European Research Council
Executive Agency

Established by the European Commission

GRANT AGREEMENT

NUMBER — 647755 — DYNPOR

This **Agreement** ('the Agreement') is **between** the following parties:

on the one part,

the **European Research Council Executive Agency (ERCEA)** ('the Agency'), under the power delegated by the European Commission ('the Commission'),

represented for the purposes of signature of this Agreement by Head of Unit, European Research Council Executive Agency (ERCEA), Grant Management Department, Consolidator Grant , Marja HENNESSY,

and

on the other part,

'the beneficiary':

***UNIVERSITEIT GENT (UNIVERSITEIT GENT)**, 248015142, established in SINT PIETERSNIEUWSTRAAT 25, GENT 9000, Belgium, BE0248015142, represented for the purposes of signing the Agreement by Rector, Anne DE PAEPE, hosting and engaging the following '**principal investigator**':*

- ***Van Speybroeck Véronique**, 30/08/1974, Belgium*

If one or more beneficiaries accede to this Agreement (see Article 56), the beneficiary hosting *and engaging* the principal investigator becomes the '**principal beneficiary**'.

The parties referred to above have agreed to enter into the Agreement under the terms and conditions below.

By signing the Agreement, the beneficiary accepts the grant and agrees to implement it under its responsibility and in accordance with the Agreement, with all the obligations and conditions it sets out.

The Agreement is composed of:

Terms and Conditions

Annex 1 Description of the action

Annex 2 Estimated budget for the action

Annex 3 Not Applicable

Annex 4 Model for the financial statements

Annex 5 Model for the certificate on the financial statements

Annex 6 Model for the certificate on the methodology

TERMS AND CONDITIONS

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CHAPTER 1 GENERAL

ARTICLE 1 — SUBJECT OF THE AGREEMENT

This Agreement sets out the rights and obligations and the terms and conditions applicable to the grant awarded to the beneficiary for implementing the action set out in Chapter 2.

CHAPTER 2 ACTION

ARTICLE 2 — ACTION TO BE IMPLEMENTED

The grant is awarded for the action entitled '***First principle molecular dynamics simulations for complex chemical transformations in nanoporous materials — DYNPOR***' **('action')**, as described in Annex 1.

ARTICLE 3 — DURATION AND STARTING DATE OF THE ACTION

The duration of the action will be ***60*** **months** as of *01/08/2015* ('**starting date of the action**').

ARTICLE 4 — ESTIMATED BUDGET AND BUDGET TRANSFERS

4.1 Estimated budget

The '**estimated budget**' for the action is set out in Annex 2.

It contains the estimated eligible costs and the forms of costs, broken down by budget category (see Articles 5, 6).

4.2 Budget transfers

The estimated budget breakdown indicated in Annex 2 may be adjusted by transfers of amounts between budget categories. This does not require an amendment according to Article 55, if the action is implemented as described in Annex 1.

However, the beneficiary may not add costs relating to subcontracts not provided for in Annex 1, unless such additional subcontracts are approved by an amendment or in accordance with Article 13.

CHAPTER 3 GRANT

ARTICLE 5 — GRANT AMOUNT, FORM OF GRANT, REIMBURSEMENT RATES AND FORMS OF COSTS

5.1 Maximum grant amount

The '**maximum grant amount**' is **EUR 1,993,750.00** (one million nine hundred and ninety three thousand seven hundred and fifty EURO).

5.2 Form of grant, reimbursement rate and forms of costs

The grant reimburses **100%** of the beneficiary's eligible costs for the action (see Article 6) ('**reimbursement of eligible costs grant**') (see Annex 2).

The estimated eligible costs of the action are EUR **1,993,750.00** (one million nine hundred and ninety three thousand seven hundred and fifty EURO).

Eligible costs (see Article 6) must be declared under the following forms ('**forms of costs**'):

(a) for **direct personnel costs**:

- as actually incurred costs ('**actual costs**') or
- on the basis of an amount per unit calculated by the beneficiary in accordance with its usual cost accounting practices ('**unit costs**').

Personnel **costs for SME owners** or **beneficiaries that are natural persons** not receiving a salary (see Article 6.2, Points A.4 and A.5) must be declared on the basis of the amount per unit set out in Annex 2 (**unit costs**);

(b) for **direct costs for subcontracting**: as actually incurred costs (**actual costs**);

(c) for **direct costs of providing financial support** to third parties: not applicable;

(d) for **other direct costs**: as actually incurred costs (**actual costs**);

(e) for **indirect costs**: on the basis of a flat-rate applied as set out in Article 6.2, Point E ('**flat-rate costs**');

(f) for **specific cost category(ies)**: not applicable.

5.3 Final grant amount — Calculation

The '**final grant amount**' depends on the actual extent to which the action is implemented in accordance with the Agreement's terms and conditions.

This amount is calculated by the Agency — when the payment of the balance is made (see Article 21.4) — in the following steps:

Step 1 – Application of the reimbursement rates to the eligible costs

Step 2 – Limit to the maximum grant amount

Step 3 – Reduction due to the no-profit rule

Step 4 – Reduction due to improper implementation or breach of other obligations

5.3.1 Step 1 — Application of the reimbursement rates to the eligible costs

The reimbursement rate(s) (see Article 5.2) are applied to the eligible costs (actual costs, unit costs and flat-rate costs; see Article 6) declared by the beneficiary (see Article 20) and approved by the Agency (see Article 21).

5.3.2 Step 2 — Limit to the maximum grant amount

If the amount obtained following Step 1 is higher than the maximum grant amount set out in Article 5.1, it will be limited to the latter.

5.3.3 Step 3 — Reduction due to the no-profit rule

The grant must not produce a profit.

'**Profit**' means the surplus of the amount obtained following Steps 1 and 2 plus the action's total receipts, over the action's total eligible costs.

The '**action's total eligible costs**' are the consolidated total eligible costs approved by the Agency.

The '**action's total receipts**' are the consolidated total receipts generated during its duration (see Article 3).

The following are considered **receipts**:

(a) income generated by the action; if the income is generated from selling equipment or other assets purchased under the Agreement, the receipt is up to the amount declared as eligible under the Agreement;

(b) financial contributions given by third parties to the beneficiary specifically to be used for the action, and

(c) in-kind contributions provided by third parties free of charge and specifically to be used for the action, if they have been declared as eligible costs.

The following are however not considered receipts:

(a) income generated by exploiting the action's results (see Article 28);

(b) financial contributions by third parties, if they may be used to cover costs other than the eligible costs (see Article 6);

(c) financial contributions by third parties with no obligation to repay any amount unused at the end of the period set out in Article 3.

If there is a profit, it will be deducted from the amount obtained following Steps 1 and 2.

5.3.4 Step 4 — Reduction due to improper implementation or breach of other obligations — Reduced grant amount — Calculation

If the grant is reduced (see Article 43), the Agency will calculate the reduced grant amount by deducting the amount of the reduction (calculated in proportion to the improper implementation of the action or to the seriousness of the breach of obligations in accordance with Article 43.2) from the maximum grant amount set out in Article 5.1.

The final grant amount will be the lower of the following two:

- the amount obtained following Steps 1 to 3 or

- the reduced grant amount following Step 4.

5.4 Revised final grant amount — Calculation

If — after the payment of the balance (in particular, after checks, reviews, audits or investigations; see Article 22) — the Agency rejects costs (see Article 42) or reduces the grant (see Article 43), it will calculate the '**revised final grant amount**'.

This amount is calculated by the Agency on the basis of the findings, as follows:

- in case of **rejection of costs**: by applying the reimbursement rate to the revised eligible costs approved by the Agency;

- in case of **reduction of the grant**: in proportion to its improper implementation of the action or to the seriousness of its breach of obligations (see Article 43.2).

In case of **rejection of costs and reduction of the grant**, the revised final grant amount will be the lower of the two amounts above.

ARTICLE 6 — ELIGIBLE AND INELIGIBLE COSTS

6.1 General conditions for costs to be eligible

'**Eligible costs**' are costs that meet the following criteria:

(a) for **actual costs**:

(i) they must be actually incurred by the beneficiary;

(ii) they must be incurred in the period set out in Article 3, with the exception of costs relating to the submission of the periodic report for the last reporting period and the final report (see Article 20);

(iii) they must be indicated in the estimated budget set out in Annex 2;

(iv) they must be incurred in connection with the action as described in Annex 1 and necessary for its implementation;

(v) they must be identifiable and verifiable, in particular recorded in the beneficiary's accounts in accordance with the accounting standards applicable in the country where the beneficiary is established and with the beneficiary's usual cost accounting practices;

(vi) they must comply with the applicable national law on taxes, labour and social security, and

(vii) they must be reasonable, justified and must comply with the principle of sound financial management, in particular regarding economy and efficiency;

(b) for **unit costs**:

(i) they must be calculated as follows:

{amounts per unit set out in Annex 2 or calculated by the beneficiary in accordance with its usual cost accounting practices (see Article 6.2, PointA)}

multiplied by

{the number of actual units};

(ii) the number of actual units must comply with the following conditions:

- the units must be actually used or produced in the period set out in Article 3;
- the units must be necessary for implementing the action or produced by it, and
- the number of units must be identifiable and verifiable, in particular supported by records and documentation (see Article 18);

(c) for **flat-rate costs**:

(i) they must be calculated by applying the flat-rate set out in Annex 2, and

(ii) the costs (actual costs or unit costs) to which the flat-rate is applied must comply with the conditions for eligibility set out in this Article.

6.2 Specific conditions for costs to be eligible

Costs are eligible if they comply with the general conditions (see above) and the specific conditions set out below for each of the following budget categories:

A. direct personnel costs;

B. direct costs of subcontracting;

C. *not applicable;*

D. other direct costs;

E. indirect costs;

F. *not applicable.*

'Direct costs' are costs that are directly linked to the action implementation and can therefore be attributed to it directly. They must not include any indirect costs (see Point E below).

'Indirect costs' are costs that are not directly linked to the action implementation and therefore cannot be attributed directly to it.

A. Direct personnel costs

<u>Types of eligible personnel costs</u>

A.1 Personnel costs are eligible, if they are related to personnel working for the beneficiary under an employment contract (or equivalent appointing act) and assigned to the action ('**costs for employees (or equivalent)**'). They must be limited to salaries (including during parental leave),

social security contributions, taxes and other costs included in the **remuneration**, if they arise from national law or the employment contract (or equivalent appointing act).

If the beneficiary is a non-profit legal entity[1], it may also declare as personnel costs **additional remuneration** for personnel assigned to the action (including payments on the basis of supplementary contracts regardless of their nature), if:

(a) it is part of the beneficiary's usual remuneration practices and is paid in a consistent manner whenever the same kind of work or expertise is required;

(b) the criteria used to calculate the supplementary payments are objective and generally applied by the beneficiary, regardless of the source of funding used.

Additional remuneration for personnel assigned to the action is eligible up to the following amount:

(a) if the person works full time and exclusively on the action during the full year: up to EUR 8 000;

(b) if the person works exclusively on the action but not full-time or not for the full year: up to the corresponding pro-rata amount of EUR 8 000, or

(c) if the person does not work exclusively on the action: up to a pro-rata amount calculated as follows:

{{EUR 8 000

divided by

the number of annual productive hours (see below)},

multiplied by

the number of hours that the person has worked on the action during the year}.

A.2 The **costs for natural persons working under a direct contract** with the beneficiary other than an employment contract are eligible personnel costs, if:

(a) the person works under the beneficiary's instructions and, unless otherwise agreed with the beneficiary, on the beneficiary's premises;

(b) the result of the work carried out belongs to the beneficiary, and

(c) the costs are not significantly different from those for personnel performing similar tasks under an employment contract with the beneficiary.

A.3 The **costs of personnel seconded by a third party against payment** are eligible personnel costs, if the conditions in Article 11.1 are met.

[1] For the definition, see Article 2.1(14) of the Rules for Participation Regulation No 1290/2013: '**non-profit legal entity**' means a legal entity which by its legal form is non-profit-making or which has a legal or statutory obligation not to distribute profits to its shareholders or individual members.

A.4 If the beneficiary is a small and medium-sized enterprise ('**SME**'), the **costs of** its **owner** who is working on the action and who does not receive a salary are eligible personnel costs, if they correspond to the amount per unit set out in Annex 2 multiplied by the number of actual hours worked on the action.

A.5 If the beneficiary is a **natural person not receiving a salary**, its **costs** are eligible personnel costs if they correspond to the amount per unit set out in Annex 2 multiplied by the number of actual hours worked on the action.

Calculation

Personnel costs must be calculated by the beneficiary as follows:

{{hourly rate

multiplied by

the number of actual hours worked on the action},

plus

for non-profit legal entities: additional remuneration to personnel assigned to the action under the conditions set out above (Point A.1)}.

The number of actual hours declared for a person must be identifiable and verifiable (see Article 18).

The total number of hours declared in EU or Euratom grants, for a person for a year, cannot be higher than the annual productive hours used for the calculations of the hourly rate. Therefore, the maximum number of hours that can be declared for the grant are:

{the number of annual productive hours for the year (see below)

minus

total number of hours declared by the beneficiary for that person in that year for other EU or Euratom grants}.

The '**hourly rate**' is one of the following:

(a) for personnel costs declared as **actual costs:** the hourly rate is the amount calculated as follows:

{actual annual personnel costs (excluding additional remuneration) for the person

divided by

number of annual productive hours}.

The beneficiary must use the annual personnel costs and the number of annual productive hours for each financial year covered by the reporting period concerned. If a financial year is not closed at the end of the reporting period, the beneficiary must use the hourly rate of the last closed financial year available.

For the 'number of annual productive hours', the beneficiary may choose one of the following:

(i) 'fixed number of hours': 1 720 hours for persons working full time (or corresponding pro-rata for persons not working full time);

(ii) 'individual annual productive hours': the total number of hours worked by the person in the year for the beneficiary, calculated as follows:

{annual workable hours of the person (according to the employment contract, applicable collective labour agreement or national law)

plus

overtime worked

minus

absences (such as sick leave and special leave)}.

'Annual workable hours' means the period during which the personnel must be working, at the employer's disposal and carrying out his/her activity or duties under the employment contract, applicable collective labour agreement or national working time legislation.

If the contract (or applicable collective labour agreement or national working time legislation) does not allow to determine the annual workable hours, this option cannot be used;

(iii) 'standard annual productive hours': the standard number of annual hours generally applied by the beneficiary for its personnel in accordance with its usual cost accounting practices. This number must be at least 90% of the 'standard annual workable hours'.

If there is no applicable reference for the standard annual workable hours, this option cannot be used.

For all options, the actual time spent on **parental leave** by a person assigned to the action may be deducted from the number of annual productive hours;

(b) for personnel costs declared on the basis of **unit costs**: the hourly rate is one of the following:

(i) for an SME owner or beneficiary that is a natural person: the hourly rate set out in Annex 2 (see Points A.4 and A.5 above), or

(ii) for personnel costs declared on the basis of the beneficiary's usual cost accounting practices: the hourly rate calculated by the beneficiary in accordance with its usual cost accounting practices, if:

- the cost accounting practices used are applied in a consistent manner, based on objective criteria, regardless of the source of funding;

- the hourly rate is calculated using the actual personnel costs recorded in the beneficiary's accounts, excluding any ineligible cost or costs included in other budget categories.

The actual personnel costs may be adjusted by the beneficiary on the basis of budgeted or estimated elements. Those elements must be relevant for calculating

the personnel costs, reasonable and correspond to objective and verifiable information;

and

- the hourly rate is calculated using the number of annual productive hours (see above).

B. Direct costs of subcontracting (including related duties, taxes and charges such as non-deductible value added tax (VAT) paid by the beneficiary) are eligible if the conditions in Article 13.1.1 are met.

C. Direct costs of providing financial support to third parties

Not applicable.

D. Other direct costs

D.1 **Travel costs and related subsistence allowances** (including related duties, taxes and charges such as non-deductible value added tax (VAT) paid by the beneficiary) are eligible if they are in line with the beneficiary's usual practices on travel.

D.2 *The **depreciation costs of equipment, infrastructure or other assets** (new or second-hand) as recorded in the beneficiary's accounts are eligible, if they were purchased in accordance with Article 10.1.1 and written off in accordance with international accounting standards and the beneficiary's usual accounting practices.*

*The **costs of renting or leasing** equipment, infrastructure or other assets (including related duties, taxes and charges such as non-deductible value added tax (VAT) paid by the beneficiary) are also eligible, if they do not exceed the depreciation costs of similar equipment, infrastructure or assets and do not include any financing fees.*

*The costs of equipment, infrastructure or other assets **contributed in-kind against payment** are eligible, if they do not exceed the depreciation costs of similar equipment, infrastructure or assets, do not include any financing fees and if the conditions in Article 11.1 are met.*

The only portion of the costs that will be taken into account is that which corresponds to the duration of the action and rate of actual use for the purposes of the action.

D.3 **Costs of other goods and services** (including related duties, taxes and charges such as non-deductible value added tax (VAT) paid by the beneficiary) are eligible, if they are:

(a) purchased specifically for the action and in accordance with Article 10.1.1 or

(b) contributed in kind against payment and in accordance with Article 11.1.

Such goods and services include, for instance, consumables and supplies, dissemination (including open access), protection of results, certificates on the financial statements (if they are required by the Agreement), certificates on the methodology, translations and publications.

D.4 **Capitalised and operating costs of 'large research infrastructure'**[2] *directly used for the action are eligible, if:*

(a) the value of the large research infrastructure represents at least 75% of the total fixed assets (at historical value in its last closed balance sheet before the date of the signature of the Agreement or as determined on the basis of the rental and leasing costs of the research infrastructure[3]*);*

*(b) the beneficiary's methodology for declaring the costs for large research infrastructure has been positively assessed by the Commission ('**ex-ante assessment**');*

(c) the beneficiary declares as direct eligible costs only the portion which corresponds to the duration of the action and the rate of actual use for the purposes of the action, and

(d) they comply with the conditions as further detailed in the annotations to the H2020 grant agreements.

E. Indirect costs

Indirect costs are eligible if they are declared on the basis of the flat-rate of 25% of the eligible direct costs (see Article 5.2 and Points A to D above), from which are excluded:

(a) costs of subcontracting and

(b) costs of in-kind contributions provided by third parties which are not used on the beneficiary's premises.

(c) *not applicable;*

(d) *not applicable.*

If the beneficiary receives an operating grant [4] financed by the EU or Euratom budget, it cannot declare indirect costs for the period covered by the operating grant.

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[2] '**Large research infrastructure**' means research infrastructure of a total value of at least EUR 20 million, for a beneficiary, calculated as the sum of historical asset values of each individual research infrastructure of that beneficiary, as they appear in its last closed balance sheet before the date of the signature of the Agreement or as determined on the basis of the rental and leasing costs of the research infrastructure.

[3] For the definition see Article 2(f) of the H2020 Framework Programme Regulation No 1291/2013 : '**Research infrastructure**' are facilities, resources and services that are used by the research communities to conduct research and foster innovation in their fields. Where relevant, they may be used beyond research, e.g. for education or public services. They include: major scientific equipment (or sets of instruments); knowledge-based resources such as collections, archives or scientific data; e-infrastructures such as data and computing systems and communication networks; and any other infrastructure of a unique nature essential to achieve excellence in research and innovation. Such infrastructures may be 'single-sited', 'virtual' or 'distributed'.

[4] For the definition, see Article 121(1)(b) of Regulation (EU, Euratom) No 966/2012 of the European Parliament and of the Council of 25 October 2012 on the financial rules applicable to the general budget of the Union and repealing Council Regulation (EC, Euratom) No 1605/2002 (OJ L 218, 26.10.2012, p.1) ('**Financial Regulation No 966/2012**'): '**operating grant**' means direct financial contribution, by way of donation, from the budget in order to finance the functioning of a body which pursues an aim of general EU interest or has an objective forming part of and supporting an EU policy.

F. *Specific cost category(ies)*

Not applicable

6.3 Conditions for costs of linked third parties to be eligible

not applicable

6.4 Conditions for in-kind contributions provided by third parties free of charge to be eligible

In-kind contributions provided free of charge are eligible direct costs (for the beneficiary), if the costs incurred by the third party fulfil — *mutatis mutandis* — the general and specific conditions for eligibility set out in this Article (Article 6.1 and 6.2) and Article 12.1.

6.5 Ineligible costs

'**Ineligible costs**' are:

(a) costs that do not comply with the conditions set out above (Article 6.1 to 6.4), in particular:

(i) costs related to return on capital;

(ii) debt and debt service charges;

(iii) provisions for future losses or debts;

(iv) interest owed;

(v) doubtful debts;

(vi) currency exchange losses;

(vii) bank costs charged by the beneficiary's bank for transfers from the Agency;

(viii) excessive or reckless expenditure;

(ix) deductible VAT;

(x) costs incurred during suspension of the implementation of the action (see Article 49);

(b) costs declared under another EU or Euratom grant (including grants awarded by a Member State and financed by the EU or Euratom budget and grants awarded by bodies other than the Agency for the purpose of implementing the EU or Euratom budget); in particular, indirect costs if the beneficiary is already receiving an operating grant financed by the EU or Euratom budget in the same period.

6.6 Consequences of declaration of ineligible costs

Declared costs that are ineligible will be rejected (see Article 42).

This may also lead to any of the other measures described in Chapter 6.

CHAPTER 4 RIGHTS AND OBLIGATIONS OF THE PARTIES

SECTION 1 RIGHTS AND OBLIGATIONS RELATED TO IMPLEMENTING THE ACTION

ARTICLE 7 — GENERAL OBLIGATION TO PROPERLY IMPLEMENT THE ACTION

7.1 General obligation to properly implement the action

The beneficiary must implement the action as described in Annex 1 and in compliance with the provisions of the Agreement and all legal obligations under applicable EU, international and national law.

The beneficiary must ensure that the action tasks described in Annex 1 are performed under the guidance of the principal investigator.

7.2 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 8 — RESOURCES TO IMPLEMENT THE ACTION — THIRD PARTIES INVOLVED IN THE ACTION

The beneficiary must have the appropriate resources to implement the action.

If it is necessary to implement the action, the beneficiary may:

- purchase goods, works and services (see Article 10);
- use in-kind contributions provided by third parties against payment (see Article 11);
- use in-kind contributions provided by third parties free of charge (see Article 12);
- call upon subcontractors to implement action tasks described in Annex 1 (see Article 13);
- call upon linked third parties to implement action tasks described in Annex 1 (see Article 14).

In these cases, the beneficiary retains sole responsibility towards the Agency for implementing the action.

ARTICLE 9 — IMPLEMENTATION OF ACTION TASKS BY BENEFICIARY NOT RECEIVING EU FUNDING

Not applicable

ARTICLE 10 — PURCHASE OF GOODS, WORKS OR SERVICES

10.1 Rules for purchasing goods, works or services

10.1.1 If necessary to implement the action, the beneficiary may purchase goods, works or services.

The beneficiary must make such purchases ensuring the best value for money or, if appropriate, the lowest price. In doing so, it must avoid any conflict of interests (see Article 35).

The beneficiary must ensure that the Agency, the Commission, the European Court of Auditors (ECA) and the European Anti-fraud Office (OLAF) can exercise their rights under Articles 22 and 23 also towards their contractors.

10.1.2 If the beneficiary is a 'contracting authority' within the meaning of Directive 2004/18/EC[5] or a 'contracting entity' within the meaning of Directive 2004/17/EC[6] it must comply with the applicable national law on public procurement.

10.2 Consequences of non-compliance

If the beneficiary breaches any of its obligations under Article 10.1.1, the costs related to the contract concerned will be ineligible (see Article 6) and will be rejected (see Article 42).

If the beneficiary breaches any of its obligations under Article 10.1.2, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 11 — USE OF IN-KIND CONTRIBUTIONS PROVIDED BY THIRD PARTIES AGAINST PAYMENT

11.1 Rules for the use of in-kind contributions against payment

If necessary to implement the action, the beneficiary may use in-kind contributions provided by third parties against payment.

The beneficiary may declare costs related to the payment of in-kind contributions as eligible (see Article 6.1 and 6.2), up to the third parties' costs for the seconded persons, contributed equipment, infrastructure or other assets or other contributed goods and services.

The third parties and their contributions must be set out in Annex 1. The Agency may however approve in-kind contributions not set out in Annex 1 without amendment (see Article 55), if:

- they are specifically justified in the periodic financial report and
- their use does not entail changes to the Agreement which would call into question the decision awarding the grant or breach the principle of equal treatment of applicants.

[5] Directive 2004/18/EC of the European Parliament and of the Council of 31 March 2004 on the coordination of procedures for the award of public work contracts, public supply contracts and public service contracts (OJ L 134, 30.04.2004, p. 114).

[6] Directive 2004/17/EC of the European Parliament and of the Council of 31 March 2004 coordinating the procurement procedures of entities operating in the water, energy, transport and postal services sectors (OJ L 134, 30.04.2004, p. 1).

The beneficiary must ensure that the Agency, the Commission, the European Court of Auditors (ECA) and the European Anti-Fraud Office (OLAF) can exercise their rights under Articles 22 and 23 also towards the third parties.

11.2 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the costs related to the payment of the in-kind contribution will be ineligible (see Article 6) and will be rejected (see Article 42).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 12 — USE OF IN-KIND CONTRIBUTIONS PROVIDED BY THIRD PARTIES FREE OF CHARGE

12.1 Rules for the use of in-kind contributions free of charge

If necessary to implement the action, the beneficiary may use in-kind contributions provided by third parties free of charge.

The beneficiary may declare costs incurred by the third parties for the seconded persons, contributed equipment, infrastructure or other assets or other contributed goods and services as eligible in accordance with Article 6.4.

The third parties and their contributions must be set out in Annex 1. The Agency may however approve in-kind contributions not set out in Annex 1 without amendment (see Article 55), if:

- they are specifically justified in the periodic financial report and
- their use does not entail changes to the Agreement which would call into question the decision awarding the grant or breach the principle of equal treatment of applicants.

The beneficiary must ensure that the Agency, the Commission, the European Court of Auditors (ECA) and the European Anti-Fraud Office (OLAF) can exercise their rights under Articles 22 and 23 also towards the third parties.

12.2 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the costs incurred by the third parties related to the in-kind contribution will be ineligible (see Article 6) and will be rejected (see Article 42).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 13 — IMPLEMENTATION OF ACTION TASKS BY SUBCONTRACTORS

13.1 Rules for subcontracting action tasks

13.1.1 If necessary to implement the action, the beneficiary may award subcontracts covering the implementation of certain action tasks described in Annex 1.

Subcontracting may cover only a limited part of the action.

The beneficiary must award the subcontracts ensuring the best value for money or, if appropriate, the lowest price. In doing so, they must avoid any conflict of interests (see Article 35).

The tasks to be implemented and the estimated cost for each subcontract must be set out in Annex 1 and the total estimated costs of subcontracting per beneficiary must be set out in Annex 2. The Agency may however approve subcontracts not set out in Annex 1 and 2 without amendment (see Article 55), if:

- they are specifically justified in the periodic financial report and

- they do not entail changes to the Agreement which would call into question the decision awarding the grant or breach the principle of equal treatment of applicants.

The beneficiary must ensure that the Agency, the Commission, the European Court of Auditors (ECA) and the European Anti-Fraud Office (OLAF) can exercise their rights under Articles 22 and 23 also towards its subcontractors.

13.1.2 The beneficiary must ensure that its obligations under Articles 35, 36, 38 and 46 also apply to the subcontractors.

If the beneficiary is a 'contracting authority' within the meaning of Directive 2004/18/EC or 'contracting entity' within the meaning of Directive 2004/17/EC, it must comply with the applicable national law on public procurement.

13.2 Consequences of non-compliance

If the beneficiary breaches any of its obligations under Article 13.1.1, the costs related to the subcontract concerned will be ineligible (see Article 6) and will be rejected (see Article 42).

If the beneficiary breaches any of its obligations under Article 13.1.2, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 14 — IMPLEMENTATION OF ACTION TASKS BY LINKED THIRD PARTIES

Not applicable

ARTICLE 15 — FINANCIAL SUPPORT TO THIRD PARTIES

Not applicable

ARTICLE 16 — PROVISION OF TRANS-NATIONAL OR VIRTUAL ACCESS TO RESEARCH INFRASTRUCTURE

Not applicable

SECTION 2 RIGHTS AND OBLIGATIONS RELATED TO THE GRANT ADMINISTRATION

ARTICLE 17 — GENERAL OBLIGATION TO INFORM

17.1 General obligation to provide information upon request

The beneficiary must provide — during implementation of the action or afterwards — any information requested in order to verify eligibility of the costs, proper implementation of the action and compliance with any other obligation under the Agreement.

17.2 Obligation to keep information up to date and to inform about events and circumstances likely to affect the Agreement

The beneficiary must keep information stored in the 'Beneficiary Register' (via the electronic exchange system; see Article 52) up to date, in particular, its name, address, legal representatives, legal form and organisation type.

The beneficiary must immediately inform the Agency of any of the following:

(a) **events** which are likely to affect significantly or delay the implementation of the action or the EU's financial interests, in particular:

  (i) changes in its legal, financial, technical, organisational or ownership situation

(b) **circumstances** affecting:

  (i) the decision to award the grant or

  (ii) compliance with requirements under the Agreement.

17.3 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 18 — KEEPING RECORDS — SUPPORTING DOCUMENTATION

18.1 Obligation to keep records and other supporting documentation

The beneficiary must — for a period of *five* years after the payment of the balance — keep records and other supporting documentation in order to prove the proper implementation of the action and the costs it declares as eligible.

It must make them available upon request (see Article 17) or in the context of checks, reviews, audits or investigations (see Article 22).

If there are on-going checks, reviews, audits, investigations, litigation or other pursuits of claims under the Agreement (including the extension of findings; see Articles 22), the beneficiary must keep the records and other supporting documentation until the end of these procedures.

The beneficiary must keep the original documents. Digital and digitalised documents are considered originals if they are authorised by the applicable national law. The Agency may accept non-original documents if it considers that they offer a comparable level of assurance.

18.1.1 Records and other supporting documentation on the scientific and technical implementation

The beneficiary must keep records and other supporting documentation on scientific and technical implementation of the action in line with the accepted standards in the respective field.

18.1.2 Records and other documentation to support the costs declared

The beneficiary must keep the records and documentation supporting the costs declared, in particular the following:

(a) for **actual costs**: adequate records and other supporting documentation to prove the costs declared, such as contracts, subcontracts, invoices and accounting records. In addition, the beneficiary' usual cost accounting practices and internal control procedures must enable direct reconciliation between the amounts declared, the amounts recorded in its accounts and the amounts stated in the supporting documentation;

(b) for **unit costs**: adequate records and other supporting documentation to prove the number of units declared. The beneficiary does not need to identify the actual eligible costs covered or to keep or provide supporting documentation (such as accounting statements) to prove the amount per unit.

In addition, **for direct personnel costs declared as unit costs calculated in accordance with the beneficiary's usual cost accounting practices**, the beneficiary must keep adequate records and documentation to prove that the cost accounting practices used comply with the conditions set out in Article 6.2, Point A.

The beneficiary may submit to the Commission, for approval, a certificate (drawn up in accordance with Annex 6) stating that its usual cost accounting practices comply with these conditions ('**certificate on the methodology**'). If the certificate is approved, costs declared in line with this methodology will not be challenged subsequently, unless the beneficiary has concealed information for the purpose of the approval.

(c) for **flat-rate costs**: adequate records and other supporting documentation to prove the eligibility of the costs to which the flat-rate is applied. The beneficiary does not need to identify the costs covered or provide supporting documentation (such as accounting statements) to prove the amount declared at a flat-rate.

In addition, for **personnel costs** (declared as actual costs or on the basis of unit costs), the beneficiary must keep **time records** for the number of hours declared. The time records must be in writing and approved by the persons working on the action and their supervisors, at least monthly. In the absence of reliable time records of the hours worked on the action, the Agency may accept alternative evidence supporting the number of hours declared, if it considers that it offers an adequate level of assurance.

As an exception, for **persons working exclusively on the action**, there is no need to keep time records, if the beneficiary signs a **declaration** confirming that the persons concerned have worked exclusively on the action.

18.2 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, costs insufficiently substantiated will be ineligible (see Article 6) and will be rejected (see Article 42), and the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 19 — SUBMISSION OF DELIVERABLES

19.1 Obligation to submit deliverables

The beneficiary must submit the '**deliverables**' identified in Annex 1, in accordance with the timing and conditions set out in it.

19.2 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the Agency may apply any of the measures described in Chapter 6.

ARTICLE 20 — REPORTING — PAYMENT REQUESTS

20.1 Obligation to submit reports

The beneficiary must submit to the Agency (see Article 52) the scientific and financial reports set out in this Article. The financial report includes the requests for payment.

The reports must be drawn up using the forms and templates provided in the electronic exchange system (see Article 52).

20.2 Scientific reporting — Reporting periods

The action is divided into the following '**scientific reporting periods**':
- SRP1: from month 1 to month 30
- *final SRP: from month 31 to 60.*

The beneficiary must submit to the Agency a:

- '**periodic scientific report**' within 60 days after the end of each period (except the last one) and
- '**final scientific report**' within 60 days after the end of the last reporting period.

The **periodic scientific report** must include:

(a) information about the **scientific progress** of the work;

(b) **achievements and results** of the action, such as publications and a declaration of any major change of scientific strategy;

(c) information on whether and how open access has been provided to these results (see Article 29);

(d) a summary of the achievements of the action for publication by the Agency.

The **final scientific report** must:

(a) present the **final results, achievements and conclusions** of the action, and how they have been disseminated (including via scientific publications) (see Article 29);

(b) contain a summary of the achievements of the action, for publication by the Agency.

20.3 Financial reporting — Payment requests — Reporting periods

The action is divided into the following '**financial reporting periods**':

- FRP1: from month 1 to month 18
- *FRP2: from month 19 to month 36*
- *FRP3: from month 37 to month 54*
- *final FRP: from month 55 to 60.*

The beneficiary must — within 60 days after the end of each period — submit to the Agency a '**financial report**' for each reporting period.

The **financial report** must contain:

(a) information on the eligible costs, including a '**breakdown of direct costs table**' and a '**budget follow-up table**';

(b) an '**individual financial statement**' (see Annex 4) from each beneficiary for the reporting period concerned.

The individual financial statement must detail the eligible costs (actual costs, unit costs and flat-rate costs [and lump sum costs]; see Article 6) for each budget category (see Annex 2).

The beneficiary must declare all eligible costs, even if — for actual costs, unit costs and flat-rate costs — they exceed the amounts indicated in the estimated budget (see Annex 2). Amounts which are not declared in a financial statement will not be taken into account by the Agency.

If an individual financial statement is not submitted for a reporting period, it may be included in the periodic financial report for the next reporting period.

The final financial statements must also detail the **receipts of the action** (see Article 5.3.3).

