or technical skills outside the normal framework of the institution's activities. Each request for subcontracting needs a approval from the programme administrator.

II. 9. EQUIPMENT

Indicate the equipment (with an estimation of the cost) that will be purchased from the IAP-budget for the coming from four years (2007-2010) and justify.

No equipment will be purchased

II. 10. SUBCONTRACTING

To be completed only if subcontracting is foreseen.

Describe and justify the tasks and/or services that will be provided by a third party.

No subcontracting is foreseen

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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION II

Information on the partners

to be completed by each network partner including the EU-partner(s)

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the partner : Marin Guy (P5) Institution : Universiteit Gent

II. 1. PARTNER CONTACT DETAILS

PARTNER N° (consult the list in Section I of Annex I) * : P5

- Family Name : Marin
- First Name : Guy
- Title (Prof., Dr., ...) : Prof.
- Institution : Universiteit Gent
- Institution's abbreviation : UGent
- Faculty/Department :Engineering
- Research Unit : Chemical Engineering
- Road/Street, n° : Krijgslaan 281 S5
- Post Code : 9000
- Town/City : Gent
- Country : Belgium
- Tel : 0032 9 264 45 17
- Tel secretariat : 0032 9 264 45 16
- Fax : 0032 9 264 49 99
- E-mail : guy.marin@ugent.be
- Website : http://www.tw12.ugent.be/LPTweb/home.html

* For Belgian partners : P1 to P13
For EU-partners : EU1 to EU4

II. 2. STAFF MEMBERS WORKING ON THE PROJECT (paid and not paid by the IAP-budget)

Staff	Number
Professor	6
Senior scientist	2
Post-doc	5
PhD student	23
Researcher without phD	/
Technician	6
Secretary	2
Other	/
TOTAL	**44**

II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, phD student, researcher without phD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name : *Guy B. Marin*
   Profile : professor
   Skills : Chemical Reaction Engineering

2. Name : Geraldine Heynderickx
   Profile : professor
   Skills : Chemical Reactor Engineering/Computational Fluid Dynamics

3. Name : Marie-Françoise Reyniers
   Profile : professor
   Skills : Catalysis/polymerization/molecular engineering

4. Name : Joris W. Thybaut
   Profile : professor
   Skills : Catalytic Reaction Engineering/multiscale modelling

5. Name : Roger De Gryse
   Profile : professor
   Skills : solid state chemistry

6. Name : Diederik Depla
   Profile : professor
   Skills : reactive sputtering

7. Name : Konstantinos Alexopoulos
   Profile : PhD student
   Skills : ab initio modelling on inorganic oxides

8. Name : Veerle Balcaen
   Profile : PhD student
   Skills : catalytic oxidation

9. Name : *Edward Baudrez*
   Profile : PhD student
   Skills : multi-scale modeling

10. Name : Indranil Choudhury
    Profile : PhD student
    Skills : micropores induced shape selectivity

11. Name : Ionel Craciun
    Profile : PhD student
    Skills : fundamental kinetic modelling

12. Name : Susana Cruz
    Profile : PhD student

Skills : high-throughput data modelling and treatment

13. Name : Thomas Davidian
Profile : postdoctoral
Skills : multi-scale modeling

14. Name : Bart De Moor
Profile : PhD student
Skills : ab initio calculations on acid catalyzed reactions

15. Name : Sandra De Schepper
Profile : PhD student
Skills : multi-scale modelling

16. Name : Abhishek Dutta
Profile : PhD student
Skills : multi-scale modelling

17. Name : Rahul Ekatpure
Profile : PhD student
Skills : *reactor engineering*

18. Name : Philippe Heynderickx
Profile : *PhD student*
Skills : catalytic oxidation

19. Name : Gisela Lozano
Profile : PhD student
Skills : fundamental kinetic modelling

20. Name : Maria Olea
Profile : senior scientist
Skills : catalytic oxidation

21. Name : Cem Ozdemir
Profile : PhD student
Skills : reactor engineering

22. Name : Periyasamy Balasubramanian
Profile : postdoctoral
Skills : fundamental kinetic modelling for high throughput methodologies

23. Name : Rado Raharintsalama
Profile : postdoctoral
Skills : ab initio calculations of microporous media

24. Name : Raf Roelant
Profile : PhD student
Skills : mathematics for transient chemical kinetics and reaction network construction

25. Name : Roberto Quintana Solorzano
Profile : PhD student
Skills : *reactions in acid microporous materials*

26. Name : Maarten Sabbe
    Profile : PhD Student
    Skills : ab initio calculations on radical reactions

27. Name : Georgios Stefanidis
    Profile : PhD student
    Skills : multi-scale modelling

28. Name : Jianjun Sun
    Profile : postdoctoral
    Skills : fundamental kinetic modelling of catalyst descriptors

29. Name : Rhona Van Borm
    Profile : PhD student
    Skills : reactions in biporous materials

30. Name : Kevin Van Geem
    Profile : PhD student
    Skills : radical reaction simulation/multi-scale modelling

31. Name : Suryanarayana Prasad Vegendla
    Profile : PhD student
    Skills : multi-scale modelling

32. Name : Jidong Wang
    Profile : PhD student
    Skills : radical reaction kinetics/ thin layer coatings

33. Name : Joris Wieme
    Profile : PhD student
    Skills : synthesis/nanostructure relations in polymers

34. Name : Hilde Poelman
    Profile : senior scientist
    Skills : oxide catalyst preparation

35. Name : Geert Silversmit
    Profile : post-doc
    Skills : X-ray photoelectron and absorption spectroscopy

36. Name : Karin Eufinger
    Profile : PhD student
    Skills : photocatalysis

37. Name : Rene De Coster
    Profile : technician
    Skills : electronics

38. Name : Michaël Lottin
    Profile : technician
    Skills : laboratory assistant

39. Name : Tom Ravelingien
    Profile : technician

Skills : electro-mechanics

40. Name : Etienne Van Damme
Profile : secretary
Skills : administration

41. Name : Georges Verenghen
Profile : technician
Skills : ICT / electronics

42. Name : Marcel Vervust
Profile : technician
Skills : electro-mechanics

43. Name : Rudi Van Paemel
Profile : technician
Skills : vacuum technology

44. Name : Marc Thys
Profile : secretary
Skills : administration

II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

A fundamental kinetic model for hydrocracking of C_8 to C_{12} alkanes on Pt/US-Y zeolites.
G.G. Martens, G.B. Marin, J.A. Martens, P.A. Jacobs, G.V. Baron.
Journal of Catalysis, 195, 253-267, 2000.

Ab initio study of radical addition reactions : addition of a primary ethylbenzene radical to ethene (I).
V. Van Speybroeck, D. Van Neck, M. Waroquier, S. Wauters, M. Saeys, G..B. Marin.
Journal of Physical Chemistry A, 104, 10939-10950, 2000.

Density functional study of benzene adsorption on Pt(111).
M. Saeys, M.-F. Reyniers, G.B. Marin, M. Neurock.
Journal of Physical Chemistry B , 106, 7489-7498, 2002.

Ab initio calculations for hydrocarbons : enthalpy of formation, transition state geometry, and activation energy for radical reactions.
M. Saeys, M.-F. Reyniers, G.B. Marin, V. Van Speybroeck, M. Waroquier.
Journal of Physical Chemistry A, 107, 9147-9159, 2003.

TAP studies on the reoxidation of some partially reduced vanadia-based catalysts.
I.Sack, M. Olea, H. Poelman, K. Eufinger, R. De Gryse, G.B. Marin
Catalysis Today, 91-92, 149-153, 2004.

Density functional theory investigation of the stereochemistry effects on ^1H and ^{13}C NMR chemical shifts of poly(vinyl chloride) oligomers.
P. d'Antuono, E. Botek, B. Champagne, J. Wieme, M.-F. Reyniers, G.B. Marin, P.J. Adriaensens, J.M. Gelan.
Chemical Physics Letters, 411, 207-213, 2005.

Estimation of intrinsic rate coefficients in vinyl chloride suspension polymerization.
T. De Roo, J. Wieme, G.J.. Heynderickx, G.B. Marin.
Polymer 46, 8340-8354, 2005.

First-principles based kinetic model for the hydrogenation of toluene.
M.Saeys, M.-F. Reyniers, J.W. Thybaut, M.Neurock, G.B. Marin.
Journal of Catalysis, 236, 129-138, 2005.

The structure of supported and unsupported vanadium oxide under calcination, reduction and oxidation determined with XAS
G. Silversmit, J.A. Van Bokhoven, H. Poelman, A. van der Eerden, G.B. Marin, M.-F. Reyniers, R. De Gryse
Applied Catalysis A: General 285/1-2 , 151-162, 2005.

Understanding the failure of direct C-C coupling in the zeolite-catalyzed Methanol-to-Olefin Process.
D. Lesthaeghe, V.V. Speybroeck, G.B. Marin, M. Waroquier,
Angewandte Chemie International Edition, Very Important Paper (VIP), 45, 1714-1719, 2006

II. 5. INTERNATIONAL CONTACTS IN THE PROJECT'S RESEARCH DOMAIN

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

Networks:
DUBBLE, the Dutch-Belgian beam line at the ESRF synchrotron facility in Grenoble. It provides privileged beam time for synchrotron related research (SAXS, WAXS, XANES, EXAFS, Interface diffraction) to all participating groups, including partner 5.

IDECAT (Integrated DEsign of CATalytic nanomaterials for a sustainable production), European Network of Excellence

TOPCOMBI (Towards OPtimized chemical processes and new materials by COMBInatorial science)

EUROKIN: a consortium of companies and universities on the use of kinetic modelling in the development of new processes and products.

CRE: Working Party of the European Federation of Chemical Engineering on " Chemical Reaction Engineering"

Collaborations:

ITME (Institute of Electronic Materials Technology), Dr. H. Tomaszewski, ceramic materials, RBS-measurements and ion implantations

Kernforschungsinstitut Julich, Prof. Wördenweber, characterization by RBS and diffraction techniques

MIT, Prof W. Green, chemical reaction engineering, multiscale modeling

University of Virginia, Prof.M. Neurock, ab initio modeling of heterogeneous catalyzed reactions

Von Humboldt University, Prof. J. Sauer, ab initio modeling of heterogeneous catalyzed reactions

TUDelft, Prof. H. van den Akker, multiscale modeling

TUDelft, Prof.F. Kapteijn/Prof. J. Moulijn, dynamic methods in kinetics

Washington University at St-Louis, Prof. G. Yablonsky, dynamic methods in kinetics

IFP, Lyon, dr P. Galtier, single event micro kinetics

TUMünchen, Prof. J. Lercher, high throughput material synthesis

ITQ-Valencia, Prof. A. Corma, high throughput material synthesis

IRC-Villeurbanne, dr. C. Mirodatos, combinatorial methodologies

Queens University Belfast, Prof. H. Stitt, catalytic reaction engineering

II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,. .).

EC
Towards optimised chemical processes and new materials by combinatorial science (TOPCOMBI) , FP6 – IP 515792-2
UGent Principal Investigator: Guy Marin
April 1, 2005 – February 28, 2010
Projectnumber: 41P092105

Network of Excellence IDECAT (Integrated Design of Catalytic Nanomaterials for a Sustainable Production)
UGent Principal Investigator: Guy Marin
1 april 2005 – na
Projectnumber: 41T08905

Federal Government
Supramolecular chemistry and supramolecular catalysis (IUAP 5).
UGent Principal Investigator: Guy Marin
January 1, 2002 - December 31, 2006
Projectnumber: 120C03C2

Supramolecular chemistry and supramolecular catalysis (IUAP 5).
UGent Principal Investigator: Roger De Gryse
January 1, 2002 - December 31, 2006
Projectnumber: 120C03C2

FWO
Kinetic models for innovation in the process industry
UGent Principal Investigator: Guy Marin
January 1, 2006 – December,31 2009
Projectnumber: 3G007106

Structural analysis of hard and soft condensed matter by means of synchrotron radiation
UGent Principal investigator: Roger De Gryse
January 1, 2003 – December 31, 2006
Projectnummer: G.0177.03

Heat and momentum transport in furnaces: three dimensional coupled simulation of flow and combustion.
UGent Principal Investigator: Geraldine Heynderickx
Januariy 1, 2003 – December, 31 2006
Projectnumber: 3G007003

Scientific Research Community "De actieve plaats van katalysator tot reactor"
Principal Investigator R. Schoonheydt, KULeuven

January 1. 2005 –December 31, 2009

Scientific Research Community " Oppervlaktemodificatie van materialen"
Principal Investigator A. Van Tomme, KULeuven
January 1. 2005 –December 31. 2009

Scientific Research Community "Structurele en Chemische Karakterisatie van materialen op micro- en nanometerschaal"
Principal Investigator N. Schryvers, UA
January 1. 2005 –December 31. 2009

IWT
Design of Bimodal porous materials for catalysis and sorption-BIPOM (SBO; IWT 030202)
UGent Principal Investigators: Guy Marin and Michel Waroquier
October 1, 2003 – September, 30 2007
Projectnumber: 174IT343

ThiFA: Roll-to-roll Processing of Textured Films for Thin Film Applications
UGent Principal investigator: Roger De Gryse
May, 1 2004 –April 30, 2007
Projectnumber: IWT040385

Mechanism of Biaxial Alignment in Thin Films, GBOU
UGent Principal investigator: Roger De Gryse
May, 1 2003 –April 30, 2007
Projectnumber: IWT020198

BOF
Elimination of volatile organic compounds (VOC's) : Development of catalytic oxidation technologies for a better environment, GOA nr. 12051603
UGent Principal Investigator: Guy Marin
April, 1 2003 – March, 31 2009
Projectnumber: 12051603

Implementation of a high-throughput platform in heterogeneous catalysis and foundation of an interuniversitary virtual centre for high-throughput experiments in heterogeneous catalysis – VIRKAT
UGent Principal Investigator: Guy Marin
October 1, 2005 - na
Projectnumber: 174PZA05

Mathematical methods in chemical kinetics and engineering (GOA nr. 01GB0405)
UGent Principal Investigator: Roger Van Keer
January 1, 2005 - October 31, 2011
Projectnumber: 01GB0405

II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: WP1, Nanodots and photonic crystals (tasks 2, 4)
2. Workpackage number and title: WP2, Organic nanostructures (coordinator) (task 1)
3. Workpackage number and title: WP3, Porous frameworks (tasks 2, 3)
4. Workpackage number and title: WP4, Hybrid materials (task 2)
5. Workpackage number and title: Workpackage number and title: WP6, Biomaterials (tasks 3)
6. Workpackage number and title: WP7, Functional coatings (task 2)
7. Workpackage number and title: WP8, Supramolecular conjugated systems (task 1)
8. Workpackage number and title:
9. Workpackage number and title:
10. Workpackage number and title:
11. Workpackage number and title:
12. Workpackage number and title:
13. Workpackage number and title:
14. Workpackage number and title:

Partner's name : Marin Guy (P 5)

II. 8. BUDGET (distribution per year) *

(in EURO)

Deleted: , without decimals

	2007	2008	2009	2010	2011	Total
Personnel	103.000,00	106.090,00	109.273,00	112.551,00	115.927,00	546.841,00
Operating costs	69.539,00	66.450,00	63.260,00	59.900,00	56.619,52	315.768,52
Equipment	0,00	0,00	0,00	0,00	Not allowed	0,00
Overheads	8.626,95	8.627,00	8.626,65	8.622,55	8.627,33	43.130,48
Subcontracting	0,00	0,00	0,00	0,00	0,00	0,00
Subtotal	181.165,95	181.167,00	181.159,65	181.073,55	181.173,85	905.740,00
EU 1 (name)	0,00	0,00	0,00	0,00	0,00	0,00
EU 2 (name)	0,00	0,00	0,00	0,00	0,00	0,00
EU 3 (name)	0,00	0,00	0,00	0,00	0,00	0,00
EU 4 (name)	0,00	0,00	0,00	0,00	0,00	0,00
Total	181.165,95	181.167,00	181.159,65	181.073,55	181.173,85	905.740,00

* This table should not be completed by the European partner as his/her budget is mentioned in the budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership

- Personnel: indexed gross remunerations; employer's social contributions; statutory insurance costs as well as any other compensation or allocation legally due in addition to the salary; the reimbursements for PhD and postdoctoral grant holders (exempt from tax and benefiting from social security). Personnel costs must account for minimum 60% of the total budget attributed to each partner of the network. The costs for the tax-free PhD grants and postdoctoral grants may not account for more than 60% of the total personnel costs.

- Operating costs: documentation; travel and accommodation; hosting of visiting foreign researchers use of computing facilities; software; telecommunications; maintenance and operation of equipment and, more generally, consumables;.

- Equipment: acquisition and installation of scientific and technical appliances and instruments, including IT equipment placed at the project's disposal. Equipment cannot be asked for during the last year of the programme.

- Overheads: general expenses of the institutions covering, on an inclusive basis, administrative, telephone, postal, maintenance, heating, electricity, rental, material depreciation and insurance costs. The total amount for this heading may not exceed 5% of total personnel and operating costs.

- Subcontracting: costs incurred by a third party in order to perform tasks or provide services necessitating specific scientific or technical skills outside the normal framework of the institution's activities. Each request for subcontracting needs a approval from the programme administrator.

II. 9. EQUIPMENT

Indicate the equipment (with an estimation of the cost) that will be purchased from the IAP-budget for the coming from four years (2007-2010) and justify.

No equipment will be purchased.

II. 10. SUBCONTRACTING

To be completed only if subcontracting is foreseen.

Describe and justify the tasks and/or services that will be provided by a third party.

No subcontracting is foreseen.

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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION II

Information on the partners

to be completed by each network partner including the EU-partner(s)

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the partner : Jonas Alain (P6) *Institution : Université Catholique de Louvain*

II. 1. PARTNER CONTACT DETAILS

PARTNER N° *(consult the list in Section I of Annex I)* * : P6

- Family Name : Jonas
- First Name : Alain
- Title (Prof., Dr., ...) : Prof.
- Institution : University Catholique de Louvain
- Institution's abbreviation : UCL
- Faculty/Department : Faculté des Sciences Appliquées
  Département de science des matériaux et procédés
  FSA / MAPR
- Research Unit : *Unité de physique et de chimie des hauts polymères* (POLY)
- Road/Street, n° : Place Croix du Sud, 1
- Post Code : 1348
- Town/City : Louvain-la-Neuve
- Country : Belgium
- Tel : 0032 10 47 37 65
- Tel secretariat : 0032 10 47 35 60
- Fax : 0032 10 45 15 93
- E-mail : alain.jonas@uclouvain.be
- Website : *http://www.mapr.ucl.ac.be/~jonas*

* For Belgian partners : P1 to P13
For EU-partners : EU1 to EU4

II. 2. STAFF MEMBERS WORKING ON THE PROJECT (paid and not paid by the IAP-budget)

Staff	Number
Professor	5
Senior scientist	4
Post-doc	11
PhD student	26
Researcher without phD	8
Technician	8.5
Secretary	3
Other	/
TOTAL	**65.5**

II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, phD student, researcher without phD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name : Christian Bailly
   Profile : Professor
   Skills : Rheometry. Polymer chemistry.

2. Name : Sophie Demoustier-Champagne
   Profile : Research Associate of F.N.R.S.
   Skills : Chemical and electrochemical synthesis of organic and hybrid nano-objects. Polymerization and grafting of bio-macromolecules in confined media. Electrochemical and electrical characterisation of functional nanomaterials.

3. Name : Yves Dufrêne
   Profile : Research Associate of F.N.R.S.
   Skills : Biosystems (biomolecules at interfaces, lipid membranes, cells) on the nanoscale: nanofabrication, nanocharacterization using atomic force microscopy, nanobiomimetic devices

4. Name : Christine Dupont
   Profile : Research Associate of F.N.R.S.
   Skills : Design of nanostructured materials surfaces, nano-organization of protein layers by self-assembly and interactions with materials surfaces, cell-material interactions, biocompatibility

5. Name : Jean-François Gohy
   Profile : Professor
   Skills : Block copolymer synthesis and assembly. Macromolecular synthesis.

6. Name : Jean-Louis Habib Jiwan
   Profile : Professor
   Skills : Supramolecular chemistry, analytical organic chemistry, spectroscopy

7. Name : Alain Jonas
   Profile : Professor
   Skills : Layer-by-layer, self- and templated assembly. Nanolithography, nano-imprint and chemical nano-patterning of surfaces. Polymer crystallization. X-ray reflectometry.

8. Name : Bernard Nysten
   Profile : Research Associate of F.N.R.S.
   Skills : Nanomechanics. Atomic force microscopy. Organic semi-conductors. Chemical nano-patterning of surfaces.

9. Name : Olivier Riant
   Profile : Professor
   Skills : Synthetic organic chemistry. Organometallic catalysis, organic materials.

10. Name : Houssein Awada

Profile : Post-doc
Skills : Thin polymer films, dewetting

11. Name : Pascal Borget
Profile : Post-doc
Skills : Polymer scaffolds, biocompatibility

12. Name : Cédric Buron
Profile : Post-doc
Skills : Chemical nanolithography, LbL assembly

13. Name : Sandrine Fleith
Profile : Post-doc
Skills : Protein adsorption, hemocompatibility

14. Name : Charles-André Fustin
Profile : Post-doc
Skills : Polymer synthesis and characterization (AFM, DLS, XPS, GPC...)

15. Name : Yann Gilbert
Profile : Post-doc
Skills : Atomic force microscopy on biomembranes, drug-membrane interactions

16. Name : Matthieu Horgnies
Profile : Post-doc
Skills : Design of smart coatings

17. Name : Zhijun Hu
Profile : Post-doc
Skills : X-ray reflectometry, nano-imprint

18. Name : Chen-Yang Liu
Profile : Post-doc
Skills : rheometry, polymer dynamics

19. Name : Delphine Magnin
Profile : Post-doc
Skills : Functionalization and characterization (mainly SEM and TEM) of nano-objects

20. Name : Halima Alem
Profile : PhD Student
Skills : Stimuli-responsive membranes. Nano-wires grown in confined media.

21. Name : Samuel Caillou
Profile : PhD Student
Skills : Activity of enzymes at interfaces

22. Name : Vincent Callegari
Profile : PhD student
Skills : Electrochemical synthesis of organic and hybrid nano-objects. Structural and electrical characterization.

23. Name : Caroline Dekeyser
Profile : PhD Student

Skills : Nanostructured surfaces, cell culture, biocompatibility

24. Name : Nadia Frederich
Profile : PhD student
Skills : Nano-patterned surfaces, fluorescence spectroscopy

25. Name : Pierre Guillet
Profile : PhD student
Skills : Polymer synthesis and characterization (TEM, DLS, GPC...)

26. Name : Nathalie Lefèvre
Profile : PhD student
Skills : Polymer characterization (AFM, TEM, DLS...)

27. Name : Pierre-Olivier Mouthuy
Profile : PhD student
Skills : Nano-patterning, transport properties of organic semi-conductors

28. Name : Cristèle Nonckreman
Profile : PhD Student
Skills : Design of nanostructured surfaces, protein adsorption, hemocompatibility

29. Name : Claire Verbelen
Profile : PhD Student
Skills : Atomic force microscopy on biomembranes, drug-membrane interactions

30. Name : Emilienne Zuyderhoff
Profile : PhD Student
Skills : Design of nanoheterogeneous surfaces, protein adsorption

31. Name : Yasmine Adriansen
Profile : Technician
Skills : X-ray photoelectron spectroscopy, electrokinetic measurements, UV-visible spectroscopy

32. Name : Françoise Blondeau
Profile : Technician
Skills : Surface functionalization and characterization. Grafting of bio-macromolecules on nano-objects.