The beneficiary must **certify** that:

- the information provided is full, reliable and true;
- the costs declared are eligible (see Article 6);
- the costs can be substantiated by adequate records and supporting documentation (see Article 18) that will be produced upon request (see Article 17) or in the context of checks, audits and investigations (see Article 22), and
- for the last reporting period: that all the receipts have been declared (see Article 5.3.3);

(c) a '**summary financial statement**' (see Annex 4), created automatically by the electronic exchange system, including the **request for interim payment** (or — for the last financial reporting period — the **request for payment of the balance**);

(d) for the last financial reporting period only: a '**certificate on the financial statements**' (see Annex 5) for the beneficiary, if it requests a total contribution of EUR 325 000 or more, as reimbursement of actual costs and unit costs calculated on the basis of its usual cost accounting practices (see Article 5.2 and Article 6.2, Point A).

20.4 Currency for financial statements and conversion into euro

Financial statements must be drafted in euro.

If the beneficiary has accounting established in a currency other than the euro, it must convert the costs recorded in their accounts into euro at the average of the daily exchange rates published in the C series of the *Official Journal of the European Union*, calculated over the corresponding reporting period.

If no daily euro exchange rate is published in the *Official Journal of the European Union* for the currency in question, they must be converted at the average of the monthly accounting rates published on the Commission's website, calculated over the corresponding reporting period.

If the beneficiary has accounting established in euro, it must convert costs incurred in another currency into euro according to its usual accounting practices.

20.5 Language of reports

All reports (scientific and financial reports, including financial statements) must be submitted in the language of the Agreement.

20.6 Consequences of non-compliance — Suspension of the payment deadline — Termination

If the reports submitted do not comply with this Article, the Agency may suspend the payment deadline (see Article 47) and apply any of the other measures described in Chapter 6.

If the beneficiary breaches its obligation to submit the reports and if it fails to comply with this obligation within 30 days following a written reminder sent by the Agency, the Agreement may be terminated (see Article 50).

ARTICLE 21 — PAYMENTS AND PAYMENT ARRANGEMENTS

21.1 Payments to be made

The following payments will be made to the beneficiary:

- one **pre-financing payment**;
- one or more **interim payments**, on the basis of the request(s) for interim payment (see Article 20), and
- one **payment of the balance**, on the basis of the request for payment of the balance (see Article 20).

21.2 Pre-financing payment — Amount — Amount retained for the Guarantee Fund

The aim of the pre-financing is to provide the beneficiary with a float.

It remains the property of the EU until the payment of the balance.

*The amount of the pre-financing payment will be EUR **498,437.50** (four hundred and ninety eight thousand four hundred and thirty seven EURO and fifty eurocents).*

The Agency will — except if Article 48 applies - make the pre-financing payment to the beneficiary within 30 days, either from the entry into force of the Agreement (see Article 58) or from 10 days before the starting date of the action (see Article 3)whichever is the latest.

*An amount of EUR **99,687.50** (ninety nine thousand six hundred and eighty seven EURO and fifty eurocents), corresponding to the 5% of the maximum grant amount (see Article 5.1), is retained by the Agency from the pre-financing payment and transferred into the '**Guarantee Fund**'.*

21.3 Interim payments — Amount — Calculation

Interim payments reimburse the eligible costs incurred for the implementation of the action during the corresponding reporting periods.

The Agency will pay to the beneficiary the amount due as interim payment within 90 days from receiving the financial report (see Article 20.3), except if Articles 47 or 48 apply.

Payment is subject to the approval of the financial report. Its approval does not imply recognition of the compliance, authenticity, completeness or correctness of its content.

The **amount due as interim payment** is calculated by the Agency in the following steps:

Step 1 – Application of the reimbursement rate

Step 2 – Limit to 90% of the maximum grant amount

21.3.1 Step 1 — Application of the reimbursement rate

The reimbursement rate (see Article 5.2) is applied to the eligible costs (actual costs, unit costs, flat-rate costs; see Article 6) declared by the beneficiary (see Article 20) and approved by the Agency (see above) for the concerned reporting period.

21.3.2 Step 2 — Limit to 90% of the maximum grant amount

The total amount of pre-financing and interim payments must not exceed 90% of the maximum grant amount specified in Article 5.1. The maximum amount for the interim payment will be calculated as follows:

{90% of the maximum grant amount (see Article 5.1)

minus

{pre-financing and previous interim payments}}.

21.4 Payment of the balance — Amount — Calculation — Release of the amount retained for the Guarantee Fund

The payment of the balance reimburses the remaining part of the eligible costs incurred by the beneficiary for the implementation of the action.

If the total amount of earlier payments is greater than the final grant amount (see Article 5.3), the payment of the balance takes the form of a recovery (see Article 44).

If the total amount of earlier payments is lower than the final grant amount, the Agency will pay the balance within 90 days from receiving the financial report and the final scientific report (see Article 20.3), except if Articles 47 or 48 apply.

Payment is subject to the approval of the financial and final scientific reports. Their approval does not imply recognition of the compliance, authenticity, completeness or correctness of their content.

The **amount due as the balance** is calculated by the Agency by deducting the total amount of pre-financing and interim payments (if any) already made, from the final grant amount determined in accordance with Article 5.3:

{{final grant amount (see Article 5.3)

minus

{pre-financing and interim payments (if any) made}}.

At the payment of the balance, the amount retained for the Guarantee Fund (see above) will be released and:

- if the balance is positive: the amount released will be paid in full to the beneficiary, together with the amount due as the balance;
- if the balance is negative (payment of the balance taking the form of recovery): it will be deducted from the amount released (see Article 44.1.2). If the resulting amount:
    - is positive, it will be paid to the beneficiary,
    - is negative, it will be recovered.

The amount to be paid may however be offset — without the beneficiary's consent — against any other amount owed by the beneficiary to the Agency, the Commission or another executive agency (under the EU or Euratom budget), up to the maximum EU contribution indicated, for the beneficiary, in the estimated budget (see Annex 2).

21.5 Notification of amounts due

When making payments, the Agency will formally notify to the beneficiary the amount due, specifying whether it concerns an interim payment or the payment of the balance.

For the payment of the balance, the notification will also specify the final grant amount.

In the case of reduction of the grant or recovery of undue amounts, the notification will be preceded by the contradictory procedure set out in Articles 43 and 44.

21.6 Currency for payments

The Agency will make all payments in euro.

21.7 Payments to the beneficiary

Payments will be made to the beneficiary.

Payments to the beneficiary will discharge the Agency from its payment obligation.

21.8 Bank account for payments

All payments will be made to the following bank account:

Name of bank: ING BELGIUM NV/SA (FORMERLY BANK BRUSSELS LAMBERT SA), BRUSS
Address of branch: 60, COURS SAINT MICHEL BRUSSELS, Belgium
Full name of the account holder: UNIVERSITEIT GENT
Full account number (including bank codes):
IBAN code: BE59390096580026

21.9 Costs of payment transfers

The cost of the payment transfers is borne as follows:

- the Agency bears the cost of transfers charged by its bank;
- the beneficiary bears the cost of transfers charged by its bank;
- the party causing a repetition of a transfer bears all costs of the repeated transfer.

21.10 Date of payment

Payments by the Agency are considered to have been carried out on the date when they are debited to its account.

21.11 Consequences of non-compliance

21.11.1 *If the Agency does not pay within the payment deadlines (see above), the beneficiary is entitled to **late-payment interest** at the rate applied by the European Central Bank (ECB) for its main refinancing operations in euros ('reference rate'), plus three and a half points. The reference rate is the rate in force on the first day of the month in which the payment deadline expires, as published in the C series of the Official Journal of the European Union.*

If the late-payment interest is lower than or equal to EUR 200, it will be paid to the beneficiary only upon request submitted within two months of receiving the late payment.

Late-payment interest is not due if the beneficiary is an EU Member State (including regional and local government authorities or other public bodies acting on behalf of a Member State for the purpose of this Agreement).

Suspension of the payment deadline or payments (see Articles 47 and 48) will not be considered as late payment.

Late-payment interest covers the period running from the day following the due date for payment (see above), up to and including the date of payment.

Late-payment interest is not considered for the purposes of calculating the final grant amount.

21.11.2 Not applicable

ARTICLE 22 — CHECKS, REVIEWS, AUDITS AND INVESTIGATIONS — EXTENSION OF FINDINGS

22.1 Checks, reviews and audits by the Agency and the Commission

22.1.1 Right to carry out checks

The Agency or the Commission will — during the implementation of the action or afterwards — check the proper implementation of the action and compliance with the obligations under the Agreement, including assessing deliverables and reports.

For this purpose the Agency or the Commission may be assisted by external persons or bodies.

The Agency or the Commission may also request additional information in accordance with Article 17. The Agency or the Commission may request the beneficiary to provide such information to it directly.

Information provided must be accurate, precise and complete and in the format requested, including electronic format.

22.1.2 Right to carry out reviews

The Agency or the Commission may — during the implementation of the action or afterwards — carry out reviews on the proper implementation of the action (including assessment of deliverables and reports), compliance with the obligations under the Agreement and continued scientific or technological relevance of the action.

Reviews may be started **up to two years after the payment of the balance**. They will be formally notified to the beneficiary and will be considered to have started on the date of the formal notification.

If the review is carried out on a third party (see Articles 10 to 16), the beneficiary must inform the third party.

The Agency or the Commission may carry out reviews directly (using its own staff) or indirectly (using external persons or bodies appointed to do so). It will inform the beneficiary of the identity of the external persons or bodies. It has the right to object to the appointment on grounds of commercial confidentiality.

The beneficiary must provide — within the deadline requested — any information and data in addition to deliverables and reports already submitted (including information on the use of resources). The Agency or the Commission may request the beneficiary to provide such information to it directly.

The beneficiary may be requested to participate in meetings, including with external experts.

For **on-the-spot** reviews, the beneficiary must allow access to its sites and premises, including to external persons or bodies, and must ensure that information requested is readily available.

Information provided must be accurate, precise and complete and in the format requested, including electronic format.

On the basis of the review findings, a '**review report**' will be drawn up.

The Agency or the Commission will formally notify the review report to the beneficiary, which has 30 days to formally notify observations ('**contradictory review procedure**').

Reviews (including review reports) are in the language of the Agreement.

22.1.3 Right to carry out audits

The Agency or the Commission may — during the implementation of the action or afterwards — carry out audits on the proper implementation of the action and compliance with the obligations under the Agreement.

Audits may be started **up to two years after the payment of the balance**. They will be formally notified to the beneficiary and will be considered to have started on the date of the formal notification.

If the audit is carried out on a third party (see Articles 10 to 16), the beneficiary must inform the third party.

The Agency or the Commission may carry out audits directly (using its own staff) or indirectly (using external persons or bodies appointed to do so). It will inform the beneficiary of the identity of the external persons or bodies. It has the right to object to the appointment on grounds of commercial confidentiality.

The beneficiary must provide — within the deadline requested — any information (including complete accounts, individual salary statements or other personal data) to verify compliance with the Agreement. The Agency or the Commission may request beneficiary to provide such information to it directly.

For **on-the-spot** audits, the beneficiary must allow access to its sites and premises, including to external persons or bodies, and must ensure that information requested is readily available.

Information provided must be accurate, precise and complete and in the format requested, including electronic format.

On the basis of the audit findings, a '**draft audit report**' will be drawn up.

The Agency or the Commission will formally notify the draft audit report to the beneficiary, which has 30 days to formally notify observations ('**contradictory audit procedure**'). This period may be extended by the Agency or the Commission in justified cases.

The '**final audit report**' will take into account observations by the beneficiary. The report will be formally notified to it.

Audits (including audit reports) are in the language of the Agreement.

The Agency or the Commission may also access the beneficiary' statutory records for the periodical assessment of unit costs or flat-rate amounts.

22.2 Investigations by the European Anti-Fraud Office (OLAF)

Under Regulations No 883/2013[9] and No 2185/96[10] (and in accordance with their provisions and procedures), the European Anti-Fraud Office (OLAF) may — at any moment during implementation of the action or afterwards — carry out investigations, including on-the-spot checks and inspections, to establish whether there has been fraud, corruption or any other illegal activity affecting the financial interests of the EU.

22.3 Checks and audits by the European Court of Auditors (ECA)

Under Article 287 of the Treaty on the Functioning of the European Union (TFEU) and Article 161 of the Financial Regulation No 966/2012[11], the European Court of Auditors (ECA) may — at any moment during implementation of the action or afterwards — carry out audits.

The ECA has the right of access for the purpose of checks and audits.

22.4 Checks, reviews, audits and investigations for international organisations

Not applicable

22.5 Consequences of findings in checks, reviews, audits and investigations —Extension of findings

22.5.1 Findings in this grant

Findings in checks, reviews, audits or investigations carried out in the context of this grant may lead to the rejection of ineligible costs (see Article 42), reduction of the grant (see Article 43), recovery of undue amounts (see Article 44) or to any of the other measures described in Chapter 6.

Rejection of costs or reduction of the grant after the payment of the balance will lead to a revised final grant amount (see Article 5.4).

Findings in checks, reviews, audits or investigations may lead to a request for amendment for the modification of Annex 1 (see Article 55).

Checks, reviews, audits or investigations that find systemic or recurrent errors, irregularities, fraud or breach of obligations may also lead to consequences in other EU or Euratom grants awarded under similar conditions (‘**extension of findings from this grant to other grants**’).

Moreover, findings arising from an OLAF investigation may lead to criminal prosecution under national law.

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[9] Regulation (EU, Euratom) No 883/2013 of the European Parliament and of the Council of 11 September 2013 concerning investigations conducted by the European Anti-Fraud Office (OLAF) and repealing Regulation (EC) No 1073/1999 of the European Parliament and of the Council and Council Regulation (Euratom) No 1074/1999 (OJ L 248, 18.09.2013, p. 1).

[10] Council Regulation (Euratom, EC) No 2185/1996 of 11 November 1996 concerning on-the-spot checks and inspections carried out by the Commission in order to protect the European Communities' financial interests against fraud and other irregularities (OJ L 292, 15.11.1996, p. 2).

[11] Regulation (EU, EURATOM) No 966/2012 of the European Parliament and of the Council of 25 October 2012 on the financial rules applicable to the general budget of the Union and repealing Council Regulation (EC, EURATOM)) No 1605/2002 (OJ L 298, 26.10.2012, p. 1).

22.5.2 Findings in other grants

The Agency or the Commission may extend findings from other grants to this grant ('**extension of findings from other grants to this grant**'), if:

(a) the beneficiary is found, in other EU or Euratom grants awarded under similar conditions, to have committed systemic or recurrent errors, irregularities, fraud or breach of obligations that have a material impact on this grant and

(b) those findings are formally notified to the beneficiary — together with the list of grants affected by the findings — no later than two years after the payment of the balance of this grant.

The extension of findings may lead to the rejection of costs (see Article 42), reduction of the grant (see Article 43), recovery of undue amounts (see Article 44), suspension of payments (see Article 48), suspension of the action implementation (see Article 49) or termination (see Article 50).

22.5.3 Procedure

The Agency or the Commission will formally notify the beneficiary the systemic or recurrent errors and its intention to extend these audit findings, together with the list of grants affected.

22.5.3.1 If the findings concern **eligibility of costs**: the formal notification will include:

(a) an invitation to submit observations on the list of grants affected by the findings;

(b) the request to submit **revised financial statements** for all grants affected;

(c) the **correction rate for extrapolation** established by the Agency or the Commission on the basis of the systemic or recurrent errors, to calculate the amounts to be rejected if the beneficiary:

(i) considers that the submission of revised financial statements is not possible or practicable or

(ii) does not submit revised financial statements.

The beneficiary has 90 days from receiving notification to submit observations, revised financial statements or to propose a duly substantiated **alternative correction method**. This period may be extended by the Agency or the Commission in justified cases.

The amounts to be rejected will be determined on the basis of the revised financial statements, subject to their approval.

If the Agency or the Commission does not receive any observations or revised financial statements, does not accept the observations or the proposed alternative correction method or does not approve the revised financial statements, it will formally notify the beneficiary the application of the initially notified correction rate for extrapolation.

If the Agency or the Commission accepts the alternative correction method proposed by the beneficiary, it will formally notify the application of the accepted alternative correction method.

22.5.3.2 If the findings concern **improper implementation** or a **breach of another obligation**: the formal notification will include:

(a) an invitation to submit observations on the list of grants affected by the findings and

(b) the flat-rate the Agency or the Commission intends to apply according to the principle of proportionality.

The beneficiary has 90 days from receiving notification to submit observations or to propose a duly substantiated alternative flat-rate.

If the Agency or the Commission does not receive any observations or does not accept the observations or the proposed alternative flat-rate, it will formally notify the beneficiary the application of the initially notified flat-rate.

If the Agency or the Commission accepts the alternative flat-rate proposed by the beneficiary, it will formally notify the application of the accepted alternative flat-rate.

22.6 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, any insufficiently substantiated costs will be ineligible (see Article 6) and will be rejected (see Article 42).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 23 — EVALUATION OF THE IMPACT OF THE ACTION

23.1 Right to evaluate the impact of the action

The Agency or the Commission may carry out interim and final evaluations of the impact of the action measured against the objective of the EU programme.

Evaluations may be started during implementation of the action and up to five years after the payment of the balance. The evaluation is considered to start on the date of the formal notification to the beneficiary.

The Agency or the Commission may make these evaluations directly (using its own staff) or indirectly (using external bodies or persons it has authorised to do so).

The beneficiary must provide any information relevant to evaluate the impact of the action, including information in electronic format.

23.2 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the Agency may apply the measures described in Chapter 6.

SECTION 3 RIGHTS AND OBLIGATIONS RELATED TO BACKGROUND AND RESULTS

SUBSECTION 1 GENERAL

ARTICLE 23a — MANAGEMENT OF INTELLECTUAL PROPERTY

23a.1 Obligation to take measures to implement the Commission Recommendation on the management of intellectual property in knowledge transfer activities

If the beneficiary is a university or other public research organisation it must take measures to implement the principles set out in Points 1 and 2 of the Code of Practice annexed to the Commission Recommendation on the management of intellectual property in knowledge transfer activities[12].

This does not change the obligations set out in Subsections 2 and 3 of this Section.

The beneficiary must ensure that researchers and third parties involved in the action are aware of them.

23a.2 Consequences of non-compliance

If the beneficiary breaches its obligations under this Article, the Agency may apply any of the measures described in Chapter 6.

SUBSECTION 2 RIGHTS AND OBLIGATIONS RELATED TO BACKGROUND

ARTICLE 24 — AGREEMENT ON BACKGROUND

Not applicable

ARTICLE 25 — ACCESS RIGHTS TO BACKGROUND

25.1 Exercise of access rights — Waiving of access rights — No sub-licensing

To exercise access rights, this must first be requested in writing ('**request for access**').

'**Access rights**' means rights to use results or background under the terms and conditions laid down in this Agreement.

Waivers of access rights are not valid unless in writing.

Unless agreed otherwise, access rights do not include the right to sub-license.

25.2 Access rights for other beneficiaries, for implementing their own tasks under the action

Not applicable

25.3 Access rights for other beneficiaries, for exploiting their own results

Not applicable

25.4 Access rights for affiliated entities

Not applicable

[12] Commission Recommendation C (2008) 1329 of 10.4.2008 on the management of intellectual property in knowledge transfer activities and the Code of Practice for universities and other public research institutions attached to this recommendation.

25.5 Access rights for third parties

Not applicable

25.6 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

SUBSECTION 3 RIGHTS AND OBLIGATIONS RELATED TO RESULTS

ARTICLE 26 — OWNERSHIP OF RESULTS

26.1 Ownership by the beneficiary that generates the results

The beneficiary owns the results it generates.

'**Results**' means any (tangible or intangible) output of the action such as data, knowledge or information — whatever its form or nature, whether it can be protected or not — that is generated in the action, as well as any rights attached to it, including intellectual property rights.

26.2 Joint ownership by several beneficiaries

Not applicable

26.3 Rights of third parties (including personnel and the principal investigator)

If third parties (including personnel and the principal investigator) may claim rights to the results, the beneficiary must ensure that it complies with its obligations under the Agreement.

If a third party generates results for the beneficiary, the beneficiary must obtain all necessary rights (transfer, licences or other) from the third party, in order to be able to respect its obligations as if those results were generated by the beneficiary itself.

If obtaining the rights is impossible, the beneficiary must refrain from using the third party to generate the results.

26.4 *Agency* ownership, to protect results

26.4.1 *The Agency* may — with the consent of the beneficiary — assume ownership of results to protect them, if the beneficiary intends — up to four years after the period set out in Article 3 — to disseminate its results without protecting them, except in any of the following cases:

(a) the lack of protection is because protecting the results is not possible, reasonable or justified (given the circumstances);

(b) the lack of protection is because there is a lack of potential for commercial or industrial exploitation, or

(c) the beneficiary intends to transfer the results to a third party established in an EU Member State or associated country[13], which will protect them.

Before the results are disseminated and unless any of the cases above under Points (a), (b) or (c) applies, the beneficiary must formally notify the Agency and at the same time inform it of any reasons for refusing consent. The beneficiary may refuse consent only if it can show that its legitimate interests would suffer significant harm.

If the Agency decides to assume ownership, it will formally notify the beneficiary within 45 days of receiving notification.

No dissemination relating to these results may before the end of this period or, if the Agency takes a positive decision, until it has taken the necessary steps to protect the results.

26.4.2 *The Agency* may — with the consent of the beneficiary — assume ownership of results to protect them, if the beneficiary intends — up to four years after the period set out in Article 3 — to stop protecting them or not to seek an extension of protection, except in any of the following cases:

(a) the protection is stopped because of a lack of potential for commercial or industrial exploitation;

(b) an extension would not be justified given the circumstances.

The beneficiary that intends to stop protecting results or not seek an extension must — unless any of the cases above under Points (a) or (b) applies — formally notify the Agency at least 60 days before the protection lapses or its extension is no longer possible and at the same time inform it of any reasons for refusing consent. The beneficiary may refuse consent only if it can show that its legitimate interests would suffer significant harm.

If the Agency decides to assume ownership, it will formally notify the beneficiary within 45 days of receiving notification.

26.5 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to the any of the other measures described in Chapter 6.

ARTICLE 27 — PROTECTION OF RESULTS — VISIBILITY OF EU FUNDING

27.1 Obligation to protect the results

The beneficiary must examine the possibility of protecting its results and must adequately protect them — for an appropriate period and with appropriate territorial coverage — if:

(a) the results can reasonably be expected to be commercially or industrially exploited and

[13] For the definition, see 2.1(3) Rules for Participation Regulation No 1290/2013: 'associated country' means a third country which is party to an international agreement with the Union, as identified Article 7 of the H2020 Framework Programme Regulation No 1291/2013. Article 7 sets out the conditions for association of non-EU countries to Horizon 2020.

(b) protecting them is possible, reasonable and justified (given the circumstances).

When deciding on protection, the beneficiary must consider its own legitimate interests.

27.2 *Agency* ownership, to protect the results

If the beneficiary intends not to protect its results, to stop protecting them or not seek an extension of protection, *The Agency* may — under certain conditions (see Article 26.4) — assume ownership to ensure their (continued) protection.

27.3 Information on EU funding

Applications for protection of results (including patent applications) filed by or on behalf of the beneficiary must — unless the Agency requests or agrees otherwise or unless it is impossible — include the following:

> "The project leading to this application has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No [number])".

27.4 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such a breach may also lead to any of the other measures described in Chapter 6.

ARTICLE 28 — EXPLOITATION OF RESULTS

28.1 General obligation to exploit the results

The beneficiary must — up to four years after the period set out in Article 3 — take measures aiming to ensure '**exploitation**' of its results (either directly or indirectly, in particular through transfer or licensing; see Article 30) by:

(a) using them in further research activities (outside the action);

(b) developing, creating or marketing a product or process;

(c) creating and providing a service, or

(d) using them in standardisation activities.

This does not change the security obligations in Article 37, which still apply.

28.2 Results that could contribute to European or international standards — Information on EU funding

If results are incorporated in a standard, the beneficiary must — unless the Agency requests or agrees otherwise or unless it is impossible — ask the standardisation body to include the following statement in (information related to) the standard:

"Results incorporated in this standard have received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No [number])".

28.3 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the grant may be reduced in accordance with Article 43.

Such a breach may also lead to any of the other measures described in Chapter 6.

ARTICLE 29 — DISSEMINATION OF RESULTS — OPEN ACCESS — VISIBILITY OF EU FUNDING

29.1 Obligation to disseminate results

Unless it goes against its legitimate interests, the beneficiary must — as soon as possible — '**disseminate**' its results by disclosing them to the public by appropriate means (other than those resulting from protecting or exploiting the results), including in scientific publications (in any medium).

This does not change the obligation to protect results in Article 27, the confidentiality obligations in Article 36, the security obligations in Article 37 or the obligations to protect personal data in Article 39, all of which still apply.

If the beneficiary intends not to protect its results, it may — under certain conditions (see Article 26.4.1) — need to formally notify the Agency before dissemination takes place.

29.2 Open access to scientific publications

The beneficiary must ensure open access (free of charge online access for any user) to all peer-reviewed scientific publications relating to its results.

In particular, it must:

(a) as soon as possible and at the latest on publication, deposit a machine-readable electronic copy of the published version or final peer-reviewed manuscript accepted for publication in a repository for scientific publications.

Moreover, the beneficiary must aim to deposit at the same time the research data needed to validate the results presented in the deposited scientific publications.

(b) ensure open access to the deposited publication — via the repository — at the latest:

(i) on publication, if an electronic version is available for free via the publisher, or

(ii) within six months of publication (twelve months for publications in the social sciences and humanities) in any other case.

(c) ensure open access — via the repository — to the bibliographic metadata that identify the deposited publication, which must include a persistent identifier.

29.3 Open access to research data

Not applicable

29.4 Information on EU funding — Obligation and right to use the EU emblem and the ERC logo

Unless the Agency requests or agrees otherwise or unless it is impossible, any dissemination of results (in any form, including electronic) must:

(a) display the EU emblem, the ERC logo and

(b) include the following text:

> "This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No [number])".

When displayed together with another logo, the EU emblem and the ERC logo must have appropriate prominence.

For the purposes of its obligations under this Article, the beneficiary may use the EU emblem and the ERC logo without first obtaining approval from the Agency.

This does not however give it the right to exclusive use.

Moreover, the beneficiary may not appropriate the EU emblem, the ERC logo or any similar trademark or logo, either by registration or by any other means.

29.5 Disclaimer excluding Agency responsibility

Any dissemination of results must indicate that it reflects only the author's view and that the Agency is not responsible for any use that may be made of the information it contains.

29.6 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such a breach may also lead to any of the other measures described in Chapter 6.

ARTICLE 30 — TRANSFER AND LICENSING OF RESULTS

30.1 Transfer of ownership

The beneficiary may transfer ownership of its results.

It must however ensure that its obligations under Articles 26.2, 26.4, 27, 28, 29, 30 and 31 also apply to the new owner and that this owner has the obligation to pass them on in any subsequent transfer.

This does not change the security obligations in Article 37, which still apply.

30.2 Granting licenses

The beneficiary may grant licences to its results (or otherwise give the right to exploit them), if:

(a) this does not impede the rights under Article 31 and

(b) *not applicable.*

This does not change the dissemination obligations in Article 29 or security obligations in Article 37, which still apply.

30.3 Agency right to object to transfers or licensing

The Agency may — up to four years after the period set out in Article 3 — object to a transfer of ownership or the exclusive licensing of results, if:

(a) it is to a third party established in a non-EU country not associated with Horizon 2020 and

(b) the Agency considers that the transfer or licence is not in line with EU interests regarding competitiveness or is inconsistent with ethical principles or security considerations.

The beneficiary that intends to transfer ownership or grant an exclusive licence must formally notify the Agency before the intended transfer or licensing takes place and:

- *identify the specific results concerned;*
- *describe in detail the new owner or licensee and the planned or potential exploitation of the results, and*
- *include a reasoned assessment of the likely impact of the transfer or licence on EU competitiveness and its consistency with ethical principles and security considerations.*

The Agency may request additional information.

If the Agency decides to object to a transfer or exclusive licence, it must formally notify the beneficiary within 60 days of receiving notification (or any additional information it has requested).

No transfer or licensing may take place in the following cases:

- *pending the Agency decision, within the period set out above;*
- *if the Agency objects;*
- *until the conditions are complied with, if the Agency objection comes with conditions.*

30.4 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such a breach may also lead to any of the other measures described in Chapter 6.

ARTICLE 31 — ACCESS RIGHTS TO RESULTS

31.1 Exercise of access rights — Waiving of access rights — No sub-licensing

The conditions set out in Article 25.1 apply.

The obligations set out in this Article do not change the security obligations in Article 37, which still apply.

31.2 Access rights for other beneficiaries, for implementing their own tasks under the action

Not applicable

31.3 Access rights for other beneficiaries, for exploiting their own results

Not applicable

31.4 Access rights of affiliated entities

Not applicable

31.5 Access rights for the EU institutions, bodies, offices or agencies and EU Member States

The beneficiary must give access to its results — on a royalty-free basis — to EU institutions, bodies, offices or agencies, for developing, implementing or monitoring EU policies or programmes.

Such access rights are limited to non-commercial and non-competitive use.

This does not change the right to use any material, document or information received from the beneficiary for communication and publicising activities (see Article 38.2).

31.6 Access rights for principal investigators

The beneficiary must — on a royalty-free basis — give access to the principal investigator to results needed for *his/her* activities under the action.

31.7 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

SECTION 4 OTHER RIGHTS AND OBLIGATIONS

ARTICLE 32 — WORKING CONDITIONS FOR THE PRINCIPAL INVESTIGATOR AND *HIS/HER* TEAM

32.1 Obligations towards the principal investigator and *his/her* team

The beneficiaries must respect the following working conditions for the principal investigator and *his/her* team:

(a) take all measures to implement the principles set out in the Commission Recommendation on the European Charter for Researchers and the Code of Conduct for the Recruitment of Researchers[14] — in particular regarding working conditions, transparent recruitment processes based on merit and career development — and ensure that the principal investigator, researchers and third parties involved in the action are aware of them;

(b) enter — before signature of the Agreement — into a '**supplementary agreement**' with the principal investigator, that specifies:

(i) the obligation of the beneficiary to meet its obligations under the Agreement;

(ii) the obligation of the principal investigator to supervise the scientific and technological implementation of the action;

(iii) the obligation of the principal investigator to assume the responsibility for the scientific reporting for the beneficiary and contribute to the financial reporting;

(iv) the obligation of the principal investigator to meet the time commitments for implementing the action as described in Annex 1;

(v) the obligation of the principal investigator to apply the beneficiary's usual management practices;

(vi) the obligation of the principal investigator to inform the beneficiary immediately of any events or circumstances likely to affect the Agreement (see Article 17), such as:

- a planned transfer of the action (or part of it) to a new beneficiary (see Article 56a);
- any personal grounds affecting the implementation of the action;
- any changes in the information that was used as a basis for signing the supplementary agreement;
- any changes in the information that was used as a basis for awarding the grant;

(vii) the obligation of the principal investigator to ensure the visibility of EU funding in communications or publications and in applications for the protection of results (see Articles 27, 28, 29 and 38);

(viii) the obligation of the principal investigator to uphold the intellectual property rights of the beneficiary during the implementation of the action and afterwards;

(ix) the obligation of the principal investigator to maintain confidentiality (see Article 36);

[14] Commission Recommendation 2005/251/EC of 11 March 2005 on the European Charter for Researchers and on a Code of Conduct for the Recruitment of Researchers (OJ L 75, 22.3.2005, p. 67).

(x) for a transfer of the action (or part of it) to a new beneficiary (see Article 56a): the obligation of the principal investigator to:

- propose to the beneficiary (in writing) to what extent the action will be transferred and the details of the transfer arrangement;

- provide a statement to the beneficiary with the detailed results of the research up to the time of transfer;

(xi) the right of the Commission and the Agency, the European Court of Auditors (ECA) and the European Anti-fraud Office (OLAF) to exercise their rights under Articles 22 and 23 also towards the principal investigator;

(xii) the applicable law and the country in which disputes must be settled;

(c) provide the principal investigator with a copy of the signed Agreement;

(d) guarantee the principal investigator scientific independence, in particular for the:

(i) use of the budget to achieve the scientific objectives;

(ii) authority to publish as senior author and invite as co-authors those who have contributed substantially to the work;

(iii) preparation of scientific reports for the action;

(iv) selection and supervision of the other team members (hosted *and engaged* by the beneficiary or other legal entities), in line with the profiles needed to conduct the research and in accordance with the beneficiary's usual management practices;

(v) possibility to apply independently for funding;

(vi) access to appropriate space and facilities for conducting the research;

(e) provide — during the implementation of the action — research support to the principal investigator and the team members (regarding infrastructure, equipment, access rights, products and other services necessary for conducting the research);

(f) support the principal investigator and provide administrative assistance, in particular for the:

(i) general management of the work and his/her team

(ii) scientific reporting, especially ensuring that the team members send their scientific results to the principal investigator;

(iii) financial reporting, especially providing timely and clear financial information;

(iv) application of the beneficiary's usual management practices;

(v) general logistics of the action;

(vi) access to the electronic exchange system (see Article 52);

(g) inform the principal investigator immediately (in writing) of any events or circumstances likely to affect the Agreement (see Article 17);

(h) ensure that the principal investigator enjoy*s* adequate:

(i) conditions for annual, sickness and parental leave;

(ii) occupational health and safety standards;

(iii) insurance under the general social security scheme, such as pension rights;

(i) allow the transfer of the Agreement to a new beneficiary ('portability'; see Article 56a)

32.2 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 33 — GENDER EQUALITY

33.1 Obligation to aim for gender equality

The beneficiary must take all measures to promote equal opportunities between men and women in the implementation of the action. It must aim, to the extent possible, for a gender balance at all levels of personnel assigned to the action, including at supervisory and managerial level.

33.2 Consequences of non-compliance

If the beneficiary breaches its obligations under this Article, the Agency may apply any of the measures described in Chapter 6.

ARTICLE 34 — ETHICS

34.1 Obligation to comply with ethical principles

The beneficiary must carry out the action in compliance with:

(a) ethical principles (including the highest standards of research integrity — as set out, for instance, in the European Code of Conduct for Research Integrity[15] — and including, in particular, avoiding fabrication, falsification, plagiarism or other research misconduct) and

[15] The European Code of Conduct for Research Integrity of ALLEA (All European Academies) and ESF (European Science Foundation) of March 2011.
http://www.esf.org/fileadmin/Public_documents/Publications/Code_Conduct_ResearchIntegrity.pdf

(b) applicable international, EU and national law.

Funding will not be granted for activities carried out outside the EU if they are prohibited in all Member States.

The beneficiary must ensure that the activities under the action have an exclusive focus on civil applications.

The beneficiary must ensure that the activities under the action do not:

(a) aim at human cloning for reproductive purposes;

(b) intend to modify the genetic heritage of human beings which could make such changes heritable (with the exception of research relating to cancer treatment of the gonads, which may be financed), or

(c) intend to create human embryos solely for the purpose of research or for the purpose of stem cell procurement, including by means of somatic cell nuclear transfer.

34.2 Activities raising ethical issues

Activities raising ethical issues must comply with the '**ethics requirements**' set out in Annex 1.

Before the beginning of an activity raising an ethical issue, the beneficiary must submit (see Article 52) to the Agency copy of:

(a) any ethics committee opinion required under national law and

(b) any notification or authorisation for activities raising ethical issues required under national law.

If these documents are not in English, the beneficiary must also submit an English summary of the submitted opinions, notifications and authorisations (containing, if available, the conclusions of the committee or authority concerned).

If these documents are specifically requested for the action, the request must contain an explicit reference to the action title. The beneficiary must submit a declaration that all the submitted documents cover the action tasks.

34.3 Activities involving human embryos or human embryonic stem cells

Activities involving research on human embryos or human embryonic stem cells may be carried out only if:

- they are set out in Annex 1 or

- the beneficiary has obtained explicit approval (in writing) from the Agency (see Article 52).

34.4 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43) and the Agreement may be terminated (see Article 50).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 35 — CONFLICT OF INTERESTS

35.1 Obligation to avoid a conflict of interests

The beneficiary must take all measures to prevent any situation where the impartial and objective implementation of the action is compromised for reasons involving economic interest, political or national affinity, family or emotional ties or any other shared interest (‘**conflict of interests**’).

It must formally notify to the Agency without delay any situation constituting or likely to lead to a conflict of interests and immediately take all the necessary steps to rectify this situation.

The Agency may verify that the measures taken are appropriate and may require additional measures to be taken by a specified deadline.

35.2 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43) and the Agreement may be terminated (see Article 50).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 36 — CONFIDENTIALITY

36.1 General obligation to maintain confidentiality

During implementation of the action and for four years after the period set out in Article 3, the parties must keep confidential any data, documents or other material (in any form) that is identified as confidential at the time it is disclosed (‘**confidential information**’).

If the beneficiary requests, the Agency may agree to keep such information confidential for an additional period beyond the initial four years.

If information has been identified as confidential only orally, it will be considered to be confidential only if this is confirmed in writing within 15 days of the oral disclosure.

Unless otherwise agreed between the parties, they may use confidential information only to implement the Agreement.

The beneficiary may disclose confidential information to its personnel or third parties involved in the action only if they:

(a) need to know to implement the Agreement and

(b) are bound by an obligation of confidentiality.

This does not change the security obligations in Article 37, which still apply.

The Agency may disclose confidential information to its staff, other EU institutions and bodies or third parties, if:

(a) this is necessary to implement the Agreement or safeguard the EU's financial interests and

(b) the recipients of the information are bound by an obligation of confidentiality.

Under the conditions set out in Article 4 of the Rules for Participation Regulation No 1290/2013[16], the Commission must moreover make available information on the results to other EU institutions, bodies, offices or agencies as well as Member States or associated countries.

The confidentiality obligations no longer apply if:

(a) the disclosing party agrees to release the other party;

(b) the information was already known by the recipient or is given to him without obligation of confidentiality by a third party that was not bound by any obligation of confidentiality;

(c) the recipient proves that the information was developed without the use of confidential information;

(d) the information becomes generally and publicly available, without breaching any confidentiality obligation, or

(e) the disclosure of the information is required by EU or national law.

36.2 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 37 — SECURITY-RELATED OBLIGATIONS

37.1 Results with a security recommendation

Not applicable

37.2 Classified results

Not applicable

37.3 Activities involving dual-use goods or dangerous materials and substances

Not applicable

37.4 Consequences of non-compliance

Not applicable

[16] Regulation (EU) No 1290/2013 of the European Parliament and of the Council of 11 December 2013 laying down the rules for participation and dissemination in "Horizon 2020 - the Framework Programme for Research and Innovation (2014-2020)" (OJ L 347, 20.12.2013 p.81).

ARTICLE 38 — PROMOTING THE ACTION — VISIBILITY OF EU FUNDING

38.1 Communication activities by the beneficiary

38.1.1 Obligation to promote the action and its results

The beneficiary must promote the action and its results, by providing targeted information to multiple audiences (including the media and the public) in a strategic and effective manner.

This does not change the dissemination obligations in Article 29, the confidentiality obligations in Article 36 or the security obligations in Article 37, all of which still apply.

Before engaging in a communication activity expected to have a major media impact, the beneficiary must inform the Agency (see Article 52).

38.1.2 Information on EU funding — Obligation and right to use the EU emblem and the ERC logo

Unless the Agency requests or agrees otherwise or unless it is impossible, any communication activity related to the action (including in electronic form, via social media, etc.) and any infrastructure, equipment and major results funded by the grant must:

(a) display the EU emblem and the ERC Logo and

(b) include the following text:

> For communication activities: “This project has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement No [number])”.
>
> For infrastructure, equipment and major results: “This [infrastructure][equipment][insert type of result] is part of a project that has received funding from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement No [number])”.

When displayed together with another logo, the EU emblem and the ERC Logo must have appropriate prominence.

For the purposes of its obligations under this Article, the beneficiary may use the EU emblem and the ERC Logo without first obtaining approval from the Agency.

This does not, however, give it the right to exclusive use.

Moreover, the beneficiary may not appropriate the EU emblem and the ERC Logo or any similar trademark or logo, either by registration or by any other means.

38.1.3 Disclaimer excluding Agency responsibility

Any communication activity related to the action must indicate that it reflects only the author's view and that the Agency is not responsible for any use that may be made of the information it contains.

38.2 Communication activities by the Agency

38.2.1 Right to use the beneficiary’s materials, documents or information

The Agency may use, for its own communication and publicising activities, information relating to the action, documents notably summaries for publication and public deliverables as well as any other material, such as pictures or audio-visual material that it receives from the beneficiary (including in electronic form).

This does not change the confidentiality obligations in Article 36 and the security obligations in Article 37, all of which still apply.

However, if the Agency's use of these materials, documents or information would risk compromising legitimate interests, the beneficiary may request the Agency not to use it (see Article 52).

The right to use a beneficiary's or principal investigator's materials, documents and information includes:

(a) **use for its own purposes** (in particular, making them available to persons working for the Agency or any other EU institution, body, office or agency or body or institutions in EU Member States; and copying or reproducing them in whole or in part, in unlimited numbers);

(b) **distribution to the public** (in particular, publication as hard copies and in electronic or digital format, publication on the internet, as a downloadable or non-downloadable file, broadcasting by any channel, public display or presentation, communicating through press information services, or inclusion in widely accessible databases or indexes);

(c) **editing or redrafting** for communication and publicising activities (including shortening, summarising, inserting other elements (such as meta-data, legends, other graphic, visual, audio or text elements), extracting parts (e.g. audio or video files), dividing into parts, use in a compilation);

(d) **translation**;

(e) giving **access in response to individual requests** under Regulation (EC) No 1049/2001[17], without the right to reproduce or exploit;

(f) **storage** in paper, electronic or other form;

(g) **archiving**, in line with applicable document-management rules, and

(h) the right to authorise **third parties** to act on its behalf or sub-license the modes of exploitation set out in points (b),(c),(d) and (f) to third parties if needed for the communication and publicising activities of the Agency.

If the right of use is subject to rights of a third party (including personnel of the beneficiary and the principal investigator), the beneficiary must ensure that it complies with its obligations under this Agreement (in particular, by obtaining the necessary approval from the third parties concerned).

Where applicable (and if provided by the beneficiary or the principal investigator), the Agency will insert the following information:

[17] Regulation (EC) No 1049/2001 of the European Parliament and of the Council of 30 May 2001 regarding public access to European Parliament, Council and Commission documents, OJ L 145, 31.5.2001, p. 43.

"© – [year] – [name of the copyright owner]. All rights reserved. Licensed to the European Research Council Executive Agency (ERCEA) under conditions."

38.3 Consequences of non-compliance

If the beneficiary breaches any of its obligations under this Article, the grant may be reduced (see Article 43).

Such breaches may also lead to any of the other measures described in Chapter 6.

ARTICLE 39 — PROCESSING OF PERSONAL DATA

39.1 Processing of personal data by the Agency and the Commission

Any personal data under the Agreement will be processed by the Agency or the Commission under Regulation No 45/2001[18] and according to the 'notifications of the processing operations' to the Data Protection Officer (DPO) of the Agency or the Commission (publicly accessible in the DPO register).

Such data will be processed by the '**data controller**' of the Agency or the Commission for the purposes of implementing, managing and monitoring the Agreement or protecting the financial interests of the EU or Euratom (including checks, reviews, audits and investigations; see Article 22).

The persons whose personal data are processed have the right to access and correct their own personal data. For this purpose, they must send any queries about the processing of their personal data to the data controller, via the contact point indicated in the 'service specific privacy statement(s) (SSPS)' that are published on the Agency and the Commission websites.

They also have the right to have recourse at any time to the European Data Protection Supervisor (EDPS).

39.2 Processing of personal data by the beneficiary

The beneficiary must process personal data under the Agreement in compliance with applicable EU and national law on data protection (including authorisations or notification requirements).

The beneficiary may grant its personnel access only to data that is strictly necessary for implementing, managing and monitoring the Agreement.

The beneficiary must inform the personnel whose personal data are collected and processed by the Agency or the Commission. For this purpose, it must provide them with the service specific privacy statement(s) (SSPS) (see above), before transmitting their data to the Agency or the Commission.

39.3 Consequences of non-compliance

If the beneficiary breaches any of its obligations under Article 39.2, the Agency may apply any of the measures described in Chapter 6.

[18] Regulation (EC) No 45/2001 of the European Parliament and of the Council of 18 December 2000 on the protection of individuals with regard to the processing of personal data by the Community institutions and bodies and on the free movement of such data (OJ L 8, 12.01.2001, p. 1).

ARTICLE 40 — ASSIGNMENTS OF CLAIMS FOR PAYMENT AGAINST THE AGENCY

The beneficiary may not assign any of its claims for payment against the Agency to any third party, except if approved by the Agency on the basis of a reasoned, written request.

If the Agency has not accepted the assignment or the terms of it are not observed, the assignment will have no effect on it.

In no circumstances will an assignment release the beneficiary from its obligations towards the Agency.

CHAPTER 5 DIVISION OF THE BENEFICIARY'S ROLES AND RESPONSIBILITIES — RELATIONSHIP WITH COMPLEMENTARY BENEFICIARIES — RELATIONSHIP WITH PARTNERS OF A JOINT ACTION

ARTICLE 41 — DIVISION OF THE BENEFICIARY'S ROLES AND RESPONSIBILITIES — RELATIONSHIP WITH COMPLEMENTARY BENEFICIARIES — RELATIONSHIP WITH PARTNERS OF A JOINT ACTION

41.1 Roles and responsibility towards the Agency

The beneficiary has full responsibility for implementing the action and complying with the Agreement.

The beneficiary is itself responsible for:

(a) monitoring that the action is implemented properly (see Article 7);

(b) informing the Agency immediately of any events or circumstances likely to affect significantly or delay the implementation of the action (see Article 17);

(c) submit the deliverables and reports to the Agency (see Articles 19 and 20);

(d) submit to the Agency in good time any documents or information required by it

and may not subcontract these tasks to any third party.

41.2 Internal division of roles and responsibilities

Not applicable

41.3 Internal arrangements

Not applicable

41.4 Relationship with complementary beneficiaries — Collaboration agreement

Not applicable

41.5 Relationship with partners of a joint action — Coordination agreement

Not applicable

CHAPTER 6 REJECTION OF COSTS — REDUCTION OF THE GRANT — RECOVERY — PENALTIES — DAMAGES — SUSPENSION — TERMINATION — FORCE MAJEURE

SECTION 1 REJECTION OF COSTS — REDUCTION OF THE GRANT — RECOVERY — PENALTIES

ARTICLE 42 — REJECTION OF INELIGIBLE COSTS

42.1 Conditions

42.1.1 The Agency will — at the time of an **interim payment, at the payment of the balance** or **afterwards** — reject any costs which are ineligible (see Article 6), in particular following checks, reviews, audits or investigations (see Article 22).

42.1.2 The rejection may also be based on the **extension of findings from other grants to this grant**, under the conditions set out in Article 22.5.2.

42.2 Ineligible costs to be rejected — Calculation — Procedure

Ineligible costs will be rejected in full.

If the Agency rejects costs **without reduction of the grant** (see Article 43) or **recovery of undue amounts** (see Article 44), it will formally notify the beneficiary the rejection of costs, the amounts and the reasons why (if applicable, together with the notification of amounts due; see Article 21.5). The beneficiary may — within 30 days of receiving notification — formally notify the Agency of its disagreement and the reasons why.

If the Agency rejects costs **with reduction of the grant** or **recovery of undue amounts** , it will formally notify the rejection in the '**pre-information letter**' on reduction or recovery set out in Articles 43 and 44.

42.3 Effects

If the Agency rejects costs at the time of an **interim payment** or **the payment of the balance**, it will deduct them from the total eligible costs declared, for the action, in the periodic or final summary financial statement (see Articles 20.3 and 20.4). It will then calculate the interim payment or payment of the balance as set out in Articles 21.3 or 21.4.

If the Agency — **after an interim payment but before the payment of the balance** — rejects costs declared in a periodic summary financial statement, it will deduct them from the total eligible costs declared, for the action, in the next periodic summary financial statement or in the final summary financial statement. It will then calculate the interim payment or payment of the balance as set out in Articles 21.3 or 21.4.

If the Agency rejects costs **after the payment of the balance**, it will deduct the amount rejected from the total eligible costs declared, in the final summary financial statement. It will then calculate the revised final grant amount as set out in Article 5.4.

ARTICLE 43 — REDUCTION OF THE GRANT

43.1 Conditions

43.1.1 The Agency may — **at the payment of the balance** or **afterwards** — reduce the maximum grant amount (see Article 5.1), if the action has not been implemented properly as described in Annex 1 or another obligation under the Agreement has been breached.

43.1.2 The Agency may also reduce the maximum grant amount on the basis of the **extension of findings from other grants to this grant**, under the conditions set out in Article 22.5.2.

43.2 Amount to be reduced — Calculation — Procedure

The amount of the reduction will be proportionate to the improper implementation of the action or to the seriousness of the breach.

Before reduction of the grant, the Agency will formally notify a '**pre-information letter**' to the beneficiary:

- informing it of its intention to reduce the grant, the amount it intends to reduce and the reasons why and

- inviting it to submit observations within 30 days of receiving notification

If the Agency does not receive any observations or decides to pursue reduction despite the observations it has received, it will formally notify **confirmation** of the reduction (if applicable, together with the notification of amounts due; see Article 21).

43.3 Effects

If the Agency reduces the grant at the time of **the payment of the balance**, it will calculate the reduced grant amount for the action and then determine the amount due as payment of the balance (see Articles 5.3.4 and 21.4).

If the Agency reduces the grant **after the payment of the balance**, it will calculate the revised final grant amount (see Article 5.4). If the revised final grant amount is lower than the final grant amount, the Agency will recover the difference (see Article 44).

ARTICLE 44 — RECOVERY OF UNDUE AMOUNTS

44.1 Amount to be recovered — Calculation — Procedure

The Agency will — **at the payment of the balance** or **afterwards** — claim back amount that was paid but is not due under the Agreement.

44.1.1 Recovery after termination of a beneficiary's participation

Not applicable

44.1.2 Recovery at payment of the balance

If the payment of the balance takes the form of a recovery (see Article 21.4), the Agency will formally notify a '**pre-information letter**' to the beneficiary:

- informing it of its intention to recover, the amount due as the balance and the reasons why;

- specifying that it intends to deduct the amount to be recovered from the amount retained for the Guarantee Fund;

- inviting it to submit observations within 30 days of receiving notification.

If no observations are submitted or the Agency decides to pursue recovery despite the observations it has received, it will **confirm recovery** (together with the notification of amounts due; see Article 21.5) and:

- pay the difference between the amount to be recovered and the amount retained for the Guarantee Fund, **if the difference is positive** or

- formally notify to the beneficiary a **debit note** for the difference between the amount to be recovered and the amount retained for the Guarantee Fund, **if the difference is negative**. This note will also specify the terms and the date for payment.

If payment is not made by the date specified in the debit note, the Agency will **recover** the amount:

(a) by '**offsetting**' it — without the beneficiary's consent — against any amounts owed to the beneficiary concerned by the Agency, the Commission or another executive agency (from the EU or Euratom budget).

In exceptional circumstances, to safeguard the EU's financial interests, the Agency may offset before the payment date specified in the debit note;

(b) by **drawing on the Guarantee Fund**. The Agency or the Commission will formally notify the beneficiary the debit note on behalf of the Guarantee Fund and recover the amount:

(i) *not applicable*

(ii) by **taking legal action** (see Article 57) or by **adopting an enforceable decision** under Article 299 of the Treaty on the Functioning of the EU (TFEU) and Article 79(2) of the Financial Regulation No 966/2012.

If payment is not made by the date in the debit note, the amount to be recovered (see above) will be increased by **late-payment interest** at the rate set out in Article 21.11, from the day following the payment date in the debit note, up to and including the date the Agency or the Commission receives full payment of the amount.

Partial payments will be first credited against expenses, charges and late-payment interest and then against the principal.

Bank charges incurred in the recovery process will be borne by the beneficiary, unless Directive 2007/64/EC applies.

44.1.3 Recovery of amounts after payment of the balance

If, the revised final grant amount (see Article 5.4) is lower than the final grant amount, the beneficiary must repay the difference to the Agency.

The Agency will formally notify a **pre-information letter** to the beneficiary:

- informing it of its intention to recover, the due amount and the reasons why and
- inviting it to submit observations within 30 days of receiving notification.

If no observations are submitted or the Agency decides to pursue recovery despite the observations it has received, it will **confirm** the amount to be recovered and formally notify to the beneficiary a **debit note**. This note will also specify the terms and the date for payment.

If payment is not made by the date specified in the debit note, the Agency will **recover** the amount:

(a) by '**offsetting**' it — without the beneficiary's consent — against any amounts owed to the beneficiary concerned by the Agency, the Commission or another executive agency (from the EU or Euratom budget).

In exceptional circumstances, to safeguard the EU's financial interests, the Agency may offset before the payment date specified in the debit note;

(b) by **drawing on the Guarantee Fund**. The Agency or the Commission will formally notify the beneficiary the debit note on behalf of the Guarantee Fund and recover the amount:

(i) *not applicable*

(ii) by **taking legal action** (see Article 57) or by **adopting an enforceable decision** under Article 299 of the Treaty on the Functioning of the EU (TFEU) and Article 79(2) of the Financial Regulation No 966/2012.

If payment is not made by the date in the debit note, the amount to be recovered (see above) will be increased by **late-payment interest** at the rate set out in Article 21.11, from the day following the date for payment in the debit note, up to and including the date the Agency or the Commission receives full payment of the amount.

Partial payments will be first credited against expenses, charges and late-payment interest and then against the principal.

Bank charges incurred in the recovery process will be borne by the beneficiary, unless Directive 2007/64/EC applies.

ARTICLE 45 — ADMINISTRATIVE AND FINANCIAL PENALTIES

45.1 Conditions

Under Articles 109 and 131(4) of the Financial Regulation No 966/2012, the Agency may impose **administrative** and **financial penalties** if a beneficiary:

(a) has committed substantial errors, irregularities or fraud or is in serious breach of its obligations under the Agreement or

(b) has made false declarations about information required under the Agreement or for the submission of the proposal (or has not supplied such information).

Under Article 109(3) of the Financial Regulation No 966/2012, the Agency or the Commission may — under certain conditions and limits — publish decisions imposing administrative or financial penalties.

45.2 Duration — Amount of penalty — Calculation

Administrative penalties exclude the beneficiary from all contracts and grants financed from the EU or Euratom budget for a maximum of five years from the date the infringement is established by the Agency.

If the beneficiary commits another infringement within five years of the date the first infringement is established, the Agency may extend the exclusion period up to 10 years.

Financial penalties will be between 2% and 10% of the maximum EU contribution in the estimated budget (see Annex 2).

If the beneficiary commits another infringement within five years of the date the first infringement is established, the Agency may increase the rate of financial penalties to between 4% and 20%.

45.3 Procedure

Before applying a penalty, the Agency will formally notify the beneficiary:

- informing it of its intention to impose a penalty, its duration or amount and the reasons why and

- inviting it to submit observations within 30 days.

If the Agency does not receive any observations or decides to impose the penalty despite of observations it has received, it will formally notify **confirmation** of the penalty to the beneficiary and — in case of financial penalties — deduct the penalty from the payment of the balance or formally notify a **debit note**, specifying the amount to be recovered, the terms and the date for payment.

If payment is not made by the date specified in the debit note, the Agency or the Commission may **recover** the amount:

(a) by '**offsetting**' it — without the beneficiary's consent — against any amounts owed to the beneficiary concerned by the Agency, the Commission or another executive agency (from the EU or Euratom budget).

In exceptional circumstances, to safeguard the EU's financial interests, the Agency may offset before the payment date specified in the debit note;

(b) by **taking legal action** (see Article 57) or by **adopting an enforceable decision** under Article 299 of the Treaty on the Functioning of the EU (TFEU) and Article 79(2) of the Financial Regulation No 966/2012.

If payment is not made by the date in the debit note, the amount to be recovered (see above) will be increased by **late-payment interest** at the rate set out in Article 21.11, from the day following the payment date in the debit note, up to and including the date the Agency or the Commission receives full payment of the amount.

Partial payments will be first credited against expenses, charges and late-payment interest and then against the principal.

Bank charges incurred in the recovery process will be borne by the beneficiary, unless Directive 2007/64/EC applies.

SECTION 2 LIABILITY FOR DAMAGES

ARTICLE 46 — LIABILITY FOR DAMAGES

46.1 Liability of the Agency

The Agency cannot be held liable for any damage caused to the beneficiary (or to third parties) as a consequence of implementing the Agreement, including for gross negligence.

The Agency cannot be held liable for any damage caused by the beneficiary or third parties involved in the action, as a consequence on implementing the Agreement.

46.2 Liability of the beneficiary

46.2.1 Conditions

Except in case of force majeure (see Article 51), the beneficiary must compensate the Agency for any damage it sustains as a result of the implementation of the action or because the action was not implemented in full compliance with the Agreement.

46.2.2 Amount of damages - Calculation

The amount the Agency can claim from the beneficiary will correspond to the damage caused by that beneficiary.

46.2.3 Procedure

Before claiming damages, the Agency will formally notify the beneficiary:

- informing it of its intention to claim damages, the amount and the reasons why and
- inviting it to submit observations within 30 days.

If the Agency does not receive any observations or decides to claim damages despite the observations it has received, it will formally notify **confirmation** of the claim for damages and a **debit note**, specifying the amount to be recovered, the terms and the date for payment.

If payment is not made by the date specified in the debit note, the Agency or the Commission may **recover** the amount:

(a) by '**offsetting**' it — without the beneficiary's consent — against any amounts owed to the beneficiary concerned by the Agency, the Commission or another executive agency (from the EU or Euratom budget).

In exceptional circumstances, to safeguard the EU's financial interests, the Agency may offset before the payment date specified in the debit note;

(b) by **taking legal action** (see Article 57) or by **adopting an enforceable decision** under Article 299 of the Treaty on the Functioning of the EU (TFEU) and Article 79(2) of the Financial Regulation No 966/2012.

If payment is not made by the date in the debit note, the amount to be recovered (see above) will be increased by **late-payment interest** at the rate set out in Article 21.11, from the day following the payment date in the debit note, up to and including the date the Agency or the Commission receives full payment of the amount.

Partial payments will be first credited against expenses, charges and late-payment interest and then against the principal.

Bank charges incurred in the recovery process will be borne by the beneficiary, unless Directive 2007/64/EC applies.

SECTION 3 SUSPENSION AND TERMINATION

ARTICLE 47 — SUSPENSION OF PAYMENT DEADLINE

47.1 Conditions

The Agency may — at any moment — suspend the payment deadline (see Article 21.2 to 21.4) if a request for payment (see Article 20) cannot be approved because:

(a) it does not comply with the provisions of the Agreement (see Article 20);

(b) the technical reports or financial reports have not been submitted or are not complete or additional information is needed, or

(c) there is doubt about the eligibility of the costs declared in the financial statements and additional checks, reviews, audits or investigations are necessary.

47.2 Procedure

The Agency will formally notify the beneficiary of the suspension and the reasons why.

The suspension will **take effect** the day notification is sent by the Agency (see Article 52).

If the conditions for suspending the payment deadline are no longer met, the suspension will be **lifted** — and the remaining period will resume.

If the suspension exceeds two months, the beneficiary may request the Agency if the suspension will continue.

If the payment deadline has been suspended due to the non-compliance of the scientific or financial reports (see Article 20) and the revised report or statement is not submitted or was submitted but is also rejected, the Agency may also terminate the Agreement (see Article 50.3.1(l)).

ARTICLE 48 — SUSPENSION OF PAYMENTS

48.1 Conditions

The Agency may — at any moment — suspend, in whole or in part, the pre-financing payment and interim payments or the payment of the balance, if the beneficiary:

(a) has committed or is suspected of having committed substantial errors, irregularities, fraud or serious breach of obligations in the award procedure or under this Agreement or

(b) has committed — in other EU or Euratom grants awarded to it under similar conditions — systemic or recurrent errors, irregularities, fraud or serious breach of obligations that have a material impact on this grant (**extension of findings from other grants to this grant**; see Article 22.5.2).

48.2 Procedure

Before suspending payments, the Agency will formally notify the beneficiary:

- informing it of its intention to suspend payments and the reasons why and

- inviting it to submit observations within 30 days of receiving notification.

If the Agency does not receive observations or decides to pursue the procedure despite the observations it has received, it will formally notify **confirmation** of the suspension. Otherwise, it will formally notify that the suspension procedure is not continued.

The suspension will **take effect** the day the confirmation notification is sent by the Agency.

If the conditions for resuming payments are met, the suspension will be **lifted**. The Agency will formally notify the beneficiary.

During the suspension, the beneficiary must not submit a periodic report(s) (see Article 20.3). When the Agency resumes payments, the beneficiary may include them in the next periodic report.

The beneficiary may suspend implementation of the action (see Article 49.1) or terminate the Agreement (see Article 50.1 and 50.2).

ARTICLE 49 — SUSPENSION OF THE ACTION IMPLEMENTATION

49.1 Suspension of the action implementation, by the beneficiary

49.1.1 Conditions

The beneficiary may suspend implementation of the action or any part of it, if exceptional circumstances — in particular *force majeure* (see Article 51) — make implementation impossible or excessively difficult.

49.1.2 Procedure

The beneficiary must immediately formally notify to the Agency the suspension (see Article 52), stating:

- the reasons why and
- the expected date of resumption.

The suspension will **take effect** the day this notification is received by the Agency.

Once circumstances allow for implementation to resume, the beneficiary must immediately formally notify the Agency and request an **amendment** of the Agreement to set the date on which the action will be resumed, extend the duration of the action and make other changes necessary to adapt the action to the new situation (see Article 55) — unless the Agreement has been terminated (see Article 50).

The suspension will be **lifted** with effect from the resumption date set out in the amendment. This date may be before the date on which the amendment enters into force.

Costs incurred during suspension of the action implementation are not eligible (see Article 6).

49.2 Suspension of the action implementation, by the Agency

49.2.1 Conditions

The Agency may suspend implementation of the action or any part of it:

(a) if the beneficiary has committed or is suspected of having committed substantial errors, irregularities, fraud or serious breach of obligations in the award procedure or under this Agreement;

(b) if the beneficiary has committed — in other EU or Euratom grants awarded to it under similar conditions — systemic or recurrent errors, irregularities, fraud or serious breach of obligations that have a material impact on this grant (**extension of findings from other grants to this grant**; see Article 22.5.2), or

(c) if the action is suspected of having lost its scientific or technological relevance.

49.2.2 Procedure

Before suspending implementation of the action, the Agency will formally notify the beneficiary:

- informing it of its intention to suspend the implementation and the reasons why and
- inviting it to submit observations within 30 days of receiving notification.

If the Agency does not receive observations or decides to pursue the procedure despite the observations it has received, it will formally notify **confirmation** of the suspension. Otherwise, it will formally notify that the procedure is not continued.

The suspension will **take effect** five days after confirmation notification is received by the beneficiary (or on a later date specified in the notification).

It will be **lifted** if the conditions for resuming implementation of the action are met.

The beneficiary will be formally notified of the lifting and the Agreement will be **amended** to set the date on which the action will be resumed, extend the duration of the action and make other changes necessary to adapt the action to the new situation (see Article 55) — unless the Agreement has already been terminated (see Article 50).

The suspension will be lifted with effect from the resumption date set out in the amendment. This date may be before the date on which the amendment enters into force.

Costs incurred during suspension are not eligible (see Article 6).

The beneficiary may not claim damages due to suspension by the Agency (see Article 46).

Suspension of the action implementation does not affect the Agency*'s* right to terminate the Agreement (see Article 50), reduce the grant or recover amounts unduly paid (see Articles 43 and 44).

ARTICLE 50 — TERMINATION OF THE AGREEMENT

50.1 Termination of the Agreement by the beneficiary

50.1.1 Conditions and procedure

The beneficiary may — with the agreement of the principal investigator — terminate the Agreement.

The beneficiary must formally notify termination to the Agency (see Article 52), stating:

- the reasons why and
- the date the termination will take effect. This date must be after the notification.

If no reasons are given or if the Agency considers the reasons do not justify termination, the Agreement will be considered to have been '**terminated improperly**'.

The termination will **take effect** on the day specified in the notification.

50.1.2 Effects

The beneficiary must — within 60 days from when termination takes effect — submit:

(i) a periodic financial report (for the open reporting period until termination; see Article 20.3) and

(ii) the final scientific report (see Article 20.3).

If the Agency does not receive the reports within the deadline (see above), only costs which are included in an approved periodic financial report will be taken into account.

The Agency will **calculate** the final grant amount (see Article 5.3) and the balance (see Article 21.4) on the basis of the reports submitted. Only costs incurred until termination are eligible. Costs relating to contracts due for execution only after termination are not eligible.

Improper termination may lead to a reduction of the grant (see Article 43).

After termination, the beneficiary' obligations (in particular Articles 20, 22, 23, Section 3 of Chapter 4, 36, 37, 38 and 40) continue to apply.

50.2 Termination of the participation of one or more beneficiaries, by the beneficiaries

Not applicable

50.3 Termination of the Agreement, by the Agency

50.3.1 Conditions

The Agency may terminate the Agreement, if:

(a) not applicable;

(b) a change to the legal, financial, scientific organisational or ownership situation of the beneficiary is likely to substantially affect or delay the implementation of the action or calls into question the decision to award the grant;

(c) not applicable;

(d) implementation of the action is prevented by force majeure (see Article 51) or suspended by the beneficiary (see Article 49.1) and either:

  (i) resumption is impossible, or

  (ii) the necessary changes to the Agreement would call into question the decision awarding the grant or breach the principle of equal treatment of applicants;

(e) the beneficiary is declared bankrupt, being wound up, having its affairs administered by the courts, has entered into an arrangement with creditors, has suspended business activities, or is subject to any other similar proceedings or procedures under national law;

(f) the beneficiary (or a natural person who has the power to represent or take decisions on its behalf) has been found guilty of professional misconduct, proven by any means;

(g) the beneficiary does not comply with the applicable national law on taxes and social security;

(h) the action — with respect to the state of the art — is no longer of scientific or technological relevance or no longer has any breakthrough potential;

(i) not applicable;

(j) not applicable;

(k) the beneficiary (or a natural person who has the power to represent or take decisions on its behalf) has committed fraud, corruption, or is involved in a criminal organisation, money laundering or any other illegal activity affecting the EU's financial interests;

(l) the beneficiary (or a natural person who has the power to represent or take decisions on its behalf) has — in the award procedure or under the Agreement — committed:

(i) substantial errors, irregularities, fraud or

(ii) serious breach of obligations, including improper implementation of the action, submission of false information, failure to provide required information, breach of ethical principles;

(m) the beneficiary has committed — in other EU or Euratom grants awarded to it under similar conditions — systemic or recurrent errors, irregularities, fraud or serious breach of obligations that have a material impact on this grant ('**extension of findings from other grants to this grant**');

(n) *the* principal investigator is no longer in the position to continue working under the action.

50.3.2 Procedure

Before terminating the Agreement, the Agency will formally notify the beneficiary:

- informing of its intention to terminate and the reasons why, and

- inviting it, within 30 days of receiving notification, to submit observations and — in case of Point (l.ii) above — to inform the Agency of the measures to ensure compliance with the obligations under the Agreement.

If the Agency does not receive observations or decides to pursue the procedure despite the observations it has received, it will formally notify to the beneficiary (with copy to the principal investigator) **confirmation** of the termination and the date it will take effect. Otherwise, it will formally notify the beneficiary (with copy to the principal investigator) that the procedure is not continued.

The termination will **take effect**:

- for terminations under Points (b), (e), (g), (h), (j), (l.ii) and (n) above: on the day specified in the notification of the confirmation (see above);

- for terminations under Points (d), (f), (i), (k), (l.i) and (m) above: on the day after notification of the confirmation is received by the beneficiary.

50.3.3 Effects

The beneficiary must — within 60 days from when termination takes effect — submit:

(i) a periodic financial report (for the last open reporting period until termination) (see Article 20.3) and

(ii) a final scientific report (see Article 20.2).

If the Agreement is terminated for breach of the obligation to submit the report(s) (see Articles 20.6 and 50.3.1(l)), the beneficiary may not submit any reports after termination.

If the Agency does not receive the report(s) within the deadline (see above), only costs which are included in an approved periodic report will be taken into account.

The Agency will **calculate** the final grant amount (see Article 5.3) and the balance (see Article 21.4) on the basis of the report(s) submitted. Only costs incurred until termination takes effect are eligible (see Article 6). Costs relating to contracts due for execution only after termination are not eligible.

This does not affect the Agency's right to reduce the grant (see Article 43) or to impose administrative and financial penalties (Article 45).

The beneficiary may not claim damages due to termination by the Agency.

After termination, the beneficiary's obligations (in particular Articles 20, 22, 23, Section 3 of Chapter 4, 36, 37, 38, and 40) continue to apply.

SECTION 4 FORCE MAJEURE

ARTICLE 51 — FORCE MAJEURE

'Force majeure' means any situation or event that:

- prevents either party from fulfilling their obligations under the Agreement,
- was unforeseeable, exceptional situation and beyond the parties' control,
- was not due to error or negligence on their part (or on the part of third parties involved in the action), and
- proves to be inevitable in spite of exercising all due diligence.