33. Name : Cédric Buron
Profile : Technician
Skills : LbL assembly, ellipsometry, AFM, silanization

34. Name : Cécile D'Haese
Profile : Technician
Skills : Polymer synthesis and characterization (TEM, DLS...), fluorescence spectroscopy, NMR

35. Name : Sylvie Derclaye
Profile : Technician
Skills : Wetting measurements, atomic force microscopy

36. Name : Michel Genet

Profile : Technician
Skills : X-ray photoelectron spectroscopy

37. Name : Van Van Trieu
Profile : Technician
Skills : Liquid chromatography methods (HPLC, MPLC) for analytical and preparative separations.

II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

1. Encoding Crystal Microstructure and Chain Folding in the Chemical Structure of Synthetic Polymers, C. Le Fevere de ten Hove, J. Penelle, D.A. Ivanov, A.M. Jonas, *Nature Materials* **2004**, *3*, 33-37.

2. Nanoscale mapping and functional analysis of individual adhesins on living bacteria, Dupres, V.; Menozzi, F.D.; Locht, C.; Clare, B.H.; Abbott, N.L.; Cuenot, S.; Bompard, C.; Raze, D.; Dufrêne, Y.F. *Nature Methods* **2005**, *2*, 515.

3. Highly Diastereo- and Enantioselective Copper-Catalyzed Domino Reduction/Aldol Reaction of Ketones with Methyl Acrylate, Julia Deschamp, Olivier Chuzel, Jérome Hannedouche, Olivier Riant, *Angew. Chem. Int. Ed. Engl.*, **2006**, *45*, 1292.

4. Nanoscale Control of Polymer Crystallization by Nanoimprint Lithography', Zhijun Hu, Gabriel Baralia, Vincent Bayot, Jean-François Gohy, and Alain M. Jonas, *Nano Letters* **2005**, *5*, 1738-1743.

5. Nano-confined polyelectrolyte multilayers, A. Pallandre, A. Moussa, B. Nysten, A.M. Jonas, *Adv. Mater.* **2006**, *18*, 481-486.

6. Nanoporous thin films from self-assembled metallo-supramolecular block copolymers, C. A. Fustin, B. G. G. Lohmeijer, A.-S. Duwez, A. M. Jonas, U. S. Schubert, J.-F. Gohy, *Adv. Mater.* **2005**, *17*, 1162-1165.

7. Supramolecular assemblies of adsorbed collagen affect the adhesion of endothelial cells, Keresztes, Z.; Rouxhet, P.G.; Remacle, C.; Dupont-Gillain, C.C. *J. Biomed. Mater. Res.* **2006**, *76A*, 223.

8. Mechanically-Linked Poly(Ethylene Terephthalate), C. A. Fustin, G. Clarkson, D. A. Leigh, F. Van Hoof, A. M. Jonas, C. Bailly , *Macromolecules* **2004**, *37*, 7884-7892.

9. Aggregation numbers of cationic oligomeric surfactants : a Time-resolved fluorescence quenching study, L. Wattebled, A. Laschewsky, A. Moussa, J-L Habib Jiwan, *Langmuir* **2006**, *22*, 2551-2557.

10. Template Electrochemical Growth of Polypyrrole and Gold-Polypyrrole-Gold Nanowire Arrays, O. Reynes, S. Demoustier-Champagne, *Journal of The Electrochemical Society* **2005**, *152* (9), 130-135.

II. 5. INTERNATIONAL CONTACTS IN THE PROJECT'S RESEARCH DOMAIN.

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

International networks

FAME, European Network of Excellence.

International contacts:

N. Abbott (University of Wisconsin-Madison, USA)
M. Blanchard-Desce (Université de Rennes)
D.G. Castner (University of Washington, USA)
P. Cebe (Tufts University, Boston, USA)
J.-L. Duvail (Institut des Matériaux de Nantes)
H. Federoff (University of Rochester, USA)
N. Gadegaard & A. Curtis (University of Glasgow, UK)
K. Glinel (CNRS-Rouen, France)
H. Gruber & P. Hinterdorfer (University of Linz, Austria)
V. Hlady (University of Utah, Salt Lake City, USA)
W.T.S. Huck (University of Cambridge, UK)
J. Klein (University of Oxford, UK)
A. Laschewsky (University of Potsdam & Fraunhofer Institute for Polymer Research)
S. Lecommandoux (Université de Bordeaux, France)
G. Leggett (University of Sheffield, UK)
C. Locht & D. Raze (Pasteur Lille, France)
J. Penelle (CNRS-Thiais, France)
C. Petit (Université Paris-6, France)
G. Reiter & D.A. Ivanov (CNRS-Mulhouse, France)
C. Roberts (University of Nottingham, UK)
T. Russell (University of Massachusetts, USA)
U. Schubert (Eindhoven University of Technology, NL)
D. Stievenard (Institut d'Electronique, de Microélectronique et de Nanotechnologies, Lille, France)
D.S. Sutherland (Chalmers University of Technology, Göteborg, Sweden)
A. Vasella (Swiss Federal Institute of Technology, Switzerland)
A. Walcarius (Université H. Poincaré Nancy I)
U. Wiesner (Cornell University, Ithaca, USA)
B. Xu (Hong Kong University of Science & Technology, Hong Kong)
D.Y. Yoon (Seoul National University, Korea)

II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,...).

2001-2006: Belgium Federal Governement: Inter-University Attraction Pole: member (level 2) of the *Supramolecular Chemistry & Supramolecular Catalysis* network

2002-2007: Wallonia Region: Nanotechnology Program: *développement d'un bio-nanosenseur* (NANOSENS).

2002-2007: Wallonia Region: Nanotechnology Program: *développement d'un modèle membranaire nanobiomimétique à usage pharmacologique* (NANOMEMB).

2002-2007: Wallonia Region: Nanotechnology Program: *nanostructuration de surface pour l'hémocompatibilité des polyoléfines* (NEH).

2003-2008: French Community of Belgium: Concerted Research Action NANOMOL *Nanoélectronique moléculaire.*

2004-2008: Wallonia Region: Network Program: *Surfaces micro- et nano-structurées auto-nettoyantes et anti-corrosion* (CORRONET).

2004-2008: Wallonia Region: Network Program: *Elaboration et mise en oeuvre de molécules électroactives pour la réalisation de transistors organiques* (ETIQUEL).

2005-2007: Wallonia Region: Excellence Program *nanoTIC: swarms of smart sensors*. Project 1 FEELING : *Molecular Recognition and Generation of the first Signal.*

2005-2008: Wallonia Region: WINNOMAT Program: *optimisation d'un biomatériau composite fibre - hydrogel - cellule destiné à promouvoir la reconstruction osseuse* (FIGELCEL).

2005-2008: European Union: METAMOS Strep: *Metallic source and drain for advanced MOS technology.*

2005-2009: Wallonia Region: WINNOMAT Program: *revêtements intelligents pour une meilleure nettoyabilité de l'acier inox* (SMARTNET).

2006-2011: French Community of Belgium: Concerted Research Action DynanoMOVE: *Controlling motion and dynamical phenomena at the nanometer scale.*

II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: WP1, Nanodots and photonic crystals (tasks 1, 2, 4)
2. Workpackage number and title: WP2, Organic nanostructures (tasks 1, 2)
3. Workpackage number and title: WP3, Porous frameworks (task 4)
4. Workpackage number and title: WP4, Hybrid Materials (tasks 1, 2)
5. Workpackage number and title: WP5, (Bio)membranes (tasks 1, 2, 4, 5)
6. Workpackage number and title: WP6, Biomolecules and Biocatalysis (task 5)
7. Workpackage number and title: WP7, Functional coatings (tasks 1, 2, 3)
8. Workpackage number and title: WP8, Supramolecular conjugated systems (task 1)
9. Workpackage number and title: WP9, Self-assembly at surfaces (tasks 1, 2)
10. Workpackage number and title:
11. Workpackage number and title:
12. Workpackage number and title:
13. Workpackage number and title:
14. Workpackage number and title:
15. Workpackage number and title:

II. 8. BUDGET (distribution per year) *

(in EURO)

	2007	2008	2009	2010	2011	Total
Personnel	98.990,00	133.930,00	124.044,00	127.765,00	111.413,86	**596.142,86**
Operating costs	45.000,00	54.000,00	63.000,00	54.000,00	45.000,00	**261.000,00**
Equipment	0,00	0,00	0,00	0,00	Not allowed	**0,00**
Overheads	7.199,50	9.396,50	9.352,20	9.088,25	7.820,69	**42.857,14**
Subcontracting	0,00	0,00	0,00	0,00	0,00	**0,00**
Subtotal	**151.189,50**	**197.326,50**	**196.396,20**	**190.853,25**	**164.234,55**	**900.000,00**
EU 1 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 2 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 3 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 4 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
Total	**151.189,50**	**197.326,50**	**196.396,20**	**190.853,25**	**164.234,55**	**900.000,00**

* This table should not be completed by the European partner as his/her budget is mentioned in the budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership

- Personnel: indexed gross remunerations; employer's social contributions; statutory insurance costs as well as any other compensation or allocation legally due in addition to the salary; the reimbursements for PhD and postdoctoral grant holders (exempt from tax and benefiting from social security). Personnel costs must account for minimum 60% of the total budget attributed to each partner of the network. The costs for the tax-free PhD grants and postdoctoral grants may not account for more than 60% of the total personnel costs.

- Operating costs: documentation; travel and accommodation; hosting of visiting foreign researchers use of computing facilities; software; telecommunications; maintenance and operation of equipment and, more generally, consumables;.

- Equipment: acquisition and installation of scientific and technical appliances and instruments, including IT equipment placed at the project's disposal. Equipment cannot be asked for during the last year of the programme.

- Overheads: general expenses of the institutions covering, on an inclusive basis, administrative, telephone, postal, maintenance, heating, electricity, rental, material depreciation and insurance costs. The total amount for this heading may not exceed 5% of total personnel and operating costs.

- Subcontracting: costs incurred by a third party in order to perform tasks or provide services necessitating specific scientific or technical skills outside the normal framework of the institution's activities. Each request for subcontracting needs a approval from the programme administrator.

II. 9. EQUIPMENT

Indicate the equipment (with an estimation of the cost) that will be purchased from the IAP-budget for the coming from four years (2007-2010) and justify.

No equipment will be purchased

II. 10. SUBCONTRACTING

To be completed only if subcontracting is foreseen.

Describe and justify the tasks and/or services that will be provided by a third party.

No subcontracting is foreseen

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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION II

Information on the partners

to be completed by each network partner including the EU-partner(s)

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the partner : Du Prez Filip (P7) Institution : Universiteit Gent

II. 1. PARTNER CONTACT DETAILS

PARTNER N° (consult the list in Section I of Annex I) * : P7

- Family Name : Du Prez
- First Name : Filip
- Title (Prof., Dr., ...) : Prof.
- Institution : Universiteit Gent
- Institution's abbreviation : UGent
- Faculty/Department : Faculty of Sciences/Department of Organic Chemistry
- Research Unit : Polymer Chemistry Research Group
- Road/Street, n° : Krijgslaan 281 S4bis
- Post Code : 9000
- Town/City : Gent
- Country : Belgium
- Tel : 0032 9 264 45 03
- Tel secretariat : 0032 9 264 44 89
- Fax : 0032 9 264 49 72
- E-mail : fillip.duprez@ugent.be
- Website : http://www.orgchem.ugent.be/PolymDup.htm

* For Belgian partners : P1 to P13
For EU-partners : EU1 to EU4

II. 2. STAFF MEMBERS WORKING ON THE PROJECT (paid and not paid by the IAP-budget)

Staff	Number
Professor	1
Senior scientist	1
Post-doc	2
PhD student	6
Researcher without phD	3
Technician	1
Secretary	1
Other	/
TOTAL	**15**

II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, phD student, researcher without phD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name : Du Prez Filip
   Profile : Prof.
   Skills : Research leader Polymer Chemistry Research Group; coordinator of work package 4

2. Name : Dr. Verbrugghe Sam
   Profile : senior scientist
   Skills : IOF Technology developer: responsible for valorisation of research results (project drafting, partnering, licensing, spin-off development)

3. Name : Van Camp Wim
   Profile : post-doctoral researcher
   Skills : Design of novel polymer supports for catalytic complexes to be used for atom transfer radical polymerization and click chemistry (related to task 5.5 and 9.2).

4. Name : Bonami Lies
   Profile : PhD
   Skills : Design and use of amine-containing metal complexing polymer networks, for example as supports for catalysts of ATRP (related to task 2.1)

5. Name : D'Hollander Stijn
   Profile : PhD
   Skills : Exploration of synthetic methods for the preparation of shape memory polymers based on multiblock copolymers for their use in several applications (related to task 2.1)

6. Name : Dervaux Bart
   Profile : PhD
   Skills : Development of new approaches to make complex polymer structures such as gradient copolymers by controlled radical polymerization techniques in a continuous way (related to task 2.1)

7. Name : Gökmen Talha
   Profile : PhD
   Skills : Design of novel kind of polymer beads by suspension polymerization with 'clickable' groups for attachment of functionalized molecules.

8. Name : De Meyer Bernhard
   Profile : Technician
   Skills : Operator of advanced equipment for the analysis of polymer materials and supramolecular assemblies (related to all tasks with involvement of partner 7)

9. Name : Denaene Ingrid
   Profile : Secretary
   Skills : financial project management, ordering, facturation, secretary work during the writing of publications and reports, logistic support for the organization of meetings and workshops.

II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

1. K. Bernaerts, F. Du Prez, "Dual/heterofunctional initiators for the combination of mechanistically distinct polymerization techniques", *Progr. Polym. Sci.*, **31**, 671-748 (2006)
2. L. Van Renterghem, X. Feng, D. Taton, Y. Gnanou, F. Du Prez, "MALDI-TOF analysis of dendrimer-like poly(ethylene oxide)s", *Macromolecules*, **38**, 10609-10613 (2005).
3. K. Van Durme, B. Van Mele, W. Loos, F. Du Prez, "Introduction of silica into thermo-responsive poly(N-isopropyl acrylamide) hydrogels: a novel approach to improve response rates", *Polymer*, **46**, 9851–9862 (2005).
4. Ivo F.J. Vankelecom, K. De Smet, Lieven E.M. Gevers, Peggy Van De Velde, Filip Du Prez, Pierre A. Jacobs, "Physico-chemical interpretation of SRNF transport mechanisms through dense silicone membranes" *J. Memb. Sci.*, **274**, 173-182 (2006).
5. B. Verdonck, J-F Gohy, E. Khousakoun, R. Jérôme, F. Du Prez, "Association behavior of thermo-responsive block copolymers based on poly(vinyl ethers) ", *Polymer,* **46**, 9899-9907 (2005).
6. W. Lequieu, N. Shtanko, F. Du Prez, "Track etched membranes with thermo-adjustable porosity and separation properties by surface immobilization of poly(N-vinylcaprolactam)", *J. Memb. Sci.*, **256**, 64-71 (2005).
7. K. Bernaerts, F. Du Prez, "Design of novel poly(methyl vinyl ether) containing AB and ABC block copolymers by the dual initiator strategy", *Polymer,* **46**, 8469-8482 (2005).
8. N. Tsarevsky, K. Bernaerts, B. Dufour, F. Du Prez, K. Matyaszewski, "Well-defined (co)polymers with 5-vinyltetrazole units via combination of atom transfer radical (co)polymerization of acrylonitrile and "click chemistry"-type postpolymerization modification", *Macromolecules*, **37**, 9308-9313 (2004).
9. W. Van Camp, S. Bon, F. Du Prez, "ATRP of 1-ethoxyalkyl(meth)acrylate: facile route towards near-monodisperse poly((meth)acrylic acid)", *Macromolecules*, 37, 6673-6675 (2004).
10. W. Lequieu, F.E. Du Prez, "Segmented Polymer Networks based on Poly(N-isopropyl acrylamide) and poly(tetrahydrofuran) as polymer membranes with thermo-responsive permeability", *Polymer*, **45**, 749-757 (2004).

II. 5. INTERNATIONAL CONTACTS IN THE PROJECT'S RESEARCH DOMAIN

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

- Partner in European network from European Science Foundation (ESF) '*STIPOMAT*' (experimental and theoretical design of *stimuli-responsive polymeric materials*, 2005-2008): regular exchange of researchers with the research groups of Prof. H. Tenhu (University of Helsinki, Finland, E-mail: heikki.tenhu@helsinki.fi) and Prof. I. Galaev (University of Lund, Sweden, E-mail: igor.galaev@biotek.lu.se)

- Prof. Kris Matyjaszewski (Carnegie Mellon University, USA, E-mail: km3b@andrew.cmu.edu): PhD-student exchanges in the field of controlled radical polymerization.

- coordinator of bilateral BOF-project (2006-2007) with Prof. V. Zubov (E-mail: zubov@mail.ibch.ru) from Moscow State University (Russia) on design of stimuli-responsive segmented structures for controllable stabilization of pigments and colloids

- Prof. Darinka Christova (Polymer institute of Bulgarian Academy of Sciences, E-mail: dchristo@mail.polymer.bas.bg): exchange of researchers within the field of polymer membranes (FWO-BAS + NATO-project)

- Prof. Yves Gnanou (University of Bordeaux, Laboratoire de Chimie des Polymères Organiques, E-mail: gnanou@enscpb.fr): student exchanges in the framework of design and advanced characterization of thermo-responsive polymer structures.

- Prof. U. Schubert (Technical University of Eindhoven, Netherlands, E-mail: u.s.schubert@tue.nl): regular PhD-student exchanges in the framework of the use of combinatorial approaches in polymer chemistry.

- Prof. Adler/Dr. Kuckling (Technical University of Dresden, Germany, E-mail: dirk.kuckling@chemie.tu-dresden.de): regular exchange of students for characterization (SPR) of stimuli-responsive hydrogel systems.

II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,...).

- "Experimental and Theoretical Design of Stimuli-Responsive Polymeric Materials", European Science Foundation (ESF), participation in European Project STIPOMAT, 2005-2008.
- "Sensing Endocrine Disrupting Chemicals: development of novel solid phase extraction systems", European Framework-6 (Marie-Curie) early stage training network, 2006-2010.
- "Blocky gradient versus block copolymers: comparison of structure-property relations", BOF-UGent (coll. with Russia), 2006-2009
- "Polymer networks and polyion complexes: synthesis, characterization and use in membrane processes", FWO, 2006-2009
- "Cs-corrected Transmission Electron Microscope for Analysis of Materials with Atomic Resolution", BOF-Flemish Community (heavy equipment), 2005
- "Multifunctional scanning probe microscope", BOF- basic equipment, 2005
- "Gradient- versus block copolymers via atom transfer radical polymerisation: continuous preparation via column reactors", FWO-fellowship B. Dervaux, 2005-2009
- "Synthesis and evaluation of shape memory materials based on multiblock copolymers", IWT-fellowship, 2004-2008
- "Synthesis and evaluation of block copolymer structures with labile segments", IWT-fellowship, 2002-2006
- "Physical cross-linking of linear polymers by means of nano-polymer networks", IWT-fellowship, 2002-2006

II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: WP2, Organic nanostructures (task 1)
2. Workpackage number and title: WP4, Hybrid materials (as coordinator) (tasks 1, 2)
3. Workpackage number and title: WP5, (Bio)membranes (task 5)
4. Workpackage number and title: WP7, Functional coatings (tasks 1, 3)
5. Workpackage number and title: WP9, Self-assembly at surfaces (task 2)
6. Workpackage number and title:
7. Workpackage number and title:
8. Workpackage number and title:
9. Workpackage number and title:
10. Workpackage number and title:
11. Workpackage number and title:
12. Workpackage number and title:
13. Workpackage number and title:
14. Workpackage number and title:
15. Workpackage number and title:

II. 8. BUDGET (distribution per year) *

(in EURO)

	2007	2008	2009	2010	2011	Total
Personnel	51.000,00	82.100,00	34.800,00	105.700,00	37.200,00	**310.800,00**
Operating costs	14.152,38	14.000,00	14.000,00	14.000,00	14.000,00	**70.152,38**
Equipment	0,00	0,00	0,00	0,00	Not allowed	**0,00**
Overheads	3.257,62	4.805,00	2.440,00	5.985,00	2.560,00	**19.047,62**
Subcontracting	0,00	0,00	0,00	0,00	0,00	**0,00**
Subtotal	**68.410,00**	**100.905,00**	**51.240,00**	**125.685,00**	**53.760,00**	**400.000,00**
EU 1 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 2 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 3 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 4 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
Total	**68.410,00**	**100.905,00**	**51.240,00**	**125.685,00**	**53.760,00**	**400.000,00**

* This table should not be completed by the European partner as his/her budget is mentioned in the budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership

- Personnel: indexed gross remunerations; employer's social contributions; statutory insurance costs as well as any other compensation or allocation legally due in addition to the salary; the reimbursements for PhD and postdoctoral grant holders (exempt from tax and benefiting from social security). Personnel costs must account for minimum 60% of the total budget attributed to each partner of the network. The costs for the tax-free PhD grants and postdoctoral grants may not account for more than 60% of the total personnel costs.

- Operating costs: documentation; travel and accommodation; hosting of visiting foreign researchers use of computing facilities; software; telecommunications; maintenance and operation of equipment and, more generally, consumables;.

- Equipment: acquisition and installation of scientific and technical appliances and instruments, including IT equipment placed at the project's disposal. Equipment cannot be asked for during the last year of the programme.

- Overheads: general expenses of the institutions covering, on an inclusive basis, administrative, telephone, postal, maintenance, heating, electricity, rental, material depreciation and insurance costs. The total amount for this heading may not exceed 5% of total personnel and operating costs.

- Subcontracting: costs incurred by a third party in order to perform tasks or provide services necessitating specific scientific or technical skills outside the normal framework of the institution's activities. Each request for subcontracting needs a approval from the programme administrator.

II. 9. EQUIPMENT

Indicate the equipment (with an estimation of the cost) that will be purchased from the IAP-budget for the coming from four years (2007-2010) and justify.

No equipment will be purchased

II. 10. SUBCONTRACTING

To be completed only if subcontracting is foreseen.

Describe and justify the tasks and/or services that will be provided by a third party.

No subcontracting is foreseen.

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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION II

Information on the partners

to be completed by each network partner including the EU-partner(s)

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the partner : Baron Gino (P8) Institution : Vrije Universiteit Brussel

II. 1. PARTNER CONTACT DETAILS

PARTNER N° (consult the list in Section I of Annex I) * : P8

- Family Name : Baron
- First Name : Gino
- Title (Prof., Dr., ...) : Prof.
- Institution : Vrije Universiteit Brussel
- Institution's abbreviation : VUB
- Faculty/Department : Applied Sciences / Department of Chemical Engineering
- Research Unit :
- Road/Street, n° : Pleinlaan 2
- Post Code : 1050
- Town/City : Brussel
- Country : Belgium
- Tel : 0032 2 629 32 46
- Tel secretariat : 0032 2 629 32 50
- Fax : 0032 2 629 32 48
- E-mail : gvbaron@vub.ac.be
- Website : http://wwwtw.vub.ac.be/chis/

* For Belgian partners : P1 to P13
For EU-partners : EU1 to EU4

II. 2. STAFF MEMBERS WORKING ON THE PROJECT (paid and not paid by the IAP-budget)

Staff	Number
Professor	4
Senior scientist	2
Post-doc	3
PhD student	18
Researcher without phD	/
Technician	2
Secretary	1
Other	/
TOTAL	**30**

II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, phD student, researcher without phD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name : Gino Baron
   Profile : Professor
   Skills : Chemical Engineering, Adsorption, Catalysis

2. Name : Gert Desmet
   Profile : Professor
   Skills : Chemical Engineering, Chromatography, DNA Analysis

3. Name : Joeri Denayer
   Profile : Professor
   Skills : Chemical Engineering, Adsorption, Catalysis

4. Name : Harry Verelst
   Profile : Professor
   Skills : Chemical Engineering, Adsorption, Catalysis

5. Name : Ksudhiram Mantri
   Profile : Senior scientist
   Skills : Catalysis, Material synthesis

6. Name : Shiping Huang
   Profile : Senior scientist
   Skills : Molecular modeling

7. Name : David Clicq
   Profile : post-doctoral
   Skills : Chromatography, Nanobiotechnology

8. Name : Piotr Gzil
   Profile : post-doctoral
   Skills : Chromatography, Computational Modelling

9. Name : Kris Papaert
   Profile : post-doctoral
   Skills : Chromatography, Nanobiotechnology

10. Name : Lisa Devriese
    Profile : PhD student
    Skills : Adsorption, diffusion, zeolites

11. Name : Eileen Dejaegere
    Profile : PhD student
    Skills : Catalysis, adsorption, GC-MS

12. Name : Vincent Finsy
    Profile : PhD student
    Skills : Adsorption, Metallo-organic frameworks, GC

13. Name : Jeroen Persoons
    Profile : PhD student
    Skills : Adsorption, diffusion, porous materials, HPLC

14. Name : Lina Ma
    Profile : PhD student
    Skills : Catalysis, synthesis

15. Name : Jeroen Billen
    Profile : PhD student
    Skills : Chromatography, Computational Modelling

16. Name : Jan De Smet
    Profile : PhD student
    Skills : Chromatography, Computational Modelling

17. Name : Wim De Malsche
    Profile : PhD student
    Skills : Micromachining, Nano-Imprinting

18. Name : Veronika Fekete
    Profile : PhD student
    Skills : Chromatography, Porous Materials

19. Name : Sander Deridder
    Profile : PhD student
    Skills : Chromatography, Computational Modelling

20. Name : Frederik Detobel
    Profile : PhD student
    Skills : DNA Microarray Analysis

21. Name : Deirdre Cabooter
    Profile : PhD student
    Skills : Chromatography

22. Name : Joris Vangelooven
    Profile : PhD student
    Skills : Chromatography, Nanobiotechnology

23. Name : Hamed Eghbali
    Profile : PhD student
    Skills : Chromatography, Porous Materials

24. Name : Ken Broeckhoven
    Profile : PhD student
    Skills : HP Chromatography

25. Name : Selm De Bruyne
    Profile : PhD student

Skills : HP Chromatography

26. Name : Alexios Harkiolakis
Profile : PhD student
Skills : Thin films, adsorptive separations

27. Name : Pierre Martin
Profile : PhD student
Skills : Data mining, adsorption

II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

Inge Daems, Alain Méthivier, Philibert Leflaive, Alain H. Fuchs, Gino V. Baron, and Joeri F. M. Denayer, Unexpected Si:Al effect on the binary mixtures liquid phase adsorption selectivities in faujasite zeolites, J. AM. CHEM. SOC. 2005, 127, 11600-11601.

Clicq, D, Pappaert, K., Vankrunkelsven, S., Vervoort, N., Baron, G. V. and Desmet, G., 2004, Shear-driven Flows: A New Approach to LC and Macro-molecular Separations, Anal. Chem. 76(23); 430A-439A.

Joeri F. M. Denayer, Refik A. Ocakoglu, Joris Thybaut, Guy Marin, Pierre Jacobs, Johan Martens, and G. V. Baron, n- and Isoalkane Adsorption Mechanisms on Zeolite MCM-22, J. Phys. Chem. B; 2006; 110(17), 8551 – 8558.

Gzil, P., Vervoort, N., Baron, G. V. and Desmet, G., 2004, General Rules for the Optimal External Porosity of LC Supports, Analytical Chemistry, 76(22); 6707-6718.

Joeri F. M. Denayer, Refik A. Ocakoglu, Ilbige C. Arik, Christine E. A. Kirschhock, Johan A. Martens, Gino V. Baron, Rotational Entropy Driven Separation of Alkane/Isoalkane Mixtures in Zeolite Cages, Angewandte Chemie International Edition, 44, 2005, 400-403.

Desmet, G., Clicq, D. and Gzil, P., 2005, Geometry-independent Plate Height Representation Methods for the Direct Comparison of the Kinetic Performance of LC Supports with a Different Size or Morphology, Anal. Chem., 77, 4058-4070.

Denayer, J.F.M., De Meyer, K., Martens, J.A., Baron, G.V., Molecular Competition Effects in Liquid Phase Adsorption of Long Chain n-Alkane Mixtures in ZSM-5 Zeolite Pores, Angewandte Chemie, 42, 2774-2777, 2003.

Desmet, G., Gzil, P., Nguyen, Dao T.-T., Guillarme, D., Rudaz S., Veuthey, J.-L. Vervoort, N., Torok, G., Cabooter, D. and Clicq, D., Including Practical Constraints In The Kinetic Plot Representation of Chromatographic Performance Data: Theory and Application To Experimental Data, Anal Chem,. 2006, 78, 2150-2162.

Sophie FM Van der Beken; Eileen Dejaegere; Kourosch A Tehrani, Johan S Paul, Pierre A Jacobs, Gino V Baron, Denayer, J.F.M., Alkylation of Deactivated Aromatic Compounds on Zeolites. Part 1: Adsorption, Deactivation and Selectivity Effects in the Alkylation of Bromobenzene and Toluene with Bifunctional Alkylating Agents, Journal of Catalysis 235 (2005) 128–138.

Vankrunkelsven, S., Clicq, D., Fekete, V., Cabooter, D., De Malsche, W., Gardeniers J. G. E. and Desmet, G, 2006, Ultra-rapid Separation of an Angiotensin Mixture in Nanochannels using Shear-driven Chromatography., Journal of Chromatography A, 1102, 96-103.

II. 5. INTERNATIONAL CONTACTS IN THE PROJECT'S RESEARCH DOMAIN

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

- Prof. A. Fuchs, LCP, Orsay (FR) (2004-...) Molecular modeling alkene – aromatic separation with zeolites
- dr. John Tomkinson (ISIS, UK) (2004-...) Inelastic neutron scattering spectroscopy: study of configuration of long alkanes in 2-D pore systems, measurement of diffusion in zeolites
- Randy Snurr, Dept. Chemical Engineering Northwestern University, Evanston (US), (2003-..). Hydrocarbon Adsorption in Liquid Phase, Molecular simulation
- Prof. Pasch, Deutsches Kunststoff-Institut (DE) (2002-...) Characterization of polymers by adsorptive separation
- Dr. P. Simell, E. Kurkela, VTT, Finland Biomass gasification high temperature gas cleaning research projects (EU)
- INSTITUT FRANCAIS du PETROLE (IFP), A. Méthivier, Ph. Leflaive, (01.03.2002-)... Adsorptive separation of paraffins and olefins on zeolites X en Y
- Prof. S. Brandani, University College London, ZLC-diffusion measurement with TOF-MS detector
- Prof. van den Berg, MESA+ Research Institute, University of Twente, Micro- and Nanolithography for the production of miniaturized bio-separation systems
- Prof. Cees Gooijer, ACAS, Vrije Universiteit Amsterdam, Ultra-sensitive Laser Based decection in Nanochannels

Prof. Peter Schoenmakers, van 't Hoff Institute for Molecuar Studies, Universiteit van Amsterdam, Characterization of Novel Chromatographic Supports

- Prof. Knut Irgum Analytical Chemistry, Umeå University, Sweden, Prof. Knut Irgum, Characterization of Polymeric Monolithic Chromatographic Supports

II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,...).

- Supramolecular chemistry and supramolecular catalysis, IUAP V-3, DWTC, 2002-2006.
- BIPOM: design of bimodal porous materials for catalysis and sorption, IWT-SBO, 2003-2007.
- Bimodal porous materials for separation, VUB (OZR), 2004-2007.
- *Gravimetric determination of packing effects in zeolites*, FWO, 2004-2006.
- VIRKAT – Virtual Center for High throughput testing in Adsorption and Catalysis (Equipment), Vlaamse Gemeenschap.
- NextChrom: Building and Using the Next Generation of Liquid Phase (Bio-)Analytical Separation Devices: Exploiting the Advantages of Maximal Column Structure Control And Maximal Process Integration ,IWT-SBO, 2006-2010.
-Molecular interactions and Transport in Confined Spaces and Ordered Structures, 2005-2009, VUB (OZR).
- Computer-Gesteund Ontwerp Van Chemische Analyse-Chips Voor (Bio-)Farmaceutische Scheidingen, VUB (OZR), 2005-2006.
- Detectie van snelle chromatografische scheidingen, single-molecule passages en target/receptor-bindingen in nano-kanalen. FWO, 2004-2006.
- Adsorptive characterization and application in liquid phase separation with thin zeolite films, FWO, 2006-2009.
- A high-throughput and combinatorial approach to synthesis/adsorption/catalysis, FWO, 2003-2006.
- Adsorptive characterization and application in liquid phase separation with thin zeolite films, VUB (OZR), 2006-2009.

II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: WP1, Nanodots and photonic crystals (task 1)
2. Workpackage number and title: WP3, Porous frameworks (tasks 2, 3)
3. Workpackage number and title: WP4, Hybrid materials (tasks 1, 2)
4. Workpackage number and title: WP5, (Bio)membranes (task 5)
5. Workpackage number and title: WP6, Biomolecules and biocatalysis (tasks 2, 4)
6. Workpackage number and title:
7. Workpackage number and title:
8. Workpackage number and title:
9. Workpackage number and title:
10. Workpackage number and title:
11. Workpackage number and title:
12. Workpackage number and title:
13. Workpackage number and title:
14. Workpackage number and title:
15. Workpackage number and title:

II. 8. BUDGET (distribution per year) *

(in EURO)

	2007	2008	2009	2010	2011	Total
Personnel	68.000,00	68.000,00	68.000,00	68.000,00	68.000,00	**340.000,00**
Operating costs	20.109,52	20.000,00	20.000,00	20.000,00	20.000,00	**100.109,52**
Equipment	0,00	0,00	0,00	0,00	Not allowed	**0,00**
Overheads	4.405,48	4.400,00	4.400,00	4.400,00	4.400,00	**22.005,48**
Subcontracting	0,00	0,00	0,00	0,00	0,00	**0,00**
Subtotal	**92.515,00**	**92.400,00**	**92.400,00**	**92.400,00**	**92.400,00**	**462.115,00**
EU 1 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 2 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 3 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 4 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
Total	**92.515,00**	**92.400,00**	**92.400,00**	**92.400,00**	**92.400,00**	**462.115,00**

* This table should not be completed by the European partner as his/her budget is mentioned in the budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership

- Personnel: indexed gross remunerations; employer's social contributions; statutory insurance costs as well as any other compensation or allocation legally due in addition to the salary; the reimbursements for PhD and postdoctoral grant holders (exempt from tax and benefiting from social security). Personnel costs must account for minimum 60% of the total budget attributed to each partner of the network. The costs for the tax-free PhD grants and postdoctoral grants may not account for more than 60% of the total personnel costs.

- Operating costs: documentation; travel and accommodation; hosting of visiting foreign researchers use of computing facilities; software; telecommunications; maintenance and operation of equipment and, more generally, consumables;.

- Equipment: acquisition and installation of scientific and technical appliances and instruments, including IT equipment placed at the project's disposal. Equipment cannot be asked for during the last year of the programme.

- Overheads: general expenses of the institutions covering, on an inclusive basis, administrative, telephone, postal, maintenance, heating, electricity, rental, material depreciation and insurance costs. The total amount for this heading may not exceed 5% of total personnel and operating costs.

- Subcontracting: costs incurred by a third party in order to perform tasks or provide services necessitating specific scientific or technical skills outside the normal framework of the institution's activities. Each request for subcontracting needs a approval from the programme administrator.

II. 9. EQUIPMENT

Indicate the equipment (with an estimation of the cost) that will be purchased from the IAP-budget for the coming from four years (2007-2010) and justify.

No equipment will be purchased.

II. 10. SUBCONTRACTING

To be completed only if subcontracting is foreseen.

Describe and justify the tasks and/or services that will be provided by a third party.

No subcontracting is foreseen.

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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION II

Information on the partners

to be completed by each network partner including the EU-partner(s)

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the partner : *De Mesmaeker-Kirsch Andrée* (P9) Institution : Université Libre de Bruxelles

.be

II. 1. PARTNER CONTACT DETAILS

PARTNER N° (consult the list in Section I of Annex I) * : P9

- Family Name : De Mesmaeker - Kirsch
- First Name : Andrée
- Title (Prof., Dr., ...) : Prof.
- Institution : Université Libre de Bruxelles
- Institution's abbreviation : ULB
- Faculty/Department : Faculty of Sciences, Department of Chemistry
- Research Unit : Chimie Organique, Photochimie et Chimie des Polymères
- Road/Street, n° : 50 av. F.D. Roosevelt
- Post Code : 1050
- Town/City : Brussels
- *Country* : *Belgium*
- Tel : 0032 2 650 30 17
- Tel secretariat : 0032 2 650 20 99
- Fax : 0032 2 650 30 18
- E-mail : akirsch@ulb.ac.be
- Website : http://www.ulb.ac.be/sciences/cop, http://www.ulb.ac.be/sciences/chimpoly/

* For Belgian partners : P1 to P13
For EU-partners : EU1 to EU4

II. 2. STAFF MEMBERS WORKING ON THE PROJECT (paid and not paid by the IAP-budget)

Staff	Number
Professor	3
Senior scientist	3
Post-doc	4
PhD student	10
Researcher without phD	9
Technician	2
Secretary	2
Other	1
TOTAL	**34**

II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, phD student, researcher without phD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name : De Mesmaeker – Kirsch, Andrée
   Profile : Professor
   Skills : DNA, oligonucleotides + Ru complexes and polynuclear, dendritic compounds

2. Name : Moucheron Cécile
   Profile : Professor
   Skills : DNA, oligonucleotides + Ru complexes and polynuclear, dendritic compounds

3. Name : Geerts, Yves
   Profile : Professor
   Skills : Discotic compounds

4. Name : Pierard, Frédéric
   Profile : Senior scientist
   Skills : Synthesis, study of self assemblies of metal ions with organic ligands and oligonucleotides

5. Name : Elias Benjamin
   Profile : Senior scientist
   Skills : Synthesis, photophysics of dinuclear, polynuclear complexes

6. Name : Mokhir, Larisa
   Profile : Post doc
   Skills : Assemblies of DNA/polymers probed by luminescent metal complexes

7. Name : Rickling Stéphane
   Profile : Post doc
   Skills : Ru-derivatized oligonucleotides, photochemistry, photophysics

8. Name : Gihzdavu, Liana
   Profile : Post doc
   Skills : Ru complexes synthesis, interaction, photoreaction with different DNA

9. Name : Boisdenghien, Arnaud
   Profile : PhD student
   Skills : Ru complexes with intercalating ligands, synthesis, photophysical study

10. Name : Claessens Nicolas
    Profile : PhD student
    Skills : Chiral metal complexes

11. Name : Deroo Stéphanie
    Profile : PhD student
    Skills : Ru-derivatized oligonucleotides, study by gel electrophoresis

12. Name : Herman Leslie

Profile : PhD student
Skills : Photophysics, laser flash photolysis of Ru complexes

13. Name : Vandeloise Robert
Profile : Technician
Skills : Electronics

14. Name : Lareppe Rita
Profile : Secretary
Skills : Secretariat

15. Name : Sergey Sergueev
Profile : Senior Scientist
Skills : Organic synthesis, supramolecular chemistry

16. Name : Eric Pouzet
Profile : Postdoc
Skills : X-ray diffraction

17. Name : Mievis Isabelle
Profile : Ph.D. Student
Skills : Polymer synthesis and characterization

18. Name : Olivier Roussel
Profile : Ph.D. Student
Skills : Liquid crystals

19. Name : Julie Leroy
Profile : Ph.D. Student
Skills : Organic synthesis and liquid crystals

20. Name : Delphine Didier
Profile : Ph.D. Student
Skills : Organic synthesis, supramolecular chemistry

21. Name : Jeremy Levin
Profile : Engineer
Skills : Organic synthesis, supramolecular chemistry

22. Name : Adrienne Remacle
Profile : Engineer
Skills : Organic synthesis, purification by HPLC

23. Name : Françoise Van Eycken
Profile : Secretary
Skills : Secretariat

II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

Photoreaction of $Ru[(HAT)_2phen]^{2+}$ with GMP and DNA : formation of new types of photoadducts.
R. Blasius, H. Nierengarten, M. Luhmer, J.F. Constant, E. Defrancq, P. Dumy, A. van Dorsselaer, C. Moucheron, A. Kirsch - De Mesmaeker
Chem. Eur. J., **11** (2005), 1507-1517.

Photoreduction of polyazaromatic Ru(II) complexes by biomolecules and possible applications.
B. Elias, A. Kirsch – De Mesmaeker.
Coordination Chem. Review. DOI : 10.1016/j.ccr.2005.11.011

Photophysical properties of Ruthenium(II) Polyazaaromatic Compounds : A theoretical Insight.
G.Pourtois, D.Beljonne, C.Moucheron, S.Schumm, A.Kirsch – De Mesmaeker, R.Lazzaroni, J.L.Brédas, *J.Am.Chem.Soc. 126(2),* 683-692, (2004)

A *nonanuclear mixed-bridging ligands* Ru(II) *dendrimer containing a trischelating core. Synthesis and* redox properties.
J. Leveque, C. Moucheron, A. Kirsch – De Mesmaeker.
F. Loiseau, S. Serroni, F. Puntoriero, S. Campagna.
H. Nierengarten, A. Van Dorsselaer.
J. Chem.Soc. Chem. Com. (RSC), (2004), 878-879.

$Ru(TAP)_3^{2+}$ photosensitized DNA cleavage studied by Atomic Force Microscopy and electrophoresis : a comparative study.
H. Uji-i, P. Foubert, F. De Schryver , S. De Feyter , E. Gicquel, A. Etoc, C. Moucheron, A. Kirsch – De Mesmaeker.
Chem.Eur.J., **12** (2006), 758-762

Tailoring Discotic Mesophases: Columnar Order Enforced with Hydrogen Bonds
R.I. Gearba, M. Lehmann, J. Levin, D.A. Ivanov, M.H.J.Koch, J. Baberá, M.G. Debije, J. Piris, Y.H. Geerts.
Adv. Mater. **15** (2003), 1614-1618.

Charge Transport Properties in Discotic Liquid Crystals: A Quantum-Chemical Insight into Structure-Property Relationships
V. Lemaur, D.A. da Silva Filho, V. Coropceanu, M. Lehmann, Y. Geerts, J. Piris, M.G. Debije, A.M. van de Craats, K. Senthilkumar, L.D.A Siebbeles, J.M. Warman, J.L. Brédas, and J. Cornil,
J. Am. Chem. Soc., **126** (2004), 3271-3279.

Electronic Delocalization in Discotic Liquid Crystals: A Joint Experimental and Theoretical Study
X. Crispin, J. Cornil, R. Friedlein, V. Lemaur, A. Crispin, G. Kestemont, M. Lehmann, M. Fahlman, R. Lazzaroni, Y. Geerts, G. Wendin, J.-L. Brédas, and W.R. Salaneck
J. Am. Chem. Soc., **126** (2004), 11889-11899.

High charge-carrier mobility in π-deficient discotic mesogens : design and structure-property relationship
Matthias Lehmann, Gaël Kestemont, Rafael Goméz Aspe, Claudine Buess-Herman, Michel J. H. Koch, Michael G. Debije, Jorge Piris, Matthijs P. de Haas, John M. Warman, Mark D. Watson, Vincent Lemaur, Jérôme Cornil, Yves Henri Geerts*, Raluca Gearba and Dimitri A. Ivanov
Chem. Eur. J., **11** (2005), 3349-3362.

Liquid Crystalline Metal-free Phthalocyanines Designed for Charge and Exciton Transport"
J. Tant, Y.H. Geerts, M. Lehmann, V. De Cupere, G. Zucchi, B. Wegge Laursen, T. Bjørnholm, V. Lemaur, V. Marcq, A. Burquel, E. Hennebicq, F. Gardebien, P. Viville, D. Beljonne, R. Lazzaroni, J.Cornil,
J. Phys. Chem. B, **43** (2005) 6166-6167.

II. 5. INTERNATIONAL CONTACTS IN THE PROJECT'S RESEARCH DOMAIN

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

COST D35, from January 2006 till December 2010, coordinator: Prof. J. Kelly, Trinity College Dublin. Network 0016/05, Profs A. De Mesmaeker and C. Moucheron, members of this network: "Networks of metal complexes and nanoparticles with electronic, magnetic and optoelectronic properties"

Laboratoire Européen Associé (LEA) between the French team (Prof. P. Dumy, Université J. Fourier, Grenoble) and the Belgian team, Profs A. De Mesmaeker and C. Moucheron, from January 2002 till December 2007. Renewable.

Current collaboration between the Belgian team with Prof's Piotr Piotrwiak at the Rutgers University (USA, N.Y.): femtosecond photochemistry of Ru complexes with telomeric DNA sequences.

Current collaboration with Dr. P Vicendo, Photochimie, Université P. Sabatier de Toulouse, France. Ru complexes and the protein SOD, flash photolysis.

Current collaboration (from previous U.E. network) with Prof. S. Campagna, Department of Chemistry, University of Messina, Italy.

Prof. Yves Geerts : Coordinator of the European research network "Self-Assembling and Self-Healing Electronic Devices Based on Mesomorphic Discotic Materials" (DISCEL), financed by the European Commission under the "sustainable growth priority" of the 5th framework program, 2001-2004

Prof. Yves Geerts : Coordinator of European integrated project "NAnoscale Integrated processing of self-organizing Multifunctional Organic Materials" (NAIMO), financed by the European Commission under the "nanotechnology priority" of the 6th framework program. 2004-2008

Prof. Yves Geerts : Member of the TECMAVER project : "Technologie et matériaux polymères innovants préservant l'environnement" financed by the Walloon Region of Belgium, 2000-2004.