The following cannot be invoked as force majeure:

- any default of a service, defect in equipment or material or delays in making them available, unless they stem directly from a relevant case of force majeure,
- labour disputes or strikes, or
- financial difficulties.

Any situation constituting force majeure must be formally notified to the other party without delay, stating the nature, likely duration and foreseeable effects.

The parties must immediately take all the necessary steps to limit any damage due to force majeure and do their best to resume implementation of the action as soon as possible.

The party prevented by force majeure from fulfilling its obligations under the Agreement cannot be considered in breach of them.

CHAPTER 7 FINAL PROVISIONS

ARTICLE 52 — COMMUNICATION BETWEEN THE PARTIES

52.1 Form and means of communication

Communication under the Agreement (information, requests, submissions, 'formal notifications', etc.) must:

- be made in writing and
- bear the number of the Agreement.

Until the payment of the balance: all communication must be made through the electronic exchange system and using the forms and templates provided there.

After the payment of the balance: formal notifications must be made by registered post with proof of delivery ('formal notification on paper').

Communications in the electronic exchange system must be made by persons authorised according to the 'Terms and Conditions of Use of the electronic exchange system'. For naming the authorised persons, the beneficiary must have designated — before the signature of this Agreement — a 'Legal Entity Appointed Representative (LEAR)'. The role and tasks of the LEAR are stipulated in his/her appointment letter (see Terms and Conditions of Use of the electronic exchange system).

If the electronic exchange system is temporarily unavailable, instructions will be given on the Agency and the Commission websites.

52.2 Date of communication

Communications are considered to have been made when they are sent by the sending party (i.e. on the date and time they are sent through the electronic exchange system).

Formal notifications through the **electronic** exchange system are considered to have been made when they are received by the receiving party (i.e. on the date and time of acceptance by the receiving party, as indicated by the time stamp). A formal notification that has not been accepted within 10 days after sending is considered to have been accepted.

Formal notifications **on paper** sent by**registered post** with proof of delivery (only after the payment of the balance) are considered to have been made on either:

- the delivery date registered by the postal service or
- the deadline for collection at the post office.

If the electronic exchange system is temporarily unavailable, the sending party cannot be considered in breach of its obligation to send a communication within a specified deadline.

52.3 Addresses for communication

The **electronic** exchange system must be accessed via the following URL:

https://ec.europa.eu/research/participants/portal/desktop/en/projects/

The Agency will formally notify the beneficiary in advance any changes to this URL.

Formal notifications on paper (only after the payment of the balance) addressed **to the Agency** must be sent to the following address:

European Research Council Executive Agency (ERCEA)
Consolidator Grant
Rue de la Loi 200
B-1049 Brussels Belgium

Formal notifications on paper (only after the payment of the balance) addressed **to the beneficiary** must be sent to its legal address as specified in the Beneficiary Register (in the electronic exchange system).

ARTICLE 53 — INTERPRETATION OF THE AGREEMENT

53.1 Precedence of the Terms and Conditions over the Annexes

The provisions in the Terms and Conditions of the Agreement take precedence over its Annexes.

Annex 2 takes precedence over Annex 1.

53.2 Privileges and immunities

Not applicable

ARTICLE 54 — CALCULATION OF PERIODS, DATES AND DEADLINES

In accordance with Regulation No 1182/71[19], periods expressed in days, months or years are calculated from the moment the triggering event occurs.

The day during which that event occurs is not considered as falling within the period.

ARTICLE 55 — AMENDMENTS TO THE AGREEMENT

55.1 Conditions

The Agreement may be amended, unless the amendment entails changes to the Agreement which would call into question the decision awarding the grant or breach the principle of equal treatment of applicants.

Amendments may be requested by any of the parties.

55.2 Procedure

The party requesting an amendment must submit a request for amendment signed in the electronic exchange system (see Article 52).

[19] Regulation (EEC, Euratom) No 1182/71 of the Council of 3 June 1971 determining the rules applicable to periods, dates and time-limits (OJ L 124, 8.6.1971, p. 1).

The request for amendment must include:

- the reasons why;

- the appropriate supporting documents;

The Agency may request additional information.

If the party receiving the request agrees, it must sign the amendment in the electronic exchange system within 45 days of receiving notification (or any additional information the Agency has requested). If it does not agree, it must formally notify its disagreement within the same deadline. The deadline may be extended, if necessary for the assessment of the request. If no notification is received within the deadline, the request is considered to have been rejected

An amendment **enters into force** on the day of the signature of the receiving party.

An amendment **takes effect** on the date agreed by the parties or, in the absence of such an agreement, on the date on which the amendment enters into force.

ARTICLE 56 — ACCESSION TO THE AGREEMENT

56.1 Addition of new beneficiaries

In justified cases, the beneficiary may request the addition of a new beneficiary.

For this purpose, the beneficiary must submit a request for amendment in accordance with Article 55. It must include an Accession Form (see Annex 3) signed by the new beneficiary in the electronic exchange system (see Article 52).

New beneficiaries must assume the rights and obligations under the Agreement with effect from the date of their accession specified in the Accession Form (see Annex 3).

If a new beneficiary is added, the grant becomes a multi-beneficiary grant and the ERC Multi-beneficiary Model Grant Agreement will apply.

ARTICLE 56a — TRANSFER OF THE AGREEMENT TO A NEW BENEFICIARY — PORTABILITY OF THE GRANT

56a.1 Conditions

The principal investigator may request the transfer of the action (or his/her part of it) to a new beneficiary, provided that the objectives of the action remain achievable.

The beneficiary may object only on the basis that the transfer is not possible under national law.

56a.2 Procedure

The beneficiary must formally notify a **request for amendment** to the Agency (see Article 55).

56a.3 Effects

The former beneficiary must agree with the principal investigator and the new beneficiary on a plan to transfer the intellectual property rights under the Agreement to the new beneficiary.

The Agency will request the former beneficiary to transfer to the new beneficiary any part of the pre-financing (see Article 21) not covered by an approved financial report.

If requested by the principal investigator, the Agency may require the former beneficiary to transfer to the new beneficiary the equipment purchased and used exclusively for the action (against reimbursement of the costs that have not yet been depreciated). The former beneficiary may object only on the basis that the transfer is not possible under national law.

ARTICLE 57 — APPLICABLE LAW AND SETTLEMENT OF DISPUTES

57.1 Applicable law

The Agreement is governed by the applicable EU law, supplemented, if necessary by the law of Belgium.

57.2 Dispute settlement

If a dispute concerning the interpretation, application or validity of the Agreement cannot be settled amicably, the General Court — or, on appeal, the Court of Justice of the European Union — has sole jurisdiction. Such actions must be brought under Article 272 of the Treaty on the Functioning of the EU (TFEU).

If a dispute concerns administrative or financial penalties, offsetting or an enforceable decision under Article 299 TFEU (see Articles 44, 45 and 46), the beneficiary must bring action before the General Court — or, on appeal, the Court of Justice of the European Union — under Article 263 TFEU. Actions against enforceable decisions must be brought against the Commission (not against the Agency).

ARTICLE 58 — ENTRY INTO FORCE OF THE AGREEMENT

The Agreement will enter into force on the day of signature by the Agency or the beneficiary, depending on which is later.

SIGNATURES

For the beneficiary

Anne DE PAEPE with ECAS id npaeanne signed in the Participant Portal on 11/03/2015 at 08:16:18 (transaction id SigId-10976-XhcL6eZqzRatfOibZzhztYqjeAEbIPPChdMlniuVFDjtzzHYIB6rwWrzYvfzMpsr1kQyUKzIXdMu7d30oZAB6eEG-PHslUMVSXYCHayJ2ruzzVqW-lhOb4OQWFvAKWMQRmxIij36c693adoZ1hKzfUzG5rsC0). Timestamp by third party at Wed Mar 11 08:16:23 CET 2015

For the Agency

Marja HENNESSY with ECAS id lehtima signed in the Participant Portal on 11/03/2015 at 14:52:33 (transaction id SigId-11959-bbWXDgGDQ93KV19OpKSmGaZFCGMzkh83pIDbXegLdUZsZzP2SMP7L5XOgB9LCdlIOKQ6RHnn5VMW6F4XrWWizNG-PHslUMVSXYCHayJ2ruzzVqW-ohjNNumk2O8nutvSphDXFSZzfO7zx2mazKojg1LKOd58). Timestamp by third party at Wed Mar 11 14:52:35 CET 2015

European Research Council
Executive Agency

Established by the European Commission

ANNEX 1 (part A)

Consolidator Grant

NUMBER — 647755 — DYNPOR

Table of Contents

1.1. The project summary

Project Number [1]	647755	Project Acronym [2]	DYNPOR

One form per project

General information	
Project title [3]	First principle molecular dynamics simulations for complex chemical transformations in nanoporous materials
Starting date [4]	01/08/2015
Duration in months [5]	60
Call (part) identifier [6]	ERC-2014-CoG
Topic	ERC-CoG-2014 ERC Consolidator Grant
Fixed EC Keywords	Heterogeneous catalysis, Chemical reactions: mechanisms, dynamics, kinetics and catalytic reactions, Theoretical and computational chemistry
Free keywords	

Abstract [7]

Chemical transformations in nanoporous materials are vital in many application domains, such as catalysis, molecular separations, sustainable chemistry,…. Model-guided design is indispensable to tailoring materials at the nanometer scale level. At real operating conditions, chemical transformations taking place at the nanometer scale have a very complex nature, due to the interplay of several factors such as the number of particles present in the pores of the material, framework flexibility, competitive pathways, entropy effects,… The textbook concept of a single transition state is far too simplistic in such cases. A restricted number of configurations of the potential energy surface is not sufficient to capture the complexity of the transformation. My objective is to simulate complex chemical transformations in nanoporous materials using first principle molecular dynamics methods at real operating conditions, capturing the full complexity of the free energy surface. To achieve these goals advanced sampling methods will be used to explore the interesting regions of the free energy surface. The number of guest molecules at real operating conditions will be derived and the diffusion of small molecules through pores with blocking molecules will be studied. New theoretical models will be developed to keep track of both the framework flexibility and entropy of the lattice. The selected applications are timely and rely on an extensive network with prominent experimental partners. The applications will encompass contemporary catalytic conversions in zeolites, active site engineering in metal organic frameworks and structural transitions in nanoporous materials, and the expected outcomes will have the potential to yield groundbreaking new insights. The results are expected to have impact far beyond the horizon of the current project as they will contribute to the transition from static to dynamically based modeling tools within heterogeneous catalysis

1.2. List of Beneficiaries

Project Number [1]	647755	Project Acronym [2]	DYNPOR

List of Beneficiaries

No	Name	Short name	Country	Project entry month[8]	Project exit month
1	UNIVERSITEIT GENT	UNIVERSITEIT GENT	Belgium	1	60

1.3. Ethics Requirements

No ethics requirements indicated

1. Project number

The project number has been assigned by the Commission as the unique identifier for your project. It cannot be changed. The project number **should appear on each page of the grant agreement preparation documents (part A and part B)** to prevent errors during its handling.

2. Project acronym

Use the project acronym as given in the submitted proposal. It can generally not be changed. The same acronym **should appear on each page of the grant agreement preparation documents (part A and part B)** to prevent errors during its handling.

3. Project title

Use the title (preferably no longer than 200 characters) as indicated in the submitted proposal. Minor corrections are possible if agreed during the preparation of the grant agreement.

4. Starting date

Unless a specific (fixed) starting date is duly justified and agreed upon during the preparation of the Grant Agreement, the project will start on the first day of the month following the entry into force of the Grant Agreement (NB : entry into force = signature by the Commission). Please note that if a fixed starting date is used, you will be required to provide a written justification.

5. Duration

Insert the duration of the project in full months.

6. Call (part) identifier

The Call (part) identifier is the reference number given in the call or part of the call you were addressing, as indicated in the publication of the call in the Official Journal of the European Union. You have to use the identifier given by the Commission in the letter inviting to prepare the grant agreement.

7. Abstract

8. Project Entry Month

The month at which the participant joined the consortium, month 1 marking the start date of the project, and all other start dates being relative to this start date.

9. Work Package number

Work package number: WP1, WP2, WP3, ..., WPn

10. Lead beneficiary

This must be one of the beneficiaries in the grant (not a third party) - Number of the beneficiary leading the work in this work package

11. Person-months per work package

The total number of person-months allocated to each work package.

12. Start month

Relative start date for the work in the specific work packages, month 1 marking the start date of the project, and all other start dates being relative to this start date.

13. End month

Relative end date, month 1 marking the start date of the project, and all end dates being relative to this start date.

14. Deliverable number

Deliverable numbers: D1 - Dn

15. Type

Please indicate the type of the deliverable using one of the following codes:

R	Document, report
DEM	Demonstrator, pilot, prototype
DEC	Websites, patent fillings, videos, etc.
OTHER	

16. Dissemination level

Please indicate the dissemination level using one of the following codes:

PU	Public

CO Confidential, only for members of the consortium (including the Commission Services)
CI Classified, as referred to in Commission Decision 2001/844/EC

17. Delivery date for Deliverable

Month in which the deliverables will be available, month 1 marking the start date of the project, and all delivery dates being relative to this start date.

18. Milestone number

Milestone number:MS1, MS2, ..., MSn

19. Review number

Review number: RV1, RV2, ..., RVn

20. Installation Number

Number progressively the installations of a same infrastructure. An installation is a part of an infrastructure that could be used independently from the rest.

21. Installation country

Code of the country where the installation is located or IO if the access provider (the beneficiary or linked third party) is an international organization, an ERIC or a similar legal entity.

22. Type of access

VA if virtual access,
TA-uc if trans-national access with access costs declared on the basis of unit cost,
TA-ac if trans-national access with access costs declared as actual costs, and
TA-cb if trans-national access with access costs declared as a combination of actual costs and costs on the basis of unit cost.

23. Access costs

Cost of the access provided under the project. For virtual access fill only the second column. For trans-national access fill one of the two columns or both according to the way access costs are declared. Trans-national access costs on the basis of unit cost will result from the unit cost by the quantity of access to be provided.

ERC Consolidator Grant 2014

First principle molecular **dyn**amics simulations for complex chemical transformations in nano**por**ous materials

DYNPOR

Veronique Van Speybroeck (PI)
Ghent University, Center for Molecular Modeling (Belgium)
60 months

Chemical transformations in nanoporous materials are vital in many application domains, such as catalysis, molecular separations, sustainable chemistry,…. Model-guided design is indispensable to tailoring materials at the nanometer scale level.

At real operating conditions, chemical transformations taking place at the nanometer scale have a **very complex nature**, due to the interplay of several factors such as the number of particles present in the pores of the material, framework flexibility, competitive pathways, entropy effects,… The textbook concept of **a single transition state is** far **too simplistic** in such cases. A restricted number of configurations of the potential energy surface is not sufficient to capture the complexity of the transformation.

My objective is **to simulate complex chemical transformations in nanoporous materials using first principle molecular dynamics methods at real operating conditions, capturing the full complexity of the free energy surface.** To achieve these goals advanced sampling methods will be used to explore the interesting regions of the free energy surface. The number of guest molecules at real operating conditions will be derived and the diffusion of small molecules through pores with blocking molecules will be studied. New theoretical models will be developed to keep track of both the framework flexibility and entropy of the lattice.

The selected applications are timely and rely on an extensive network with prominent experimental partners. The applications will encompass contemporary **catalytic conversions in zeolites, active site engineering in metal organic frameworks and structural transitions in nanoporous materials,** and the expected outcomes will have the potential to yield groundbreaking new insights.

The results are expected to have impact far beyond the horizon of the current project as they will contribute to the transition from static to dynamically based modeling tools within heterogeneous catalysis.

Section a: Extended Synopsis

Situating the proposal and stating the objectives

Nanoporous materials are vital for various applications such as catalysis, molecular separations, energy storage…. [1] They are tractable due to their characteristic pore dimensions, high surface area, porosity, diversity. In this proposal, focus is set on **chemical transformations** taking place in nanoporous materials, encompassing catalytic reactions, active site engineering by intentional creation of defects, but also processes involving structural transitions in which the chemical architecture of the framework changes. There is a rapid growth in the range of new materials being synthesized, each with their own characteristic features. Zeolites are the most popular, but other intriguing materials have entered the scene during the last decades such as metal organic frameworks (MOFs). [2] Model-guided design is essential to progress further towards new applications and to optimize current processes which do not yet explore their full potential. [3]

Within the framework of my ERC starting grant "First principle chemical kinetics in nanoporous materials" I have contributed substantially to the level of maturity that molecular modelling has reached today in predicting rate coefficients and barriers for catalytic reactions occurring at a well defined active site and for a well defined elementary reaction. [4] Various seminal contributions have appeared in the past years by leading scientists. [5]

However, it is now the right moment to take **the next leap within the field of catalysis in nanoporous materials.** To date most theoretical methods rely on a static approach where information is extracted from discrete points on the potential energy surface at 0K, apart from some notable exceptions. [6]. The static approach has its merits, but fails in describing the complexity of the chemical conversion under real operating conditions. The **complexity** originates from the interplay of several factors such as high loadings of guest molecules in the pores of the material, framework flexibility, entropy effects and competitive pathways. (Figure 1) Under these circumstances, the reaction coordinate can no longer be described with a limited number of geometrical variables. Rather than focussing on one single transition state, one has to describe a chemical transformation as a transition from one stable free energy basin to another, thereby passing through a bottleneck region. Transitions may be not only energetically but also entropically hampered. A proper description of entropy driving forces in nanoporous materials poses a huge problem with currently available routines.

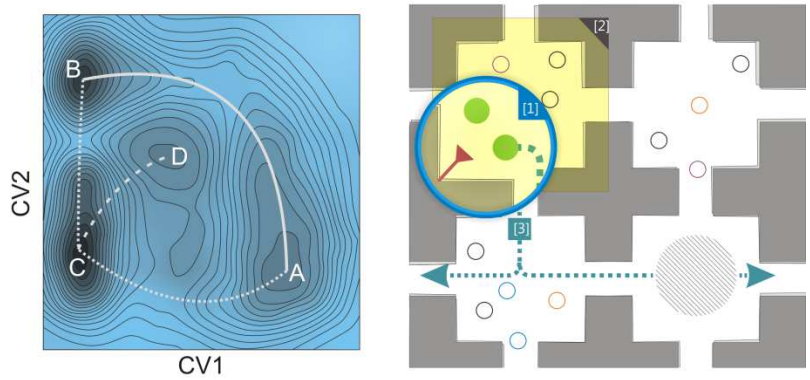

Figure 1 : Left panel : complex 2D free energ surface with indication of several reaciton pathways. Right panel : Schematic representation of complex chemical transformations and various levels in this proposal.

Unravelling complex phenomena requires methods that go beyond state of the art and allow sampling the configuration space efficiently. Molecular dynamics (MD) methods and Monte Carlo (MC) simulations have grown into extremely powerful and versatile tools to sample configuration space and could in principle do the job. [7] MC methods are the methods of choice to transport the system from one high likelihood region to another without sampling the bottleneck regions. MD methods should be used to sample also the higher free energy regions of phase space. Such approach is valid provided the interesting regions are sampled with high enough probabilities. As we focus on processes in which chemical bonds are broken or formed, we need methods that enable the description of a strongly varying electronic structure. Thus, quantum mechanical based methods are mandatory, at least for the part in which the chemical transformation takes place.

Objectives

The major research challenge of this proposal is to gain a greater understanding of the chemical transformations in nanoporous materials under real operating conditions using first principle molecular dynamics methods, capturing the full complexity of the free energy surface. The applications to be focused on are situated in zeolite catalysis and transformations in Metal-Organic-Frameworks (MOF) and are

inspired by an extensive network with prominent experimental partners. To pursue these ambitious goals, the workflow of the project is defined in two platforms: a methodology and an application platform (Figure 2). The interaction between new model developments, applications and experimental results is an essential is key to achieving ground-breaking research results. The outcome of this project should have impact on the longer term as it is expected to contribute substantially to the transition from using static methods to dynamically based modelling tools in nanoporous materials.

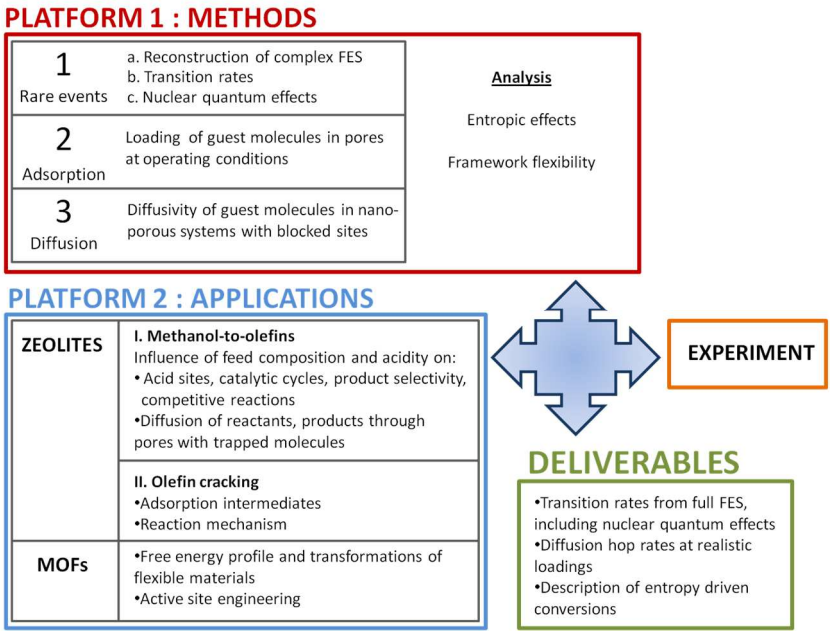

Figure 2 : Workflow of the project

Methods Platform

Simulating a highly complex rare event (**Level 1a**) requires usage of enhanced sampling methods in combination with ab initio MD techniques to explore interesting parts of the free energy surface (FES). At present advanced algorithms have been developed but most applications are situated in the field of (bio)chemistry. Recently, a limited number of papers appeared in the field of catalysis using advanced MD approaches. [6] Within the framework of my ERC Starter program I succeeded into simulating the methylation of benzene in H-ZSM-5 using the metadynamics method as introduced by Laio and Parrinello. [8] That work was an eye-opener for me and gave me an inspiration for this proposal. I am fully convinced of the huge potential of advanced MD techniques in the field of catalytic conversions in nanoporous materials, which can further be exploited in applications with ever growing complexity.

The concept of metadynamics is well known and is schematically shown in Figure 3. It relies on adding a bias potential to the PES. [8] Key for a successful metadynamics run is the choice of proper collective variables that describe the chemical transformations. In applications with multiple guest molecules (Figure 3), the number of collective variables can easily increase to 3 or 4. Powerful analysis methods have been developed such as the committor analysis to check the validity of the choice of the collective variables.[9] The methodology is not yet available for chemical transformations in nanoporous materials, and will be developed within the framework of this project. This will be performed in collaboration with the UvA group in Amsterdam (E.J. Meijer, P. Bolhuis, B. Ensing), which is a renowned group for its seminal work on rare events in biosystems and in homogeneous catalysis and with whom I have established research collaborations in the past two years. Additionally, the METAGUI interface developed by Laio will be used, which also enables us to keep track of the enormous amounts of structures

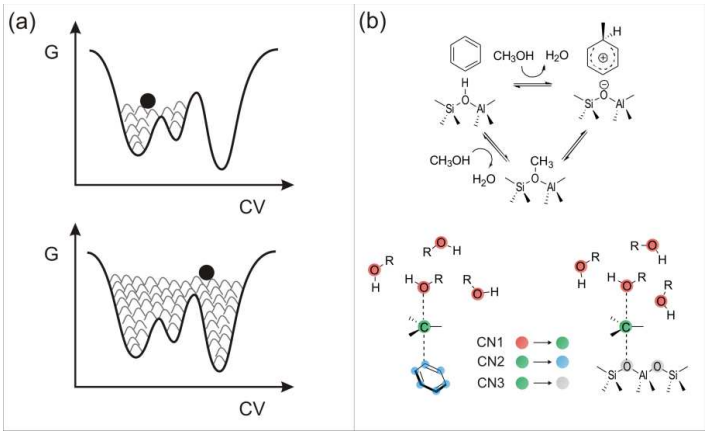

Figure 3 : Gaussian hills construct the bias potential during a metadynamics run (a). To describe competing reaction paths, a high number of atoms should be included in the collective variables as illustrated for a methylation pathway.

generated through a metadynamics run. [10] Apart from previous methods, other innovative methods such as generation of quasi-classical trajectories (QCT) starting from a transition state will be tested. [6(e)]

Once the FES is constructed, it is essential to calculate the transition rates between stable minima on the surface. This has been recently performed by Tiwary and Parrinello by extending the scope of the metadynamics method.[11] Within this proposal I will test this new method for various reactions in nanoporous materials (**Level Ib**) and compare initially the transition rates with our earlier chemical accurate kinetics values. If successful this would be the first full dynamical exploration of chemical transitions in nanoporous materials also giving transition rates. Achieving this will be far from straightforward but would have a high impact.

For reactions in which light atoms are involved nuclear quantum effects during the molecular dynamics run will grow in importance (**Level Ic**). Very recently Ceriotti and co-workers applied path integral molecular dynamics simulations in combination with electronic structure programs. [12] I plan to test the i-PI interface in conjunction with CP2K for the simulation of elusive intermediates in zeolite chemistry. The transfer of these methodologies to nanoporous materials will certainly create obstacles, which we will have to overcome based on our physical and chemical insights.

To simulate the system under real operating conditions, knowledge of the number of guest molecules present in the pores is an essential ingredient in MD simulations (**Level 2**). In the molecular dynamics simulations so far, this number was guessed on basis of chemical intuition and available space. A more straightforward method is to extract this information from adsorption isotherms, calculated using GCMC calculations and force fields.[7] Within this proposal, a two step procedure will be used to calculate the adsorption isotherms at operating conditions, thus accounting for the framework flexibility. Using first principle dynamics simulations, a series of snapshots of the material will be generated, which will be used in a second step as input for the Monte Carlo simulations. The latter simulations will be performed by dedicated programs such as RASPA [13] (D. Dubbeldam et al.) or COTA (B. Smit et al.). An ongoing collaboration with these groups guarantees success of this part of the research program.

In **Level 3**, the hindered diffusion of small reactant and product molecules through the pores of nanoporous materials is investigated. Diffusion through pores containing blocking molecules has large repercussions on activity and product selectivity. The trapped molecules could act as gating molecules, i.e. blocking the pores depending on their orientation. At first instance, I will study the diffusion barriers under realistic conditions of loadings, temperatures and active sites using the free energy methods developed in **Level 1**. This will give first principle determined hop rates in operating conditions, which is unprecedented so far. Special attention will be given to the diffusion mechanisms at higher loadings where molecules could diffuse in a concerted way or as duo or rather as individual randomly moving particles. The force fields, developed by my group in collaboration with R.Schmid (Bochum) and G.Sastre (Valencia), will be used for the molecular dynamics runs. Knowledge of the hop rates can also serve as input for kinetic Monte Carlo methods to calculate the diffusivity. [14] These goals are a very high risk, but with the competence of my team, enlarged with complementary expertise of other theoretical groups, they should be feasible.

Effects of entropy and framework flexibility:

Nanoporous materials are often much more flexible than generally assumed [15]. Proper understanding of flexibility requires an adequate description of the entropy of the lattice. The extraction of entropy or entropy differences from atomistic simulations poses a huge challenge. Within this framework methods will be implemented and developed to extract the framework's entropy from MD and MC simulations. Within the field of biomolecular systems a series of methods have been introduced such as the thermodynamic integration methods, free energy perturbation methods and integration of the heat capacity in terms of temperature. [16] This part of the proposal is essential to simulate entropy driven processes.

Application Platform : Rationale for selected materials and chemical transformations:

The applications selected in this proposal are situated in the field of **zeolite catalysis** and **transformations in Metal-Organic-Frameworks.** The rationale for this choice is inspired by the fact (i) that my group has built substantial experience in these areas over several years, and has achieved a prominent position on the international scene, (ii) and that I can maintain the fruitful existing collaborations with international top experimental groups in catalysed chemical reactions over zeolites and MOF's.

Each topic shows all ingredients to fully explore the capacities of the advanced MD techniques proposed in the methods section. A strong interaction between theory and experiment is key to making ground-breaking achievements, making it possible to get an in depth knowledge of the targeted applications and to pose topical questions with state of the art methodologies.

Zeolite catalysis:

Within zeolite catalysis, the **conversion of methanol to hydrocarbons** and **cracking of olefins** over acidic zeolites will be studied. Both processes are of relevance in the search for alternative processes to produce hydrocarbon products and are from theoretical modelling point of view very challenging. Within MTO chemistry (Figure 4), the catalyst has a supramolecular nature with hydrocarbons trapped in the zeolite pores and for cracking of olefins there is serious debate on the nature of the intermediates in terms of the process conditions. The interactions with our experimental partners have revealed that there are unresolved questions which may not be solved using static based approaches.

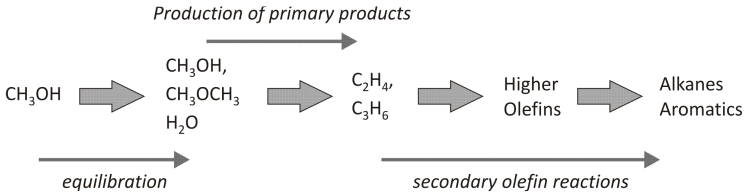

Figure 4 : Schematic illustration of the conversion of methanol to olefins over a solid acid zeolite catalyst.

Influence of feed composition, acidity on acid sites, catalytic cycles, product selectivities, competitive reactions within MTO catalysis.

- ***Influence of water on the availability of active sites and active routes in zeolites with different acidity, topology (H-ZSM-5, H-SAPO-34, H-SSZ-13, H-SAPO-5, H-SSZ-24,…) :***

It is unclear how water – always present in the methanol feed - influences the nature of the active sites, by formation of protonated clusters with methanol or dimethylether. Water also affects the product selectivity. (in collaboration with B.Weckhuysen (Utrecht)).

- ***Influence of catalyst acid strength on the active routes:***

Isostructural materials such as H-SSZ-24 and H-SAPO-5 (both AFI topology, with different acidity) show distinct behaviour during methanol conversion due to their different acid strengths. In particular, for the methylation of benzene, distinct variations in product selectivity and complex reactions orders for both reactants are experimentally observed. [17] (in collaboration with the Catalysis group at the University of Oslo (U.Olsbye))

- ***Kinetics and mechanisms for methylations of benzene, toluene and xylene over H-ZSM-5:***

Bhan et al. reported on the impact of complex formation on experimentally observed rates for methylation of benzene, xylene and toluene over H-ZSM-5 using dimethylether as methylating agent. [18] A hypothesis has been put forward that relies on the formation of adsorption complexes that depends on the nature of the aromatic involved. The proposed methodology here enables to study the various competitive pathways contributing to the observed variations in reaction orders.

Diffusion of small guest molecules such as ethene, propene in zeolites with distinct variations in topology and including hydrocarbon pool species (MTO process):

To explain the observed variations in selectivity from experimental point of view, it is essential to get track on the hop rates of small molecules in the nanoporous pore system. First principle based diffusion hop rates will be calculated at real operating conditions. (in collaboration with experimental group of J. Denayer (VUB-Brussels).

Cracking of olefins in ZSM-5: (in collaboration with J.Lercher (TU Munchen))

I will study the adsorption of alkenes in H-ZSM-5 within a full dynamical approach including framework flexibility, conformational freedom at realistic process temperatures. It will reveal essential information on the competition between physisorption and chemisorption with side reactions such as isomerizations, dimerizations, …. The complex free energy surface for the cracking reactions will be constructed using the battery of techniques developed within this proposal.

MOFs :

Free energy profiles and transformations of flexible materials: Some MOFs have the capacity to undergo large structural deformations upon external stimuli, such as temperature, pressure, guest molecules. The MIL-53(X) have received most attention within this respect. [19] Energy profiles in terms of the breathing angle using QM methods are not sufficient to understand the flexible behavior. A proper understanding of the entropy is mandatory. The methods developed within this project will enable us to go beyond current state of the art. I plan to apply a metadynamics approach, with an appropriate choice of collective variables, which should be well-thought as it might be anticipated that many degrees of freedom will contribute to the overall

observed transition. Generating such a free energy profile for flexible MOFs would be truly ground-breaking for the MOF community. (in collaboration with G.Maurin(Montpellier))

Active site engineering for catalysis in MOFs: Recently it was shown that tailor-made modifications in MOFs can substantially increase the catalytic activity for Lewis and acid based catalysis in MOFs. [20] Together with D. De Vos (KULeuven) we showed a successful modulation approach for the UiO-66(Zr) type of material. This is a typical problem for which physical and chemical transformations are closely intertwined. Depending on the modulation, chemical integrity could be preserved or not. In any case usage of advanced theoretical tools to estimate the free energies associated with a modulation approach is mandatory to guide experimental design. (in collaboration with D.De Vos (COK-KULeuven))

High Risk/High Gain profile and perspectives on the longer term :

This project relies partly on the transfer of MD methods to the field of nanoporous materials and on the development of new theoretical algorithms in my own group. Each of the applications is very challenging on its own and have not been tackled with the integrated degree of complexity foreseen here. Based on my solid network with experimental partners and continuous interaction with them, I am convinced that we will be able to go beyond current state of the art. Insights will be obtained which are unprecedented so far. I have no doubt that we will be able to publish the work in leading journals. Maybe even more important, I foresee that the outcome of the project will be influential on the longer term. If successful I will be able to show that complex chemical conversions in nanoporous materials may be simulated on the fly. Some parts of the projects are very high risky such as the calculation of transition rates from MTD simulations with many collective variables, the inclusion of nuclear quantum effects, first principle diffusion hop rates and entropies of the lattices. I realise that I will have invest strongly to overcome the hurdles, but I believe my chances are high in achieving these ambitious goals. First of all I will rely on my own physical background, the cross fertilization of chemists, physicists and material scientists within the CMM and my strong communication skills to set up new collaborations to stimulate gain of knowledge to my team. So far in my career, I was especially attracted towards taking major challenges. I also learnt that setting major milestones are key towards very good science and that investment on the longer term is very rewarding towards excellence.

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Section b: Curriculum Vitae

Personal Information:

Date of birth : 30th August 1974
Nationality : Belgian
Civil Status : Married and mother of two children :
Marcus de Paepe (°04/06/2002) and Alexander de Paepe (°23/06/2004)

Current Professional Affiliation: Full professor and Head of the Center for Molecular Modeling (CMM), Ghent University, Belgium. URL: molmod.ugent.be, with a prominent research profile, which is rather exceptional and only granted to excellent scientists on an extremely competitive basis.