Prof. Yves Geerts : Member of the SOLPLAST project : "Conception et élaboration de cellules solaires plastiques" financed by the Walloon Region of Belgium, 2003-2005.

Prof. Yves Geerts : Member of the Technology Attraction Pole SOLTEX: "Flexible, organic solar cells for power generating textiles" financed by the Federal Governement of Belgium, 2003-2005.

Prof. Yves Geerts : Member of a Concerted Research Action (ARC) : "Surface Orientation and Polymerisation of Discotic Molecules", French Community of Belgium, 2000-2005.

Prof. Yves Geerts : Member of the ETIQUEL project : "Elaboration et mise en oeuvre de molécules électroactives pour la réalisation de transistors organiques" financed by the Walloon Region of Belgium, 2004-2008.

Current collaboration with Prof. Klaus Müllen and Prof. Hans-Wolfgang Spiess, Max-Planck-Institute for Polymer Research, Mainz, Germany.

Current collaboration with Dr. Fabio Biscarini, CNR-Bologna, Italy

Current collaboration with Prof. Martin Nielsen, University of Copenhagen, Denmark.

Current collaboration with Prof. Jean-Luc Brédas, Georgia Institute of Technology, USA

Current collaboration with Prof. Sir Richard Friend, University of Cambridge, United Kingdom.

Current collaboration with Prof. William Salaneck and Prof. Xavier Crispin, Linköping University, Sweden

Current collaboration with Prof. Kotohiro Nomura, Nara Institute of Technology, Japan

Current collaboration with Prof. Jun-Il Jin, Korea Advanced Institute of Science and Technology, Korea

II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,...).

PAI 5/3, pole B, corresponding partner. Supramolecular Chemistry and supramolecular catalysis. From January 2002 till December 2006.

Action de Recherche Concertée 02/07-286, from September 2002 till August 2007 (A. De Mesmaeker, C. Moucheron and M. Luhmer) "Chimie Supramoléculaire Organométallique: conception et étude de nouveaux senseurs moléculaires photo-activables".

FRFC-FNRS (conv. 2.4554.02), "Biomolecular engineering: recognition of structures and particular bases sequences of DNA by metallic complexes, tethered or not to oligonucleotides". From January 2002 till December 2007.

WALEO 2, N° 0616289, "Carcinom", "Treatment of skin's carcinomes by original phototherapy" From 1 March 2006 till 28 February 2011.

European integrated project "NAnoscale Integrated processing of self-organizing Multifunctional Organic Materials" NAIMO, N° NMP4-CT-2004-500355, financed by the European Commission under the "nanotechnology priority" of the 6th framework program. 2004-2008

ETIQUEL, N° 04/1/5706 : "Elaboration et mise en oeuvre de molécules électroactives pour la réalisation de transistors organiques" financed by the Walloon Region of Belgium, 2004-2008.

II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: WP6, Biomolecules and biocatalysis (task 2)
2. Workpackage number and title: WP8, Supramolecular conjugated systems (task 1)
3. Workpackage number and title: WP9, Self-assembly at surfaces (tasks 1, 2)
4. Workpackage number and title:
5. Workpackage number and title:
6. Workpackage number and title:
7. Workpackage number and title:
8. Workpackage number and title:
9. Workpackage number and title:
10. Workpackage number and title:
11. Workpackage number and title:
12. Workpackage number and title:
13. Workpackage number and title:
14. Workpackage number and title:
15. Workpackage number and title:

II. 8. BUDGET (distribution per year) *

(in EURO)

	2007	2008	2009	2010	2011	Total
Personnel	29.104,00	61.206,00	59.796,00	64.070,00	25.824,00	**240.000,00**
Operating costs	14.856,00	37.182,00	37.182,00	34.502,00	17.230,38	**140.952,38**
Equipment	0,00	0,00	0,00	0,00	Not allowed	**0,00**
Overheads	2.198,00	4.919,40	4.848,90	4.928,60	2.152,72	**19.047,62**
Subcontracting	0,00	0,00	0,00	0,00	0,00	**0,00**
Subtotal	**46.158,00**	**103.307,40**	**101.826,90**	**103.500,60**	**45.207,10**	**400.000,00**
EU 1 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 2 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 3 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 4 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
Total	**46.158,00**	**103.307,40**	**101.826,90**	**103.500,60**	**45.207,10**	**400.000,00**

* This table should not be completed by the European partner as his/her budget is mentioned in the budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership

- Personnel: indexed gross remunerations; employer's social contributions; statutory insurance costs as well as any other compensation or allocation legally due in addition to the salary; the reimbursements for PhD and postdoctoral grant holders (exempt from tax and benefiting from social security). Personnel costs must account for minimum 60% of the total budget attributed to each partner of the network. The costs for the tax-free PhD grants and postdoctoral grants may not account for more than 60% of the total personnel costs.

- Operating costs: documentation; travel and accommodation; hosting of visiting foreign researchers use of computing facilities; software; telecommunications; maintenance and operation of equipment and, more generally, consumables;.

- Equipment: acquisition and installation of scientific and technical appliances and instruments, including IT equipment placed at the project's disposal. Equipment cannot be asked for during the last year of the programme.

- Overheads: general expenses of the institutions covering, on an inclusive basis, administrative, telephone, postal, maintenance, heating, electricity, rental, material depreciation and insurance costs. The total amount for this heading may not exceed 5% of total personnel and operating costs.

- Subcontracting: costs incurred by a third party in order to perform tasks or provide services necessitating specific scientific or technical skills outside the normal framework of the institution's activities. Each request for subcontracting needs a approval from the programme administrator.

II. 9. EQUIPMENT

Indicate the equipment (with an estimation of the cost) that will be purchased from the IAP-budget for the coming from four years (2007-2010) and justify.

No equipment will be purchased

II. 10. SUBCONTRACTING

To be completed only if subcontracting is foreseen.

Describe and justify the tasks and/or services that will be provided by a third party.

No subcontracting is foreseen

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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION II

Information on the partners

to be completed by each network partner including the EU-partner(s)

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the partner : Wouters Johan (P10) Institution : Facultés Universitaires Notre-Dame de la Paix

II. 1. PARTNER CONTACT DETAILS

PARTNER N° (consult the list in Section I of Annex I) * : P10

- Family Name : Wouters
- First Name : Johan
- Title (Prof., Dr., ...) : Prof.
- Institution : Facultés Universitaires Notre-Dame de la Paix
- Institution's abbreviation : FUNDP
- Faculty/Department :Department de Chimie
- Research Unit : Laboratoire de chimie biologique structurale
- Road/Street, n° : rue de Bruxelles, 61
- Post Code : 5000
- Town/City : Namur
- Country : Belgium
- Tel : 0032 81 72 45 50
- Tel secretariat : 0032 81 72 54 67
- Fax : 0032 81 72 45 30
- E-mail : johan.wouters@fundp.ac.be
- Website : http://www.fundp.ac.be/universite/personnes/page_view/NR000247/

* For Belgian partners : P1 to P13
For EU-partners : EU1 to EU4

II. 2. STAFF MEMBERS WORKING ON THE PROJECT (paid and not paid by the IAP-budget)

Staff	Number
Professor	2
Senior scientist	2
Post-doc	3
PhD student	2
Researcher without phD	/
Technician	1
Secretary	/
Other	/
TOTAL	**10**

II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, phD student, researcher without phD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name : CHAMPAGNE Benoît
   Profile : Research Director of the FNRS
   Skills : Theoretical chemist – elaboration and applications of quantum chemistry tools to predict and interpret electronic, optical, and vibrational properties of molecules, polymers, and solids.

2. Name : BOTEK Edith
   Profile : post-doc
   Skills : Theoretical chemist – Elaboration of quantum chemistry methods to describe the properties of molecules/aggregates under the influence of electric and magnetic fields.

3. Name : WOUTERS Johan
   Profile : Professor
   Skills : Structural biology (crystallography of small molecules and protein, molecular modelling), establishment of structure-function relationships

4. Name : VERCAUTEREN Daniel
   Profile : Professor
   Skills : Theoretical chemist – Application of molecular modelling techniques (molecular mechanics, molecular dynamics, ab initio methods) for determining structure-function relationships in catalysis and drug design.

5. Name : d'ANTUONO Philippe
   Profile : PhD Student
   Skills : Theoretical chemist – Modelling and interpreting NMR spectra of molecules and polymers

6. Name : GUILLAUME Maxime
   Profile : post-doc
   Skills : Theoretical chemist – Elaboration of quantum chemistry methods for simulating and interpreting the optical spectra of molecules and molecular crystals/aggregates.

7. Name : MICHAUX Catherine
   Profile : post-doc FNRS
   Skills : Molecular modelling, structures of proteins, establishment of structure-function relationships

8. Name : LEHERTE Laurence
   Profile : Senior Scientist
   Skills : Theoretical chemist – molecular mechanics and neural networks

9. Name : NORBERG Bernadette
   Profile : Technician
   Skills : Responsible for small molecule crystallography data collection and analysis

10. Name : STAELENS Nicolas
    Profile : PhD Student
    Skills : Theoretical Chemist – Molecular mechanics and molecular dynamics of supramolecular systems

II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

D. Truffier-Boutry, X.A. Gallez, S. Demoustier-Champagne, J. Devaux, M. Mestdagh, B. Champagne, and G. Leloup, « Identification of Free Radicals Trapped in Solid Methacrylated Resins », J. Polym. Sci. : Part A : Polym. Chem. 41, 1691-1699 (2003).

B. Champagne, J.M. André, E. Botek, E. Licandro, S. Maiorana, A. Bossi, K. Clays, and A. Persoons, « Theoretical Design of Substituted Tetrathia-[7]-Helicenes with Large Second-Order Nonlinear Optical Responses », ChemPhysChem 5, 1438-1442 (2004).

S. Masuo, T. Vosch, M. Cotlet, P. Tinnefeld, S. Habuchi, T.D.M. Bell, I. Oesterling, D. Beljonne, B. Champagne, K. Müllen, M. Sauer, J. Hofkens, and F.C. De Schryver, « Multichromophoric Dendrimers as Single Photon Sources : A Single-Molecule Study », J. Phys. Chem. B 108, 16686-16696 (2004).

V. Liégeois, O. Quinet, and B. Champagne, « Vibrational Raman Optical Activity as a Mean for Revealing the Helicity of Oligosilanes. A Quantum Chemical Investigation », J. Chem. Phys. 122, 214304 (8 pages) (2005).

Ph. D'Antuono, E. Botek, B. Champagne, J. Wieme, M.F. Reyniers, G.B. Marin, P.J. Adriaensens, and J. M. Gelan, « Density Functional Theory Investigation of the Stereochemistry Effects on 1H and 13C NMR Chemical Shifts of Poly(vinyl chloride) Oligomers », Chem. Phys. Lett. 411, 207-213 (2005).

E. Botek, M. Spassova, B. Champagne, I. Asselberghs, A. Persoons, and K. Clays, « Evaluation of hyper-Rayleigh Hyperpolarizabilities in Neutral and Charged Helicenes », Chem. Phys. Lett. 412, 274-279 (2005).

M. Guillaume and B. Champagne, « Modeling the Electric Field Third-Order Nonlinear Responses of an Infinite Aggregate of Hexatriene Chains using the Electrostatic Interaction Model », Phys. Chem. Chem. Phys. 7, 3284 - 3289 (2005).

B. Champagne and B. Kirtman, « Comment on Physical Limits on Electronic Nonlinear Molecular Susceptibilities, M.G. Kuzyk [Phys. Rev. Lett. 85, 001218 (2000)] », Phys. Rev. Lett., 95 109401 (2005).

M. Elanany, D.P. Vercauteren, M. Koyama, M. Kubo, P. Selvam, E. Broclawik, and. A. Miyamoto, « H-MOR: Density Functional Investigation for the Relative Strength of Bronsted Acid Sites and Dynamics Simulation of NH3 Protonation-Deprotonation », J. Mol. Catal. A, 243, 1-7 (2006).

M. Nakano, R. Kishi, N. Nakagawa, S. Ohta, H. Takahashi, S.I. Furukawa, T. Kubo, K. Kamada, K. Ohta, B. Champagne, E. Botek, S. Yamada, and K. Yamaguchi, « Second Hyperpolarizabilities ( ) of Bisimidazole and Bistriazole Benzenes : Diradical Character and Spin State Dependences », J. Phys. Chem. A 110, 4238-4243 (2006).

II. 5. INTERNATIONAL CONTACTS IN THE PROJECT'S RESEARCH DOMAIN

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

Bernie KIRTMAN (UCSB, Santa Barbara, USA)
Frédéric CASTET and Vincent RODRIGUEZ (LPCM, Bordeaux I, FRANCE)
Masayoshi NAKANO and kizashi YAMAGUCHI (Osaka, JAPAN)
Milena SPASSOVA, Pavletta DENKOVA, and Venelin ENCHEV (Bulgarian Academy of Sciences, Sofia, BULGARIA)
Kenneth RUUD (Tromsø, NORWAY)
Werner HUG (Fribourg, SWITZERLAND)
Magdalena PECUL and Joanna SADLEJ (Warsaw, POLAND)
Yuriko AOKI (Kyushu, JAPAN)
Weitao YANG (Durham, North Carolina, USA)
Yngve ÖHRN and So HIRATA (Gainesville, Florida, USA)
Raphaël SCHNEIDER and Alain WALCARIUS (Nancy, FRANCE)
David M. BISHOP (Ottawa, CANADA)
Jacopo TOMASI (Pisa, ITALY)
Stan van GISBERGEN and Evert-Jan BAERENDS (Amsterdam, THE NETHERLANDS)
Peer FISHER (Harvard, Massachussetts, USA)
Armand SOLDERA (Sherbrooke, CANADA)
Lilian JACQUAMET (Grenoble, FRANCE)
A. ZECCHINA and C. LAMBERTI (Torino, ITALY)
Alexander LARIN and D.N. TRUBNIKOV (Moscow, RUSSIA)
Claude LECOMTE and F. PORCHER (Nancy, FRANCE)
Joachim SAUER and Marek SIERKA (Berlin, GERMANY)

II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,...).

COST D26 Action « Integrative Computational Chemistry», working group D26/0010/02 « Experiment-oriented quantum chemistry tools for spectroscopies based on electric, magnetic, and vibrational phenomena» with H. Ågren (Stockholm), R. Cammi (Parma), W. Hug (Fribourg), J. Jokisaari (Oulu), P. Lazzeretti (Modena), A. Peremans (FUNDP), K. Ruud (Tromsø), J. Tomasi (Pisa), and J. Vaara (Helsinki). 2002 –2007.

CGRI-CNRS-FNRS Project with the Laboratoire de Physico-Chimie Moléculaire de l'Université de Bordeaux I (France) on « Etude des propriétés optiques et vibrationelles, lineaires et non-lineaires de structures hélicoïdales », 2005 – 2006.

CGRI-DRI Project with le Centre d'Etudes des Matériaux Optiques et Photonique of Sherbrooke Université (Québec, Canada) on « Conception de nouveaux matériaux optiques performants pour l'optique non-linéaire », 2005 – 2007.

FNRS-FRFC Project "Etude par simulations numériques des mécanismes d'autoassemblage moléculaire pour la synthèse de matériaux aux propriétés physiques hors-normes et pour la conception de dispositifs électroniques et photoniques, linéaires et nonlinéaires », Convention n° 2.4578.02, 2002 – 2006.

CGRI-CNRS-FNRS Project with the Theoretical Chemistry Lab of the Bulgarian Academy of Sciences (Sofia, Bulgaria) on « Étude théorique d'assemblages supramoléculaires organiques pour la photonique et l'électronique », 2005 –2006.

II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: WP1, Nanodots and photonic crystals (tasks 1, 3, 4)
2. Workpackage number and title: WP2, Organic nanostructures (tasks 1, 2)
3. Workpackage number and title: WP3, Porous frameworks (task 3)
4. Workpackage number and title: WP4, Hybrid materials (task 2)
5. Workpackage number and title: WP5, (Bio)membranes (tasks 1, 3, 5)
6. Workpackage number and title: WP6, Biomolecules and biocatalysis (task 1)
7. Workpackage number and title: WP8, Supramolecular conjugated systems (tasks 1)
8. Workpackage number and title: WP9, Self-assembly at surfaces (tasks 1, 2)
9. Workpackage number and title:
10. Workpackage number and title:
11. Workpackage number and title:
12. Workpackage number and title:
13. Workpackage number and title:
14. Workpackage number and title:
15. Workpackage number and title:

II. 8. BUDGET (distribution per year) *

(in EURO)

	2007	2008	2009	2010	2011	Total
Personnel	62.000,00	64.000,00	66.000,00	68.000,00	70.000,00	**330.000,00**
Operating costs	5.500,00	5.700,00	5.900,00	6.100,00	6.300,00	**29.500,00**
Equipment	5.300,00	5.500,00	5.700,00	6.025,00	Not allowed	**22.525,00**
Overheads	3.375,00	3.485,00	3.595,00	3.705,00	3.815,00	**17.975,00**
Subcontracting	0,00	0,00	0,00	0,00	0,00	**0,00**
Subtotal	**76.175,00**	**78.685,00**	**81.195,00**	**83.830,00**	**80.115,00**	**400.000,00**
EU 1 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 2 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 3 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 4 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
Total	**76.175,00**	**78.685,00**	**81.195,00**	**83.830,00**	**80.115,00**	**400.000,00**

* This table should not be completed by the European partner as his/her budget is mentioned in the budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership

- Personnel: indexed gross remunerations; employer's social contributions; statutory insurance costs as well as any other compensation or allocation legally due in addition to the salary; the reimbursements for PhD and postdoctoral grant holders (exempt from tax and benefiting from social security). Personnel costs must account for minimum 60% of the total budget attributed to each partner of the network. The costs for the tax-free PhD grants and postdoctoral grants may not account for more than 60% of the total personnel costs.

- Operating costs: documentation; travel and accommodation; hosting of visiting foreign researchers use of computing facilities; software; telecommunications; maintenance and operation of equipment and, more generally, consumables;.

- Equipment: acquisition and installation of scientific and technical appliances and instruments, including IT equipment placed at the project's disposal. Equipment cannot be asked for during the last year of the programme.

- Overheads: general expenses of the institutions covering, on an inclusive basis, administrative, telephone, postal, maintenance, heating, electricity, rental, material depreciation and insurance costs. The total amount for this heading may not exceed 5% of total personnel and operating costs.

- Subcontracting: costs incurred by a third party in order to perform tasks or provide services necessitating specific scientific or technical skills outside the normal framework of the institution's activities. Each request for subcontracting needs a approval from the programme administrator.

II. 9. EQUIPMENT

Indicate the equipment (with an estimation of the cost) that will be purchased from the IAP-budget for the coming from four years (2007-2010) and justify.

It mostly consists of computers, for both production of data and their analysis. It is therefore a sketch of what can be acquired in the coming years since the computer business is changing very fast.

1) hardware to add to the iSCF computing centre [11 800 Euros]

Sun Fire X4100 Dual Opteron 254 @ 2.8 GHz, 8Gb RAM, 2 disks of 73GB 10kRPM SAS.
estimated cost: 5000 Euros. (x 2).

ProcessorIntel Pentium 4 630 @ 3GHz, Intel SE7230HN1-E, 1GB RAM, hard disk 80GB SATA 7200RPM, RAID5 Adaptec 2410SA, 4 disks SATA 250GB 7200RPM.
estimated cost: 1800 Euros.

2) computers for analyzing the data [10 725 Euros]

MacBookPro, 2Gb SDRAM, 160 GB ATA Drive
estimated cost: 3200 Euros

MacPro, 2.66 GHz, 2Gb RAM, 250 Gb Serial ATA hard disk
estimated cost: 3800 Euros

PRIMINFO'5 1Gb DDR, 160Gb, flat screen
estimated cost: 925 Euros

PRIMINFO ASUS, portable, 1Gb DDR, 160 Gb
estimated cost: 1400 Euros (x 2)

These computers are necessary to achieve our different "theoretical chemistry" tasks in the IAP program, both from the high-performance computing side and from the data treatment side. Note that the project will also benefit from the access to the iSCF computing centre, encompassing currently 80 V60x biprocessors, 19 V20z biprocessors, and 2 V880 octoprocessors.

II. 10. SUBCONTRACTING

To be completed only if subcontracting is foreseen.

Describe and justify the tasks and/or services that will be provided by a third party.

No subcontracting is foreseen

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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION II

Information on the partners

to be completed by each network partner including the EU-partner(s)

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the partner : Vanderzande Dirk (P11) Institution : Universiteit Hasselt

II. 1. PARTNER CONTACT DETAILS

PARTNER N° (consult the list in Section I of Annex I) * : P11

- Family Name : Vanderzande
- First Name : Dirk
- Title (Prof., Dr., ...) : Prof
- Institution : Universiteit Hasselt
- Institution's abbreviation : UHasselt
- Faculty/Department : Sciences/SBG
- Research Unit : Institute for Material Research (IMO)
- Road/Street, n° : Agoralaan, Bld D
- Post Code : 3590
- Town/City : Hasselt
- Country : Belgium
- Tel : 0032 11 26 83 21
- Tel secretariat : 0032 11 26 83 64
- Fax : 0032 11 26 83 01
- E-mail : dirk.vanderzande@uhasselt.be
- Website : http://www.uhasselt.be

* For Belgian partners : P1 to P13
For EU-partners : EU1 to EU4

II. 2. STAFF MEMBERS WORKING ON THE PROJECT (paid and not paid by the IAP-budget)

Staff	*Number*
Professor	4
Senior scientist	2
Post-doc	2
PhD student	12
Researcher without phD	1
Technician	3
Secretary	1
Other	
TOTAL	**25**

II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, phD student, researcher without phD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name : Vanderzande Dirk
   Profile : *Professor*
   Skills : Organic synthesis, polymer chemistry specifically on conjugated polymers, developer of new synthetic routes toward materials with special electronic or optical properties.

2. Name : Gelan Jan
   Profile : Professor
   Skills : NMR-Spectroscopy, study of multiphase behaviour of polymeric systems, MRI of materials and biological systems

3. Name : Ameloot Marcel
   Profile : *Professor*
   Skills : Microfluorimetric techniques in biological systems, time-resolved fluorescence, fluorescence anisotropy, global analysis of multidimensional fluorescence decay data surfaces, identifiability of photophysical models in time-resolved fluorescence

4. Name : Thomas Cleij
   Profile : Professor
   Skills : Electrochemistry of conjugated systems, in situ spectro-electrochemical characterisation of conjugated polymers

5. Name : Adriaensens Peter
   Profile : Senior scientist
   Skills : NMR-Spectroscopy, study of multiphase behaviour of polymeric systems, MRI of materials and biological systems

6. Name : Martin vandeVen
   Profile : Senior scientist
   Skills : steady-state and time-resolved fluorescence and fluorescence anisotropy spectroscopy, global and image analysis of multidimensional fluorescence decay data surfaces, image correlation analysis, identifiability of photophysical models in time-resolved fluorescence

7. Name : Wibren Oosterbaan
   Profile : Postdoc
   Skills : Synthesis of semi-conductive conjugated polymers, use of reductive polymerization techniques for synthesis of said polymers

8. Name : Kristof Colladet
   Profile : Postdoc
   Skills : Synthesis of multifunctional semi-conductive conjugated polymers

9. Name . Hanne Diliën
   Profile : PhD-student
   Skills : Synthesis of multifunctional conjugated polymers

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10. Name : Arne Palmaerts
    Profile : PhD-student
    Skills : Synthesis of conjugated polymers containing substructures of C60

    Name : Joke Vandenbergh
    Profile : PhD-student
    Skills : Synthesis of low band gap polymers

    Name : Raoul Mens
    Profile : PhD-student
    Skills : NMR spectroscopy of polymer blends

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II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

Arne Palmaerts, Michael van Haren, Laurence Lutsen, Thomas J. Cleij and Dirk Vanderzande, "Synthesis and Properties of Poly(*p*-fluoranthene vinylene): A Novel Conjugated Polymer with Nonalternant Repeating Units", Macromolecules (2006), *39*, 2438-2440.

Kesters E, Vanderzande D, Lutsen L, Penxten H, Carleer R, "Study of the thermal elimination and degradation processes of n-alkylsulfinyl-PPV and -OC1C10-PPV precursor polymers with in situ spectroscopic techniques", Macromolecules (2005), 38, 1141-1147.

Henckens A, Colladet K, Fourier S, Cleij TJ, Lutsen L, Gelan J, Vanderzande D, "Synthesis of 3,4-diphenyl-substituted poly(thienylene vinylene) low-band-gap polymers via the dithiocarbamate route", Macromolecules (2005), 38, 19-26.

Riedel, I; Parisi, J; Dyakonov, V; Lutsen, L; Vanderzande, D; Hummelen, JC; "Effect of temperature and illumination on the electrical characteristics of polymer-fullerene bulk-heterojunction solar cells", Advanced Functional Materials; (2004), 14, 38-44.

M. A. Acasandrei, R. E. Dale, M. vandeVen, M. Ameloot, "Two-dimensional Förster resonance energy transfer (2-D FRET) and the membrane raft hypothesis.", Chemical Physics Letters (2006) 419, 469-473.

Boens N, Novikov E, Szubiakowski J, Ameloot M, "Identifiability of Models for Intramolecular Two-State Excited-State Processes with Added Quencher and Coupled Species-Dependent Rotational Diffusion", J Phys Chem A Mol Spectrosc Kinet Environ Gen Theory.; (2005) 109(51), 11655-11664.

d'Antuono P, Botek E, Champagne B, Wieme J, Marin G, Reyniers M P, Adriaensens P, Gelan J, "Density Functional Theory investigation of the stereochemistry effects on ^{1}H and ^{13}C NMR chemical shifts of poly(vinyl chloride) oligomers", Chemical Physics Letters, (2005) 411, 207-213.

Roex H, Adriaensens P, Vanderzande D, Gelan J, "Identification and quantification of polymerization defects in ^{13}C-labeled sulphinyl and Gilch OC_1C_{10}-PPV by NMR spectroscopy", Macromolecules, (2003) 36, 5613-5622.

Kotzev A, Laschewsky A, Adriaensens P and Gelan J, "Micellar polymers with hydrocarbon and fluorocarbon hydrophobic chains. A strategy to multicompartment micelles", Macromolecules, (2002) 35,1091.

Adriaensens P, Storme L, Carleer R, Gelan J, Du Prez F E, "Comparative morphological study of poly(dioxolane)/poly(methyl methacrylate) segmented networks and blends by ^{13}C solid state NMR and thermal analysis", Macromolecules, (2002) 35, 3965.

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II. 5. INTERNATIONAL CONTACTS IN THE PROJECT'S RESEARCH DOMAIN

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

ESF/PESC Research Networking Programme New generation of organic based photovoltaic devices (ORGANISOLAR), Duration 2006-2010

Prof. Dr. R. Janssen; Molecular Materials and Nanosystems, Laboratory of Macromolecular and Organic Chemistry, Eindhoven University of Technology, Eindhoven, The Netherlands

Prof. Dr. U. Scherf, Bergische Universität Wuppertal, Makromolekulare Chemie, Gaussstrasse 20, Bld. U, 42119 Wuppertal, Germany

Prof. Dr. N. Martin, Departamento de Quimica Organica, Facultad de Quimica, Universidad Complutense, Madrid. Spain

Prof. Dr. V. Dyakonov, Experimental Physics VI, Faculty of Physics and Astronomy, University of Würzburg, Würzburg, Germany

Prof. Dr. P. Blom, Physics of Organic Semiconductors, Materials Science Centre, University of Groningen, Groningen, The Netherlands

Prof. Dr. D. Bradley, Head of Experimental Solid State Physics Group, Deputy Director of the Centre for Electronic Materials and Devices, The Blackett Laboratory, Imperial College London, London, UK

Prof. Dr. T. Torres; Department of Organic Chemistry, Universidad Autonoma de Madrid, Madrid. Spain

Prof. Dr. A. Holmes, ARC Federation and VESKI Fellow, Bio21 Institute and CSIRO Molecular and Health Technologies, University of Melbourne, Australia

Dr. R. E. Dale, King's College London, School of Biomedical and Health Sciences, Randall Division for Cell and Molecular Biophysics, 3rd Floor, New Hunt's House, Guy's Hospital Campus, London SE1 1UL, United Kingdom

Prof. Dr. E. Gratton, The Henry Samueli School of Engineering, Dept. of Biomedical Engineering , Natural Sciences Bldg II, University of California at Irvine, Irvine, CA 92697-2715, U.S.A.

II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,...).

SBO *Nanosolar*: "*Nano-gestructureerde hybride materiaalsystemen en integratie in innovatieve* fotovoltaische concepten"; okt.2003-okt.2007, Flemisch Government (IWT)

IUAP-V-project "Supramolecular Chemistry and supramolecular catalysis"; 2002 – 2006, Federal Government (DWTC).

EU BIOPOLTRONIX European Project Marie-Curie Host fellowships for the Transfer of Knowledge n° MTKD-CT-2004-509233_FP6; "Development and Characterisation of new Semi-Conducting Polymers Soluble in Environmentally Friendly Solvent for Self-assembled Nanostructured and Application in Advanced Electronic devices, Chemical and Biological Sensors", 2004-2006, European Union

EU MOLYCELL European Project n°SES6-CT-2003-502783_FP6; "Molecular Orientation, Low Band Gap and new Hydrid device Concepts for the Improvement of Flexible Organic Solar Cells", 2004-2006, European Union

FWO project "Studie van moleculaire dynamica en nanomorfologie van elektro-actieve polymeren door middel van vaste stof NMR relaxometrie"; 2003-2006, Flemisch Government (FWO)

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II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: WP1, Nanodots and photonic crystals (tasks 3, 5)
2. Workpackage number and title: WP2, Organic nanostructures (tasks 1 , 2)
3. Workpackage number and title: WP3, Porous Frameworks (task 3)
4. Workpackage number and title: WP5, (Bio)membranes (tasks 1, 2, 4)
5. Workpackage number and title: WP6, Biomolecules and biocatalysis (task 1)
6. Workpackage number and title: WP8, Supramolecular conjugated systems (task 1)
7. Workpackage number and title: WP9, Self-assembly at surfaces (task 2)
8. Workpackage number and title:
9. Workpackage number and title:
10. Workpackage number and title:
11. Workpackage number and title:
12. Workpackage number and title:
13. Workpackage number and title:
14. Workpackage number and title:
15. Workpackage number and title:

Deleted: ; Task 1.3 Peptide stabilized fluorescent silver/gold atomic clusters as probes for single molecule spectroscopy and task 1.5 Semiconductor and metal clusters in OLEDS and solar cells.

Deleted: Task 2.1: Multifunctional copolymers and task 2.2: Organic nanodots

Deleted: Task 3.3: Mapping and modelling of diffusion and catalytic activity in zeolites and mesoporous molecular sieves

Deleted: Task 5.1: Organization of lipid membranes: characterization of structure and dynamics of "rafts" ; task 5.2: Dynamics of bacterial biofilms and structure function analysis of bacterial surfaces containing lipoteichoic acids and task 5.4: Biomimetic polymer membranes

Deleted: Task 6.1: Autofluorescent and photoswitchable proteins and use as probes

II. 8. BUDGET *(distribution per year)* *

(in EURO)

	2007	2008	2009	2010	2011	Total
Personnel	50.000,00	123.000,00	30.000,00	74.000,00	44.000,00	**321.000,00**
Operating costs	10.000,00	10.000,00	10.000,00	10.000,00	10.000,00	**50.000,00**
Equipment	10.450,00	0,00	0,00	0,00	Not allowed	**10.450,00**
Overheads	3.000,00	6.650,00	2.000,00	4.200,00	2.700,00	**18.550,00**
Subcontracting	0,00	0,00	0,00	0,00	0,00	**0,00**
Subtotal	**73.450,00**	**139.650,00**	**42.000,00**	**88.200,00**	**56.700,00**	**400.000,00**
EU 1 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 2 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 3 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 4 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
Total	**73.450,00**	**139.650,00**	**42.000,00**	**88.200,00**	**56.700,00**	**400.000,00**

* *This table should not be completed by the European partner as his/her budget is mentioned in the* budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership

- Personnel: indexed gross remunerations; employer's social contributions, statutory insurance costs as well as any other compensation or allocation legally due in addition to the salary; the reimbursements for PhD and postdoctoral grant holders (exempt from tax and benefiting from social security). Personnel costs must account for minimum 60% of the total budget attributed to each partner of the network. The costs for the tax-free PhD grants and postdoctoral grants may not account for more than 60% of the total personnel costs.

- Operating costs: documentation; travel and accommodation; hosting of visiting foreign researchers use of computing facilities; software; telecommunications; maintenance and operation of equipment and, more generally, consumables;.

- Equipment: *acquisition and installation of scientific and technical appliances and instruments*, including IT equipment placed at the project's disposal. Equipment cannot be asked for during the last year of the programme.

- Overheads: general expenses of the institutions covering, on an inclusive basis, administrative, telephone, postal, maintenance, heating, electricity, rental, material depreciation and insurance costs. The total amount for this heading may not exceed 5% of total personnel and operating costs.

- Subcontracting: costs incurred by a third party in order to perform tasks or provide services necessitating specific scientific or technical skills outside the normal framework of the institution's activities. Each request for subcontracting needs a approval from the programme administrator.

II. 9. EQUIPMENT

Indicate the equipment (with an estimation of the cost) that will be purchased from the IAP-budget for the coming from four years (2007-2010) and justify.

10 450 Euro available budget on IUAP· DAWN HELEOS Peltier heated cooled option (15.000€) Peltier-driven temperature regulation for the read head that permits control of the cell from approximately -15°C to +80°C (±0.1°C). The budget will be added to the equipment budget available from the UHasselt as basic financement of the research group.
The polymeric materials synthesized in the project will be analyzed with Gel Permeation Chromatography with advanced detectors. To improve the quality of the measurements a heating element is needed to be able to analyse the samples at constant temperature

II. 10. SUBCONTRACTING

To be completed only if subcontracting is foreseen.

Describe and justify the tasks and/or services that will be provided by a third party.

No subcontracting is foreseen

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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION II

Information on the partners

to be completed by each network partner including the EU-partner(s)

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the partner : Vanderleyden Jozef (P12) Institution : Katholieke Universiteit Leuven

II. 1. PARTNER CONTACT DETAILS

PARTNER N° (consult the list in Section I of Annex I) * : P12

- Family Name : Vanderleyden
- First Name : Jozef
- Title (Prof., Dr., ...) : Prof.
- Institution : Katholieke Universiteit Leuven
- Institution's abbreviation : K.U.Leuven
- Faculty/Department : Department of Microbial and Molecular Systems
- Research Unit : Centre of Microbial and Plant Genetics
- Road/Street, n° : Kasteelpark Arenberg 20
- Post Code : 3001
- Town/City : Heverlee
- Country : Belgium
- Tel : 0032 16 32 96 79
- Tel secretariat : 0032 16 32 16 31
- Fax : 0032 16 32 19 63
- E-mail : jozef.vanderleyden@biw.kuleuven.be
- *Website : http://www.cmpg.be*

* For Belgian partners : P1 to P13
For EU-partners : EU1 to EU4

II. 2. STAFF MEMBERS WORKING ON THE PROJECT (paid and not paid by the IAP-budget)

Staff	Number
Professor	5
Senior scientist	4
Post-doc	7
PhD student	20
Researcher without phD	/
Technician	14
Secretary	1
Other	/
TOTAL	**51**

II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, phD student, researcher without phD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name : Jozef Vanderleyden
   Profile : Professor
   Skills : Signalling in bacterial populations. Use of green fluorescent protein as a tool to monitor gene expression, protein trafficking and cellular localization of proteins. Adhesion patterns of proteins and cells to surfaces.

2. Name : Ann Vande Broek
   Profile : Senior scientist
   Skills : Site directed mutagenesis. Expression of oligopeptide libraries in membrane proteins (e.g outer membrane protein, flagellin) of bacteria.

3. Name : Sigrid. De Keersmaecker
   Profile : Postdoc
   Skills : Molecular microbiology of gastro-intestinal bacteria. Use of gene fusions with green fluorescent protein in combination with Fluorescence Assisted Cell Sorting (FACS) to monitor differential gene expression in microbial populations. Study of bacterial determinants in biofilm formation and biofouling.

4. Name : Ellen Somers
   Profile : Postdoc
   Skills : Molecular microbiology of plant root colonizing bacteria. Developing methodologies for biofilm formation and signalling in biofilms.

5. Name : Joost Janssens
   Profile : Ph.D student
   Skills : Chemical synthesis of molecules used by bacteria for quorum sensing, and determing the Structure Activity Relation (SAR) of these molecules using various bioscreens.

6. Name : Stijn Spaepen
   Profile : Ph.D. student
   Skills : Biochemistry of decarboxylases with carbo-ligase activity: structural, kinetic and mutational analysis.

7. Name : Monica Perea Velez
   Profile : Ph.D student
   Skills : Surface analysis of lactic acid bacteria, using various microscopic techniques. Structural analysis of lipoteichoic acids. Coculture of bacteria and human intestinal cell lines.

8. Name : Sarah Lebeer
   Profile : Ph.D. student
   Skills : Signaling in lactic acid bacteria. Immunology. Use of *in vitro* and *in vitro* models for testing immunomodulatory properties of lactic acid bacteria.

9. Name : Hans Steenackers
   Profile : Ph.D. student

Skills : Synthesis and screening for biological activity of halogenated furanones. Molecular docking.

10. Name : Jos Desair
    Profile : Technician
    Skills : High performance liquid chromatography for purification of proteins and cellular metabolites.

11. Name : Geert Schoofs
    Profile : Technician
    Skills : Various separation techniques (chromatography, electrophoresis) for cellular proteins. Analysis of metabolic pathways in bacteria using metabolomics and proteomics.

12. Name : Tine Verhoeven
    Profile : Technician
    Skills : Culture of human intestinal cell lines. Molecular genetic analysis of *Escherichia coli*, *Salmonella typhimurium*, and *Lactobacillus* spp.

13. Name : David De Coster
    Profile : Technician
    Skills : Heterologous overexpression of proteins in various bacterial expression systems. Analysis of small RNAs in catalysis and gene regulation.

14. Name : Anita Vermassen
    Profile : Secretary
    Skills : Financial management of projects using SAP. Editing project proposals and scientific reports

II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

Vande Broek,A., Lambrecht,M., and Vanderleyden,J. (1999) Auxins upregulate expression of the indole-3-pyruvate decarboxylase gene from *Azospirillum brasilense*. *J.Bacteriol.* **181** 1338-1342.

Cotlet,M., Hofkens,J., Habuchi,S., Dirix,G., Van Guyse,M., Michiels,J., Vanderleyden,J., and De Schryver,F. (2001) Identification of different emitting species in the red fluorescent protein DsRed by means of ensemble and single-molecule spectroscopy. *Proc.Nat.Acad.Sci.USA* **98** 14398-14403.

Lerouge,I. and Vanderleyden,J. (2002) O-antigen structural variation: mechanisms and possible roles in animal/plant-microbe interactions. *FEMS Microbiol.Rev.* **26** (1), 17-47.

Habuchi,S., Cotlet,M., Gronheid,R., Dirix,G., Michiels,J., Vanderleyden,J., De Schryver,F.C., and Hofkens,J. (2003) Single-molecule surface enhanced resonance raman spectroscopy of the enhanced green fluorescent protein. *J.Am.Chem.Soc.* **125** (28), 8446-8447.

Daniels,R., Vanderleyden,J., and Michiels,J. (2004) Quorum sensing and swarming migration in bacteria. *FEMS Microbiol.Rev.* **28** 261-289.

De Keersmaecker,S., Varszegi,C., van Boxel,N., Habel,L., Metzger,K., Daniels,R., Marchal,K., De Vos,D., and Vanderleyden,J. (2005) Chemical synthesis of (*S*)-4,5-Dihydroxy-2,3-pentanedione, a bacterial signal molecule precursor, and validation of its activity in *Salmonella typhimurium*. *J.Biol.Chem.* **280** (20), 19563-19568.

Dombrecht,B., Heusdens,C., Beullens,S., Verreth,C., Mulkers,E., Proost,P., Vanderleyden,J., and Michiels,J. (2005) Defense of *Rhizobium etli* bacteroids against oxidative stress requires a complexly regulated atypical 2-Cys peroxiredoxin. *Mol.Microbiol.* **55** (4), 1207-1221.

Habuchi,S., Cotlet,M., Gensch,T., Bednarz,T., Haber-Pohlmeier,S., Rozenski,J., Dirix,G., Michiels,J., Vanderleyden,J., Heberle,J., De Schryver,F.C., and Hofkens,J. (2005) Evidence for the isomerization and decarboxylation in the photoconversion of the red fluorescent protein DsRed. *J.Am.Chem.Soc.* **127** 8977-8984.

Rediers,H., Rainey,P.B., Vanderleyden,J., and De Mot,R. (2005) Unraveling the secret lives of bacteria: use of in vivo expression technology and differential fluorescence induction promoter traps as tools for exploring niche-specific gene expression. *Microbiol.Mol.Biol.Rev.* **69** (2), 217-261.

Verhaert,J., Vanderleyden,J., and Michiels,J. (2005) Bacterial endocytic systems in plants and animals: Ca^{2+} as a common theme? *Crit.Rev.Plant Sci.* **24** 283-308.

II. 5. INTERNATIONAL CONTACTS IN THE PROJECT'S RESEARCH DOMAIN

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

A. Internationale contacten
A.1. Prof. Guido Bloemberg, Institute of Biology, Leiden University, the Netherlands

A.2. Dr. Martina Pohl, Institute for Molecular Enzyme Technology, Forschungszentrum Jülich, Germany

A.3. Prof. Michael McClelland, Sidney Kimmel Cancer Research Institute, San Diego, USA

A.4. Prof. A. Geyer, Philipps-Universität Marburg, Fachbereich Organische Chemie, Marburg/Lahn, Germany

B. Internationale netwerken
B.1. COST Action 631: Modelling Plant Soil Interactions in the Rhizosphere Environment

B.2. COST Action 856: Denitrification - Systems Biology Approach

II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,...).

Supramolecular Chemistry and Supramolecular Catalysis (IUAP P5/03). 01.01.2002 – 31.12.2006. Belgian Science Policy

Signals and signal transduction pathways in microbe-plant interactions (GOA/2003/09). 1.10.2002 – 30.09.2007. Bijzonder Onderzoeksfonds K.U.Leuven

Molecular and computational biology of quorum signaling in bacterial pathogens: Salmonella's Quorum Sensing to Attach Disease (SQUAD). (GBOU-IWT Project 020160). 1.01.2003 – 31.03.2007. IWT

Regulation of bacterial auxin biosynthesis (G.0085.03). 1.1.2003 – 31.12.2006. FWO

PROMETA: Interfaculty Center for proteomics and metabolomics. 01.10.2005 – 30.09.2010. Fonds Minister Van Mechelen Zware Apparatuur en matching fund K.U.Leuven Zware Apparatuur

Synthesis and biological screening of halogenated furanones and analogues to interfere with bacterial cell-cell communication. SB/0441310. IWT specialisatiebeurs

Arabinoxylan oligosaccharides with impact on man and animal (IMPAXOS) (IDO/03/005). Financieringsbron is Bijzonder Onderzoeksfonds K.U.Leuven

II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: WP1, Nanodots and photonic crystals (task 3)
2. Workpackage number and title: WP5, (Bio)membranes (tasks 2, 3, 4)
3. Workpackage number and title: WP6, Biomolecules and Biocatalysis (tasks 1, 3, 5)
4. Workpackage number and title: WP7, Functional coatings (task 3)
5. Workpackage number and title: WP9, Self-assembly at surfaces (task 2)
6. Workpackage number and title:
7. Workpackage number and title:
8. Workpackage number and title:
9. Workpackage number and title:
10. Workpackage number and title:
11. Workpackage number and title:
12. Workpackage number and title:
13. Workpackage number and title:
14. Workpackage number and title:
15. Workpackage number and title:

II. 8. BUDGET (distribution per year) *

(in EURO)

	2007	2008	2009	2010	2011	Total
Personnel	58.700,00	51.000,00	53.200,00	60.500,00	62.000,00	**285.400,00**
Operating costs	8.000,00	14.000,00	15.000,00	10.000,00	13.980,95	**60.980,95**
Equipment	13.300,00	10.000,00	8.000,00	5.000,00	Not allowed	**36.300,00**
Overheads	3.335,00	3.250,00	3.410,00	3.525,00	3.799,05	**17.319,05**
Subcontracting	0,00	0,00	0,00	0,00	0,00	**0,00**
Subtotal	**83.335,00**	**78.250,00**	**79.610,00**	**79.025,00**	**79.780,00**	**400.000,00**
EU 1 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
Feijen	10.000,00	10.000,00	10.000,00	10.000,00	10.000,00	**50.000,00**
EU 3 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 4 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
Total	**93.335,00**	**88.250,00**	**89.610,00**	**89.025,00**	**89.780,00**	**450.000,00**

* *This table should not be completed by the European partner as his/her budget is mentioned in the* budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership

- Personnel: indexed gross remunerations; employer's social contributions; statutory insurance costs as well as any other compensation or allocation legally due in addition to the salary; the reimbursements for PhD and postdoctoral grant holders (exempt from tax and benefiting from social security). Personnel costs must account for minimum 60% of the total budget attributed to each partner of the network. The costs for the tax-free PhD grants and postdoctoral grants may not account for more than 60% of the total personnel costs.

- Operating costs: documentation; travel and accommodation; hosting of visiting foreign researchers use of computing facilities; software; telecommunications; maintenance and operation of equipment and, more generally, consumables;.

- Equipment: acquisition and installation of scientific and technical appliances and instruments, including IT equipment placed at the project's disposal. Equipment cannot be asked for during the last year of the programme.