Education

- **Ph.D. in Engineering**, 5th October 2001, Ghent University, "Study of chemical reactions with static and dynamic molecular methods", Supervisor Prof.M.Waroquier
- **Master in Engineering, Applied Physics**, July 1997, magna cum laude ("met grote onderscheiding"), Ghent University

Professional experience:

Oct 2012 – present : Full Professor and Head of Center for Molecular Modeling (CMM)
- Faculty of Engineering and Architecture of the Ghent University
Oct 2007 – Sept 2012 : Associate Professor with a prominent research mandate for 10 years at Ghent University
Oct 2002 – Sept 2007: Postdoctoral fellow of the Fund for Scientific Research Flanders (FWO)
Oct 2001 – Sept 2002: Postdoctoral Fellow (Special Research Fund – Ghent University)
Oct 1997 – Sept 2001: PhD Fellow (Special Research Fund- Ghent University)
July 1997 – Sep 1997: Research fellow at DSM Research, Geleen, The Netherlands.

Research Grants and Fellowships :

- **ERC starting grant** (Call ERC-2009-StG) awarded on a subject on first principle chemical kinetics in nanoporous materials (KINPOR)**.** Total budget: 1.150 kEuro
- **Principal investigator of various research grants** funded by several agencies such as ESA and FP7 (EU), BELSPO (Belgian Science Policy), FWO and IWT (Flemish government) and BOF (Research Fund UGent). Total budget : 1.960 kEuro , PhD grants: total months: 276, Postdocs: total months: 180
- **Current composition of my research group:** 5 postdoctoral researchers and 16 PhD. Most of them have obtained a personal grant at the FWO. The rest is funded by the awarded projects.

Awards:

- **May 2012 : Elected as full member of Royal (Flemish) Academy for Science and the Arts of Belgium (www.kvab.be)** – The KVAB assembles distinguished scientists of Flanders, which are elected on basis of their excellent scientific achievements and careers.
- **December 2011** : Laureate 2011 of the **Royal (Flemish) Academy for Science and the Arts of Belgium.** Yearly price awarded to a prominent scientist younger than 40 years and for his/her excellent achievements. Prize award : 10 kEuro. (www.kvab.be)
- Supervisor of various Master and PhD theses which have been awarded (DSM Award North 2007, International Club of Flanders award "Andreas De Leenheer 2010, Umicore Award 2010 and ArcelorMittal Award 2010, Solvay Award 2011 - IE-net prijs 2011 – Jozef Plateauprijs 2011)

Scientific Leadership Profile:

Supervisor of completed PhD dissertations : 12

7 with former PhD supervisor : (Peter Van Steenkiste, UGent 2006, Karen Hemelsoet, UGent 2007, Karen Van Cauter, UGent 2007, Toon Verstraelen, UGent 2007, Bart De Sterck, UGent 2010, Matthias Vandichel, UGent 2012, Marc Vanhouteghem, UGent 2013)

5 without former PhD supervisor : (David Lesthaeghe, UGent, 2007, Isa Degirmenci Joint PhD between UGent and Bogazici University, Kurt Lejaeghere, UGent 2014, Jeroen Van der Mynsbrugge, UGent, 2014.)

3 have obtained an individual FWO postdoc position under my supervision.

2 have applied for an individual FWO postdoc position under my supervision.

Supervisor of completed master theses : 31
13 with my former PhD supervisor
18 without my former PhD supervisor
13 of them have decided to do a PhD under my supervision.

Current position :
I am head of the CMM (I was also co-founder) responsible for daily operation including organizational, logistics and personnel affairs. I replaced Prof. M. Waroquier, who officially retired since October 2012. Within the CMM I have since many years my own research line on Computational Molecular Modeling, which has grown steadily in recent years. My research group currently consists of 5 postdoctoral fellows, 16 PhD students and various master students. The scientific progress of all my team members is discussed in research meetings on a daily basis. I am organizing on a weekly basis Friday Morning Lectures of about 20 minutes to stimulate cross pollination among the various group members.

Teaching activities:
Lecturer or co-lecturer of following Master Courses belonging to the study programs of the Faculty of Engineering and the Faculty of Science :
" Atomic and Molecular Physics" from October 2007 – present
"Molecular Modeling of industrial processes" from October 2004 – present
"Chemistry of Industrial Processes" from October 2011 - present
Lecturer or co-lecturer of Bachelor Courses belonging to the study programs of the Faculty of Engineering, including Statistical Physics (since 2009), Thermodynamics(since 2009) , Molecular Structure, Advanced Quantum Mechanics (since October 2013).

Activities to enhance impact of science on society:
- Selected as role model of action "**Richting Morgen**" of the Flemish government to promote science, technology and innovation (www.richtingmorgen.be) to youngsters
- Invited member by the Flemish government of the **STEM-Platform**. The Platform was installed by the government to promote Science, Technology, Engineering and Mathematics training and careers. The Platform consists of 15 distinguished members of various industry and academic stakeholders which are committed to stimulate youngsters to develop careers in science, technology and innovation to young people.

Organisation of Scientific Meetings:
- 1-6 April 2012, Ghent: Main organizer of **Challenges in Density Matrix and Density Functional Theory**, # of participants ≈ 100.
- 26 - 30 June 2012, Vlissingen : co-organiser of 14th International Conference on Theoretical Aspects of Catalysis ICTAC14 (# of participants ≈ 200)
- 14 May 2007, Ghent : co-organiser of fundamental and applied aspects of Density Functional Theory; bio-applications of Density Functional Theory (# of participants ≈ 100)

Commissions of trust – academic services:
- Member of the Research Board of the Ghent University since 1 January 2013.
- Member of the Research Board of the Antwerp University since 1 January 2013
- Member of the FWO Committee W&T3 (Condensed Matter and Physical Chemistry) since January 2011
- Member of IWT Committees for evaluation of doctoral grants
- Member of the Examination Jury of about 15 Doctoral Dissertations including Examination Jury abroad (TUEindhoven – Main Opponent doctoral thesis University Oslo,…)
- Editorial board ChemPlusChem
- Reviewer on very regular basis for a broad variety of journals
- Editorial board ChemPluschem
- Member of the American Chemical Society (ACS), American Institute of Chemical Engineers (AICHE), World Association of theoretically oriented Chemists (WATOC; Life Member)
- Member of three scientific Research Communities of the Fund for Scientific Research Flanders (FWO) "The active site : from catalyst to reactor", "Computational modelling of materials" en "Density Functional Theory and Applications".
- Member of the Koninklijke Vlaamse Ingenieursvereniging (KVIV)

Appendix: All on-going and submitted grants and funding of the PI (Funding ID)

Projects - Funding:
Currently, I am involved in about 20 projects, funded by national and international organisations. I am the principal investigator in about half of these projects, and in three quarters of the projects I collaborate with an external partner. In most of the cases it concerns experimental partners, as they form the ideal complement of a computational, theoretical research group.

The most prestigious project was the acquisition of an ERC starting grant in 2010 on a topic "First principle chemical kinetics in nanoporous materials". This grant gave me true independence to establish a research team for which I had the full responsibility, and to work towards a label of excellence at the national and international scene. The grant initiated a multiplication effect and on top of the funding many excellent researchers which could obtain a personal grant joined my team.

I also have close contacts with several industrial partners and have given a lot of presentations of my research work at industrial meetings in research divisions of international companies.

On-going Grants

Project Title	*Funding source*	*Amount (Euros)*	*Period*	*Role of the PI*	*Relation to current ERC proposal*
First Principle Chemical Kinetics in Nanoporous Materials (KINPOR)	ERC	1.150.000	1/1/2010 - 31/12/2014	supervision with several work discussions	chemical kinetics using static methods has been developed, I will build on this knowledge but there is no direct overlap
Safe ExploitAtion Related CHemistry for HLM reactors (SEARCH)	EC-FP7	160.000	1/11/2011 - 31/10/2014	supervision	none
Functional Supramolecular Systems (FS2)	BELSPO IAP VII/5	500.000	1/4/2012 - 30/9/2017	Head and spokesperson of CMM part in network	Outcome of the ERC proposal, could potentially be applied on some themes of the IAP project
Simulation of electronic excitation and emission spectra using advanced molecular dynamics combined with TD-DFT	FWO	160.000	1/1/2014 - 31/12/2017	co-supervisor	Molecular dynamics methods are used to simulate spectra, no chemical conversions are studied in the program, thus no direct overlap.
Combined experimental and computational study of electronically modulated MOF catalysts	FWO	280.000	1/1/2012 - 31/12/2015	supervision	On the application side, it will provide some data that will be useful but there will be no direct overlap, since only static methods have been applied
Model based synthesis of a new generation metal organic	BOF-GOA	250.000	01/01/2010 to 31/12/2015	supervisor	Outcome of the ERC proposal, could potentially be applied on some themes of the

frameworks (MOFs) for catalytic applications					project
First Principle Chemical Kinetics in Nanoporous Materials	BOF/N24	193.000	01/10/2009 - 30/09/2014	supervisor	chemical kinetics using static methods has been developed, I will build on this knowledge but there is no direct overlap
POXilation asnext generation PEGylation	SBO-IWT	120.000	1/2/2013 - 31/01/2014	supervision	none

Besides on-going grants for projects, many members of my team obtained an individual grant as PhD fellowship (4 years) or as postdoctoral researcher (3 years). Under my direct supervision there are currently 5 PhD FWO fellowships and 4 Postdoctoral grants on going.

Applications

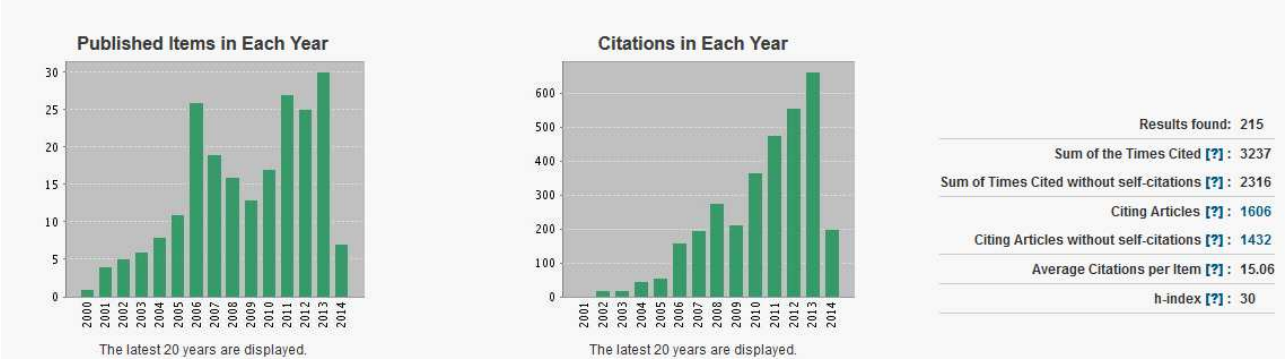
Project Title	*Funding source*	*Amount (Euros)*	*Period*	*Role of the PI*	*Relation to current ERC proposal*
Defect Network materials science and engineering	Call : H2020-MSCA-ITN-2014	1.5 PhD student	Pending	Supervisor Coordinator : Prof. R. Fischer Ruhr- University Bochum	Force field development for describing defects in metal-organic frameworks

Some applications for individual PhD and Postdoc grants are on-going. This year I was involved as main supervisor in 3 proposals for aspirant (PhD fellowship at the FWO) and 2 proposals as co-supervisor. In addition I had 3 applications for FWO-postdoctoral grants as main supervisor.

Section c: Early achievements track-record

Summary of scientific publications :

- **220 a1 papers (**most in so-called Q1 journals and about 20 in top 5% ranked journals)
- **26 a1 papers without my PhD supervisor of which 23 the last three years**, demonstrating the full independence of the research performed.
- Corresponding author/last author for about half of my publications.
- **h-index = 30**
- Sum of citations = 3237, without self-citations = 2316
- Substantial number of publications in **highest ranked journals** such as **Chemical Society Reviews (3x) Angewandte Chemie IC (6 x)**, **JACS (5 x), Nature Materials (1 x), Physical Review Letters (1x),** Journal of Catalysis (8 x), Chemistry -A European Journal (10 x), Chemical Communications (4 x), etc. Full bibliography available at https://molmod.ugent.be/members/prof-dr-ir-veronique-van-speybroeck .
- I have always been especially attracted to working **across disciplines** and have found the cross pollination from various fields very inspiring. My strong communication skills with people not belonging to my own discipline lie on the basis of some major breakthroughs.



Short description of selected key publications along the whole scientific career (corresponding author is underlined – those without my PhD supervisor highlighted)

- Insight into the formation and reactivity of framework-bound methoxide species in H-ZSM-5 from static and dynamic molecular simulations, J. Van der Mynsbrugge, S. Moors, K. De Wispelaere, **V. Van Speybroeck**, just accepted in **ChemCatChem**, DOI : 10.1002/cctc.201402146R1, IF: 5.181 *Representative for my current research in zeolite catalysis and a true achievement of my independent research team that I established within the framework of my ERC starting grant.*
- S.L.C. Moors, K. De Wispelaere, J. Van der Mynsbrugge, M. Waroquier, **V. Van Speybroeck**, Molecular Dynamics Kinetic Study on the Zeolite-Catalyzed Benzene Methylation in ZSM-5, **ACS Catalysis**, 3 (11), 2556-2567, **2013** (IF: 5.265) *First paper using metadynamics to calculate first principle chemical kinetics in nanoporous materials including guest molecules.*
- Ranking the stars: A refined Pareto approach to computational materials design, K. Lejaeghere, S. Cottenier, **V. Van Speybroeck**, Physical Review Letters, 111 (7), 075501, **2013**, IF: 7.943, Ranking : 5/83 *This publication shows that I am able to publish research of my own independent team in the highest impact journals within the multidisciplinary field of physics. Nature Materials, devoted its 'Material Witness' column to this article. (Nature Mater. 12, 876 (2013))*
- Methylation of benzene by methanol: single-site kinetics over H-ZSM-5 and H-beta zeolite catalysts, J. Van der Mynsbrugge, M. Visur, U. Olsbye, P. Beato, M. Bjørgen, **V. Van Speybroeck**, S. Svelle, **Journal of Catalysis**, 292, 201-212, **2012**, IF: 5.787, Times cited: 10 *Publication performed in the framework of my ERC starting grant. We predicted rate coefficients with chemical accuracy, compared them with new experiments conducted in the group of Prof. U. Olsbye (University of Oslo)*
- Mn-salen@MIL101(Al) a heterogeneous, enantioselective catalyst using a 'bottle around the ship' approach, T. Bogaerts, A. Van Yperen-De Deyne, Y-Y Liu, F. Lynen, **V. Van Speybroeck**, P. Van der Voort, **Chemical Communications**, **2013** (49), 8021-8023, 2013, IF: 6.378.
- Entropy-Driven Chemisorption of NOx on Phosphotungstic Acid, S. Heylen, L. Joos, V. Van Speybroeck, C. Kirschhock, J.A. Martens, **Angewandte Chemie int. Ed.**, **2012**, 51 (44), 11010-11013, 2012, IF: 13.734
- Electronic effects of linker substitution on Lewis acid catalysis with Metal-organic frameworks, F. Vermoortele, M. Vandichel, B. Van de Voorde, R. Ameloot, M. Waroquier, **V. Van Speybroeck**, D. De Vos, **Angewandte Chemie int. Ed.**, 51(20), 4887-4890, 2012 ((IF= 13.734, 7/152; Cited: 36)
- Design of zeolite by inverse sigma transformation, E. Verheyen, L. Joos, K. Van Havenbergh, N. Kasian, E. Gobechiya, K. Houthoofd, M. Hinterstein, E. Breynaerts, **V. Van Speybroeck**, M. Waroquier, S.

Bals, G. Van Tendeloo, C. Kirschhock, J.A. Martens, **Nature Materials**, 11 (12), 1059-1064, **2012**, (IF: 35.749; Times Cited: 12) *The four publications show that I have the ability to collaborate successfully with prominent experimental partners and that such interactions allow to publish the results in the highest ranked journal.*

- First principle kinetic studies of zeolite-catalyzed methylation reactions, **V.Van Speybroeck**, J. Van der Mynsbrugge, M. Vandichel, K. Hemelsoet, D. Lesthaeghe, A. Ghysels, G.B. Marin, M. Waroquier, **Journal of the American Chemical Society**, Vol.133, 888-899, **2011**, (IF=10.677; Times Cited : 35) *This publications is a key reference for the accurate calculation of chemical kinetics in nanoporous materials. I fully conducted the research myself.*
- 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 (46), 10939-10950, **2000** (IF=2.765, Times Cited=110) *My first paper in which I presented a new model to treat internal rotors in macromolecules and their contribution to entropic effects.*
- Understanding the failure of direct C-C coupling in the zeolite-catalyzed methanol-to-olefin process, David Lesthaeghe, **V. Van Speybroeck**, G. B. Marin, M. Waroquier, **Angewandte Chemie - International Edition**, Vol.45 (11), 1714 – 1719 (selected as VIP paper), **2006** (IF=10.031, Times Cited=81)
- D. McCann, D. Lesthaeghe, P.W.Kletnieks, D.R.Guenther, M.J.Hayman, **V. Van Speybroeck**, M.Waroquier and J. F.Haw, A complete catalytic cycle for MTO catalysis with rate constants from theoretical modeling of an entire cage and contents, **Angewandte Chemie, Int.Ed**., 47 (28), 5179-5182, 2008 (IF: 10.031, Times Cited: 92) *Two seminal papers for the work on the Methanol-to-Olefin process. The papers received many citations so far. I was daily supervisor of the PhD student who performed the work (D. Lesthaeghe)*
- The calculation of thermodynamic properties in molecules, **V. Van Speybroeck**, R. Gani, R.J. Meier, Chemical Society Reviews, 39, 1764-1779,2010, IF=30.181, Times cited :24.
- Error estimates for solid-state density-functional theory predictions: an overview by means of the ground-state elemental crystals, K. Lejaeghere, **V. Van Speybroeck**, G. Van Oost, S. Cottenier, **Critical Reviews in Solid State and Materials Sciences**, 39 (1), 1-24, **2014**, IF: 5.947, Times cited: 8
- Mn-salen@MIL101(Al) a heterogeneous, enantioselective catalyst using a 'bottle around the ship' approach, T. Bogaerts, A. Van Yperen-De Deyne, Y-Y Liu, F. Lynen, **V. Van Speybroeck**, P. Van der Voort, Chemical Communications, 2013 (49), 8021-8023, **2013**, IF: 6.378.
- Bimetallic–Organic Framework as a Zero-Leaching Catalyst in the Aerobic Oxidation of Cyclohexene, Y-Y Liu, K. Leus, T. Bogaerts, K. Hemelsoet, E. Bruneel, **V. Van Speybroeck**, P. Van der Voort, **ChemCatChem,** 5 (12), 3657–3664, **2013**, IF: 5.181.
- Investigating the Halochromic Properties of Azo Dyes in an Aqueous Environment by Using a Combined Experimental and Theoretical Approach , T. De Meyer, K. Hemelsoet, L . Van der Schueren, E. Pauwels, K. De Clerck, **V. Van Speybroeck**, Chemistry – A European Journal, 18, 8120-8129 , 2012, IF: 5.83, Times cited: 7

International recognition / Major Collaborations:

- 29 invited talks on international conferences, prominent research institutes and universities.
- I encourage my researchers to actively participate in international conferences with oral and poster presentations. I am strongly involved in the preparation of these talks, giving them an intensive training in communication skills. The number of posters will easily exceed 200.

The CMM has an extensive international network with leading scientists from all over the world (Prof. L. Radom, Australia; Prof. J. Haw, USA, Prof. V. Aviyente, Turkey; Prof. P. Ayers, Canada; Prof. R. Van Santen, the Netherlands; Prof. Dr. B. Brooks, USA, Prof. Dr. J. Hutter, Switserland, Prof. Dr. R.J. Meier, the Netherlands). All of these collaborations have led to common research papers in which I am involved.
Since my appointment as research professor in 2007 I **personally extended the network of academic collaborations with prominent research teams**, mostly within the field of heterogeneous catalysis. I have adapted a modus operandi, in which I go regularly on side visits of a few days to external labs and invite my collaborators to my group for a short period. Such visits are very intensive, but allow to develop the roadmap for future common projects. I encourage my researchers to spend longer periods at renowned institutes such as the UC Berkeley, UvA (Prof. E.J. Meijer Amsterdam), Oslo (Prof.U.Olsbye, Prof.S.Svelle), Berlin (Prof.J.Sauer), Eindhoven (Prof.R.van Santen), Utrecht (Prof.B.Wechhuysen), Montpellier (Prof.G.Maurin), Munchen (Prof.J.Lercher), Valencia (Dr.G.Sastre), Bochum (Dr.R.Schmid), etc. To stimulate transfer of knowledge to my group, I hosted various postdocs from top institutes for shorter or longer periods in my group

ERC Consolidator Grant 2014

Section a. State-of-the-art and objectives

Chemical conversions in nanoporous materials are omnipresent in a broad versatility of application domains such as energy storage, energy conversions, sustainable chemistry, biomedical applications,…[1-3] More specifically, heterogeneous catalysis using nanoporous materials is inherently part of daily industry. [4-7] Zeolites are today's workhorses in industrial catalysis but also other intriguing materials have entered the scene during the last decades such as metal organic frameworks (MOFs), covalent organic frameworks (COFs), carbon nanotubes,… [8-14]
Nanoporous materials can either be categorized into microporous (diameter<2nm) or mesoporous materials (diameter from 2 to 50nm), and are tractable due their high surface area, porosity and chemical versatility. Experimentally new materials are being synthesized at a considerable pace, using the most advanced methods to tailor materials at the nanometer scale level. Model-guided design is an essential part in this overall process to guide the experimentalists, towards new applications and to optimize current processes to their full potential. [15-17]

Strictly speaking, chemical transformations are not restricted to catalysis, but encompass any transformation in which chemical bonds are broken or formed. Given this definition, processes such as defect formation or structural transitions in which the chemical architecture of the framework changes, are also under our attention. A noteworthy example in the field of metal organic frameworks, is the intentional creation and modulation of defects to tune the catalytic activity of Lewis based catalysts. Together with Dirk De Vos (Centre for Surface Chemistry and Catalysis, KULeuven), I performed seminal work on the unexpected catalytic activity of the seemingly coordinatively saturated UiO-66 material. The catalytic activity of the material is due to missing linkers in the structure and can be significantly increased by placing electron-withdrawing groups on the linkers (Figure 1). [18-20]

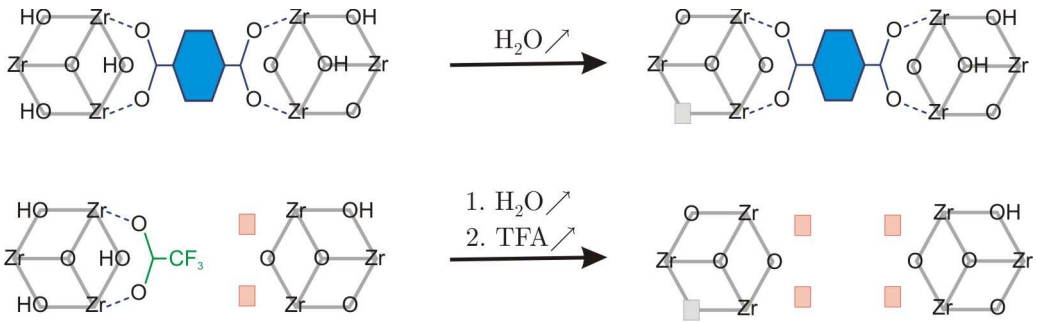


Figure 1 : Creation of defects by dehydroxylation of UiO-66(Zr) and of TFA (trifluoroacetate) modulated UiO-66(Zr)

Within this zoo of materials, rational design of nanoporous materials is of utmost importance and molecular modelling plays an indispensable role herein. In the last decade, enormous progress has been made from the methodological side, which in combination with a steady increase in computer power, contributed to the fact that many properties are now routinely calculated with high accuracy.[16, 17] One major breakthrough of the last five years - which is particularly relevant for this proposal - is the fact that theoretical methods have matured to a level where **rate coefficients of elementary reactions can now be calculated with near chemical accuracy provided the reaction takes place at a well defined active site and provided the mechanism is known.** Within the framework of my ERC starting grant "First principle chemical kinetics in nanoporous materials", I contributed substantially to this result together with other leading scientists.[21, 22] To come to this point some essential hurdles had to be overcome, such as proper inclusion of the material's topology, account for long range interactions,…

However, it is not the time to be too optimistic for theoreticians as we are still confronted with a huge number of challenges. This is especially the case when emphasis is on describing processes relevant for transformations at experimental conditions. Weckhuysen et al. illustrated nicely in his review on spatial heterogeneities in catalytic solids at different length and time scales, that the observed function of a material is the result of a multi-scale nature of phenomena. [23]

Irrespective hereof, when focus is set at the reaction taking place at the atomistic scale, which is spatially confined within the (sub)**nanometer** scale, the routinely applied methods are far too limited to mimic operational conditions. Most theoretical procedures to date describing chemical transformations at the nanometer level still rely on **static methods**, in which information is obtained from a limited number of configurations on the potential energy surface. There only a few notable exceptions [24-26] Such static representation is a huge oversimplification. Indeed at real operating conditions, the scene is far **more complex** and one can not simply speak about one single transition state that captures all information.[26] In most cases, various competitive routes are operational, which are critical for explaining product selectivities. Moreover, various guest molecules are present in the pores of the material and each of them can take an active role depending on the operating conditions, such as pressure, temperature,… Sometimes these intermediates are very close in free energy. Furthermore some conversions are entropically driven. In the latter case, any analysis should start by exploring **the free energy surface (FES)** and one should be able to localize the passages which are representative for making the transition from one to another stable basin. The situation is illustrated for a hypothetical free energy map which is comparable to a topographical map used when hiking the mountains. (Figure 2)

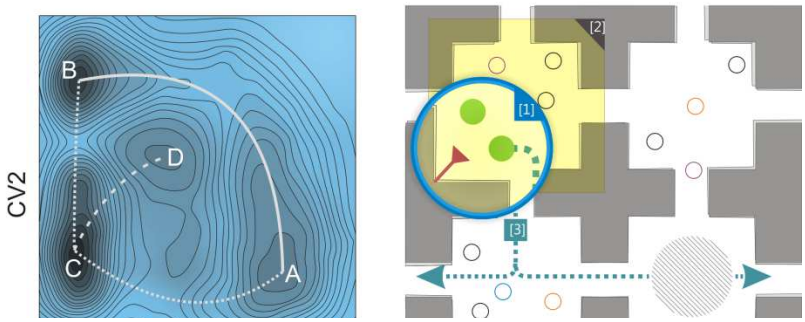


Figure 2 : Left panel : complex 2D free energy surface with indication of several reaction pathways. Right panel : Schematic representation of complex chemical transformations occurring in a nanoporous framework and various levels in this proposal.

Given this complexity, it is my strong belief that time has come to take the **next leap within modelling of nanoporous materials** that accounts for the **full complexity of the free energy surface** at **operating conditions**. Very recently I came across various timely applications which require a higher level of complexity in simulations methods. One illustrative example, which is worth mentioning is our recent publication on the methylation of benzene in H-ZSM-5 in presence of various guest molecules such as methanol,…[25] We used the metadynamics approach developed by Laio and Parrinello with only two collective variables. [27-29] It was concluded that a simple view of a localized Brønsted acid site at which the reaction occurs is far too simplistic. Using static approaches, essential factors are not taken into account such as possibility of cluster formation, the diffusivity of such clusters through the pores of the material. This application was an eye-opener as I realised that there is a huge potential for advanced MD techniques within catalytic conversions and that more advanced tools are necessary to answer timely question posed by experimentalists. To firmly make the transition from static based methods to dynamical approaches within the nanoporous materials field, major bottlenecks need to be overcome. A concerted investment and vision is required to take this next major leap.

This is precisely the objective of this proposal **: to gain a greater understanding of complex chemical transformations in nanoporous materials under real operating conditions using first principle molecular dynamics methods, capturing the full complexity of the free energy surface.**

The applications are situated in **zeolite catalysis** and transformations in **Metal-Organic-Frameworks (MOF)** and are inspired by an extensive network with prominent experimental partners. Each application is carefully selected, as detailed mechanistic insight at the atomistic level is very hard to obtain and new methods are mandatory to reach a higher level of understanding.

To pursue these ambitious goals, the workflow of the project is defined in two platforms: a methodology and an application platform (Figure 3). The interaction between new model developments, applications and experimental results is key to achieving ground-breaking research results. The outcome of this project should have impact on the longer term as it is expected to contribute substantially to the transition from using static methods to dynamically based modelling tools in nanoporous materials.

In various aspects the proposal is very challenging and poses a **high level of risk**, but if successful the impact should be very high. Following deliverables would come within reach :

- **Transition rates based on full exploration of the free energy surface** including **nuclear quantum** effects. As a result insight into **competitive pathways** would be obtained
- **Diffusion hop rates** at real operating conditions, including formation of clusters, collective motions
- Description of **entropy driven processes**. Adequate description of entropy of the lattice is unprecedented so far but essential to describe structural transitions.
- Estimate of loading of material at operating conditions of temperature, pressure including flexibility.

The proposal relies on usage, implementation and development of state-of-the-art methodologies and applications on extremely challenging problems within the field of heterogeneous catalysis, phase transformations of materials,…

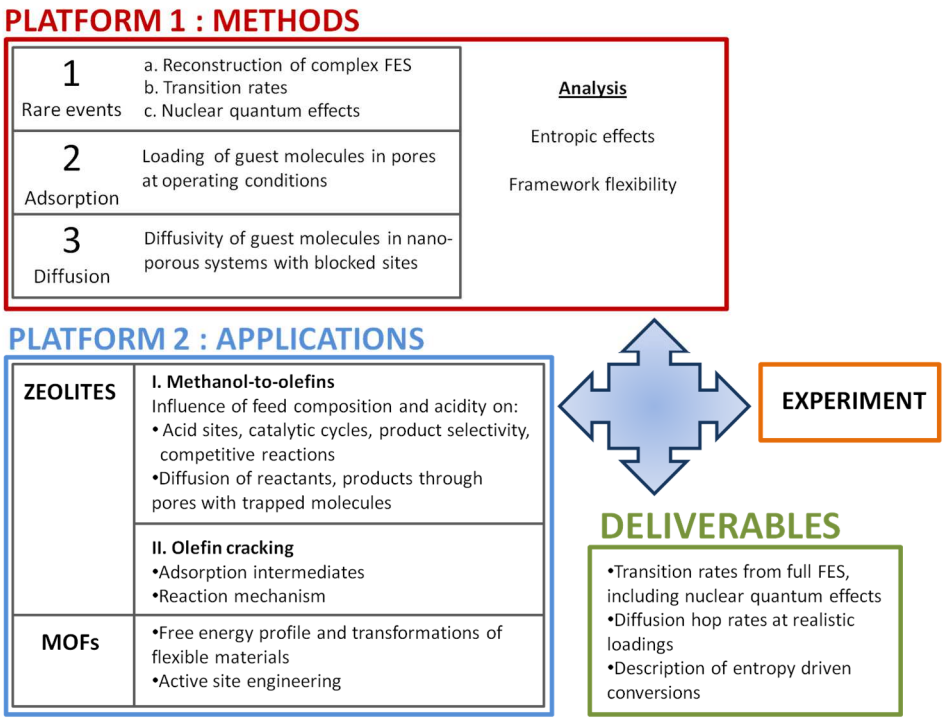


Figure 3 : Workflow of the project

Section b. Methodology

The proposal is organised in two platforms (Figure 3). The applications in PL2 will benefit from continuous methodological progress in PL1 and vice versa will the applications be the driving force for new model development.

Short survey of key components of current methodologies :

The starting point of the current workflow is the plethora of methods available in literature. It is impossible to give an exhaustive overview here. Only a few necessary components which are essential for the further outline of this proposal, are briefly mentioned below. I have recently submitted a review on invitation for Chemical Society Reviews which gives an overview of currently available methodologies.

- **Taking into account the topology of the nanoporous material** : A proper modelling of any chemical transformation in nanoporous materials should account for the material's topology. This may be accomplished using either a periodic model, where one or more unit cells are taken up in the molecular model and infinitely repeated by imposing periodic boundary conditions, or a finite cluster model, where a part is cut out of the periodic structure. Modelling chemical reactions using static approaches extensively use cluster models, as the numerical algorithms to search for transition states are very well developed. In this proposal it is the intention to go beyond a static approach and it is necessary to account for the full flexibility of the material. Therefore a periodic approach using supercells is necessary.

- **Taking into account long-range interactions** : For all systems under investigation long-range dispersion interactions play an essential role. Modelling dispersion interactions is a research domain on its own and also its application in nanoporous materials received considerable attention. [30-35] Within the framework of this proposal we will apply the arsenal of methods currently available such as DFT-D methods, advanced DFT functionals including dispersion interactions, appropriate QM/MM schemes,… It is obvious that I will follow the literature in this domain and will also apply new promising methods as they appear along the execution of the project.

PL1 : METHODOLOGY / MODEL DEVELOPMENT

The methods section relies on three levels, discriminating between various levels of complexity that need to be accounted for to accurately model a chemical conversion at operational conditions. The three levels are also schematically shown in Figure 3.

Level 1a: Simulating a rare event with high degree of complexity

The free energy surface of chemical transformations in nanoporous materials has a very complex nature and it is particularly challenging to sample the interesting parts of the configuration space and to focus on those degrees of freedom which are essential for the phenomena one wants to study. Both molecular dynamics (MD) and Monte Carlo (MC) methods have grown to powerful tools to sample the configuration space. MC can enhance the sampling efficiency, while MD should be used to simulate trajectories in time. [36] Overall the dynamics of the system spans a wide range of characteristic time scales. In MD, the dynamics of the system is followed through discrete integration of the Newtonian's equations of motions. The time step may not be chosen too large in order to sample the fastest motions of the system appropriately. Chemical transformations are rare events as their probability of occurring is very low, although once it occurs the event may be followed during a regular MD run of a few ps. To enhance sampling of interesting regions of the free energy surface a multitude of methods has been developed. [37] The metadynamics (MTD) method developed by Laio and Parrinello [27, 38] will be extensively used for the execution of this proposal. It relies on the choice of a limited number of collective variables along which the free energy landscape is filled up with Gaussian hills to accelerate sampling of events. Afterwards the sum of the Gaussians defines a bias potential for the simulations which can be used to reconstruct the free energy surface. The concept is illustrated in Figure 4. To date the method is well developed and implemented in a series of computer packages such as CP2K, CHARMM, ….The usage however of the method for applications in nanoporous materials is very limited [25]. Furthermore for the simulation of chemical transformations the potential energy surface need to be constructed using first principle based methods, rather than classical force fields.