- Overheads: general expenses of the institutions covering, on an inclusive basis, administrative, telephone, postal, maintenance, heating, electricity, rental, material depreciation and insurance costs. The total amount for this heading may not exceed 5% of total personnel and operating costs.

- Subcontracting: costs incurred by a third party in order to perform tasks or provide services necessitating specific scientific or technical skills outside the normal framework of the institution's activities. Each request for subcontracting needs a approval from the programme administrator.

II. 9. EQUIPMENT

Indicate the equipment (with an estimation of the cost) that will be purchased from the IAP-budget for the coming from four years (2007-2010) and justify.

2007
RI detector for HPLC detector: 8.500 Euro
HPLC columns (separating macro-molecules): 4.800 Euro

2008
Gradient PCR apparatus: 10.000 Euro

2009
Nano Photometer: 8.000 Euro

2010
HPLC columns (separating macro-molecules): 5.000 Euro

II. 10. SUBCONTRACTING

To be completed only if subcontracting is foreseen.

Describe and justify the tasks and/or services that will be provided by a third party.

No subcontracting is foreseen.

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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION II

Information on the partners

to be completed by each network partner including the EU-partner(s)

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the partner : Waroquier Michel (P13) Institution : Universiteit Gent

II. 1. PARTNER CONTACT DETAILS

PARTNER N° (consult the list in Section I of Annex I) * : P13

- Family Name : Waroquier
- First Name : Michel
- Title (Prof., Dr., ...) : Prof.
- Institution : Universiteit Gent
- Institution's abbreviation : UGent
- Faculty/Department : Sciences
- Research Unit : Center Molecular Modeling (CMM)
- Road/Street, n° : Proeftuinstraat, 86
- Post Code : 9000
- Town/City : Gent
- Country : Belgium
- Tel : 0032 9 264 65 59
- Tel secretariat : 0032 9 264 65 28
- Fax : 0032 9 264 66 97
- E-mail : michel.waroquier@UGent.be
- Website : http://molmod.ugent.be

* For Belgian partners : P1 to P13
For EU-partners : EU1 to EU4

II. 2. STAFF MEMBERS WORKING ON THE PROJECT (paid and not paid by the IAP-budget)

Staff	Number
Professor	2
Senior scientist	/
Post-doc	2
PhD student	10
Researcher without phD	/
Technician	/
Secretary	/
Other	/
TOTAL	**14**

II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, phD student, researcher without phD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name : Waroquier Michel
   Profile : *Professor and head CMM*
   Skills : Molecular Modeling – Model development -

2. Name : Van Speybroeck Veronique
   Profile : Postdoc FWO
   Skills : Computational Molecular Modeling – Heterogeneous Catalysis – Design New Materials – Free Radical Polymerizatin Reactions – Heterocyclic Chemistry – *Thermal Cracking of hydrocarbons – Cokes formation - EPR of paramagnetic defects* in periodic lattices – QM/MM development -

3. Name : Lesthaeghe David
   Profile : PhD Student
   Skills : Heterogeneous Catalysis – MTO Process – QM/MM development

4. Name : Verstraelen Toon
   Profile : PhD Student
   Skills : Design new materials – development new Force Fields for zeolites

5. Name : De Sterck Bart
   Profile : PhD Student
   Skills : Heterocyclic Chemistry – Heterogeneous Catalysis

6. Name : Van Cauter Karen
   Profile : PhD Student
   Skills : Free Radical Polymerization Reactions

7. Name : Hemelsoet Karen
   Profile : PhD Student
   Skills : Reactivity – Polyaromatic Hydrocarbons

8. Name : Van Steenkiste Peter
   Profile : PhD Student - Postdoc from 1st July 2006
   Skills : Internal Modes -- Hindered Rotor Model – Adsorption processes - Diffusion

9. Name : Ghysels An
   Profile : *PhD Student*
   Skills : QM/MM – normal frequencies

10. Name : Van Neck Dimitri
    Profile : Professor
    Skills : Theoretical Model Development – New Functionals - Electron correlations

11. Name : Declerck Reinout
    Profile : PhD Student
    Skills : EPR implementation in periodic codes (CPMD-CP2K) – Molecular Dynamics

12. Name : Pauwels Ewald
    Profile : Postdoc FWO
    Skills : EPR in sugars , organic crystals

13. Name : De Cooman Hendrik
    Profile : PhD Student
    Skills : EPR in sugars

14. Name : Verdonck Stijn
    Profile : PhD Student
    Skills : Electron Correlations

II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

- Applicability of the hindered rotor scheme to the puckering mode in four-membered rings, P.Vansteenkiste, V.Van Speybroeck, G.Verniest, N.De Kimpe and M.Waroquier, **Journal of Physical Chemistry A, Vol 110, 3838 - 3844, 2006.**

- Understanding the failure of direct C-C coupling in the zeolite-catalyzed methanol-to-olefin process, David Lesthaeghe, Veronique Van Speybroeck, Guy B. Marin and Michel Waroquier, **Angewandte Chemie - International Edition, Vol.45 (11), 1714 – 1719** (selected to be highlighted in the frontispiece), **2006.**

- *Non-expected four-membered over six-membered ring formation during the synthesis of azaheterocyclic* phosphonates : experimental and theoretical evaluation., Veronique Van Speybroeck, Kristof Moonen, Karen Hemelsoet, Christian V.Stevens and Michel Waroquier, **Journal of the American Chemical Society**, in press.

- An assessment of theoretical procedures for predicting the thermochemistry and kinetics of hydrogen-abstraction by methyl radical from benzene., Karen Hemelsoet, Damian Moran, Veronique Van Speybroeck, Michel Waroquier and Leo Radom, **Journal of Physical Chemistry A**, in press.

- Bifunctional acid-base catalyzed reactions in zeolites from the HSAB viewpoint, Karen Hemelsoet, David Lesthaeghe, Veronique Van Speybroeck and Michel Waroquier, **Chemical Physics Letters, 419, 10-15, 2006.**

- Regio- and stereospecific ring opening of 1-alkyl-2-(aryloxymethyl)aziridinium salts by bromide, Matthias D'hooghe, Veronique van Speybroeck, Michel Waroquier, Norbert De Kimpe, **Chemical Communications, 1554 – 1556, 2006.**

- Ab initio study of free-radical polymerization: polyethylene propagation kinetics, Karen Van Cauter, *Veronique Van Speybroeck, Peter Vansteenkiste, Marie-Francoise Reyniers and Michel Waroquier*, **ChemPhysChem, Vol. 7 (1), 131 - 140, 2006.**

- What role do oxonium ions and oxonium ylides play in the ZSM-5 catalysed methanol-to-olefin process?, David Lesthaeghe, Veronique Van Speybroeck, Guy B. Marin and Michel Waroquier, **Chemical Physics Letters, 417, 309 - 315, 2006.**

- DFT investigation of aloxide versus alkylammonium formation in amine-substituted zeolites., *D. Lesthaeghe, V. Van Speybroeck, G.B. Marin, M. Waroquier*. **Journal of Physical Chemistry B, 109 (16), 7952-7960, 2005**.

- Efficient use of bifunctional acid-base properties for alkylammonium formation in amine-substituted zeolites. *D. Lesthaeghe, V. Van Speybroeck, M. Waroquier*. **J. Am. Chem. Soc.,126 (30), 9162-9163 , 2004**.

II. 5. INTERNATIONAL CONTACTS IN THE PROJECT'S RESEARCH DOMAIN

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

Prof.Dr. Jim Haw
Ray R. Irani, Chairman of Occidental Petroleum, Chair in Chemistry
University of Southern California
Skill : Heterogeneous Catalysis

Prof.Dr.Leo Radom
School of Chemistry
University of Sydney
Sydney, NSW 2006
Australia

Chair of the WATOC
Skill : Molecular Modeling

Prof.Dr.Viktoria Aviyente
Chemistry Department
Boğaziçi University, 34342
Bebek, Istanbul,Turkey
Skill : Computational Structural Biology and Biomaterials. Free radical polymerization.

Prof.Dr.Ursula Rothlisberger
Laboratory of Computational Chemistry and Biochemistry
Swiss Federal Institute of Technology EPF Lausanne
Switzerland
Skill : ab initio and QM/MM molecular dynamics

Prof.Dr.Juerg Hutter
Fachbereich Chemie-Biochemie
Universität Zürich
Winterthurerstrasse 190
8057 Zürich
Switzerland
Skill : head consortium CPMD and CP2K

Prof.Dr.Paul Ayers
Canada Research Chair in Theoretical Chemistry and Chemical Biology
Department of Chemistry
McMaster University
Hamilton, ON L8S 4M1, CANADA
Skill : force field parameters

Prof.Dr.Hans De Vries
DSM Research, P.O.Box 18, 6160 MD Geleen, The Netherlands

Prof.Dr.Rob Meier
DSM Research, P.O.Box 18, 6160 MD Geleen, The Netherlands

II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,...).

FWO research project : G.Marin and M.Waroquier , 1/1/06 – 31/12/09
Kinetic models for innovation in the process industry

FWO research project : M.Waroquier and D.Van Neck , 1/1/02 – 31/12/06
Study of electron correlations by means of Green's function techniques and density functional theory

GOA research project : N.De Kimpe , M.Waroquier and V.Van Speybroeck , 1/1/06 – 31/12/11
Exploration of fundamental reactions on heterocyclic compounds guided by ab initio molecular modeling.

ESF research project SIMBIOMA : M.Waroquier and V.Van Speybroeck, 29/5/06 – 31/5/10
Simulation of Biomolecules and Materials.
M.Waroquier is also member of the Steering Committee.

SBO research project BIPOM : M.Waroquier and V.Van Speybroeck , 1/11/03 – 31/10/07
Coordinator : Prof.Dr.Pierre Jacobs – KULeuven

II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: WP1, Nanodots and photonic crystals (tasks 2, 4)
2. Workpackage number and title: WP2, Organic nanostructures (task 1)
3. Workpackage number and title: WP3, Porous frameworks (tasks 1, 2, 3)
4. Workpackage number and title: WP4, Hybrid materials (task 3)
5. Workpackage number and title: WP6, Biomolecules and biocatalysis (task 3)
6. Workpackage number and title:
7. Workpackage number and title:
8. Workpackage number and title:
9. Workpackage number and title:
10. Workpackage number and title:
11. Workpackage number and title:
12. Workpackage number and title:
13. Workpackage number and title:
14. Workpackage number and title:
15. Workpackage number and title:

II. 8. BUDGET (distribution per year) *

(in EURO)

	2007	2008	2009	2010	2011	Total
Personnel	39.000,00	151.000,00	88.000,00	35.000,00	35.500,00	**348.500,00**
Operating costs	6.000,00	6.547,62	6.000,00	6.000,00	6.000,00	**30.547,62**
Equipment	0,00	0,00	52.000,00	0,00	Not allowed	**52.000,00**
Overheads	2.250,00	7.877,38	4.700,00	2.050,00	2.075,00	**18.952,38**
Subcontracting	0,00	0,00	0,00	0,00	0,00	**0,00**
Subtotal	**47.250,00**	**165.425,00**	**150.700,00**	**43.050,00**	**43.575,00**	**450.000,00**
EU 1 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 2 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 3 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
EU 4 (name)	0,00	0,00	0,00	0,00	0,00	**0,00**
Total	**47.250,00**	**165.425,00**	**150.700,00**	**43.050,00**	**43.575,00**	**450.000,00**

* This table should not be completed by the European partner as his/her budget is mentioned in the budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership

- Personnel: indexed gross remunerations; employer's social contributions; statutory insurance costs as well as any other compensation or allocation legally due in addition to the salary; the reimbursements for PhD and postdoctoral grant holders (exempt from tax and benefiting from social security). Personnel costs must account for minimum 60% of the total budget attributed to each partner of the network. The costs for the tax-free PhD grants and postdoctoral grants may not account for more than 60% of the total personnel costs.

- Operating costs: documentation; travel and accommodation; hosting of visiting foreign researchers use of computing facilities; software; telecommunications; maintenance and operation of equipment and, more generally, consumables;.

- Equipment: acquisition and installation of scientific and technical appliances and instruments, including IT equipment placed at the project's disposal. Equipment cannot be asked for during the last year of the programme.

- Overheads: general expenses of the institutions covering, on an inclusive basis, administrative, telephone, postal, maintenance, heating, electricity, rental, material depreciation and insurance costs. The total amount for this heading may not exceed 5% of total personnel and operating costs.

- Subcontracting: costs incurred by a third party in order to perform tasks or provide services necessitating specific scientific or technical skills outside the normal framework of the institution's activities. Each request for subcontracting needs a approval from the programme administrator.

II. 9. EQUIPMENT

Indicate the equipment (with an estimation of the cost) that will be purchased from the IAP-budget for the coming from four years (2007-2010) and justify.

Geavanceerde computerinfrastructuur is noodzakelijk om moleculaire modellering op hoog niveau te kunnen uitvoeren.
In 2009 wordt een budget voorzien van 52000 Euro, wat zeer minimaal is en onvoldoende om sommige in 2009 verouderde workstations te vervangen. Verwacht wordt dat een budget van 200.000 Euro meer dan noodzakelijk is maar het hier gevraagde bedrag kan al een substantiële bijdrage betekenen (25 %) van het geheel.

II. 10. SUBCONTRACTING

To be completed only if subcontracting is foreseen.

Describe and justify the tasks and/or services that will be provided by a third party.

No subcontracting is foreseen

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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION II

Information on the partners

to be completed by each network partner including the EU-partner(s)

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the partner : Müllen Klaus (EU1) Institution : Max-Planck-Institute for Polymer Research

II. 1. PARTNER CONTACT DETAILS

PARTNER N° (consult the list in Section I of Annex I) * : EU

- Family Name : Müllen
- First Name : Klaus
- Title (Prof., Dr., ...) : Prof.
- Institution : Max-Planck-Institute for Polymer Research
- Institution's abbreviation : MPG-P
- Faculty/Department : Polymer Synthesis
- Research Unit :
- Road/Street, n° : Ackermannweg 10
- Post Code : 55128
- Town/City : Mainz
- Country : Germany
- Tel : +49-6131-379150
- Tel secretariat : +49-6131-379150
- Fax : +49-6131-379-350
- E-mail : muellen@mpip-mainz.mpg.de
- Website : http://www.mpip-mainz.mpg.de/

* For Belgian partners : P1 to P13
For EU-partners : EU1 to EU4

II. 2. STAFF MEMBERS WORKING ON THE PROJECT (paid and not paid by the IAP-budget)

Staff	Number
Professor	16
Senior scientist	6
Post-doc	16
PhD student	29
Researcher without phD	4
Technician	7
Secretary	2
Other	4
TOTAL	**69**

II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, phD student, researcher without phD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name : Klaus Müllen
   Profile : professor
   Skills : new polymer-forming reactions including methods of organometallic chemistry; dye cheimstry, multi-dimensional polymers with, e.g., ribbon-type, sheet-type or shape-persistent three-dimensional structures; chemistry with single molecules; charge-transport properties of polymers and related oligomers including doping mechanisms and charge-storage capacity; supramolecular chemistry, molecular materials with liquid crystalline properties.

2. Name : Frank Dierschke
   Profile : senior scientist
   Skills : Conjugated polymers, LED materials, photovoltaics blockcopolymers, metal induced coupling reactions

3. Name : Markus Klapper
   Profile : senior scientist
   Skills : Polymer chemistry, nanocomposites, hybrid materials, radical and ionic polymerization, emulsion polymerisation, blockcopolymers, nanoparticles, fuel cells

4. Name : Andreas Herrmann
   Profile : senior scientist
   Skills : dye chemistry, DNA-conjugates, blockcopolymers, aggregation behaviour of polymers

5. Name : Tanja Weil
   Profile : senior scientist
   Skills : biological membranes, dendrimers, gen transfection

6. Name : Daniel Egbe
   Profile : Post-doctoral
   Skills : conjugated polymers, LED materials, photovoltaics

7. Name : Georgui Mihov
   Profile : Post-doctoral
   Skills : Synthesis of dendrimers

8. Name : Yuri Avlasevich,
   Profile : Post doctoral
   Skills : Organic chemistry, dye chemistry

9. Name : Jiaoli Li
   Profile : PhD
   Skills : Photovoltaics, Build-up of solar cells, characterization of devices

10. Name : Ming Zhang
    Profile : Postdoctoral

Skills : Blockcopolymerisation, conjugated polymers, characterisation of the aggregation of polymers, AFM, Build up of photovoltaic devices

11. Name : Tobias Schnitzler
Profile : PhD
Skills : organic chemistry, dye stuff chemistry

12. Name : Kalina Peneva
Profile : PhD
Skills : organic chemistry, dye stuff chemistry

II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

1. Grimsdale AC. Müllen K. The chemistry of organic nanomaterials, Angewandte Chemie-International Edition. 44(35):5592-5629, 2005.
2. De Schryver FC. Vosch T. Cotlet M. Van der Auweraer M. Müllen K. Hofkens J. Energy dissipation in multichromophoric single dendrimers, Accounts of Chemical Research. 38(7):514-522, 2005
3. Jung C. Muller BK. Lamb DC. Nolde F. Müllen K. Brauchle C. A new photostable terrylene diimide dye for applications in single molecule studies and membrane labeling. Journal of the American Chemical Society. 128(15):5283-5291, 2006
4. Mihov G. Grebel-Koehler D. Lubbert A. Vandermeulen GWM. Herrmann A. Klok HA. Müllen K. Polyphenylene dendrimers as scaffolds for shape-persistent multiple peptide conjugates. Bioconjugate Chemistry. 16(2):283-293, 2005
5. John H. Bauer R. Espindola P. Sonar P. Heinze J. Müllen K. 3D-hybrid networks with controllable electrical conductivity from the electrochemical deposition of terthiophene-functionalized polyphenylene dendrimers. Angewandte Chemie-International Edition. 44(16):2447-2451, 2005.
6. Pschirer NG. Kohl C. Nolde T. Qu JQ. Müllen K. Pentarylene- and hexarylenebis(dicarboximide)s: Near-infrared-absorbing polyaromatic dyes. Angewandte Chemie-International Edition. 45(9):1401-1404, 2006.
7. El Hamaoui B. Zhi LJ. Wu JS. Kolb U. Müllen K. Uniform carbon and carbon/cobalt nanostructures by solid-state thermolysis of polyphenylene dendrimer/cobalt complexes. Advanced Materials. 17(24):2957-+, 2005 Dec 16.
8. Li JL. Dierschke F. Wu JS. Grimsdale AC. Müllen K. Poly(2,7-carbazole) and perylene tetracarboxydiimide: a promising donor/acceptor pair for polymer solar cells.] Journal of Materials Chemistry. 16(1):96-100, 2006.
9. Khrenov V. Klapper M. Koch M. Müllen K. Surface functionalized ZnO particles designed for the use in transparent nanocomposites. Macromolecular Chemistry & Physics. 206(1):95-101, 2005
10. Debije MG. Piris J. de Haas MP. Warman JM. Tomovic Z. Simpson CD. Watson MD. Müllen K. The optical and charge transport properties of discotic materials with large aromatic hydrocarbon cores, Journal of the American Chemical Society. 126(14):4641-4645, 2004

II. 5. INTERNATIONAL CONTACTS IN THE PROJECT'S RESEARCH DOMAIN

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

Prof. Dr. Richard Friend, University of Cambridge, Dept. of Physics, Cavendish Lab., Madingley Road, UK-Cambridge CB3 OHE, phone: (+44) 12 23 33 72 18, fax (+44) 12 23 35 33 97, rhf10@cus.cam.ac.uk

Prof. Dr. Roberto Lazzaroni, University of Mons, phone: (+32) 65 37 33 01

Prof. Dr. Frans DeSchryver, Katholieke Universität Leuven, Dept. of Chemistry, Celestijnenlaan 200F, B-3001 Heverlee (Leuven), phone (+32) 16 32 74 05, fax (+32) 16 32 79 89, Frans.DeSchryver@chem.kuleuven.be

Prof. Dr. Jürgen Rabe, Institut für Physik, Physik von Makromolekülen, Newtonstraße 15, D-12489 Berlin, phone (+49) 30 20 93 77 88, fax (+49) 30 20 93 76 32

Prof. Dr. Paolo Samori, Instituto per la Sintesi Organica e la Fotoreattivita, Consiglio Nazionale delle Richerche, Via Gobetti 101, I-40129 Bologna, phone (+39) 051 63 99 829, fax (+39) 051 63 99 844, samori@alma.unito.it, or Institut de Science et d'Ingenierie Supramoleculaires (I.S.I.S.), Université Louis Pasteur, 8 allée Gaspard Mouge, B. P. 70028, F-67083 Strasbourg, phone (+33) 3902 45 160, fax (+33) 3 902 45 161

Prof. Dr. Bruno Samori, Dipartimento di Biochemica, Università degli Studi di Bologna, Via Irnerio 48, I-40126 Bologna, phone (+39) 051 209 4387, samori@alma.unito.it

Prof. Dr. Emil J.W. List, c/o Technische Universität Graz, Institut für Festkörperphysik, Petersgasse 16, A-8010 Graz; phone (+43) 316 873 8475, fax (+43) 316 873 8478, e.list@TUGraz.at

RADSAS Rational Design and Characterisation of Supramolecular Architectures on Surfaces
NMP3-CT-2004-001561 1.10.2004-30.9.2008 European Commission

NAIMO: Nanoscale integrated processing of self-organizing multifunctional organic materials
NMP4-CT-2004-500355: 2004-04-01- 2008-03-31 European Commission

II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,...).