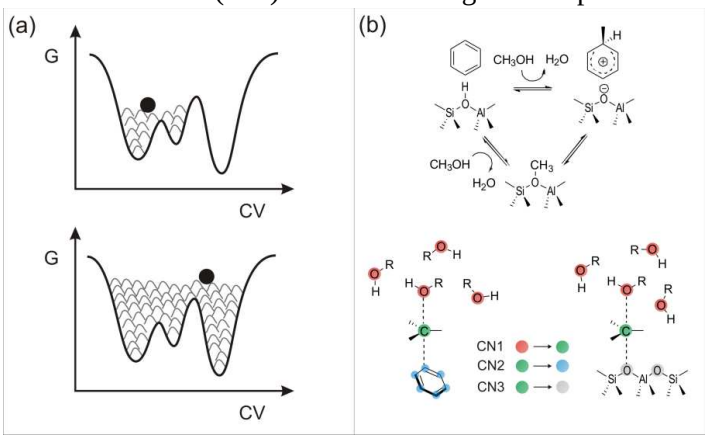


Figure 4: Gaussian hills construct the bias potential during a metadynamics run (a). To describe competing reaction paths, a high number of atoms should be included in the collective variables as illustrated for a methylation pathway (b)

Metadynamics simulations / Choice of collective variables

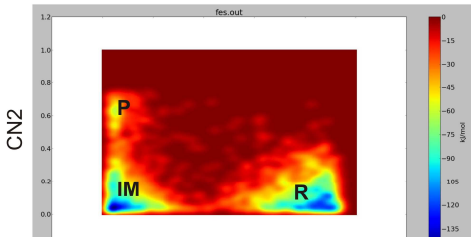


Figure 5 : FES of the methylation of benzene in H-SSZ-24 showing that next to basins R and P there is an extra basin corresponding with intermediate IM

For the applications foreseen here, the choice of the collective variables is far from obvious, as they need to capture all essential features that lead the system from one basin to another. This point can be nicely illustrated for the methylation of benzene in H-SSZ-24 (Figure 4(b)). While simulating this reaction step, one wants to sample paths that directly connect basin R with basin P (Figure 5). If however, an extra free energy minimum exists corresponding with an intermediate structure (IM) of which the formation and reaction is not explicitly sampled by the CVs, the MTD simulation gets trapped in this minimum and a proper sampling of the reaction from R to P is no longer possible. This is the case when only the collective variables CN1 and CN2 from Figure 4b are taken into account.

Within the framework of this proposal, we will need to find the right balance between a reasonable number of collective variables, that are able to capture the chemical transformations. The number of collective variables should be relatively small to avoid exceedingly long filling times of the hills. The simulation time scales exponentially with the number of collective variables. In applications with multiple guest molecules (schematically shown in Figure 2b), the number of collective variables can easily increase to 3 or 4 and a multidimensional FES is obtained. Given this complexity, it is necessary to apply automated tools to analyse a posteriori the proper choice of the collective variables. A proposed analysis method in literature, which will be used here is the committor analysis. [39] The concept relies on generation of a few hundreds of configurations starting from a given point on the free energy surface. The committor gives the conditional probability that a trajectory ends up in a particular state. The methods is available in the open source code PLUMED.[40] Very recently B. Ensing (UvA – Amsterdam) adapted the scripts to be used in conjunction with the CP2K code. Within this project the methodology will be used for chemical transformations in nanoporous materials and possibly adapted in terms of the needs. This will be performed in collaboration with the UvA group in Amsterdam with E.J. Meijer, P. Bolhuis and B. Ensing [41-43]. The group is renowned for its seminal work on rare events in biosystems and homogeneous catalysis. In the last year I have established a research collaboration with the UvA group through an exchange visit of one of my PhD students. The available scripts will be adapted to be used in conjunction with the CP2K code. The latter code will be used as a main vehicle to perform our simulations due to its attractive scaling of computational time in terms of the number of atoms involved. The CMM has very good contacts with the CP2K developer's team and we also implemented in the past new theoretical methods in the code.

Furthermore the METAGUI interface developed by Laio [44] will be used which also allows to keep track of the enormous amounts of structures generated through a MTD run. The software relies on partitioning the huge number of structures into a set of microstates characterized by similar values of the collective variables. By means of a weighted-histogram procedure relative free energies may be obtained of microstates. Where necessary, we will modify and extend the current implementations to make the method fully operational in conjunction with ab initio molecular dynamics simulations performed within CP2K.

In cases where proper definition of collective variables is problematic, we will test the transition path sampling method. [39] Hereby an ensemble of transition paths is created on basis of an initial trajectory and this may lead to discovery of new reaction paths. The method is however computationally very expensive and will only be used in for well defined cases, where other methods fail to provide the right insight.

Another method which potentially interesting, is the generation of quasi-classical trajectories (QCT) starting from a transition state. The initial atomic velocities are generated by exciting the normal modes with quantum mechanical vibrational populations. After that nuclear motion is treated classically. The method was successfully used by Bell and co-workers [26] to predict intermediates and product selectivities in cracking of alkanes over H-MFI. We will also test the method for some reactions under investigation here.

Level 1b: Transition rates between stable basins on FES.

Once the FES is reconstructed transition rates between stable minima on the surface can be calculated. The easiest method to do so is to use transition state theory where the free energy of activation is calculated as the difference between the free energy of the transition state ensemble and the free energy of the reactants region. The multidimensional free energy surface should thus be mapped in terms of a low-dimensional reaction coordinate. For simple cases this may be done using visual inspection. Within the framework of my ending ERC program I succeeded to simulate the methylation of benzene in H-ZSM-5 using the MTD. [25] The difference between two collective variables and the free energy of activation was calculated after projecting the 2D surface onto an 1D surface, as illustrated Figure 6.

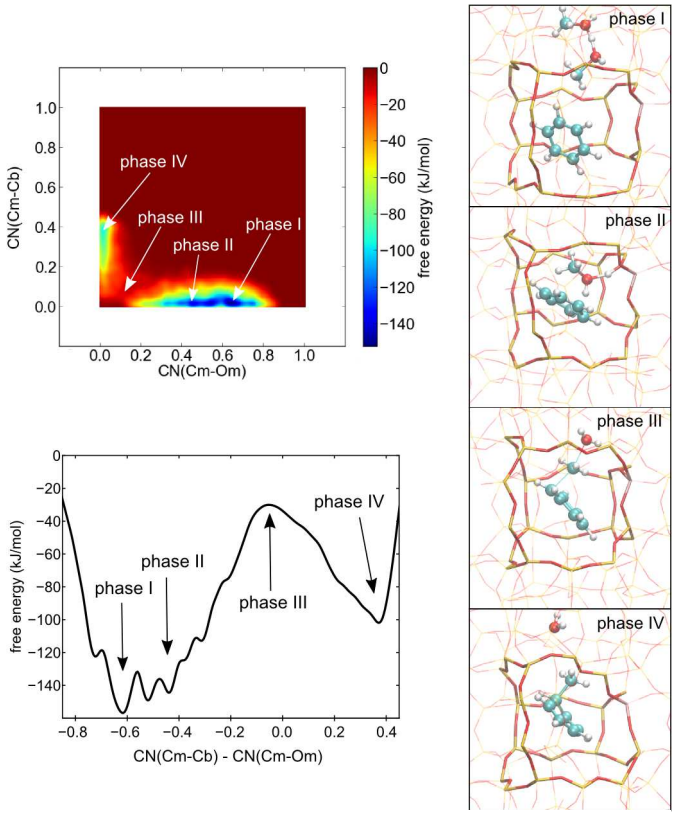


Figure 6 : 2D (top left) and 1D (bottom left) free energy profile for the methylation of benzene in H-ZSM-5 with 5 methanol molecules with selected conformations representing the four phases along the reaction pathway (shown right). Methanol molecules that do not participate in the reaction are not shown.

For the applications with multiple reaction channels and a larger number of collective variables, an automated procedure needs to be adopted. Within the framework of this proposal I will use the lowest free energy path method proposed by Ensing. [43] One starts from a stable minimum on the FES, and defines a coarse path leading us from minimum A to B. The final minimum free energy path is obtained by correcting for the width of the valley. The dimensions perpendicular to the path are integrated out, which results in the lowest free energy path in collective variable space.

Rates of transitions directly from metadynamics run : Tiwary and Parrinello recently extended the scope of the MTD method to directly calculate the transition rates between (metastable) minimum free energy states. [45] Plain MTD is capable of giving free energy barriers, but no rates, as the added Gaussian hills disturb the time information (the dynamics). The crux of their extended method relies in avoiding filling with Gaussian hills in the transition state region. The method does not require any previous knowledge of transition states or reaction coordinates and should thus be very generally applicable. The only condition is to properly choose a set of collective variables that is able to distinguish between the various minima on the FES. In this proposal I will test their new method for reactions in nanoporous materials. First of all, the obtained MTD rates will be benchmarked with our earlier chemically accurate rate coefficients.[22] If successful, it would be the first full metadynamical exploration of a chemical conversion on the fly in nanoporous materials also giving transition rates. The method has a lot of potential for the highly complex applications envisaged in PL2.

Level 1c : Including nuclear quantum effects during the molecular dynamics run

One point that is often overlooked in QM molecular dynamics runs, is the importance of nuclear quantum effects. For reaction in which light atoms are involved such effects will grow in importance. The path integral formalism is very promising but has to date not been applied extensively in combination with QM molecular dynamics simulations. Very recently Ceriotti and co-workers developed a Python interface for using path integral MD simulations in combination with electronic structure programs. [46] It is our intention to test the i-PI interface in conjunction with CP2K for the simulation of elusive intermediates in zeolite chemistry.

Level 2 : Loading of guest molecules in pores at operating conditions

The transition rates obtained in the previous sections give information on the chemical transition occurring at the active site itself. Prerequisite for these simulations is the estimation of the number of guest molecules present in the pores at operating conditions. [47, 48] Moreover, we need to estimate the adsorption capacity of the molecules at the active sites. In the MD simulations performed so far, the number of molecules in the pores of the material was guessed upon chemical intuition and space availability.[25]

In this proposal, a more straightforward approach is used to extract the distribution of guest molecules – including mixtures – from adsorption isotherms, calculated using Grand-Canonical Monte Carlo (GCMC) calculations with force fields in a fixed volume (V), fixed temperature (T) and fixed chemical potential (μ). The number of particles may vary during the simulation. [49-51] Dedicated programs have been developed by renowned groups. For the execution of this part of the proposal I will rely on two collaborations I have set up recently : (i) the group of D.Dubbeldam (UvA) who is one of the developers together with S. Calero and R. Snurr of the RASPA code.[52] One of my current PhD students has spent six months in the MOLSIM group at

the UvA. (ii) the MOLSIM group of B.Smit (Berkeley), where another PhD student of my group is currently spending one year and learns to work with the COTA code.

Such GCMC simulations are performed using classical force fields and considering a rigid framework. Simulations in the (μ,p,T) ensemble, which allow volume fluctuations by fixing the pressure p, do not always succeed in reproducing experimental isotherms due to shortcomings of the presently available flexible force fields. [53, 54] Especially, at higher temperatures - valid for some processes under consideration here - framework flexibility may have a substantial influence on the adsorption of guest particles. We propose a two step QM/MM procedure to calculate the adsorption isotherms at operating conditions, thus accounting for the framework flexibility. Using first principle dynamics simulations in the NpT ensemble, a series of snapshots of the material will be generated, which will be used in a second step as input for the Monte Carlo simulations. The latter simulations will be performed by dedicated programs such as RASPA or COTA. Repeating the MC calculations for different volumes, a set of adsorption-isotherms is obtained that account for the framework flexibility.
From the adsorption isotherms, other information may be obtained such as the distribution of guest molecules through the nanoporous materials and densities. [50, 55, 56] Very recently I have built up expertise in predicting radial distribution functions in solvents for a variety of molecules including protic molecules such as water, ethanol, methanol,… [57] It is the intention to extend the methodologies developed therein to nanoporous materials. Adaptation will be necessary as spherical symmetry is broken at the edges. Within liquid structure distinction was made between inter- en intramolecular RDF's. In analogy we will construct some adsorbate-adsorbent distribution functions.

As a result of these simulations, the average loading of guest molecules may be determined in the nanoporous material at representative conditions for the catalytic reaction at hand, thus at realistic partial pressures, temperatures.

Level 3 : Diffusivity of guest molecules in nanoporous systems with blocked sites
In this level I will study a selected number of topics which relate to diffusion of guest molecules through the pores of the materials. Diffusion is a phenomenon that takes place at larger length and time scales and is typically studied using force field based approaches. Diffusion constitutes a research domain on its own and I will only focus on those aspects that are relevant for this proposal and allow an integrated approach to describe a complex chemical conversion. It concerns the diffusion of guest molecules in the presence of trapped molecules in the pores of the material. This is particularly relevant for Methanol to Olefin (MTO) chemistry where a hydrocarbon pool species is trapped in the pores of the zeolites. There is clear experimental evidence that product selectivity might be partially ascribed to this effect. [58] The study of such blocking diffusion would be truly innovative.
The derivation of the diffusion constant is well established using molecular dynamics simulations, which track the position of the molecule over time. If however the diffusion barriers are too high, molecular dynamics runs are too slow to efficiently generate particle trajectories over the time-scales of the diffusion process. As such diffusion itself becomes a rare event and may be viewed as a hopping process between large cages separated by narrow windows. We recently studied such hopping for the diffusion of propene through small pore zeolites, containing 8-rings as the largest and indeed discovered that the diffusion process itself is a rare event (illustrated in Figure 7). A range of techniques have been suggested to also treat diffusion in these conditions, including dynamically corrected Transition State Theory, a kinetic Monte Carlo approach… [59] . Particularly interesting are the techniques suggested to simulate diffusion under various loadings of the molecules in the pores, which enable also to simulate collective-diffusion.

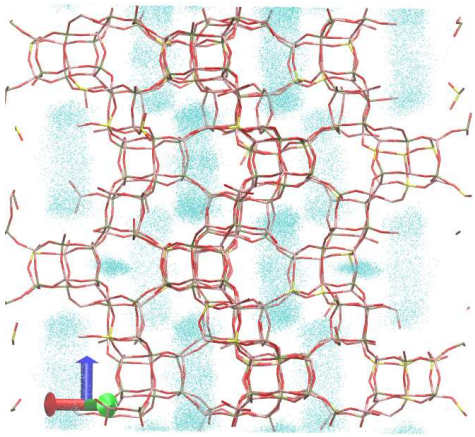


Figure 7 : Trajectories of the diffusion of propylene at 300K in H-SAPO-56. Each dot represents a propene molecule at a certain time step. The total simulation time amounts to 10 ns.

Within the framework of this proposal I will use the plethora of techniques available in literature to estimate the self-diffusion and collective-diffusion under diverse conditions of loading, presence of trapped molecules and concentration of active sites in the material. Diffusion is usually performed using classical force fields, but for the chemical transformations under study here (see PL2) under real operating conditions (high temperature and high loading), where specific

interactions take place, we propose to calculate the hop rates from first principles, using the free energy methods developed in Level 1 and 2. This will be done on selected cases of individual molecules and clusters of molecules and accounting for blocking sites. Determination of hop rates using advanced QM sampling methods will be truly innovative, which is nearly unprecedented. [60] It also will create the possibility to create a deeper understanding of product selectivities in catalysed chemical reactions. First some benchmark studies will be performed on systems where extensive method testing has been performed by renowned groups in this field. The force fields, developed by my group in collaboration with R.Schmid (Bochum) and G.Sastre (Valencia), will be used for the molecular dynamics runs. G.Sastre is an expert in theoretical modeling of nanoporous materials and their specific characteristics, such as acidity and diffusion and adsorption capabilities. [61]

In any case the overall chemical conversion is the result of three conditional processes : adsorption, diffusion and reaction itself. The integrated approach proposed here, is designed to enable us to understand observed selectivity in nanoporous materials to a deeper level than thus far performed.

Effects of entropy and framework flexibility

Nanoporous materials are often much more flexible than generally assumed. A striking experimental illustration that gas molecules with a Lennard-Jones diameter larger than the time-averaged narrow sodalite windows could still diffuse through the sodalite zeolite. [62, 63] The flexibility can therefore affect diffusivities by orders of magnitude. [50, 51, 55, 56] To understand flexibility, one needs to resort to free energy methods because it is of utmost importance to correctly describe the effects of entropy. While it is straightforward to deduce the internal energy from a molecular dynamics simulation, it is far from trivial to calculate the entropy or entropy differences from atomistic simulations. For almost all applications in this proposal, this knowledge is essential. A few examples are entropy driven processes, or structural transformations of flexible materials (PL2). In this proposal, we will implement and develop theoretical models to extract the framework's entropy from MD and MC simulations. A short resume of methods to be tested is given in Figure 8. As such we will go beyond the Harmonic Oscillator approximation that is today the standard method to estimate effects of entropy but fails in accounting correctly for the contribution of low lying collective motions of the lattice.

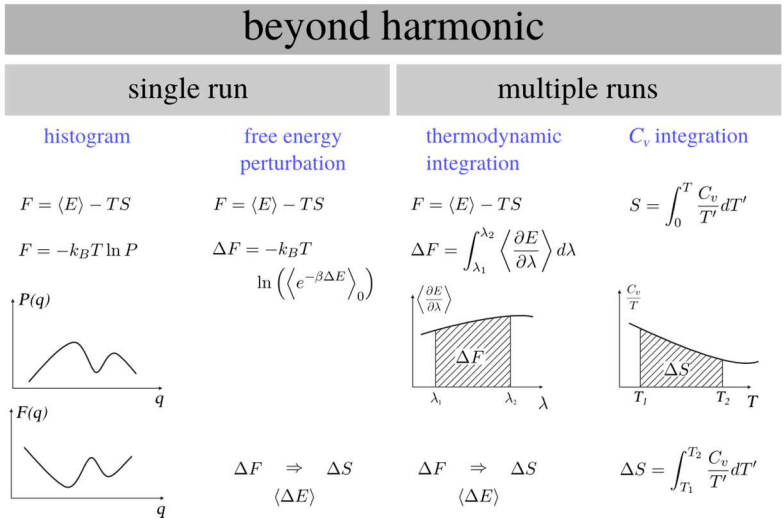


Figure 8 : Several methods to compute the entropy profile as a function of the reaction coordinate *q*, from a single or multiple runs, if necessary by first computing the free energy and next subtracting the average energy. The *histogram method* converts the histogram along the reaction coordinate to the free energy. The *free energy perturbation method* calculates the free energy change due to a perturbation in the direction of the reaction coordinate, while only sampling the reference system. *Thermodynamic integration* adiabatically varies the reaction coordinate in small steps and accumulates the small free energy changes along this path. Computing *Clausius' integral* , i.e. integrating the ratio of heat capacity over temperature, gives the entropy directly.

These methods will be adapted and extended to yield the entropy of the nanoporous solids from first principles. At first instance the methods will be tested and implemented in our own in house developed YAFF software code, which is a force field based code.[https://molmod.ugent.be/software] Currently YAFF is capable of performing MD simulation in a versatile range of thermodynamic ensembles. To reach the goals of the project some YAFF should be extended in some aspects. The advantage of using our own open source simulation code is that it allows absolute control over the modeling settings. Once the methods have been tested and operational, we will use them in other software codes for large scale applications such as DL_POLY, CP2K,… [64] This part of the proposal is very challenging from a theoretical point of view as it needs theoretical derivations, implementations and testing. It is obvious that my physical background will be necessary to accomplish the foreseen deliverables. If successful the outcome will certainly have a large impact for the simulation of nanoporous materials.

PL2 : APPLICATIONS

Rationale for selected materials and conversion processes :

The applications are situated in the field of **zeolite catalysis** and **transformations in Metal-Organic-Frameworks.** The rationale for this choice is inspired on one hand by the fact that my group is prominently active on the international scene in these areas with results published in the top journals of chemistry, material science and physics. The current achieved position is ideally suited to generate major impact using the novel approach put forward in this research program. On the other hand I can fully rely on existing collaborations with international top experimental groups in catalysed chemical reactions over zeolites and MOF's.

Each topic is carefully selected and shows all ingredients to fully explore the capacities of the advanced MD techniques proposed in the methods section. A strong interaction between theory and experiment is key towards making ground-breaking achievements, making it possible to get an in depth knowledge of the targeted applications and to tackle topical questions with state of the art methodologies.

Zeolite catalysis

Within zeolite catalysis, the **conversion of methanol to hydrocarbons** and **cracking of olefins** over acidic zeolites will be studied. Both processes are of relevance in the search for alternative processes to produce hydrocarbon products and are from theoretical modelling point of view very challenging.

The **Methanol to Olefin (MTO) process** has experimentally been developed in the past 3-4 decades and is currently being industrialized.[65] Starting from a methanol source, light olefins are produced such as ethene, propene but also some medium weight hydrocarbons (C4,C5, C6 olefins and heavier compounds) (see scheme in Figure 9). Methanol can be obtained from coal, natural gas by the production of synthesis gas which is then further processed to produce methanol. Currently the MTO process is often combined with an **olefin cracking process** (OCP) unit to further crack the higher fraction hydrocarbons to C2 and C3 species. [65, 66] Such yield improvements of ethene and propene significantly improves the return of the MTO process. From industrial technical point of view both the conversion of methanol to olefins and the cracking of olefins are thus very timely.

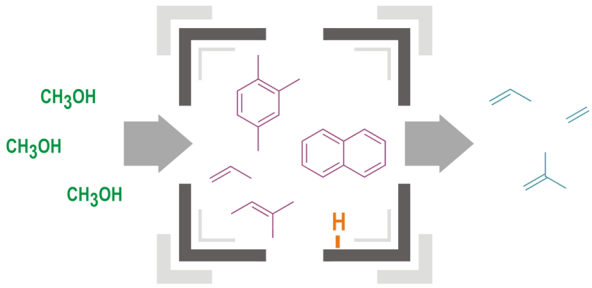


Figure 9 : Schematic representation of the supramolecular nature and framework flexibility of the MTO catalyst.

The MTO chemistry mechanism is probably one of the most disputed processes within heterogeneous catalysis from mechanistic point of view. For more than 30 years it was believed that two C1 species couple directly to form the first carbon-carbon bond. Currently there is a consensus that a hydrocarbon pool mechanism operates in which an organic center is trapped in the zeolite pores and acts as co-catalyst, as schematically shown in Figure 9. The hydrocarbon pool may be of aromatic type but also alkenes itself can take up this role. In some materials a dual cycle operates depending on the operating conditions. In that case alkenes itself may be successively methylated after which by cracking lower olefins are produced. Thus also from this viewpoint we are interested in olefin cracking reactions. Moreover, the cracking of long hydrocarbon chains is of more general interest in view of the industrially important Olefin Cracking Process (OCP) unit – often combined with the MTO process – and the Fluid Catalytic Cracking (FCC) process.

From interactions with our experimental partners, it has become clear that current static approaches are insufficient to resolve some topical issue for both processes. An overview of the topics which will be studied within the framework of this proposal is hereafter given.

Influence of feed composition and acidity on acid sites, catalytic cycles, product selectivity, competitive reactions.

- Influence of water on the availability of active sites and active routes within MTO chemistry : Water is always present in the methanol feed in various concentrations depending on the origin of the methanol source. The precise influence of water on various aspects of the catalytic cycle is yet unknown. There is evidence that water forms protonated clusters with methanol but also with dimethylether which is easily formed in the equilibrium phase. This poses challenges on the availability of acid sites in the zeolite materials. It is obvious that static methods are incapable of

describing the complex free energy surface one is confronted in this problem. In a recent publication of my group we discovered that protonated methanol clusters could also initiate the key methylation reactions. [25] Within this proposal a dedicated first principle molecular dynamics study will be performed on the influence of water on the availability of acid sites, the active catalytic cycles and eventually the product selectivity. The study will be performed in a variety of materials with different acid strength and for which the mechanistic cycles are known to differ (H-ZSM-5, H-SAPO-34, H-SSZ-13, H-SAPO-5, H-SSZ-24,…) However, care will be taken not to simulate steaming conditions under which dealumination or desilication of the catalyst materials occur. This topic is conducted in collaboration with the Catalysis group of B.Weckhuysen of the Utrecht University. I have a successful collaboration with this group which resulted already in various common papers. The group is internationally leading in the field of heterogeneous catalysis, in particular on in-situ characterization of catalytic solids. The most advanced spectroscopic tools are used to keep track of the various intermediates during the catalytic cycle.

- Influence of catalyst acid strength on MTO chemistry : Isostructural materials such as H-SSZ-24 and H-SAPO-5 (both AFI topology) show distinct variations in product distributions, reaction orders for methylation reactions of aromatic species,… H-SSZ-24 is an aluminosilicate and H-SAPO-5 is a silicoaluminophosphate exhibiting differences in the strength of the Brønsted acidic site. These materials are prototypes to elucidate the effects of acid strength as the AFI topology allows co-feed reactions with little steric constraints, in contrast to the severe diffusional constraints within the archetypical H-SAPO-34 catalyst. Herein larger aromatics may not be fed due to the small 8-ring windows.
  The materials are under investigation with our experimental partners at the Catalysis group in Oslo (U. Olsbye, S.Svelle). There are clear experimental evidences that the difference in acidic strength leads to distinct variations in the product selectivity and the prominent reaction mechanism.[67] Kinetic studies on the co-reactions of benzene revealed that the reaction orders with respect to methanol and benzene critically depend on the acid strength of the material. Using the flow scheme of this proposal we will unravel the nature of the complex free energy surface for the systems at hand. Product selectivity will be investigated by means of the QCT method (see methodology), based on the various transition states detected on the free energy surface.

Diffusion of reactants, products through pores with trapped molecules.

Using the free energy methods developed within this proposal we will study the diffusion of small molecules such as ethene, propene but also the reactant molecules in presence of hydrocarbon pool species trapped in the pores of the zeolite. We will systematically add another level of complexity to the problem. First we will perform a systematic investigation for a variety of small pore, medium pore and large pore zeolites, which will allow assessing the importance of size of the zeolite rings on the diffusivity. A non-exhaustive series of materials which are relevant within the MTO context are Beta, SAPO-5, ZSM-5, ZSM-22, SAPO-34, SAPO-18, SAPO-35. The importance of the zeolite flexibility will be systematically investigated using the entropy methods of the methods platform.

Apart from diffusion of small molecules also diffusion of some clusters (such as protonated clusters) will be studied. At second instance systematically larger hydrocarbon pool species will be introduced in the lattice and the hop rates will be calculated using the first principle methods outlined in the methodology section under realistic loadings with other guest molecules. The results obtained hereof are certainly groundbreaking and highly challenging. Diffusivities from first principle methods at operating conditions are not yet reported before as advanced free energy methods are necessary which take into account all levels of complexity.

For this item I will collaborate with the group of J. Denayer (VUB- Brussels) who is an expert in the experimental part of this problem.

Olefin cracking

Adsorption complexes of cracking intermediates : Physisorption and chemisorption of the reactants inside the pores of the zeolite catalyst are the initial steps of any catalytic process. A wealth of literature is available on the calculation of adsorption enthalpies from static methods. [68, 69]

Recently important papers of Hafner and co-workers show that finite temperature effects may become important when no strong binding exists between the adsorbate and the zeolite host. [33, 70] In this proposal we focus on the pentene cracking in H-ZSM-5 in view of an ongoing experimental collaboration with the Catalysis group of L.Lercher (TUMunchen). The topic is very challenging as depending on the nature of the alkene and operating conditions such as temperature, physisorption and chemisorption occur in competition with side-reactions such as isomerization, dimerization, making it very difficult to extract accurate experimental data.

Within this proposal a full dynamical approach including framework flexibility, conformational freedom at realistic process temperatures and accounting for the flexibility of the lattice will be conducted to get track of the relevant intermediates and adsorption complexes. Preliminary results on adsorption of pentene in H-ZSM-5 already reveal distinct differences between static and dynamic predictions of the various adsorption complexes.
Reaction mechanism : The reaction counts a lot of intermediates such as alkoxy species, carbenium ions, and other complexes, each with their specific stability and lifetime dependent on the operating conditions. In addition a multitude of competitive reactions appears, such as isomerizations, oligomerizations and beta-scissions. Within this proposal the complex free energy surface will be constructed using the advanced MTD approach . The objective is very challenging, recently various theoretical studies have appeared and the stability of various intermediates is crucially dependent on the model used to describe the material. [71-73]

Metal organic Frameworks

Free energy profile and transformations of flexible materials

Metal-organic frameworks (MOFs) have attracted an enormous attention the last decade due to their versatility but also to their extraordinary properties. A property which is very intriguing is the breathing capacity of these materials, i.e. their ability to undergo large structural deformations upon external stimuli. [12, 74] The highly flexible nanoporous MIL-53 type of materials (MIL for Material of Institut Lavoisier) has received considerable attention within this respect. It is however very difficult to get track of the intrinsic breathing profile in terms of various conditions such as temperature, pressure, …without the inclusion of guest molecules. [75, 76] Energy profiles in terms of the breathing angle may be obtained using quantum mechanics based, but the missing link concerns the entropy of the lattice. The methods developed within this proposal enable to go beyond the state of the art. The various entropy based methods for nanoporous solids will be used to generate the free energy profiles. In addition a first principle based MTD approach will be used to generate the free energy profile. The choice of collective variables is far from obvious as many degrees of freedom are anticipated to contribute to the transition from one phase to the other. The appropriate collective variables will be tested in a force field based approach using our in house developed YAFF code and force field for this type of materials. [76] The generation of a first principle dynamical based free energy profile for these type of materials in terms of various metals and linkers would be truly ground breaking for the MOF community. A wealth of experimental data is available for the MIL-53 type of material, thus it serves as an ideal benchmark system. Moreover the research will be performed in close collaboration with G. Maurin (CNRS - Institut Charles Gerhardt, Montpellier, France). If successful the methods may be applied to other interesting flexible systems such as the MIL-68 series which are closely related but for which chemical breakage of the framework may occur. [77]
The methods explored here also create perspectives for applications on structural transformations in the zeolite family. I am currently collaborating with the group of J.Martens, C.Kirschhock (COK,KULeuven) where it was observed that a periodically interrupted OKO framework (-COK-14) can transform to a fully connected OKO zeolite (COK-14) with high temperature (> 700 K), and that it hydrolysed again to the initial interrupted structure with warm water. It is an example of a chemical and physical transformation, that also needs to be tackled with ab initio MD techniques as proposed here, as entropy effects and flexibility will have a decisive role.

Active site engineering within MOF catalysis

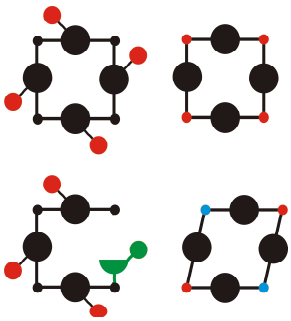


Figure 10 : Schematic representation of possible modulations in MOFs

The focus of this application part lies on the modulation and engineering of the active sites by **tailor-made modification in the structure of the material**. Emphasis is put on increasing the catalytic activity and possibly selectivity towards product distributions. A schematic overview of possible modifications is given in Figure 1. The research is inspired by a very successful collaboration with the Catalysis group of D. De Vos (KULeuven) where we showed that the catalytic activity of the UiO-66(Zr) material could be substantially improved by a modulation approach. Modulation should be interpreted in the broad sense encompassing, functionalization of the linkers, intentional removal of linkers, modulation of the electron density of the lattice through use of various metals at nodal points,…. (Figure 10). We have shown in the last two years together with our experimental partners that intentional creation of defects may substantially add to the catalytic function of the materials. [19, 20] Upon now, the free energies for creation of open sites, removal of linkers and catalytic activity was estimated on basis of a limited cluster approach or periodic approach neglecting important entropy effects and flexibility effects.

Within this proposal, I want to further build on the successful collaboration established by using more advanced theoretical tools that allow to give a representative free energy estimate for the variations modulations imposed by the experimental partners. This is also a typical problem where physical and chemical transformations are closely intertwined : sometimes transformations of the lattice are observed which preserve the chemical integrity, whereas eventually some bonds may be broken due to modulation of sites. Various acid and base catalysed reactions will be studied in materials such as the UiO-66(Zr) type of materials, the MOF-74(M) type of materials (M=Mg, Ni, Co, Zn, Mn, Cu, Fe) in collaboration with D.De Vos (COK-KULeuven)

Research vision and planning

The execution of the tasks belonging to the two platforms is closely intertwined, as schematically shown in the time table below. For some highly risk tasks, such as generation of first principle based free energy profiles for flexible materials, initiation is foreseen by a postdoc with enough maturity. The postdoc should also allow to initiate new topics, such as determination of first principle based diffusion hop rates and loading of guest molecules in the pores of the material. A close interaction with my experimental network and with various theoretical groups will be necessary. One PhD student, preferably with a physical background will work on the topics related with entropy and flexibility of the material (PhD1). The person should start from the onset of the program, to allow transfer of his/her knowledge towards the team during the execution of the project. Another PhD student (PhD3) should work for four years on rare events with the goal to determine transition rates in nanoporous materials. I foresee quite some time for this task, as it is the intention to benchmark with our earlier theoretically determined accurate kinetic rate constants. The person should also interact closely with the PhD student (PhD2) working on MTO and cracking mechanisms, to lift their applications to a higher level. The person (PhD3) should start the second year to swiftly tackle those methodological bottlenecks encountered during the first year in the applications. Such special point of attention could be the inclusion of nuclear quantum effects for some complexes in zeolite catalysis, in which light atoms are involved. PhD4 works on active site engineering in MOFs and will benefit from method developments performed by the postdoc and PhD1 working on flexible materials.

ERC Consolidator Project DYNPOR Planning scheme																					
Integration PL1/PL2	Research activities		Year 1				Year 2				Year 3				Year 4				Year 5			
Method development	MOFS	Entropy / Flexibility + Application on flexible materials	PhD1																			
Methods + Applications	MOFS	Flexible materials + First principle based free energy profiles	Postdoc																			
Methods + Applications	Zeolites - MTO	Influence of water	PhD2																			
		Influence of acidity					PhD2															
		Loading of guest molecules in pores at operating conditions					Postdoc															
		First principle based diffusion hop rates									Postdoc											
	Zeolites - cracking	Adsorption + Mechanism									PhD2											
Methods + Applications	Zeolites + MOFs	Rare events/ Transition rates/ Nuclear quantum effects					PhD3															
Applications	MOFs	Active site engineering					PhD4															

The successful execution of the project critically relies on an interdisciplinary and concerted effort of a team of about five researchers, which is coached on a daily basis by myself. I should be able to attract people with different background to my team and furthermore it will be essential for them to be integrated in my already existing team, to bounce their new ideas off. I am quite confident that I will be able to motivate such the new team of researchers for this challenging project with a clear set of milestones on the longer term. The integrated approach of methods/applications foreseen here, is especially attractive as major challenges have to be overcome. Each application on its own is very challenging and the transfer of the MD methodology to a new application field will pose obstacles that we will have to overcome. I will personally engage myself very strongly to overcome the hurdles and I will rely on my strong physical background, interactions with chemists and strong communication skills to stimulate my team and enable gain of knowledge towards my group. If successful, the outcome of this proposal on the long term will impact the catalysis and nanoporous community and provides new methods to simulate chemical transformations.

Apart from the list of experimental partners mentioned above, the project will also greatly benefit from interaction with various theoretical groups, who have complementary expertise and who are very well suited for exchange visits for various of my researchers. It is a fortiori the intention to extend and strengthen my network with new experimental and theoretical partners, within the framework of this proposal. My modus operandi of the past years in which I am continuously extending my network and inviting prominent partners to my group has been very fruitful.

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Section c. Resources (including project costs)

The total requested budget is **1993750 Euro**, which can be subdivided in a large fraction reserved for personnel, another large fraction is necessary for having access to high performance computing services and the rest is reserved for other costs related to travel, small consumables,…

Personnel

The key personnel involved in this research programme will be the PI, a postdoctoral fellow for 4,5 years and four PhD students. Given the ambitious research program both on the methodological and application front such large investment in high qualified researchers is mandatory to pursue the goals of the proposal. Note that I (as PI) am directly paid by the Ghent University, and, hence, this personnel cost is not taken up in the table. Thus overall 3 to 5 scientific collaborators paid by the grant will work full time on the project. They will receive full scientific support from the other members of the Center for Molecular Modeling in which my research group is embedded. I have one full time administrative personnel member which assists in daily managing tasks, personnel affairs, ….

A postdoctoral researcher is necessary for about the whole duration of the program, as a substantial number of new topics need to be tackled. To guarantee success, a qualified researcher with ample experience is needed, who is able to interact on a daily basis with other prominent groups. I will launch an international call to attract researchers with very good CVs to my group to strengthen the knowledge of my group.

Simultaneously two PhD students will start from the beginning, preferably having a different background allowing physical and chemical impulses in various topics of the proposal. In any case there will be an open call, guaranteeing the recruitment of the most suitable candidates. In the second year I plan to attract another two PhD students and the planned research activities should reach their full capacity from that year on.

In view of the strong interactions with experimental partners, all research members should be willing to do exchange visits for shorter and longer time in institutions of my research network. I will also visit on a regular basis the research groups with whom I collaborate to organize work discussions on various items. I think this is crucial to make sufficient progress in the various areas. Four years are scheduled for the PhD projects, which is typical in Belgium. The team will be complemented by 2 additional PhD students in year 2. A total duration of 3 years is foreseen for the postdoctoral fellow. A second mandate of 1 1/2 years is scheduled in year 4 to ensure continuity in the research activities. The personnel cost of a PhD amounts to 40000 Euro yearly (average over 4 years) , 80000 Euro for a postdoc.

Other direct costs:

The successful completion of the work program is critically dependent on the availability of intensive computer capacities. It must be noted that the calculations foreseen here, are all very time consuming. At the onset of the proposal an investment of 200000 Euro is foreseen in high performance computers which are managed by the ICT department of our university but partly financed by research groups. The local clusters belong to the TIER-2 level in the perspective of the computational infrastructure in Europe. [HPC UGent, “High Performance Computing infrastructure”, http ://www.ugent.be/hpc/en/]. Investment in this cluster is necessary to dispose of a local equipment which can be used on a flexible basis.

At the Flemish level, we dispose of a TIER-1 computer infrastructure, the Flemish Supercomputer Center (VSC). Access to this infrastructure is granted on basis of proposal submissions but is also charged following net pricing: 11.57 Euro/nodeday (using one node onTier 1 for one day). For research projects financed by the EU, the full cost will be charged.

One DFT metadynamics simulation requires 60 node days. 10 MTD simulations are needed per full application in a zeolite . Adding 10 standard MD simulations, one complete study requires 900 node days. An MD simulation of diffusion of small molecules through zeolites requires 15 node days with the DL_POLY Classic simulation package. A typical computational study needs 10 zeolite materials with 4 different diffusion molecules per zeolite, and 4 different loadings per molecule. In total such a calculation of a single diffusion study demands 2400 node days. Summarizing with the average personnel occupation, we need at least 2x900+2400 = 4200 node days/year or 48594 Euro/year for usage of Tier 1. Therefore a cost of 50000 Euro is requested per year for computing time at the TIER1 infrastructure. If necessary we will also submit proposals to request computing time at TIER-0 infrastructure at the European Level.

Travel costs are budgeted 15000 Euro per year, including the expenses of the PI. In view of the high number of collaborations with external research teams, several short period stays abroad are foreseen and also essential for successful execution of the project.

Publication costs should also be budgeted as ERC demands open-access for all papers publishing research results financing by the grant. For immediate availability the open-access fee amounts to 2000 $ for ACS journals. I budgeted the total cost for 5 papers/year which is a minimum.

For the above cost table, please indicate the % of working time the PI dedicates to the project over the period of the grant:	**50 %**

I will commit at least 50% of my time to the execution of the DYNPOR program. The other part of my time is devoted to fulfill the commitments to other running projects, teaching duties and providing some scientific community service.

PART A: BUDGET TABLE FOR BENEFICIARY UNIVERSITEIT GENT

Please enter duration in months [1]	60

Please indicate the % of working time the PI dedicates to the project over the period of the grant	50.00

Estimated eligible costs (per budget category)	month 1 to 18	month 19 to 36	month 37 to 54	month 55 to 60	Total
A. Direct Personnel costs:					
P.I.	0.00	0.00	0.00	0.00	
Senior Staff	0.00	0.00	0.00	0.00	
Post docs	200000.00	80000.00	80000.00	40000.00	
Students	120000.00	240000.00	200000.00	40000.00	
Other	0.00	0.00	0.00	0.00	
Total Personnel:	320000.00	320000.00	280000.00	80000.00	1000000.00
D. Other Direct Costs:					
D.1 Travel	22500.00	22500.00	22500.00	7500.00	
D.2 Equipment	60000.00	60000.00	60000.00	20000.00	
D.3 Other goods and services (i.e. consumables, publications)	96000.00	96000.00	96000.00	32000.00	
D.4 Costs of large research infrastructure	0.00	0.00	0.00	0.00	
Total Other Direct Costs:	178500.00	178500.00	178500.00	59500.00	595000.00
Total Direct Costs:					
E. Indirect Costs (25% of Direct Costs)	124625.00	124625.00	114625.00	34875.00	398750.00
B.Subcontracting Costs (No indirect costs)	0.00	0.00	0.00	0.00	0.00
Costs of in-kind contributions not used on premises (No indirect costs)	0.00	0.00	0.00	0.00	0.00
Total Estimated Budget (by reporting period and total):	623125.00	623125.00	573125.00	174375.00	1993750.00

[1] Duration of the action (see Article 3)

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PART B: ESTIMATED BUDGET FOR THE ACTION

	Estimated eligible[1] costs (per budget category)								EU contribution			Additional information		
	A. Direct personnel costs				B. Direct costs of subcontractin	D. Other direct costs	E. Indirect costs[2]	Total costs	Reimburseme rate %	Maximum EU contribution[3]	Maximum grant amount[4]	Information for indirect costs:	Information for auditors:	Other information:
	A.1 Employees (or equivalent) A.2 Natural persons under direct contract A.3 Seconded persons [A.6 Personnel for providing access to research infrastructure]		A.4 SME owners without salary A.5 Beneficiaries that are natural persons without salary			D.1 Travel D.2 Equipment D.3 Other goods and services D.4 Costs of large research infrastructure						Costs of inkind contributions not used on premises	Declaration of costs under Point D.4	Estimated costs of beneficiaries/ linked third parties not receiving EU funding
Form of costs[5]	Actual	Unit[6]	Unit[7] EUR/hour		Actual	Actual	Flat-rate[8] 25%							
	a	Total b	No hours	Total c	d	e	(f)=0,25x (a+b+ c+e-k)	(g)= a+b+c + d+e+f+	h	i	j	k	Yes/No	
1. UNIVER GENT	1000000.00	0.00			.00	595000.00	398750.00	1993750.00		1993750.00	1993750.00	0.00	No	

1 See Article 6 for the eligibility conditions
2 The indirect costs covered by the operating grant (received under any EU or Euratom funding programme; see Article 6.5.(b)) are ineligible under the GA. Therefore, a beneficiary that receives an operating grant during the action's duration cannot declare indirect costs for the year(s)/reporting period(s) covered by the operating grant (see Article 6.2.E).
3 This is the theoretical amount of EU contribution that the system calculates automatically (by multiplying all the budgeted costs by the reimbursement rate). This theoretical amount is capped by the 'maximum grant amount' (that the Commission/Agency decided to grant for the action) (see Article 5.1).
4 The 'maximum grant amount' is the maximum grant amount decided by the Commission/Agency. It normally corresponds to the requested grant, but may be lower.
5 See Article 5 for the forms of costs
6 Unit : hours worked on the action; costs per unit (hourly rate) : calculated according to beneficiary's usual accounting practice
7 See Annex 2a 'Additional information on the estimated budget' for the details (costs per hour (hourly rate)).
8 Flat rate : 25% of eligible direct costs, from which are excluded: direct costs of subcontracting and costs of in-kind contributions not used on premises (see Article 6.2.E)
9 See Article 9 for beneficiaries not receiving EU funding
10 Only for linked third parties that receive EU funding

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MODEL ANNEX 4 FOR H2020 ERC MGA — MULTI

FINANCIAL STATEMENT FOR BENEFICIARY [name]/ LINKED THIRD PARTY [name] FOR REPORTING PERIOD [reporting period]

	Eligible[1] costs (per budget category)									Receipts	EU contribution			Additional information
	A. Direct personnel costs				B. Direct costs of subcontracting	D. Other direct costs		E. Indirect costs[2]	Total costs	Receipts	Reimbursement rate %	Maximum EU contribution[3]	Requested EU contribution	Information for indirect costs :
	A.1 Employees (or equivalent) A.2 Natural persons under direct contract A.3 Seconded persons		A.4 SME owners without salary A.5 Beneficiaries that are natural persons without salary			D.1 Travel D.2 Equipment D.3 Other goods and services	*[D.4 Costs of large research infrastructure]*			Receipts of the action, to be reported in the last reporting period, according to Article 5.3.3				Costs of in-kind contributions not used on premises
Form of costs[4]	Actual	Unit	Unit		Actual	Actual	Actual	Flat-rate[5] 25%						
	a	Total b	No hours	Total c	d	e	*[f]*	g=0,25x(a+b+c+*[f]* -m)	h = a+b+c+d+e+*[f]* +g	i	j	k	l	m
[short name beneficiary/linked third party]														

The beneficiary/linked third party hereby confirms that:
The information provided is complete, reliable and true.
The costs declared are eligible (see Article 6).
The costs can be substantiated by adequate records and supporting documentation that will be produced upon request or in the context of checks, reviews, audits and investigations (see Articles 17, 18 and 22).
For the last reporting period: that all the receipts have been declared (see Article 5.3.3).

ⓘ Please declare all eligible costs, even if they exceed the amounts indicated in the estimated budget (see Annex 2). Only amounts that were declared in your individual financial statements can be taken into account lateron, in order to replace other costs that are found to be ineligible.

[1] See Article 6 for the eligibility conditions

[2] The indirect costs claimed must be free of any amounts covered by an operating grant (received under any EU or Euratom funding programme; see Article 6.2.E). If you have received an operating grant during this reporting period, you cannot claim any indirect costs.

[3] This is the *theoretical* amount of EU contribution that the system calculates automatically (by multiplying the reimbursement rate by the total costs declared). The amount you request (in the column 'requested EU contribution') may have to be less (e.g. if you and the other beneficiaries are above budget, if the 90% limit (see Article 21) is reached, etc).

[4] See Article 5 for the forms of costs

[5] Flat rate : 25% of eligible direct costs, from which are excluded: direct costs of subcontracting and costs of in-kind contributions not used on premises (see Article 6.2.E)

ANNEX 5

MODEL FOR THE CERTIFICATE ON THE FINANCIAL STATEMENTS

- **For options [*in italics in square brackets*]: choose the applicable option. Options not chosen should be deleted.**
- **For fields in [grey in square brackets]: enter the appropriate data**

TABLE OF CONTENTS

Terms of Reference for an Independent Report of Factual Findings on costs declared under a Grant Agreement financed under the Horizon 2020 Research and Innovation Framework Programme

This document sets out the '**Terms of Reference (ToR)**' under which

[OPTION 1: [insert name of the beneficiary] ('the Beneficiary')] [OPTION 2: [insert name of the linked third party] ('the Linked Third Party'), third party linked to the Beneficiary [insert name of the beneficiary] ('the Beneficiary')]

agrees to engage

[**insert legal name of the auditor**] ('the Auditor')

to produce an independent report of factual findings ('the Report') concerning the Financial Statement(s)[1] drawn up by the *[Beneficiary] [Linked Third Party]* for the Horizon 2020 grant agreement [insert number of the grant agreement, title of the action, acronym and duration from/to] ('the Agreement'), and

to issue a Certificate on the Financial Statements' ('CFS') referred to in Article 20.4 of the Agreement based on the compulsory reporting template stipulated by the Commission.

The Agreement has been concluded under the Horizon 2020 Research and Innovation Framework Programme (H2020) between the Beneficiary and *[OPTION 1: the European Union, represented by the European Commission ('the Commission')][OPTION 2: the European Atomic Energy Community (Euratom,) represented by the European Commission ('the Commission')][OPTION 3: the [Research Executive Agency (REA)] [European Research Council Executive Agency (ERCEA)] [Innovation and Networks Executive Agency (INEA)] [Executive Agency for Small and Medium-sized Enterprises (EASME)] ('the Agency'), under the powers delegated by the European Commission ('the Commission').]*

[1] By which costs under the Agreement are declared (see template 'Model Financial Statements' in Annex 4 to the Grant Agreement).

The *[Commission] [Agency]* is mentioned as a signatory of the Agreement with the Beneficiary only. The *[European Union][Euratom][Agency]* is not a party to this engagement.

1.1 Subject of the engagement

The coordinator must submit to the *[Commission][Agency]* the final report within 60 days following the end of the last reporting period which should include, amongst other documents, a CFS for each beneficiary and for each linked third party that requests a total contribution of EUR 325 000 or more, as reimbursement of actual costs and unit costs calculated on the basis of its usual cost accounting practices (see Article 20.4 of the Agreement). The CFS must cover all reporting periods of the beneficiary or linked third party indicated above.

The Beneficiary must submit to the coordinator the CFS for itself and for its linked third party(ies), if the CFS must be included in the final report according to Article 20.4 of the Agreement..

The CFS is composed of two separate documents:

- The Terms of Reference ('the ToR') to be signed by the *[Beneficiary] [Linked Third Party]* and the Auditor;
- The Auditor's Independent Report of Factual Findings ('the Report') to be issued on the Auditor's letterhead, dated, stamped and signed by the Auditor (or the competent public officer) which includes the agreed-upon procedures ('the Procedures') to be performed by the Auditor, and the standard factual findings ('the Findings') to be confirmed by the Auditor.

If the CFS must be included in the final report according to Article 20.4 of the Agreement, the request for payment of the balance relating to the Agreement cannot be made without the CFS. However, the payment for reimbursement of costs covered by the CFS does not preclude the *[Commission,][Agency,]* the European Anti-Fraud Office and the European Court of Auditors from carrying out checks, reviews, audits and investigations in accordance with Article 22 of the Agreement.

1.2 Responsibilities

The *[Beneficiary] [Linked Third Party]:*

- must draw up the Financial Statement(s) for the action financed by the Agreement in compliance with the obligations under the Agreement. The Financial Statement(s) must be drawn up according to the *[Beneficiary's] [Linked Third Party's]* accounting and book-keeping system and the underlying accounts and records;
- must send the Financial Statement(s) to the Auditor;
- is responsible and liable for the accuracy of the Financial Statement(s);
- is responsible for the completeness and accuracy of the information provided to enable the Auditor to carry out the Procedures. It must provide the Auditor with a written representation letter supporting these statements. The written representation letter must state the period covered by the statements and must be dated;
- accepts that the Auditor cannot carry out the Procedures unless it is given full access to the *[Beneficiary's] [Linked Third Party's]* staff and accounting as well as any other relevant records and documentation.

The Auditor:

- *[Option 1 by default:* is qualified to carry out statutory audits of accounting documents in accordance with Directive 2006/43/EC of the European Parliament and of the Council of 17 May 2006 on statutory audits of annual accounts and consolidated accounts, amending Council Directives 78/660/EEC and 83/349/EEC and repealing Council Directive 84/253/EEC or similar national regulations*]*.
- *[Option 2 if the Beneficiary or Linked Third Party has an independent Public Officer:* is a competent and independent Public Officer for which the relevant national authorities have established the legal capacity to audit the Beneficiary*].*
- *[Option 3 if the Beneficiary or Linked Third Party is an international organisation:* is an [internal] [external] auditor in accordance with the internal financial regulations and procedures of the international organisation*].*

The Auditor:

- must be independent from the Beneficiary *[and the Linked Third Party]*, in particular, it must not have been involved in preparing the *[Beneficiary's] [Linked Third Party's]* Financial Statement(s);
- must plan work so that the Procedures may be carried out and the Findings may be assessed;
- must adhere to the Procedures laid down and the compulsory report format;
- must carry out the engagement in accordance with this ToR;
- must document matters which are important to support the Report;
- must base its Report on the evidence gathered;
- must submit the Report to the *[Beneficiary] [Linked Third Party]*.

The Commission sets out the Procedures to be carried out by the Auditor. The Auditor is not responsible for their suitability or pertinence. As this engagement is not an assurance engagement, the Auditor does not provide an audit opinion or a statement of assurance.

1.3 Applicable Standards

The Auditor must comply with these Terms of Reference and with[2]:

- the International Standard on Related Services ('ISRS') 4400 *Engagements to perform Agreed-upon Procedures regarding Financial Information* as issued by the International Auditing and Assurance Standards Board (IAASB);
- the *Code of Ethics for Professional Accountants* issued by the International Ethics Standards Board for Accountants (IESBA). Although ISRS 4400 states that independence is not a requirement for engagements to carry out agreed-upon procedures, the *[Commission][Agency]* requires that the Auditor also complies with the Code's independence requirements.

The Auditor's Report must state that there is no conflict of interests in establishing this Report between the Auditor and the Beneficiary *[and the Linked Third Party]*, and must specify - if the service is invoiced - the total fee paid to the Auditor for providing the Report.

1.4 Reporting

The Report must be written in the language of the Agreement (see Article 20.7).

Under Article 22 of the Agreement, the [*Commission*] [*Agency*], the European Anti-Fraud Office and the Court of Auditors have the right to audit any work that is carried out under the action and for which costs are declared from [*the European Union*] [*Euratom*] budget. This includes work related to this engagement. The Auditor must provide access to all working papers (e.g. recalculation of hourly rates, verification of the time declared for the action) related to this assignment if the *[Commission] [Agency]*, the European Anti-Fraud Office or the European Court of Auditors requests them.

1.5 Timing

The Report must be provided by *[*dd Month yyyy*]*.

[2] Supreme Audit Institutions applying INTOSAI-standards may carry out the Procedures according to the corresponding International Standards of Supreme Audit Institutions and code of ethics issued by INTOSAI instead of the International Standard on Related Services ('ISRS') 4400 and the Code of Ethics for Professional Accountants issued by the IAASB and the IESBA.

1.6 Other terms

[*The [Beneficiary] [Linked Third Party] and the Auditor can use this section to agree other specific terms, such as the Auditor's fees, liability, applicable law, etc. Those specific terms must not contradict the terms specified above.*]

[legal name of the Auditor]	[legal name of the *[Beneficiary][Linked Third Party]*]
[name & function of authorised representative]	[name & function of authorised representative]
[dd Month yyyy]	[dd Month yyyy]
Signature of the Auditor	Signature of the *[Beneficiary][Linked Third Party]*

Independent Report of Factual Findings on costs declared under Horizon 2020 Research and Innovation Framework Programme

(To be printed on the Auditor's letterhead)

To

[name of contact person(s)], [Position]

[[*Beneficiary's*] [*Linked Third Party's*] name]

[Address]

[dd Month yyyy]

Dear [Name of contact person(s)],

As agreed under the terms of reference dated [dd Month yyyy]

with *[OPTION 1: [insert name of the beneficiary] ('the Beneficiary')] [OPTION 2: [insert name of the linked third party] ('the Linked Third Party'), third party linked to the Beneficiary [insert name of the beneficiary] ('the Beneficiary')],*

we

[name of the auditor] ('the Auditor'),

established at

[full address/city/state/province/country],

represented by

[name and function of an authorised representative],

have carried out the procedures agreed with you regarding the costs declared in the Financial Statement(s)[3] of the *[Beneficiary] [Linked Third Party]* concerning the grant agreement

[insert grant agreement reference: number, title of the action and acronym] ('the Agreement'),

with a total cost declared of

[total amount] EUR,

and a total of actual costs and 'direct personnel costs declared as unit costs calculated in accordance with the [*Beneficiary's*] [*Linked Third Party's*] usual cost accounting practices' declared of

[sum of total actual costs and total direct personnel costs declared as unit costs calculated in accordance with the *[Beneficiary's] [Linked Third Party's]* usual cost accounting practices] EUR

and **hereby provide our Independent Report of Factual Findings ('the Report')** using the compulsory report format agreed with you.

The Report

Our engagement was carried out in accordance with the terms of reference ('the ToR') appended to this Report. The Report includes the agreed-upon procedures ('the Procedures') carried out and the standard factual findings ('the Findings') examined.

The Procedures were carried out solely to assist the [*Commission*] [*Agency*] in evaluating whether the [*Beneficiary's*] [*Linked Third Party's*] costs in the accompanying Financial Statement(s) were declared in accordance with the Agreement. The *[Commission] [Agency]* draws its own conclusions from the Report and any additional information it may require.

[3] By which the Beneficiary declares costs under the Agreement (see template 'Model Financial Statement' in Annex 4 to the Agreement).

The scope of the Procedures was defined by the Commission. Therefore, the Auditor is not responsible for their suitability or pertinence. Since the Procedures carried out constitute neither an audit nor a review made in accordance with International Standards on Auditing or International Standards on Review Engagements, the Auditor does not give a statement of assurance on the Financial Statements.

Had the Auditor carried out additional procedures or an audit of the *[Beneficiary's] [Linked Third Party's]* Financial Statements in accordance with International Standards on Auditing or International Standards on Review Engagements, other matters might have come to its attention and would have been included in the Report.

Not applicable Findings

We examined the Financial Statement(s) stated above and considered the following Findings not applicable:

Explanation (to be removed from the Report):

*If a Finding was not applicable, it must be marked as '**N.A**.' ('Not applicable') in the corresponding row on the right-hand column of the table and means that the Finding did not have to be corroborated by the Auditor and the related Procedure(s) did not have to be carried out.*

The reasons of the non-application of a certain Finding must be obvious i.e.

i) if no cost was declared under a certain category then the related Finding(s) and Procedure(s) are not applicable;

ii) if the condition set to apply certain Procedure(s) are not met the related Finding(s) and those Procedure(s) are not applicable. For instance, for 'beneficiaries with accounts established in a currency other than euro' the Procedure and Finding related to 'beneficiaries with accounts established in euro' are not applicable. Similarly, if no additional remuneration is paid, the related Finding(s) and Procedure(s) for additional remuneration are not applicable.

List here all Findings considered not applicable for the present engagement and explain the reasons of the non-applicability.

….

Exceptions

Apart from the exceptions listed below, the *[Beneficiary] [Linked Third Party]* provided the Auditor all the documentation and accounting information needed by the Auditor to carry out the requested Procedures and evaluate the Findings.

Explanation (to be removed from the Report):

- *If the Auditor was not able to successfully complete a procedure requested, it must be marked as '**E**' ('Exception') in the corresponding row on the right-hand column of the table. The reason such as the inability to reconcile key information or the unavailability of data that prevents the Auditor from carrying out the Procedure must be indicated below.*
- *If the Auditor cannot corroborate a standard finding after having carried out the corresponding procedure, it must also be marked as '**E**' ('Exception') and, where possible, the reasons why the Finding was not fulfilled and its possible impact must be explained here below.*

List here any exceptions and add any information on the cause and possible consequences of each exception, if known. If the exception is quantifiable, include the corresponding amount.

….

Example (to be removed from the Report):

1. *The Beneficiary was unable to substantiate the Finding number 1 on … because ….*
2. *Finding number 30 was not fulfilled because the methodology used by the Beneficiary to calculate unit costs was different from the one approved by the Commission. The differences were as follows: …*
3. *After carrying out the agreed procedures to confirm the Finding number 31, the Auditor found a difference of _____ EUR. The difference can be explained by …*

Further Remarks

In addition to reporting on the results of the specific procedures carried out, the Auditor would like to make the following general remarks:

Example (to be removed from the Report):

1. *Regarding Finding number 8 the conditions for additional remuneration were considered as fulfilled because …*
2. *In order to be able to confirm the Finding number 15 we carried out the following additional procedures: ….*

Use of this Report

This Report may be used only for the purpose described in the above objective. It was prepared solely for the confidential use of the *[Beneficiary] [Linked Third Party]* and the [*Commission*] [*Agency*], and only to be submitted to the [*Commission*] [*Agency*] in connection with the requirements set out in Article 20.4 of the Agreement. The Report may not be used by the *[Beneficiary] [Linked Third Party]* or by the [*Commission*] [*Agency*] for any other purpose, nor may it

be distributed to any other parties. The [*Commission*] [*Agency*] may only disclose the Report to authorised parties, in particular to the European Anti-Fraud Office (OLAF) and the European Court of Auditors.

This Report relates only to the Financial Statement(s) submitted to the *[Commission] [Agency]* by the *[Beneficiary] [Linked Third Party]* for the Agreement. Therefore, it does not extend to any other of the [*Beneficiary's*] [*Linked Third Party's*] Financial Statement(s).

There was no conflict of interest[4] between the Auditor and the Beneficiary *[and Linked Third Party]* in establishing this Report. The total fee paid to the Auditor for providing the Report was EUR _____ (including EUR_____ of deductible VAT).

We look forward to discussing our Report with you and would be pleased to provide any further information or assistance.

[legal name of the Auditor]

[name and function of an authorised representative]

[dd Month yyyy]

Signature of the Auditor

[4] A conflict of interest arises when the Auditor's objectivity to establish the certificate is compromised in fact or in appearance when the Auditor for instance:
- was involved in the preparation of the Financial Statements;
- stands to benefit directly should the certificate be accepted;
- has a close relationship with any person representing the beneficiary;
- is a director, trustee or partner of the beneficiary; or
- is in any other situation that compromises his or her independence or ability to establish the certificate impartially.

Agreed-upon procedures to be performed and standard factual findings to be confirmed by the Auditor

The European Commission reserves the right to i) provide the auditor with additional guidance regarding the procedures to be followed or the facts to be ascertained and the way in which to present them (this may include sample coverage and findings) or to ii) change the procedures, by notifying the Beneficiary in writing. The procedures carried out by the auditor to confirm the standard factual finding are listed in the table below.

If this certificate relates to a Linked Third Party, any reference here below to 'the Beneficiary' is to be considered as a reference to 'the Linked Third Party'.

The 'result' column has three different options: 'C', 'E' and 'N.A.':

- 'C' stands for 'confirmed' and means that the auditor can confirm the 'standard factual finding' and, therefore, there is no exception to be reported.
- 'E' stands for 'exception' and means that the Auditor carried out the procedures but cannot confirm the 'standard factual finding', or that the Auditor was not able to carry out a specific procedure (e.g. because it was impossible to reconcile key information or data were unavailable),
- 'N.A.' stands for 'not applicable' and means that the Finding did not have to be examined by the Auditor and the related Procedure(s) did not have to be carried out. The reasons of the non-application of a certain Finding must be obvious i.e. i) if no cost was declared under a certain category then the related Finding(s) and Procedure(s) are not applicable; ii) if the condition set to apply certain Procedure(s) are not met then the related Finding(s) and Procedure(s) are not applicable. For instance, for 'beneficiaries with accounts established in a currency other than the euro' the Procedure related to 'beneficiaries with accounts established in euro' is not applicable. Similarly, if no additional remuneration is paid, the related Finding(s) and Procedure(s) for additional remuneration are not applicable.

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
A	**ACTUAL PERSONNEL COSTS AND UNIT COSTS CALCULATED BY THE BENEFICIARY IN ACCORDANCE WITH ITS USUAL COST ACCOUNTING PRACTICE**		