IAP European Partnership P5/03 1.1.2002-31.12.2006 (Belgium's Federal Government)

RADSAS Rational Design and Characterisation of Supramolecular Architectures on Surfaces
NMP3-CT-2004-001561 1.10.2004-30.9.2008 European Commission

NAIMO: Nanoscale integrated processing of self-organizing multifunctional organic materials
NMP4-CT-2004-500355: 2004-04-01- 2008-03-31 European Commission

Sonderforschungsbereich 625: Von einzelnen Molekülen zu nanoskopischen Materialien (From single molecules to nanoscopic materials) 1.7. 2002-30.6.2008 (DFG = German Research Foundation)

BIONICS (SONS-program) 1.10.2004-30.9.2008 (EPF, DFG (German Research Foundation)

II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: WP1, Nanodots and photonic crystals (tasks 1, 2, 4, 5)
2. Workpackage number and title: WP2, Organic nanostructures (tasks 1, 2)
3. Workpackage number and title: WP3, Porous frameworks (tasks 3, 4)
4. Workpackage number and title: WP5, (Bio)membranes (tasks 1, 2, 4, 5)
5. Workpackage number and title: WP6, Biomolecules and biocatalysis (tasks 1, 3)
6. Workpackage number and title: WP8, Supramolecular conjugated systems
7. Workpackage number and title: WP9, Self-assembly at surfaces (tasks 1, 2)
8. Workpackage number and title:
9. Workpackage number and title:
10. Workpackage number and title:
11. Workpackage number and title:
12. Workpackage number and title:
13. Workpackage number and title:
14. Workpackage number and title:
15. Workpackage number and title:

II. 8. BUDGET (distribution per year) *

(in EURO)

The budget of the European partner is mentioned in the budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership (see Annex III)

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2007 – 2011

ANNEX I

TO CONTRACT P6/27

TECHNICAL SPECIFICATIONS : SECTION II

Information on the partners

to be completed by each network partner including the EU-partner(s)

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the partner : Feijen Jan (EU2) Institution : Universiteit Twente

II. 1. PARTNER CONTACT DETAILS

PARTNER N° (consult the list in Section I of Annex I) * : EU2

- Family Name : Feijen
- First Name : Jan
- Title (Prof., Dr., ...) : Prof. Dr.
- Institution : University of Twente
- Institution's abbreviation : UT
- Faculty/Department : Faculty of Science and Technology
- Research Unit : Dept. of Polymer Chemistry and Biomaterials
- Road/Street, n° : Drienerlolaan 5
- Post Code : 7522 NB
- Town/City : Enschede
- Country : The Netherlands
- Tel : 0031 53 4892976
- Tel secretariat : 0031 53 4892968
- Fax : 0031 53 4893823
- E-mail : j.feijen@tnw.utwente.nl
- Website : http://pbm.tnw.utwente.nl/

* For Belgian partners : P1 to P13
For EU-partners : EU1 to EU4

II. 2. STAFF MEMBERS WORKING ON THE PROJECT *(paid and not paid by the IAP-budget)*

Staff	Number
Professor	5
Senior scientist	4
Post-doc	4
PhD student	18
Researcher without phD	6
Technician	7
Secretary	1
Other	1
TOTAL	**46**

II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, phD student, researcher without phD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name : Prof. Dr J. Feijen
   Profile : Professor
   Skills : Polymer Chemistry and Biomaterials, biodegradable materials, biocompatible surfaces/surface engineering, drug delivery systems, tissue engineering

2. Name : Prof. Dr J.F.J. Engbersen
   Profile : Professor
   Skills : Biomedical chemistry, molecular biotechnology, non-viral gene transfer systems

3. Name : Prof. Dr W. Kruijer
   Profile : Professor
   Skills : Molecular cell biology, stem cells, regenerative medicine, tissue reconstruction, gene therapy

4. Name : Prof. Dr I. Vermes
   Profile : Professor
   Skills : Molecular aspects of cell and tissue engineering, physiology, clinical biochemistry, mechanical diagnosis, tissue engineering, cancer research

5. Name : Professor Dr D.W. Grijpma
   Profile : Professor
   Skills : Polymer synthesis and properties, structure properties relationships, biomaterials, tissue engineering

6. Name : Dr P.J. Dijkstra
   Profile : Senior Scientist
   Skills : Biodegradable polymers

7. Name : Dr A.A. Poot
   Profile : Senior scientist
   Skills : Cell biology, blood compatibility, tissue engineering, biochemistry

8. Name : Dr Z. Zhong
   Profile : Senior scientist
   Skills : DNA delivery vehicles for gene therapy, peptide-based "smart" hydrogels for tissue engineering, controlled and stereo selective polymerization of lactides

9. Name : Dr J.N. Post
   Profile : Senior scientist
   Skills : Molecular cell biology, stem cell differentiation, chromatin remodelling , chromatin structure function, signal transduction

10. Name : Dr F. Meng
    Profile : Post-doctoral
    Skills : Block-copolymers, biodegradable polymersomes

11. Name : Dr Z. Zhang
    Profile : Post-doctoral
    Skills : *Biodegradable polymer networks, tissue engineering, controlled drug delivery*

12. Name : Dr S.P. Nalawade
    Profile : Post-doctoral
    Skills : Synthesis of polylactides and copolymers, stereocomplexation of polylactides and copolymers, supercritical CO_2 processing.

13. Name : *Dr M.A. Mateos Timoneda*
    Profile : Post-doctoral
    Skills : Gene therapy, non-viral vectors, biodegradable polymers

14. Name : E. Bat
    Profile : PhD
    Skills : Structure-properties relations in polymers, hybranched polymers

15. Name : M.R. ten Breteler
    Profile : PhD
    Skills : Functional hydrogels, bioactive hydrogels, artificial extra cellular matrix components, cartilage tissue engineering

16. Name : C. Hiemstra
    Profile : PhD
    Skills : Stereo complexation, hydrogel, artificial extracellular matrix, tissue engineering, cartilage

17. Name : R. Jin
    Profile : PhD
    Skills : Injectable biodegradable hydrogels, cartilage tissue engineering

18. Name : C. Lin
    Profile : PhD
    Skills : Biodegradable polymers, gene delivery, gene therapy

19. Name : A.D. van der Meer
    Profile : PhD
    Skills : Cellular mechanosensing, signal transduction, molecular cell biology

20. Name : F.P.W. Melchels
    Profile : PhD
    Skills : Bone tissue engineering, porous polymer scaffolds, microstructure, release systems

21. Name : E.H.A. Nijhuis
    Profile : PhD
    Skills : Hyperhermia, apoptosis, tumour control, non-invasive

22. Name : F. Rusmini
    Profile : PhD
    Skills : Biochips for Multi-Analyte Diagnostics

23. Name : M. Piest
    Profile : PhD
    Skills : Novel boronated polyamidoamines as multifunctional vectors of siRNA delivery

24. Name : S. Schüller
    Profile : PhD
    Skills : Stereolithography, advanced microstructures, photo polymerized networks

25. Name : B. Siebum
    Profile : PhD
    Skills : Hematopoiesis, tissue engineering, stem cells, collagen

26. Name : N.J. Sijbrandi
    Profile : PhD
    Skills : Synthesis and self-assembly properties of polyester-amide and polyether-amide triblock copolymers

27. Name : Y. Song
    Profile : PhD
    Skills : Tissue engineering, injectable hydrogels, stem cells, small calibre blood vessels

28. Name : I.W. Velthoen
    Profile : PhD
    Skills : Hyperbranched polymers, thermosensitive hydrogels, biodegradable polymers

29. Name : H.H. Weekamp
    Profile : PhD
    Skills : Tissue engineering, mesenchymal stem cells, autologous vascular grafts

30. Name : L. Yang
    Profile : PhD
    Skills : Procollagen molecules, tissue structure, mechanical properties of collagen, techniques of micromechanical analysis

31. Name : W. Zhou
    Profile : PhD
    Skills : Polymersomes, non-invasive molecular imaging biodegradability

32. Name : S.V.N. de Vos
    Profile : Researcher without PhD
    Skills : Medical device start-up, PTMC, anti adhesion barriers, Biopartner First Stage Grant

II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

1. 'Biological characterization of vascular grafts cultured in a bioreactor', P. Engbers-Buijtenhuijs, L. Buttafoco, A.A. Poot, P.J. Dijkstra, R.A.I. Vos, L.M.Th. Sterk, R.H. Geelkerken, I. Vermes, J. Feijen, Biomaterials, 27 (11), 2390-2397 (2006).

2. 'Enzymatic surface erosion of poly(trimethylene carbonate) films studied by Atomic Force Microscopy', Z. Zhang, S. Zou, G.J. Vancso, D.W. Grijpma, J. Feijen, Biomacromolecules, 6 (6), 3404-3409 (2005).

3. 'Low molecular weight linear polyethylenimine-*b*-poly(ethylene glycol)-*b*-polyethylenimine triblock copolymers: synthesis, characterization and *in vitro* gene transfer properties', Z. Zhong, J. Feijen, M.C. Lok, W.E. Hennink, L.V. Christensen, J.W. Yockman, Yong-Hee Kim, Sung Wan Kim, Biomacromolecules, 6 (6), 3440-3448 (2005).

4. 'A versatile family of degradable non-viral gene carriers based on hyperbranched poly(ester amine)s', Z. Zhong, Y. Song, J.F.J. Engbersen, M.C. Lok, W.E. Hennink, J. Feijen, Journal of Controlled Release (special issue on the occasion of the 12th Int. Symp. On Recent Advances in Drug Delivery Systems; in honor of Professor Jan Feijen, 21-24 Febr. 2005, Salt Lake City, USA), 109 (1-3), 317-329 (2005).

5. 'Biodegradable polymersomes as a basis for artificial cells: encapsulation, release and targeting', F. Meng, G.H.M. Engbers, J. Feijen, special issue Journal of Controlled Release (Proceedings of the Eighth European Symposium on Controlled Drug Delivery, April 7-9, 2004, Noordwijk aan Zee), 101 (1-3), 187 – 198 (2005).

6. 'Stereocomplex mediated gelation of PEG-(PLA)2 and PEG-(PLA)8 block copolymers', C. Hiemstra, Z. Zhong, P.J. Dijkstra, J. Feijen, Macromolecular Symposia, Bio-Based Polymerers: Recent Progress (Symp. 8th World Conference on Biodegradable Polymers and Plastics (BDPP8), Seoul, Korea, April 2004), 224, p 119-131(2005).

7. 'Single-site calcium catalysts for the controlled ring-opening polymerisation of lactides and lactones', Z. Zhong, S. Schneiderbauer, P.J. Dijkstra, M. Westerhausen, J. Feijen, Polymer Bulletin, 51, 175-182 (2003).

8. '*Controlled and Stereoselective Polymerization of Lactide: Kinetics, Selectivity and* Microstructures', Z. Zhong, P.J. Dijkstra, J. Feijen, Journal of the American Chemical Society (JACS), 125, 11291-11298 (2003).

9. '[(salen Al]-mediated, controlled and stereoselective ring-opening polymerization of lactide in solution and without solvent: Synthesis of highly isotactic polylactide stereocopolymers from racemic D,L-lactide', Z. Zhong, P.J. Dijkstra, J. Feijen, Angewandte Chemie, Communications, 41 (23), 4510 – 4513 (2002).

10. 'Synthesis and aqueous phase of thermoresponsive biodegradable poly(D,L-3-methyl glycolide)-*b*-poly(ethylene glycol)-*b*-poly(D,L-3-methyl glycolide) triblock copolymers', Z. Zhong, P.J. Dijkstra, J. Feijen, Y.M. Kwon, Y.H. Bae, S.W. Kim, *Macromolecular Chemistry and Physics*, 203, 1797-1803 (2002).

II. 5. INTERNATIONAL CONTACTS IN THE PROJECT'S RESEARCH DOMAIN

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

Professor Dr Sung Wan Kim
Department of Pharmaceutics and Pharmaceutical Chemistry
Skaggs Hall 301
30 South 2000 East BPRB rm 201
USA-SALT LAKE CITY, UT 84112-5820
UNITED STATES OF AMERICA

Professor Dr T. Okano
Institute of Biomedical Engineering
Tokyo Women's Medical College
8-1 Kawada-cho
Shinjuku-ku
JAP-TOKYO 162 JAPAN

Professor Dr Kazunori Kataoka
The University of Tokyo
Department of Materials Science
Graduate School of Engineering
7-3-1 Hongo, Bunkyo-ku
JAP-TOKYO 113-8656 JAPAN

Prof. Dr. E. Chiellini
University of Pisa
Department of Chemistry & Industrial Chemistry University of Pisa
Via Risorgimento 35
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Prof. Dr A.S. Hoffman
Bioengineering Department
USA Box 352255 AER Bldg.
Rooms 334-338
University of Washington
Seattle WA 98195 United States of America

Professor M.A. Barbosa
Laboratório de Biomateriais
INEB - Instituto de Engenharia Biomédica
Universidade do Porto
Rua do Campo Alegre, 823
4150-180 PORTO PORTUGAL

II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,...).

1/01/05 – 1/01/09
DPTE (Dutch Program for Tissue Engineering)
'Trimethylene carbonate based polymers and structures for tissue engineering'

1/01/06 – 1/01/10
DPTE (Dutch Program for Tissue Engineering)
Thermoreversible hydrogels for the release of growth factors

15/04/05 – 15/04/09
DPTE (Dutch Program for Tissue Engineering)
'Injectable hydrogels for the delivery and differentiation of stem cells'

15/01/06 – 15/01/10
DPTE (Dutch Program for Tissue Engineering)
'Hybrid hydrogels as synthetic extracellular matrices for cartilage tissue engineering'

1/11/05 – 1/11/09
DPTE (Dutch Program for Tissue Engineering)
'Cardiac tissue engineering for the treatment of heart failure'

1/04/05 – 1/04/09
DPTE (Dutch Program for Tissue Engineering)
'Tissue engineering of small-caliber blood vessels'

1/09/02 – 1/09/06
STW (Dutch Technology Foundation)
'Growing blood: from fiction to fact'

15/08/03 – 15/08/07
STW (Dutch Technology Foundation)/ZonMW (the Netherlands organization for Health Research and Development)
An artificial extra cellular matrix for the regeneration of cartilage'

15/10/02 – 15/10/06
NWO-CW(Netherlands organization for scientific research – Chemical Sciences
Assembly of synthetic and natural polymers. An artificial extra cellular matrix'

1/01/04 – 1/01/08
Medtronic/Bakken Research Center
Stimuli-responsive polymer systems for local therapy delivery

1/10/05 – 1/10/07
DPI (Dutch Polymer Institute)
'Bioactive scaffolds for the tissue engineering of cardiovascular substitutes

II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: WP2, Organic nanostructures (task 1)
2. Workpackage number and title: WP4, Hybrid materials (task 1)
3. Workpackage number and title: WP5, (Bio)membranes (task 4)
4. Workpackage number and title: WP6, Biomolecules and Biocatalysis (task 2)
5. Workpackage number and title: WP7, Functional coatings (task 3)
6. Workpackage number and title: WP9, Self-assembly at surfaces (task 1)
7. Workpackage number and title:
8. Workpackage number and title:
9. Workpackage number and title:
10. Workpackage number and title:
11. Workpackage number and title:
12. Workpackage number and title:
13. Workpackage number and title:
14. Workpackage number and title:
15. Workpackage number and title:

II. 8. BUDGET (distribution per year) *

(in EURO)

The budget of the European partner is mentioned in the budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership (see Annex III)

Annexe II au contrat P6/27 / Bijlage II bij het contract P6/27

Institution Instelling	*Promoteur* *Promotor*	tranche/schijf : 2007	2008	2009	2010	2011	solde/soldij 2012	Budget
KULeuven								
	JACOBS	156.845,00	225.120,00	242.685,00	261.620,00	282.020,00	81.710,00	**1.250.000,00**
	VAN DER AUWERAER	156.845,00	225.120,00	242.685,00	261.620,00	282.020,00	81.710,00	**1.250.000,00**
	VANDERLEYDEN	50.190,00	72.040,00	77.660,00	83.715,00	90.245,00	26.150,00	**400.000,00**
	MULLEN	6.275,00	9.005,00	9.705,00	10.465,00	11.280,00	3.270,00	**50.000,00**
	FEIJEN	6.275,00	9.005,00	9.705,00	10.465,00	11.280,00	3.270,00	**50.000,00**
ULg								
	JÉRÔME	100.380,00	144.075,00	155.315,00	167.435,00	180.495,00	52.300,00	**800.000,00**
UMH								
	LAZZARONI	94.330,00	135.395,00	145.955,00	157.350,00	169.615,00	49.133,00	**751.778,00**
UGent								
	MARIN	113.650,00	163.120,00	175.845,00	189.570,00	204.350,00	59.205,00	**905.740,00**
	DU PREZ	50.190,00	72.040,00	77.660,00	83.715,00	90.245,00	26.150,00	**400.000,00**
	WAROQUIER	56.465,00	81.045,00	87.365,00	94.185,00	101.530,00	29.410,00	**450.000,00**
UCL								
	JONAS	112.930,00	162.090,00	174.730,00	188.365,00	203.055,00	58.830,00	**900.000,00**
VUB								
	BARON	57.985,00	83.225,00	89.720,00	96.720,00	104.260,00	30.205,00	**462.115,00**
ULB								
	DE MESMAEKER	50.190,00	72.040,00	77.660,00	83.715,00	90.245,00	26.150,00	**400.000,00**
FUNDP								
	WOUTERS	50.190,00	72.040,00	77.660,00	83.715,00	90.245,00	26.150,00	**400.000,00**
UHasselt								
	VANDERZANDE	50.190,00	72.040,00	77.660,00	83.715,00	90.245,00	26.150,00	**400.000,00**
					Financement du réseau / Financiering van het			*8.869.633,00*

BELGIAN SCIENCE POLICY
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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX III

TO CONTRACT P6/27

EUROPEAN PARTNERSHIP

to be completed for each European partner

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the EU-partner : Müllen Klaus (EU1) Institution : Max Planck Institute for Polymer Research Mainz

1. THE EUROPEAN PARTNER

Partner N° (EU1 to EU4 : consult the list in Annex I – Section I): EU1

Name of the European partner: Müllen Klaus

Institution: Max Planck Institute for Polymer Research Mainz

2. THE BUDGET ALLOCATED BY THE IAP PROGRAMME FOR THE PARTNERSHIP WITH THE EUROPEAN PARTNER (without the 50% contribution of the EU-partner)

50 000 EUR

3. THE BELGIAN PARTNER

In agreement with all the network members, the IAP-budget allocated for this partnership will be added to the IAP-budget of the following Belgian partner under the heading "European partnership:

Name of the Belgian partner: Van Der Auweraer Mark

Institution: Katholieke Universiteit Leuven

4. TOTAL BUDGET FOR THE PARTNERSHIP

BUGDET allocated by the IAP programme **(a)**	50 000 EUR
BUDGET allocated by the EU-partner **(b)**	50 000 EUR
TOTAL BUDGET	100 000 EUR

5. a) DESCRIPTION OF THE USE OF THE BUDGET ALLOCATED BY THE IAP PROGRAMME FOR THE EUROPEAN PARTNERSHIP (personal and operating costs only)

The budget will be used for personnel only. Two Ph.D. students will be working on the project (Larissa Puhl, Ralph Rieger); Larissa Puhl will be charged for 10.000 euros/year on the budget of EU1.
Dr. Manfred Wagner, a senior postdoc researcher of EU1, will coordinate the work of EU1.

b) DESCRIPTION OF THE USE OF THE BUDGET ALLOCATED BY THE EU-PARTNER FOR THE EUROPEAN PARTNERSHIP

The budget will be used to contribute to the program as defined in the final application.
Work package 1.1: Photonic crystals
Work package 1.2: Catalytic metal nanoparticles
Work package 1.4: Nonmetallic inorganic nanodots as catalysts, and as diagnostic or therapeutic agents
Work package 1.5: Semiconductor and metal clusters in OLEDS and solar cells
Work package 2.1: Multifunctional copolymers
Work package 2.2: Organic nanodots
Work package 3.3: Mapping and modelling of diffusion and catalytic activity in zeolites and mesoporous molecular sieves
Work package 3.4: Layered porous materials
Work package 5.1: Organization of lipid membranes: characterization of structure and dynamics of "rafts"
Work package 5.2: Dynamics of bacterial biofilms and structure function analysis of bacterial surfaces containing lipoteichoic acids
Work package 5.4: Biomimetic polymer membranes
Work package 5.5: Functional nanoporous membranes
Work package 6.1: Autofluorescent and photoswitchable proteins and use as probes
Work package 6.3: Biocatalysis with proteins and RNAs
Work package 8.1: Joint control of the optical, transport, and morphological properties
Work package 9.1: Molecular-scale studies of the structure, dynamics, and electronic properties in adsorbed monolayers
Work package 9.2: Controlling the spatial localization of functional systems at surfaces

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Interuniversity Attraction Poles (IAP)
Phase VI

2007 – 2011

ANNEX III

TO CONTRACT P6/27

EUROPEAN PARTNERSHIP

to be completed for each European partner

Title of the project : FUNCTIONAL SUPRAMOLECULAR SYSTEMS (FS2)
Name of the EU-partner : Feijen Jan (EU2) Institution : Universiteit Twente

1. THE EUROPEAN PARTNER

Partner N° (EU1 to EU4 : consult the list in Annex I – Section I):

Name of the European partner: Feijen Jan

Institution: Universiteit Twente

2. THE BUDGET ALLOCATED BY THE IAP PROGRAMME FOR THE PARTNERSHIP WITH THE EUROPEAN PARTNER (without the 50% contribution of the EU-partner)

50 000 EUR

3. THE BELGIAN PARTNER

In agreement with all the network members, the IAP-budget allocated for this partnership will be added to the IAP-budget of the following Belgian partner under the heading "European partnership:

Name of the Belgian partner: Vanderleyden Jos

Institution: Katholieke Universiteit Leuven

4. TOTAL BUDGET FOR THE PARTNERSHIP

BUGDET allocated by the IAP programme **(a)**	50 000 EUR
BUDGET allocated by the EU-partner **(b)**	50 000 EUR
TOTAL BUDGET	100 000 EUR

5. a) DESCRIPTION OF THE USE OF THE BUDGET ALLOCATED BY THE IAP PROGRAMME FOR THE EUROPEAN PARTNERSHIP (personal and operating costs only)

The budget is Euro 20.000 per year for a period of 5 years, including 50% matching.
This budget will be used for personal costs to support the activities of EU2 in the program.
Participants will be:

Dr. P. J. Dijkstra	75 hrs/per year	Euro 55/hr	total/year	Euro 4125
Ing. M.Ankone	300 hrs/per year	Euro 32/hr	total/year	Euro 9600
Prof. Dr. J. Feijen	40 hrs/per year	Euro 97/hr	total/year	Euro 3880
Prof. Dr. J.F.J.Engbersen	40 hrs/per year	Euro75/hr	total/year	Euro 3000

b) DESCRIPTION OF THE USE OF THE BUDGET ALLOCATED BY THE EU-PARTNER FOR THE EUROPEAN PARTNERSHIP

The budget will be used to contribute to the program as defined in the final application.
Work package 2.1. Multifunctional copolymers
Work package 4.1 Multiresponsive nanogels
Work package 5.4 Biomimetic polymer membranes
Work package 6.2 DNA and oligonucleotides
Work package 7.3 Biomimetic and protein repellent coatings

WO-Fiche

Pieter Van Mulders (09)264 95 06

WBS-Element:	B/07831/03	Fonds	IV2	Gecreeerd/gewijzigd door	Pascale BLANCQUAERT	09 264 30 39	
Kredietcode:	120C51B7	Begindatum:	01/01/2007		Datum:	13/07/2007	Vak Administratie
Kredietnaam:	IUAP VI - Waroquier	Einddatum	31/12/2011		Financieringsbron:	4106	
Kredietgever:	POD-Wetenschapsbeleid				Vakgroepnummer:	WE05	
Contractnummer	P6/KUL/27	Titel:		Functional supramolecular systems			
Promotor	Prof M Waroquier						
Copromotor 1:					Gekoppelde	Kredietcodes:	120C51C7
Copromotor 2:		WO-Fiche:	vervangt vorige fiche dd.	prefin vervalt	Gekoppelde	WBS-elementen.	B/07831/02-B/08028
Copromotor 3.		Versie:	2		Promotor.		Prof. F. Du Prez - G. Marin

Contractueel Overhead-regime: procentueel — CTRL+N = nieuwe versie WO-fiche — CTRL+S = kopie extern budget naar SAP

Budgetdrager	EXTERN			INTERN			Toe te kennen budget	SAP	
	Netto-Budget (Excl. Overhead)	OH (contract)	Bedrag OH	Netto-Budget (Excl. Overhead)	OH (intern)	Bedrag OH	Budget	Budget	WBS-element
Werking	30.547,62	5,00%	1.527,38	30 547,62	5.00%	1.527,38	30.547,62		
Recuperatie OH				0,00	0.00%	0.00			
2007	6.000,00		300,00	6.000,00		300,00	6.000,00	0,00	B/07831/03
2008	6.547,62		327,38	6.547,62		327,38	6.547,62	6 547,62	
2009	6.000,00		300,00	6.000,00		300,00	6 000,00	6.000,00	
2010	6.000,00		300,00	6.000,00		300,00	6 000,00	6.000,00	
2011	6.000,00		300,00	6.000,00		300,00	6 000,00	6.000,00	
	0,00			0,00				0.00	
Person	348.500,00	5,00%	17 425,00	348.500,00	5,00%	17 425,00	348 500,00		
2007	39.000,00		1.950,00	39.000,00		1 950,00	39 000,00	39.000,00	B/07831/03
2008	151.000,00		7.550,00	151.000,00		7 550,00	151 000,00	151.000,00	0
2009	88.000,00		4.400,00	88.000,00		4 400,00	88 000,00	88 000,00	0
2010	35 000,00		1.750,00	35.000,00		1.750,00	35 000,00	35 000,00	0
2011	35 500,00		1.775,00	35.500,00		1.775,00	35.500,00	35 500,00	0
0	0,00			0,00				0,00	0
Investering	52 000,00	0 00%	0,00	52 000,00	0,00%	0,00	52 000,00		
2007	0,00			0,00				0,00	B/07831/04
2008	0,00			0,00				0,00	
2009	52.000,00		0,00	52 000,00		0,00	52.000,00	52.000,00	0
2010	0,00			0,00				0,00	0
2011	0,00			0,00				0,00	0
0	0,00			0,00				0,00	0
	0,00	0,00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0,00	
2008	0,00			0,00				0,00	0
2009	0,00			0,00				0,00	0
2010	0,00			0,00				0,00	0
2011	0,00			0,00				0,00	0
0	0,00			0,00				0,00	0
	0,00	0,00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0,00	0
2008	0,00			0,00				0,00	0
2009	0,00			0,00				0,00	0
2010	0,00			0,00				0,00	0
2011	0,00			0,00				0,00	0
0	0,00			0,00				0.00	0
Netto-Inkomsten	431.047,62	4,396818%	18.952,38	431.047,62	4.396818%	18.952,38	431 047,62	Netto-Inkomsten	
Overhead financier	18.952,38			18.952,38			18.952,38	OH in SAP	
Bruto-Inkomsten	450.000,00			450.000,00			450 000.00	Bruto-Inkomsten	
Gem. OH-% op te nemen in SAP									

4,40%

Omzetting vreemde munt

=

www.tijd.be/koersen/index.asp?page=wisselkoersen&view=

Datum:

Brutobedrag	OH-Percentage	Nettobedrag	OH
0 00	0.00%	0,0000	0.0000
0.00	0,00%	0,0000	0.0000
OH (vast bedrag)	**Brutobedrag**	**Nettobedrag**	**OH-Percentage**
0,00	0.00	0,0000	
0,00	0.00	0,0000	0,0000%

Moeten de inkomsten ingegeven worden in SAP? JA

Totaalbudget=450.000 EUR prefinanciering vervalt
niet BTW pplichtig fundamenteel onderzoek

WO-Fiche

WBS-Element	B/07831/02	Fonds:	IV2	Gecreëerd/gewijzigd door	Pascale BLANCQUAERT	09 264 30 39	
Kredietcode	120C51C7	Begindatum:	01/01/2007	Datum.	13/07/2007		Vak Administratie
Kredietnaam.	IUAP VI - Du Prez	Einddatum:	31/12/2011	Financieringsbron.	4106		
Kredietgever:	POD-Wetenschapsbeleid			Vakgroepnummer	WE07		
Contractnummer	P6/KUL/27	Titel.	Functional supramolecular systems				
Promotor	Prof. F. Du Prez						
Copromotor 1.				Gekoppelde	Kredietcodes:	120C51AB	
Copromotor 2:		WO-Fiche	vervangt vorige fiche dd.	prefin vervalt	Gekoppelde	WBS-elementen: B/07831/03-B/08028	
Copromotor 3		Versie:	5		Promotor	Prof M Waroquier-G. Mann	
Contractueel Overhead-regime:		procentueel	CTRL+N = nieuwe versie WO-fiche		CTRL+S = kopie extern budget naar SAP		

Budgetdrager	EXTERN			INTERN			Toe te kennen budget	SAP	
	Netto-Budget (Excl. Overhead)	OH (contract)	Bedrag OH	Netto-Budget (Excl. Overhead)	OH (intern)	Bedrag OH	Budget	Budget	WBS-element
Werking	70.152,38	5,00%	3.507,62	70.152,38	5,00%	3 507,62	70.152,38		
Recuperatie OH				0,00	0,00%	0,00			
2007	14.152,38		707,62	14.152,38		707,62	14.152,38	0,38	B/07831/02
2008	14.000,00		700,00	14.000,00		700,00	14 000,00	14.000,00	B/07831/02
2009	14 000,00		700,00	14.000,00		700,00	14 000,00	14.000,00	B/07831/02
2010	14 000,00		700,00	14.000,00		700,00	14 000,00	14.000,00	B/07831/02
2011	14 000,00		700,00	14.000,00		700,00	14 000,00	14.000,00	B/07831/02
	0,00			0,00				0,00	B/07831/02
Person	310.800,00	5,00%	15.540,00	310.800,00	5,00%	15.540,00	310 800,00		
2007	51 700,00		2.585,00	51.700,00		2.585,00	51 700,00	-6.570,00	B/07831/02
2008	81 400,00		4.070,00	81.400,00		4.070,00	81 400,00	66 400,00	B/07831/02
2009	34.800,00		1.740,00	34.800,00		1.740,00	34.800,00	34 800,00	B/07831/02
2010	105.700,00		5.285,00	105.700,00		5.285,00	105 700,00	105 700,00	B/07831/02
2011	37.200,00		1.860,00	37 200,00		1.860,00	37.200,00	37 200,00	B/07831/02
0	0,00			0,00				0,00	B/07831/02
Investering	0,00	0,00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0,00	B/07831/02
2008	0,00			0,00				0,00	B/07831/02
2009	0,00			0,00				0,00	B/07831/02
2010	0,00			0,00				0,00	B/07831/02
2011	0,00			0,00				0,00	B/07831/02
0	0,00			0,00				0,00	B/07831/02
	0,00	0,00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0,00	B/07831/02
2008	0,00			0,00				0,00	B/07831/02
2009	0,00			0,00				0,00	B/07831/02
2010	0,00			0,00				0,00	B/07831/02
2011	0,00			0,00				0,00	B/07831/02
0	0,00			0,00				0,00	B/07831/02
	0,00	0,00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0,00	B/07831/02
2008	0,00			0,00				0,00	B/07831/02
2009	0,00			0,00				0,00	B/07831/02
2010	0,00			0,00				0,00	B/07831/02
2011	0,00			0,00				0,00	B/07831/02
0	0,00			0,00				0,00	B/07831/02
Netto-inkomsten	380.952,38	5,000000%	19.047,62	380.952,38	5,000000%	19.047,62	380.952,38	Netto-inkomsten	Moeten de inkomsten ingegeven worden in SAP? JA
Overhead financier	19 047,62			19 047,62			19.047,62	OH in SAP	
Bruto-inkomsten	400.000,00			400.000,00			400.000,00	Bruto-inkomsten	

Gem. OH-% op te nemen in SAP

5,00%

Omzetting vreemde munt

=

www.tijd.be/koersen/index asp?page=wisselkoersen&view=

Datum.

Brutobedrag	OH-Percentage	Nettobedrag	OH
0.00	0.00%	0,0000	0,0000
0.00	0.00%	0,0000	0,0000

OH (vast bedrag)	Brutobedrag	Nettobedrag	OH-Percentage
0.00	0,00	0,0000	
0.00	0,00	0,0000	0,0000%

Totaalbudget=400 000 EUR prefinanciering vervalt - inbegrepen overdracht P2008 naar P2007 van 700 EUR cfr IUAP reglement
niet BTW plichtig: fundamenteel onderzoek

belspo

Federaal Wetenschapsbeleid

INGEKOMEN
DOZA
27 JULI 2010
NR.: .....

3ff

B/07831/03
B/07831/04
120C51B7
- 05/474202
- 05/474203

Professor Michel Waroquier
Universiteit Gent
Center Molecular Modeling (CMM)
Proeftuinstraat, 86
9000 Gent

uw kenmerk	ons kenmerk	bijlage(n)
	p6/I/ Waroquier0607	1

contactpersoon	e-mail	telefoon	datum
Veronique Feys	feys@belspo.be	02 2383486	06.07.2010

IUAP-overeenkomst P6/27 - overdracht van kredieten.

Geachte Professor,

Wij hebben uw aanvraag tot overdracht van kredieten voor het jaar 2009 goed ontvangen, waarvoor onze dank.

Na onderzoek van uw dossier kunnen wij bevestigen dat het Federale Wetenschapsbeleid akkoord gaat met uw aanvraag.

U vindt in bijlage de tabel met de nieuwe verdeling van de jaarlijkse budgetten.

Met de meeste hoogachting,

0100010082600003
Prjdef: 8/07831 Doctyp: Contract

Veronique Feys
Opdrachthouder

cc. : financiële dienst

CONTRACT IUAP Nr. P6/27
UGent
Center Molecular Modeling
Professor M. Waroquier

VOORZIENE UITGAVEN NA AUTOMATISCHE OVERDRACHTEN JAAR 2007 (in euro)

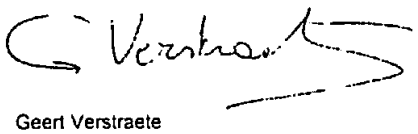
	2007	2008	2009	2010	2011	Totaal
Personeel	14 770,67	175 229,33	88 000,00	35 000,00	35 500,00	348 500,00
Werking	466,49	12 081,13	6 000,00	6 000,00	6 000,00	30 547,62
Uitrusting	0,00	0,00	52 000,00	0,00	niet toegestaan	52 000,00
Overheads	761,86	9 365,52	4 700,00	2 050,00	2 075,00	18 952,38
Onderaanneming	0,00	0,00	0,00	0,00	0,00	0,00
Subtotaal	**15 999,02**	**196 675,98**	**150 700,00**	**43 050,00**	**43 575,00**	**450 000,00**
Europees partnerschap 1	0,00	0,00	0,00	0,00	0,00	0,00
Europees partnerschap 2	0,00	0,00	0,00	0,00	0,00	0,00
Europees partnerschap 3	0,00	0,00	0,00	0,00	0,00	0,00
Europees partnerschap 4	0,00	0,00	0,00	0,00	0,00	0,00
Totaal	**15 999,02**	**196 675,98**	**150 700,00**	**43 050,00**	**43 575,00**	**450 000,00**

VOORZIENE UITGAVEN AANVRAAG OVERDRACHTEN DD 30/06/10 (in euro)

	2007	2008	2009	2010	2011	Totaal	
Personeel	14 770,67	175 229,33	88 000,00	35 000,00	35 500,00	348 500,00	103
Werking	466,49	11 429,21	6 000,00	6 000,00	6 000,00	29 895,70	103
Uitrusting	0,00	684,51	52 000,00	0,00	niet toegestaan	52 684,51	104
Overheads	761,86	9 332,93	4 700,00	2 050,00	2 075,00	18 919,79	
Onderaanneming	0,00	0,00	0,00	0,00	0,00	0,00	
Subtotaal	**15 999,02**	**196 675,98**	**150 700,00**	**43 050,00**	**43 575,00**	**450 000,00**	
Europees partnerschap 1	0,00	0,00	0,00	0,00	0,00	0,00	
Europees partnerschap 2	0,00	0,00	0,00	0,00	0,00	0,00	
Europees partnerschap 3	0,00	0,00	0,00	0,00	0,00	0,00	
Europees partnerschap 4	0,00	0,00	0,00	0,00	0,00	0,00	
Totaal	**15 999,02**	**196 675,98**	**150 700,00**	**43 050,00**	**43 575,00**	**450 000,00**	

Datum: 05/07/2010

Handtekening:



Geert Verstraete
Financieel beheerder

INITIEEL BUDGET

	2007	2008	2009	2010	2011	Totaal
Personeel	39 000,00	151 000,00	88 000,00	35 000,00	35 500,00	348 500,00
Werking	6 000,00	6 547,62	6 000,00	6 000,00	6 000,00	30 547,62
Uitrusting	0,00	0,00	52 000,00	0,00	niet toegestaan	52 000,00
Overheads	2 250,00	7 877,38	4 700,00	2 050,00	2 075,00	18 952,38
Onderaanneming	0,00	0,00	0,00	0,00	0,00	0,00
Subtotaal	**47 250,00**	**165 425,00**	**150 700,00**	**43 050,00**	**43 575,00**	**450 000,00**
Europees partnerschap 1	0,00	0,00	0,00	0,00	0,00	0,00
Europees partnerschap 2	0,00	0,00	0,00	0,00	0,00	0,00
Europees partnerschap 3	0,00	0,00	0,00	0,00	0,00	0,00
Europees partnerschap 4	0,00	0,00	0,00	0,00	0,00	0,00
Totaal	47 250,00	165 425,00	150 700,00	43 050,00	43 575,00	450 000,00

WBS-Element:	B/07831/03	Fonds:	IV2	Gecreëerd/gewijzigd door:	Pascale BLANCQUAERT	09 264 30 39	
Kredietcode:	120C51B7	Begindatum:	01/01/2007	Datum:	28/07/2010		Vak Administratie
Kredietnaam:	IUAP VI - Waroquier	Einddatum:	31/12/2011	Financieringsbron:	4106		
Kredietgever:	POD-Wetenschapsbeleid			Vakgroepnummer:	WE05		
Contractnummer:	P6/KUL/51	Titel:		Functional supramolecular systems			
Promotor:	Prof. M. Waroquier						
Copromotor 1:				Gekoppelde	Kredietcodes:	120C51C7	
Copromotor 2:		WO-Fiche:	vervangt vorige fiche dd. 13/07/2007	Gekoppelde	WBS-elementen:	B/07831/02-B/08028	
Copromotor 3:		Versie:	3	Promotor:	Prof. F. Du Prez - G. Marin		

Contractueel Overhead-regime: procentueel

CTRL+N = nieuwe versie WO-fiche — CTRL+S = kopie extern budget naar SAP

Budgetdrager	EXTERN			INTERN			Toe te kennen budget	SAP	
	Netto-Budget (Excl. Overhead)	OH (contract)	Bedrag OH	Netto-Budget (Excl. Overhead)	OH (intern)	Bedrag OH	Budget	Budget	WBS-element
Werking	29.895,70	5,00%	1.494,79	29.895,70	5,00%	1.494,79	29.895,70		
Recuperatie OH				0,00	0,00%	0,00			
2007	466,49		23,32	466,49		23,32	466,49	466,49	B/07831/03
2008	11.429,21		571,46	11.429,21		571,46	11.429,21	11.429,21	
2009	6.000,00		300,00	6.000,00		300,00	6.000,00	6.000,00	
2010	6.000,00		300,00	6.000,00		300,00	6.000,00	6.000,00	
2011	6.000,00		300,00	6.000,00		300,00	6.000,00	6.000,00	
	0,00			0,00				0,00	
Person	348.500,00	5,00%	17.425,00	348.500,00	5,00%	17.425,00	348.500,00		
2007	14.770,67		738,53	14.770,67		738,53	14.770,67	14.770,67	B/07831/03
2008	175.229,33		8.761,47	175.229,33		8.761,47	175.229,33	175.229,33	0
2009	88.000,00		4.400,00	88.000,00		4.400,00	88.000,00	88.000,00	0
2010	35.000,00		1.750,00	35.000,00		1.750,00	35.000,00	35.000,00	0
2011	35.500,00		1.775,00	35.500,00		1.775,00	35.500,00	35.500,00	0
0	0,00			0,00				0,00	0
Investering	52.684,51	0,00%	0,00	52.684,51	0,00%	0,00	52.684,51		
2007	0,00			0,00				0,00	B/07831/04
2008	684,51		0,00	684,51		0,00	684,51	684,51	
2009	52.000,00		0,00	52.000,00		0,00	52.000,00	52.000,00	0
2010	0,00			0,00				0,00	0
2011	0,00			0,00				0,00	0
0	0,00			0,00				0,00	0
	0,00	0,00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0,00	
2008	0,00			0,00				0,00	0
2009	0,00			0,00				0,00	0
2010	0,00			0,00				0,00	0
2011	0,00			0,00				0,00	0
0	0,00			0,00				0,00	0
	0,00	0,00%	0,00	0,00	0,00%	0,00	0,00		
2007	0,00			0,00				0,00	0
2008	0,00			0,00				0,00	0
2009	0,00			0,00				0,00	0
2010	0,00			0,00				0,00	0
2011	0,00			0,00				0,00	0
0	0,00			0,00				0,00	0
Netto-inkomsten	431.080,21	4,388925%	18.919,79	431.080,21	4,388925%	18.919,79	431.080,21	Netto-inkomsten	Moeten de inkomsten ingegeven worden in SAP?
Overhead financier	18.919,79			18.919,79			18.919,79	OH in SAP	
Bruto-inkomsten	450.000,00			450.000,00			450.000,00	Bruto-inkomsten	

Gem. OH-% op te nemen in SAP: **4,39%**

Omzetting vreemde munt

=

www.tijd.be/koersen/index.asp?page=wisselkoersen&view=

Datum:

Brutobedrag	OH-Percentage	Nettobedrag	OH
0,00	0,00%	0,0000	0,0000
0,00	0,00%	0,0000	0,0000
OH (vast bedrag)	**Brutobedrag**	**Nettobedrag**	**OH-Percentage**
0,00	0,00	0,0000	
0,00	0,00	0,0000	0,0000%

Totaalbudget=450.000 EUR prefinanciering vervalt
niet BTW pplichtig: fundamenteel onderzoek
Cfr. Nieuwe tabel dd. 06/07/2010

belspo

Federaal Wetenschapsbeleid

B/07831 *
- or/521652
- or/521653
- or/521654.
- or/521655.
- or/521656.

Professor Filip Du Prez
UGent
Polymer Chemistry Research Group
Krijgslaan 281 S4bis
9000 Gent

uw kenmerk	ons kenmerk		bijlage(n)
	p6/I/ DuPrez0109		1
contactpersoon	**e-mail**	**telefoon**	**datum**
Veronique Feys	feys@belspo.be	02 2383486	15.09.2010

IUAP-overeenkomst P6/27 - overdracht van kredieten.

Geachte Professor,

Wij hebben uw aanvraag tot overdracht van kredieten voor het jaar 2009 goed ontvangen, waarvoor onze dank.

Na onderzoek van uw dossier kunnen wij bevestigen dat het Federale Wetenschapsbeleid akkoord gaat met uw aanvraag.

U vindt in bijlage de tabel met de nieuwe verdeling van de jaarlijkse budgetten.

Met de meeste hoogachting,

Veronique Feys
Opdrachthouder

cc. : financiële dienst

0100010082600002
Prjdef: B/07831 Doctyp: Contract

CONTRACT IUAP Nr. P6/27
UGent
Polymer Chemistry Research Group
Professor F. Du Prez

VOORZIENE UITGAVEN NA AANVRAAG OVERDRACHTEN DD 15/04/09 (In euro)

	2007	2008	2009	2010	2011	Totaal
Personeel	41 155,21	16 451,81	110 292,98	105 700,00	37 200,00	310 800,00
Werking	7 897,25	7 777,53	20 627,47	14 000,00	14 000,00	64 302,25
Uitrusting	6 142,64	0,00	0,00	0,00	niet toegestaan	6 142,64
Overheads	2 452,62	1 211,47	6 546,02	5 985,00	2 560,00	18 755,11
Onderaanneming	0,00	0,00	0,00	0,00	0,00	0,00
Subtotaal	**57 647,72**	**25 440,81**	**137 466,47**	**125 685,00**	**53 760,00**	**400 000,00**
Europees partnerschap 1	0,00	0,00	0,00	0,00	0,00	0,00
Europees partnerschap 2	0,00	0,00	0,00	0,00	0,00	0,00
Europees partnerschap 3	0,00	0,00	0,00	0,00	0,00	0,00
Europees partnerschap 4	0,00	0,00	0,00	0,00	0,00	0,00
Totaal	57 647,72	25 440,81	137 466,47	125 685,00	53 760,00	400 000,00

VOORZIENE UITGAVEN NA AANVRAAG OVERDRACHTEN DD 06/07/10 (in euro)

	2007	2008	2009	2010	2011	Totaal
Personeel	41 155,21	16 451,81	110 292,98	105 700,00	37 200,00	310 800,00
Werking	7 897,25	6 916,55	20 627,47	14 000,00	14 000,00	63 441,27
Uitrusting	6 142,64	904,03	0,00	0,00	niet toegestaan	7 046,67
Overheads	2 452,62	1 168,42	6 546,02	5 985,00	2 560,00	18 712,06
Onderaanneming	0,00	0,00	0,00	0,00	0,00	0,00
Subtotaal	**57 647,72**	**25 440,81**	**137 466,47**	**125 685,00**	**53 760,00**	**400 000,00**
Europees partnerschap 1	0,00	0,00	0,00	0,00	0,00	0,00
Europees partnerschap 2	0,00	0,00	0,00	0,00	0,00	0,00
Europees partnerschap 3	0,00	0,00	0,00	0,00	0,00	0,00
Europees partnerschap 4	0,00	0,00	0,00	0,00	0,00	0,00
Totaal	57 647,72	25 440,81	137 466,47	125 685,00	53 760,00	400 000,00

Datum: 03/08/2010

Handtekening:

Geert Verstraete
Financieel beheerder

INITIEEL BUDGET

	2007	2008	2009	2010	2011	Totaal
Personeel	51 000,00	82 100,00	34 800,00	105 700,00	37 200,00	310 800,00
Werking	14 152,38	14 000,00	14 000,00	14 000,00	14 000,00	70 152,38
Uitrusting	0,00	0,00	0,00	0,00	niet toegestaan	0,00
Overheads	3 257,62	4 805,00	2 440,00	5 985,00	2 560,00	19 047,62
Onderaanneming	0,00	0,00	0,00	0,00	0,00	0,00
Subtotaal	**68 410,00**	**100 905,00**	**51 240,00**	**125 685,00**	**53 760,00**	**400 000,00**
Europees partnerschap 1	0,00	0,00	0,00	0,00	0,00	0,00
Europees partnerschap 2	0,00	0,00	0,00	0,00	0,00	0,00
Europees partnerschap 3	0,00	0,00	0,00	0,00	0,00	0,00
Europees partnerschap 4	0,00	0,00	0,00	0,00	0,00	0,00
Totaal	68 410,00	100 905,00	51 240,00	125 685,00	53 760,00	400 000,00