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	The Auditor draws a sample of persons whose costs were declared in the Financial Statement(s) to carry out the procedures indicated in the consecutive points of this section A. (*The sample should be selected randomly so that it is representative. Full coverage is required if there are fewer than 10 people (including employees, natural persons working under a direct contract and personnel seconded by a third party), otherwise the sample should have a minimum of 10 people, or 10% of the total, whichever number is the highest)* The Auditor sampled _____ people out of the total of _____ people.		
A.1	**PERSONNEL COSTS** <u>For the persons included in the sample and working under an employment contract or equivalent act (general procedures for individual actual personnel costs and personnel costs declared as unit costs)</u> To confirm standard factual findings 1-5 listed in the next column, the Auditor reviewed following information/documents provided by the Beneficiary: ○ a list of the persons included in the sample indicating the period(s) during which they worked for the action, their position (classification or category) and type of contract; ○ the payslips of the employees included in the sample; ○ reconciliation of the personnel costs declared in the Financial Statement(s) with the accounting system (project accounting and general ledger) and payroll system; ○ information concerning the employment status and employment conditions of personnel included in the sample, in particular their employment contracts or equivalent;	1) The employees were i) directly hired by the Beneficiary in accordance with its national legislation, ii) under the Beneficiary's sole technical supervision and responsibility and iii) remunerated in accordance with the Beneficiary's usual practices.	
		2) Personnel costs were recorded in the Beneficiary's accounts/payroll system.	
		3) Costs were adequately supported and reconciled with the accounts and payroll	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	○ the Beneficiary's usual policy regarding payroll matters (e.g. salary policy, overtime policy, variable pay); ○ applicable national law on taxes, labour and social security and ○ any other document that supports the personnel costs declared. The Auditor also verified the eligibility of all components of the retribution (see Article 6 GA) and recalculated the personnel costs for employees included in the sample.	records.	
		4) Personnel costs did not contain any ineligible elements.	
		5) There were no discrepancies between the personnel costs charged to the action and the costs recalculated by the Auditor.	
	Further procedures if 'additional remuneration' is paid To confirm standard factual findings 6-9 listed in the next column, the Auditor: ○ reviewed relevant documents provided by the Beneficiary (legal form, legal/statutory obligations, the Beneficiary's usual policy on additional remuneration, criteria used for its calculation…); ○ recalculated the amount of additional remuneration eligible for the action based on the supporting documents received (full-time or part-time work, exclusive or non-exclusive dedication to the action, etc.) to arrive at the applicable FTE/year and pro-rata rate (see data collected in the course of carrying out the procedures under A.2 'Productive hours' and A.4 'Time recording system').	6) The Beneficiary paying "additional remuneration" was a non-profit legal entity.	
		7) The amount of additional remuneration paid corresponded to the Beneficiary's usual remuneration practices and was consistently paid whenever the same kind of work or expertise was required.	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	IF ANY PART OF THE REMUNERATION PAID TO THE EMPLOYEE IS NOT MANDATORY ACCORDING TO THE NATIONAL LAW OR THE EMPLOYMENT CONTRACT ("ADDITIONAL REMUNERATION") AND IS ELIGIBLE UNDER THE PROVISIONS OF ARTICLE 6.2.A.1, THIS CAN BE CHARGED AS ELIGIBLE COST TO THE ACTION UP TO THE FOLLOWING AMOUNT: *(A) IF THE PERSON WORKS FULL TIME AND EXCLUSIVELY ON THE ACTION DURING THE FULL YEAR: UP TO EUR 8 000/YEAR;* *(B) IF THE PERSON WORKS EXCLUSIVELY ON THE ACTION BUT NOT FULL-TIME OR NOT FOR THE FULL YEAR: UP TO THE CORRESPONDING PRO-RATA AMOUNT OF EUR 8 000, OR* *(C) IF THE PERSON DOES NOT WORK EXCLUSIVELY ON THE ACTION: UP TO A PRO-RATA AMOUNT CALCULATED IN ACCORDANCE TO ARTICLE 6.2.A.1.*	8) The criteria used to calculate the additional remuneration were objective and generally applied by the Beneficiary regardless of the source of funding used.	
		9) The amount of additional remuneration included in the personnel costs charged to the action was capped at EUR 8,000 per FTE/year (up to the equivalent pro-rata amount if the person did not work on the action full-time during the year or did not work exclusively on the action).	
	Additional procedures in case "unit costs calculated by the Beneficiary in accordance with its usual cost accounting practices" is applied: Apart from carrying out the procedures indicated above to confirm standard factual findings 1-5 and, if applicable, also 6-9, the Auditor carried out following procedures to confirm standard factual findings 10-13 listed in the next column:	10) The personnel costs included in the Financial Statement were calculated in accordance with the Beneficiary's usual cost accounting practice. This methodology was consistently used in all H2020 actions.	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	○ obtained a description of the Beneficiary's usual cost accounting practice to calculate unit costs;. ○ reviewed whether the Beneficiary's usual cost accounting practice was applied for the Financial Statements subject of the present CFS; ○ verified the employees included in the sample were charged under the correct category (in accordance with the criteria used by the Beneficiary to establish personnel categories) by reviewing the contract/HR-record or analytical accounting records; ○ verified that there is no difference between the total amount of personnel costs used in calculating the cost per unit and the total amount of personnel costs recorded in the statutory accounts; ○ verified whether actual personnel costs were adjusted on the basis of budgeted or estimated elements and, if so, verified whether those elements used are actually relevant for the calculation, objective and supported by documents.	11) The employees were charged under the correct category.	
		12) Total personnel costs used in calculating the unit costs were consistent with the expenses recorded in the statutory accounts.	
		13) Any estimated or budgeted element used by the Beneficiary in its unit-cost calculation were relevant for calculating personnel costs and corresponded to objective and verifiable information.	
	<u>For natural persons included in the sample and working with the Beneficiary under a direct contract other than an employment contract, such as consultants (no subcontractors).</u> To confirm standard factual findings 14-18 listed in the next column the Auditor reviewed following information/documents provided by the Beneficiary: ○ the contracts, especially the cost, contract duration, work description, place of work, ownership of the results and reporting obligations to the Beneficiary;	14) The natural persons reported to the Beneficiary (worked under the Beneficiary's instructions).	
		15) They worked on the Beneficiary's premises (unless otherwise agreed with the Beneficiary).	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	○ the employment conditions of staff in the same category to compare costs and; ○ any other document that supports the costs declared and its registration (e.g. invoices, accounting records, etc.).	16) The results of work carried out belong to the Beneficiary.	
		17) Their costs were not significantly different from those for staff who performed similar tasks under an employment contract with the Beneficiary.	
		18) The costs were supported by audit evidence and registered in the accounts.	
	<u>For personnel seconded by a third party and included in the sample (not subcontractors)</u> To confirm standard factual findings 19-22 listed in the next column, the Auditor reviewed following information/documents provided by the Beneficiary: ○ their secondment contract(s) notably regarding costs, duration, work description, place of work and ownership of the results; ○ if there is reimbursement by the Beneficiary to the third party for the resource made available (in-kind contribution against payment): any documentation that supports the costs declared (e.g. contract, invoice, bank payment, and proof of registration in its accounting/payroll, etc.) and reconciliation of the Financial Statement(s) with the accounting system (project accounting and general ledger) as well as any proof that the amount invoiced by the third party did not include any profit;	19) Seconded personnel reported to the Beneficiary and worked on the Beneficiary's premises (unless otherwise agreed with the Beneficiary).	
		20) The results of work carried out belong to the Beneficiary.	
		If personnel is seconded against payment: 21) The costs declared were supported with documentation and recorded in the	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	○ if there is no reimbursement by the Beneficiary to the third party for the resource made available (in-kind contribution free of charge): a proof of the actual cost borne by the Third Party for the resource made available free of charge to the Beneficiary such as a statement of costs incurred by the Third Party and proof of the registration in the Third Party's accounting/payroll; ○ any other document that supports the costs declared (e.g. invoices, etc.).	Beneficiary's accounts. The third party did not include any profit.	
		If personnel is seconded free of charge: 22) The costs declared did not exceed the third party's cost as recorded in the accounts of the third party and were supported with documentation.	
A.2	**PRODUCTIVE HOURS** To confirm standard factual findings 23-28 listed in the next column, the Auditor reviewed relevant documents, especially national legislation, labour agreements and contracts and time records of the persons included in the sample, to verify that: ○ the annual productive hours applied were calculated in accordance with one of the methods described below, ○ the full-time equivalent (FTEs) ratios for employees not working full-time were correctly calculated.	23) The Beneficiary applied method [*choose one option and delete the others*] [**A**: 1720 hours] [**B**: the 'total number of hours worked'] [**C**: 'annual productive hours' used correspond to usual accounting practices]	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	If the Beneficiary applied method B, the auditor verified that the correctness in which the total number of hours worked was calculated and that the contracts specified the annual workable hours. If the Beneficiary applied method C, the auditor verified that the 'annual productive hours' applied when calculating the hourly rate were equivalent to at least 90 % of the 'standard annual workable hours'. The Auditor can only do this if the calculation of the standard annual workable hours can be supported by records, such as national legislation, labour agreements, and contracts. *BENEFICIARY'S PRODUCTIVE HOURS' FOR PERSONS WORKING FULL TIME SHALL BE ONE OF THE FOLLOWING METHODS:* ***A.*** *1720 ANNUAL PRODUCTIVE HOURS (PRO-RATA FOR PERSONS NOT WORKING FULL-TIME)* ***B.*** *THE TOTAL NUMBER OF HOURS WORKED BY THE PERSON FOR THE BENEFICIARY IN THE YEAR (THIS METHOD IS ALSO REFERRED TO AS 'TOTAL NUMBER OF HOURS WORKED' IN THE NEXT COLUMN). THE CALCULATION OF THE TOTAL NUMBER OF HOURS WORKED WAS DONE AS FOLLOWS: ANNUAL WORKABLE HOURS OF THE PERSON ACCORDING TO THE EMPLOYMENT CONTRACT, APPLICABLE LABOUR AGREEMENT OR NATIONAL LAW PLUS OVERTIME WORKED MINUS ABSENCES (SUCH AS SICK LEAVE OR SPECIAL LEAVE).*	24) Productive hours were calculated annually.	
		25) For employees not working full-time the full-time equivalent (FTE) ratio was correctly applied.	
		If the Beneficiary applied method B. 26) The calculation of the number of 'annual workable hours', overtime and absences was verifiable based on the documents provided by the Beneficiary.	
		If the Beneficiary applied method C. 27) The calculation of the number of 'standard annual workable hours' was verifiable based on the documents provided by the Beneficiary.	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	C. THE STANDARD NUMBER OF ANNUAL HOURS GENERALLY APPLIED BY THE BENEFICIARY FOR ITS PERSONNEL IN ACCORDANCE WITH ITS USUAL COST ACCOUNTING PRACTICES (THIS METHOD IS ALSO REFERRED TO AS 'TOTAL ANNUAL PRODUCTIVE HOURS' IN THE NEXT COLUMN). THIS NUMBER MUST BE AT LEAST 90% OF THE STANDARD ANNUAL WORKABLE HOURS. *'ANNUAL WORKABLE HOURS' MEANS THE PERIOD DURING WHICH THE PERSONNEL MUST BE WORKING, AT THE EMPLOYER'S DISPOSAL AND CARRYING OUT HIS/HER ACTIVITY OR DUTIES UNDER THE EMPLOYMENT CONTRACT, APPLICABLE COLLECTIVE LABOUR AGREEMENT OR NATIONAL WORKING TIME LEGISLATION.*	28) The 'annual productive hours' used for calculating the hourly rate were consistent with the usual cost accounting practices of the Beneficiary and were equivalent to at least 90 % of the 'annual workable hours'.	
A.3	**HOURLY PERSONNEL RATES** <u>I) For unit costs calculated in accordance to the Beneficiary's usual cost accounting practice (unit costs):</u> If the Beneficiary has a "Certificate on Methodology to calculate unit costs " (CoMUC) approved by the Commission, the Beneficiary provides the Auditor with a description of the approved methodology and the Commission's letter of acceptance. The Auditor verified that the Beneficiary has indeed used the methodology approved. If so, no further verification is necessary. If the Beneficiary does not have a "Certificate on Methodology" (CoMUC) approved by the	29) The Beneficiary applied [*choose one option and delete the other*]: [Option I: "Unit costs (hourly rates) were calculated in accordance with the Beneficiary's usual cost accounting practices"] [Option II: Individual hourly rates were applied]	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	Commission, or if the methodology approved was not applied, then the Auditor: o reviewed the documentation provided by the Beneficiary, including manuals and internal guidelines that explain how to calculate hourly rates; o recalculated the unit costs (hourly rates) of staff included in the sample following the results of the procedures carried out in A.1 and A.2. II) For individual hourly rates: The Auditor: o reviewed the documentation provided by the Beneficiary, including manuals and internal guidelines that explain how to calculate hourly rates; o recalculated the hourly rates of staff included in the sample following the results of the procedures carried out in A.1 and A.2. *"UNIT COSTS CALCULATED BY THE BENEFICIARY IN ACCORDANCE WITH ITS USUAL COST ACCOUNTING PRACTICES":* *IT IS CALCULATED BY DIVIDING THE TOTAL AMOUNT OF PERSONNEL COSTS OF THE CATEGORY TO WHICH THE EMPLOYEE BELONGS VERIFIED IN LINE WITH PROCEDURE A.1 BY THE NUMBER OF FTE AND THE ANNUAL TOTAL PRODUCTIVE HOURS OF THE SAME CATEGORY CALCULATED BY THE BENEFICIARY IN ACCORDANCE WITH PROCEDURE A.2.* *HOURLY RATE FOR INDIVIDUAL ACTUAL PERSONAL COSTS:* *IT IS CALCULATED BY DIVIDING THE TOTAL AMOUNT OF PERSONNEL COSTS OF AN EMPLOYEE VERIFIED IN LINE WITH*	*For option I concerning unit costs and if the Beneficiary applies the methodology approved by the Commission (CoMUC):* 30) The Beneficiary used the Commission-approved methodology to calculate hourly rates. It corresponded to the organisation's usual cost accounting practices and was applied consistently for all activities irrespective of the source of funding.	
		For option I concerning unit costs and if the Beneficiary applies a methodology not approved by the Commission: 31) The unit costs re-calculated by the Auditor were the same as the rates applied by the Beneficiary.	
		For option II concerning individual hourly rates:	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	PROCEDURE A.1 BY THE NUMBER OF ANNUAL PRODUCTIVE HOURS VERIFIED IN LINE WITH PROCEDURE A.2.	32) The individual rates re-calculated by the Auditor were the same as the rates applied by the Beneficiary.	
A.4	**TIME RECORDING SYSTEM** To verify that the time recording system ensures the fulfilment of all minimum requirements and that the hours declared for the action were correct, accurate and properly authorised and supported by documentation, the Auditor made the following checks for the persons included in the sample that declare time as worked for the action on the basis of time records: o description of the time recording system provided by the Beneficiary (registration, authorisation, processing in the HR-system); o its actual implementation; o time records were signed at least monthly by the employees (on paper or electronically) and authorised by the project manager or another manager; o the hours declared were worked within the project period; o there were no hours declared as worked for the action if HR-records showed absence due to holidays or sickness (further cross-checks with travels are carried out in B.1 below) ;	33) All persons recorded their time dedicated to the action on a **daily/ weekly/ monthly** basis using a **paper/computer-based** system. (*delete the answers that are not applicable)*	
		34) Their time-records were authorised at least monthly by the project manager or other superior.	
		35) Hours declared were worked within the project period and were consistent with the presences/absences recorded in HR-records.	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	○ the hours charged to the action matched those in the time recording system. *ONLY THE HOURS WORKED ON THE ACTION CAN BE CHARGED. ALL WORKING TIME TO BE CHARGED SHOULD BE RECORDED THROUGHOUT THE DURATION OF THE PROJECT, ADEQUATELY SUPPORTED BY EVIDENCE OF THEIR REALITY AND RELIABILITY (SEE SPECIFIC PROVISIONS BELOW FOR PERSONS WORKING EXCLUSIVELY FOR THE ACTION WITHOUT TIME RECORDS).*	36) There were no discrepancies between the number of hours charged to the action and the number of hours recorded.	
	<u>If the persons are working exclusively for the action and without time records</u> For the persons selected that worked exclusively for the action without time records, the Auditor verified evidence available demonstrating that they were in reality exclusively dedicated to the action and that the Beneficiary signed a declaration confirming that they have worked exclusively for the action.	37) The exclusive dedication is supported by a declaration signed by the Beneficiary's and by any other evidence gathered.	
B	**COSTS OF SUBCONTRACTING**		
B.1	**The Auditor obtained the detail/breakdown of subcontracting costs and sampled _____ cost items selected randomly** (*full coverage is required if there are fewer than 10 items, otherwise the sample should have a minimum of 10 item, or 10% of the total, whichever number is highest*). To confirm standard factual findings 38-42 listed in the next column, the Auditor reviewed the	38) The use of claimed subcontracting costs was foreseen in Annex 1 and costs were declared in the Financial Statements under the subcontracting category.	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	following for the items included in the sample: o the use of subcontractors was foreseen in Annex 1; o subcontracting costs were declared in the subcontracting category of the Financial Statement; o supporting documents on the selection and award procedure were followed; o the Beneficiary ensured best value for money (key elements to appreciate the respect of this principle are the award of the subcontract to the bid offering best price-quality ratio, under conditions of transparency and equal treatment. In case an existing framework contract was used the Beneficiary ensured it was established on the basis of the principle of best value for money under conditions of transparency and equal treatment). In particular, i. if the Beneficiary acted as a contracting authority within the meaning of Directive 2004/18/EC or of Directive 2004/17/EC, the Auditor verified that the applicable national law on public procurement was followed and that the subcontracting complied with the Terms and Conditions of the Agreement. ii. if the Beneficiary did not fall under the above-mentioned category the Auditor verified that the Beneficiary followed their usual procurement rules and respected the Terms and Conditions of the Agreement..	39) There were documents of requests to different providers, different offers and assessment of the offers before selection of the provider in line with internal procedures and procurement rules. Subcontracts were awarded in accordance with the principle of best value for money. *(When different offers were not collected the Auditor explains the reasons provided by the Beneficiary under the caption "Exceptions" of the Report. The Commission will analyse this information to evaluate whether these costs might be accepted as eligible)*	
	For the items included in the sample the Auditor also verified that: o the subcontracts were not awarded to other Beneficiaries in the consortium;	40) The subcontracts were not awarded to other Beneficiaries of the consortium.	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	○ there were signed agreements between the Beneficiary and the subcontractor; ○ there was evidence that the services were provided by subcontractor;	41) All subcontracts were supported by signed agreements between the Beneficiary and the subcontractor.	
		42) There was evidence that the services were provided by the subcontractors.	
C	**COSTS OF PROVIDING FINANCIAL SUPPORT TO THIRD PARTIES**		
C.1	**The Auditor obtained the detail/breakdown of the costs of providing financial support to third parties and sampled _____ cost items selected randomly** (*full coverage is required if there are fewer than 10 items, otherwise the sample should have a minimum of 10 item, or 10% of the total, whichever number is highest*). The Auditor verified that the following minimum conditions were met: a) the maximum amount of financial support for each third party did not exceed EUR 60 000, unless explicitly mentioned in Annex 1; b) the financial support to third parties was agreed in Annex 1 of the Agreement and the other provisions on financial support to third parties included in Annex 1 were	43) All minimum conditions were met	

Ref	Procedures	Standard factual finding	Result (C / E / N.A.)
	respected.		

D	OTHER ACTUAL DIRECT COSTS		
D.1	**COSTS OF TRAVEL AND RELATED SUBSISTENCE ALLOWANCES** **The Auditor sampled _____ cost items selected randomly** (*full coverage is required if there are fewer than 10 items, otherwise the sample should have a minimum of 10 item, or 10% of the total, whichever number is the highest*). The Auditor inspected the sample and verified that: ○ travel and subsistence costs were consistent with the Beneficiary's usual policy for travel. In this context, the Beneficiary provided evidence of its normal policy for travel costs (e.g. use of first class tickets, reimbursement by the Beneficiary on the basis of actual costs, a lump sum or per diem) to enable the Auditor to compare the travel costs charged with this policy; ○ travel costs are correctly identified and allocated to the action (e.g. trips are directly linked to the action) by reviewing relevant supporting documents such as minutes of meetings, workshops or conferences, their registration in the correct project account, their consistency with time records or with the dates/duration of the workshop/conference; ○ no ineligible costs or excessive or reckless expenditure was declared.	44) Costs were incurred, approved and reimbursed in line with the Beneficiary's usual policy for travels.	
		45) There was a link between the trip and the action.	
		46) The supporting documents were consistent with each other regarding subject of the trip, dates, duration and reconciled with time records and accounting.	
		47) No ineligible costs or excessive or reckless expenditure was declared.	
D.2	**DEPRECIATION COSTS FOR EQUIPMENT, INFRASTRUCTURE OR OTHER ASSETS** **The Auditor sampled _____ cost items selected randomly** (*full coverage is required if there are fewer than 10 items, otherwise the sample should have a minimum of 10 item, or 10% of the total, whichever number is the highest*). For “equipment, infrastructure or other assets” [from now on called “asset(s)”] selected in the	48) Procurement rules, principles and guides were followed.	
		49) There was a link between the grant agreement and the asset charged to the action.	

	sample the Auditor verified that: ○ the assets were acquired in conformity with the Beneficiary's internal guidelines and procedures; ○ they were correctly allocated to the action (with supporting documents such as delivery note invoice or any other proof demonstrating the link to the action) ○ they were entered in the accounting system; ○ the extent to which the assets were used for the action (as a percentage) was supported by reliable documentation (e.g. usage overview table); The Auditor recalculated the depreciation costs and verified that they were in line with the applicable rules in the Beneficiary's country and with the Beneficiary's usual accounting policy (e.g. depreciation calculated on the acquisition value). The Auditor verified that no ineligible costs such as deductible VAT, exchange rate losses, excessive or reckless expenditure were declared (see Article 6.5 GA).	50) The asset charged to the action was traceable to the accounting records and the underlying documents. 51) The depreciation method used to charge the asset to the action was in line with the applicable rules of the Beneficiary's country and the Beneficiary's usual accounting policy. 52) The amount charged corresponded to the actual usage for the action. 53) No ineligible costs or excessive or reckless expenditure were declared.	
D.3	**COSTS OF OTHER GOODS AND SERVICES** **The Auditor sampled _____ cost items selected randomly** (*full coverage is required if there are fewer than 10 items, otherwise the sample should have a minimum of 10 item, or 10% of the total, whichever number is highest*). For the purchase of goods, works or services included in the sample the Auditor verified that: ○ the contracts did not cover tasks described in Annex 1;	54) Contracts for works or services did not cover tasks described in Annex 1. 55) Costs were allocated to the correct action and the goods were not placed in the inventory of durable equipment.	

	○ they were correctly identified, allocated to the proper action, entered in the accounting system (traceable to underlying documents such as purchase orders, invoices and accounting); ○ the goods were not placed in the inventory of durable equipment; ○ the costs charged to the action were accounted in line with the Beneficiary's usual accounting practices; ○ no ineligible costs or excessive or reckless expenditure were declared (see Article 6 GA). In addition, the Auditor verified that these goods and services were acquired in conformity with the Beneficiary's internal guidelines and procedures, in particular: ○ if Beneficiary acted as a contracting authority within the meaning of Directive 2004/18/EC or of Directive 2004/17/EC, the Auditor verified that the applicable national law on public procurement was followed and that the procurement contract complied with the Terms and Conditions of the Agreement. ○ if the Beneficiary did not fall into the category above, the Auditor verified that the Beneficiary followed their usual procurement rules and respected the Terms and Conditions of the Agreement. For the items included in the sample the Auditor also verified that: ○ the Beneficiary ensured best value for money (key elements to appreciate the respect of this principle are the award of the contract to the bid offering best price-quality ratio, under conditions of transparency and equal treatment. In case an existing framework contract was used the Auditor also verified that the Beneficiary ensured it was established on the basis of the principle of best value for money under conditions of transparency and equal treatment); *SUCH GOODS AND SERVICES INCLUDE, FOR INSTANCE, CONSUMABLES AND SUPPLIES, DISSEMINATION (INCLUDING OPEN ACCESS), PROTECTION OF RESULTS, SPECIFIC EVALUATION OF THE ACTION IF IT IS REQUIRED BY THE*	56) The costs were charged in line with the Beneficiary's accounting policy and were adequately supported. 57) No ineligible costs or excessive or reckless expenditure were declared. For internal invoices/charges only the cost element was charged, without any mark-ups. 58) Procurement rules, principles and guides were followed. There were documents of requests to different providers, different offers and assessment of the offers before selection of the provider in line with internal procedures and procurement rules. The purchases were made in accordance with the principle of best value for money. *(When different offers were not collected the Auditor explains the reasons provided by the Beneficiary under the*	

	AGREEMENT, CERTIFICATES ON THE FINANCIAL STATEMENTS IF THEY ARE REQUIRED BY THE AGREEMENT AND CERTIFICATES ON THE METHODOLOGY, TRANSLATIONS, REPRODUCTION.	*caption "Exceptions" of the Report. The Commission will analyse this information to evaluate whether these costs might be accepted as eligible)*	
D.4	**AGGREGATED CAPITALISED AND OPERATING COSTS OF RESEARCH INFRASTRUCTURE** The Auditor ensured the existence of a positive ex-ante assessment (issued by the EC Services) of the cost accounting methodology of the Beneficiary allowing it to apply the guidelines on direct costing for large research infrastructures in Horizon 2020. ***In the cases that a positive ex-ante assessment has been issued*** *(see the standard factual findings 59-60 on the next column)****,*** The Auditor ensured that the beneficiary has applied consistently the methodology that is explained and approved in the positive ex ante assessment; ***In the cases that a positive ex-ante assessment has NOT been issued*** *(see the standard factual findings 61 on the next column),* The Auditor verified that no costs of Large Research Infrastructure have been charged as direct costs in any costs category;	59) The costs declared as direct costs for Large Research Infrastructures (in the appropriate line of the Financial Statement) comply with the methodology described in the positive ex-ante assessment report. 60) Any difference between the methodology applied and the one positively assessed was extensively described and adjusted accordingly. 61) The direct costs declared were free from any indirect costs items related to the Large Research Infrastructure.	

	In the cases that a draft ex-ante assessment report has been issued with recommendation for further changes *(see the standard factual findings 61 on the next column),* • The Auditor followed the same procedure as above (when a positive ex-ante assessment has NOT yet been issued) and paid particular attention (testing reinforced) to the cost items for which the draft ex-ante assessment either rejected the inclusion as direct costs for Large Research Infrastructures or issued recommendations.		
E	**USE OF EXCHANGE RATES**		
E.1	a) For Beneficiaries with accounts established in a currency other than euros **The Auditor sampled _____ cost items selected randomly and verified that the exchange rates used for converting other currencies into euros were in accordance with the following rules established in the Agreement** (*full coverage is required if there are fewer than 10 items, otherwise the sample should have a minimum of 10 item, or 10% of the total, whichever number is highest)*: *COSTS INCURRED IN ANOTHER CURRENCY SHALL BE CONVERTED INTO EURO AT THE AVERAGE OF THE DAILY EXCHANGE RATES PUBLISHED IN THE C SERIES OF OFFICIAL JOURNAL OF THE EUROPEAN UNION (https://www.ecb.int/stats/exchange/eurofxref/html/index.en.html), DETERMINED OVER THE CORRESPONDING REPORTING PERIOD.* *IF NO DAILY EURO EXCHANGE RATE IS PUBLISHED IN THE OFFICIAL JOURNAL OF THE EUROPEAN UNION FOR THE CURRENCY IN QUESTION, CONVERSION SHALL BE MADE AT THE AVERAGE OF THE MONTHLY ACCOUNTING RATES ESTABLISHED BY THE COMMISSION AND PUBLISHED ON ITS WEBSITE (http://ec.europa.eu/budget/contracts_grants/info_contracts/inforeuro/inforeuro_en.cfm),*	62) The exchange rates used to convert other currencies into Euros were in accordance with the rules established of the Grant Agreement and there was no difference in the final figures.	

	DETERMINED OVER THE CORRESPONDING REPORTING PERIOD.		
	b) For Beneficiaries with accounts established in euros **The Auditor sampled _____ cost items selected randomly and verified that the exchange rates used for converting other currencies into euros were in accordance with the following rules established in the Agreement** (*full coverage is required if there are fewer than 10 items, otherwise the sample should have a minimum of 10 item, or 10% of the total, whichever number is highest)*: *COSTS INCURRED IN ANOTHER CURRENCY SHALL BE CONVERTED INTO EURO BY APPLYING THE BENEFICIARY'S USUAL ACCOUNTING PRACTICES.*	63) The Beneficiary applied its usual accounting practices.	

[legal name of the audit firm]

[name and function of an authorised representative]

[dd Month yyyy]

<Signature of the Auditor>

ANNEX 6

MODEL FOR THE CERTIFICATE ON THE METHODOLOGY

- **For options [*in italics in square brackets*]: choose the applicable option. Options not chosen should be deleted.**
- **For fields in [grey in square brackets]: enter the appropriate data.**

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Terms of reference for an audit engagement for a methodology certificate in connection with one or more grant agreements financed under the Horizon 2020 Research and Innovation Framework Programme

This document sets out the '**Terms of Reference (ToR)**' under which

[OPTION 1: [insert name of the beneficiary] ('the Beneficiary')] [OPTION 2: [insert name of the linked third party] ('the Linked Third Party'), third party linked to the Beneficiary [insert name of the beneficiary] ('the Beneficiary')]

agrees to engage

[**insert legal name of the auditor**] ('the Auditor')

to produce an independent report of factual findings ('the Report') concerning the *[Beneficiary's] [Linked Third Party's]* usual accounting practices for calculating and claiming direct personnel costs declared as unit costs ('the Methodology') in connection with grant agreements financed under the Horizon 2020 Research and Innovation Framework Programme.

The procedures to be carried out for the assessment of the methodology will be based on the grant agreement(s) detailed below:

[title and number of the grant agreement(s)] ('the Agreement(s)')

The Agreement(s) has(have) been concluded between the Beneficiary and *[OPTION 1: the European Union, represented by the European Commission ('the Commission')][OPTION 2: the European Atomic Energy Community (Euratom,) represented by the European Commission ('the Commission')][OPTION 3: the [Research Executive Agency (REA)] [European Research Council Executive Agency (ERCEA)] [Innovation and Networks Executive Agency (INEA)] [Executive Agency for Small and Medium-sized Enterprises (EASME)] ('the Agency'), under the powers delegated by the European Commission ('the Commission').]*.

The *[Commission] [Agency]* is mentioned as a signatory of the Agreement with the Beneficiary only. The *[European Union] [Euratom] [Agency]* is not a party to this engagement.

1.1 Subject of the engagement

According to Article 18.1.2 of the Agreement, beneficiaries *[and linked third parties]* that declare direct personnel costs as unit costs calculated in accordance with their usual cost accounting practices may submit to the *[Commission] [Agency]*, for approval, a certificate on the methodology ('CoMUC') stating that there are adequate records and documentation to prove that their cost accounting practices used comply with the conditions set out in Point A of Article 6.2.

The subject of this engagement is the CoMUC which is composed of two separate documents:

- the Terms of Reference ('the ToR') to be signed by the *[Beneficiary] [Linked Third Party]* and the Auditor;

- the Auditor's Independent Report of Factual Findings ('the Report') issued on the Auditor's letterhead, dated, stamped and signed by the Auditor which includes; the standard statements ('the Statements') evaluated and signed by the *[Beneficiary] [Linked Third Party]*, the agreed-upon procedures ('the Procedures') performed by the Auditor and the standard factual findings ('the Findings') assessed by the Auditor. The Statements, Procedures and Findings are summarised in the table that forms part of the Report.

The information provided through the Statements, the Procedures and the Findings will enable the Commission to draw conclusions regarding the existence of the *[Beneficiary's] [Linked Third Party's]* usual cost accounting practice and its suitability to ensure that direct personnel costs claimed on that basis comply with the provisions of the Agreement. The Commission draws its own conclusions from the Report and any additional information it may require.

1.2 Responsibilities

The parties to this agreement are the *[Beneficiary] [Linked Third Party]* and the Auditor.

The *[Beneficiary] [Linked Third Party]:*

- is responsible for preparing financial statements for the Agreement(s) ('the Financial Statements') in compliance with those Agreements;
- is responsible for providing the Financial Statement(s) to the Auditor and enabling the Auditor to reconcile them with the *[Beneficiary's] [Linked Third Party's]* accounting and bookkeeping system and the underlying accounts and records. The Financial Statement(s) will be used as a basis for the procedures which the Auditor will carry out under this ToR;
- is responsible for its Methodology and liable for the accuracy of the Financial Statement(s);
- is responsible for endorsing or refuting the Statements indicated under the heading 'Statements to be made by the Beneficiary/ Linked Third Party' in the first column of the table that forms part of the Report;
- must provide the Auditor with a signed and dated representation letter;
- accepts that the ability of the Auditor to carry out the Procedures effectively depends upon the *[Beneficiary] [Linked Third Party]* providing full and free access to the *[Beneficiary's] [Linked Third Party's]* staff and to its accounting and other relevant records.

The Auditor:

- *[Option 1 by default: is qualified to carry out statutory audits of accounting documents in accordance with Directive 2006/43/EC of the European Parliament and of the Council of 17 May 2006 on statutory audits of annual accounts and consolidated accounts, amending Council Directives 78/660/EEC and 83/349/EEC and repealing Council Directive 84/253/EEC or similar national regulations]*.
- *[Option 2 if the Beneficiary or Linked Third Party has an independent Public Officer: is a competent and independent Public Officer for which the relevant national authorities have established the legal capacity to audit the Beneficiary]*.
- *[Option 3 if the Beneficiary or Linked Third Party is an international organisation: is an [internal] [external] auditor in accordance with the internal financial regulations and procedures of the international organisation]*.

The Auditor:

- must be independent from the Beneficiary *[and the Linked Third Party]*, in particular, it must not have been involved in preparing the Beneficiary's *[and Linked Third Party's]* Financial Statement(s);
- must plan work so that the Procedures may be carried out and the Findings may be assessed;
- must adhere to the Procedures laid down and the compulsory report format;
- must carry out the engagement in accordance with these ToR;
- must document matters which are important to support the Report;
- must base its Report on the evidence gathered;
- must submit the Report to the *[Beneficiary] [Linked Third Party]*.

The Commission sets out the Procedures to be carried out and the Findings to be endorsed by the Auditor. The Auditor is not responsible for their suitability or pertinence. As this engagement is not an assurance engagement the Auditor does not provide an audit opinion or a statement of assurance.

1.3 Applicable Standards

The Auditor must comply with these Terms of Reference and with[1]:

- the International Standard on Related Services ('ISRS') 4400 *Engagements to perform Agreed-upon Procedures regarding Financial Information* as issued by the International Auditing and Assurance Standards Board (IAASB);
- the *Code of Ethics for Professional Accountants* issued by the International Ethics Standards Board for Accountants (IESBA). Although ISRS 4400 states that independence is not a requirement for engagements to carry out agreed-upon procedures, the Commission requires that the Auditor also complies with the Code's independence requirements.

The Auditor's Report must state that there was no conflict of interests in establishing this Report between the Auditor and the Beneficiary *[and the Linked Third Party]* that could have a bearing on the Report, and must specify – if the service is invoiced - the total fee paid to the Auditor for providing the Report.

1.4 Reporting

The Report must be written in the language of the Agreement (see Article 20.7 of the Agreement).

Under Article 22 of the Agreement, the Commission, *[the Agency]*, the European Anti-Fraud Office and the Court of Auditors have the right to audit any work that is carried out under the action and for which costs are claimed from [*the European Union*] [*Euratom*] budget. This includes work related to this engagement. The Auditor must provide access to all working papers related to this assignment if the Commission*, [the Agency]*, the European Anti-Fraud Office or the European Court of Auditors requests them.

1.5 Timing

The Report must be provided by [dd Month yyyy].

[1] Supreme Audit Institutions applying INTOSAI-standards may carry out the Procedures according to the corresponding International Standards of Supreme Audit Institutions and code of ethics issued by INTOSAI instead of the International Standard on Related Services ('ISRS') 4400 and the Code of Ethics for Professional Accountants issued by the IAASB and the IESBA.

1.6 Other Terms

[The [Beneficiary] [Linked Third Party] and the Auditor can use this section to agree other specific terms, such as the Auditor's fees, liability, applicable law, etc. Those specific terms must not contradict the terms specified above.]

[legal name of the Auditor]	[legal name of the [Beneficiary] [Linked Third Party]]
[name & title of authorised representative]	[name & title of authorised representative]
[dd Month yyyy]	[dd Month yyyy]
Signature of the Auditor Signature	Signature of the *[Beneficiary] [Linked Third Party]*

Independent report of factual findings on the methodology concerning grant agreements financed under the Horizon 2020 Research and Innovation Framework Programme

(To be printed on letterhead paper of the auditor)

To

[name of contact person(s)], [Position]

[[Beneficiary's] [Linked Third Party's] name]

[Address]

[dd Month yyyy]

Dear [Name of contact person(s)],

As agreed under the terms of reference dated [dd Month yyyy]

with *[OPTION 1: [insert name of the beneficiary] ('the Beneficiary')] [OPTION 2: [insert name of the linked third party] ('the Linked Third Party'), third party linked to the Beneficiary [insert name of the beneficiary] ('the Beneficiary')]*,

we

[name of the auditor] ('the Auditor'),

established at

[full address/city/state/province/country],

represented by

[name and function of an authorised representative],

have carried out the agreed-upon procedures ('the Procedures') and provide hereby our Independent Report of Factual Findings ('the Report'), concerning the *[Beneficiary's] [Linked Third Party's]* usual accounting practices for calculating and declaring direct personnel costs declared as unit costs ('the Methodology').

You requested certain procedures to be carried out in connection with the grant(s)

[title and number of the grant agreement(s)] ('the Agreement(s)').

The Report

Our engagement was carried out in accordance with the terms of reference ('the ToR') appended to this Report. The Report includes: the standard statements ('the Statements') made by the *[Beneficiary] [Linked Third Party]*, the agreed-upon procedures ('the Procedures') carried out and the standard factual findings ('the Findings') confirmed by us.

The engagement involved carrying out the Procedures and assessing the Findings and the documentation requested appended to this Report, the results of which the Commission uses to draw conclusions regarding the acceptability of the Methodology applied by the *[Beneficiary] [Linked Third Party]*.

The Report covers the methodology used from [dd Month yyyy]. In the event that the *[Beneficiary] [Linked Third Party]* changes this methodology, the Report will not be applicable to any Financial Statement[2] submitted thereafter.

The scope of the Procedures and the definition of the standard statements and findings were determined solely by the Commission. Therefore, the Auditor is not responsible for their suitability or pertinence.

Since the Procedures carried out constitute neither an audit nor a review made in accordance with International Standards on Auditing or International Standards on Review Engagements, we do not

[2] Financial Statement in this context refers solely to Annex 4 of the Agreement by which the Beneficiary declares costs under the Agreement.

give a statement of assurance on the costs declared on the basis of the *[Beneficiary's] [Linked Third Party's]* Methodology. Had we carried out additional procedures or had we performed an audit or review in accordance with these standards, other matters might have come to its attention and would have been included in the Report.

Exceptions

Apart from the exceptions listed below, the *[Beneficiary] [Linked Third Party]* agreed with the standard Statements and provided the Auditor all the documentation and accounting information needed by the Auditor to carry out the requested Procedures and corroborate the standard Findings.

List here any exception and add any information on the cause and possible consequences of each exception, if known. If the exception is quantifiable, also indicate the corresponding amount.

…..

Explanation of possible exceptions in the form of examples (to be removed from the Report):

i. the [Beneficiary] [Linked Third Party] did not agree with the standard Statement number … because…;

ii. the Auditor could not carry out the procedure … established because …. (e.g. due to the inability to reconcile key information or the unavailability or inconsistency of data);

iii. the Auditor could not confirm or corroborate the standard Finding number … because ….

Remarks

We would like to add the following remarks relevant for the proper understanding of the Methodology applied by the [Beneficiary] [Linked Third Party] or the results reported:

Example (to be removed from the Report):

Regarding the methodology applied to calculate hourly rates …

Regarding standard Finding 15 it has to be noted that …

The [Beneficiary] [Linked Third Party] explained the deviation from the benchmark statement XXIV concerning time recording for personnel with no exclusive dedication to the action in the following manner: …

Annexes

Please provide the following documents to the auditor and annex them to the report when submitting this CoMUC to the Commission:

1. Brief description of the methodology for calculating personnel costs, productive hours and hourly rates;
2. Brief description of the time recording system in place;
3. An example of the time records used by the [*Beneficiary] [Linked Third Party*];
4. Description of any budgeted or estimated elements applied, together with an explanation as to why they are relevant for calculating the personnel costs and how they are based on objective and verifiable information;
5. A summary sheet with the hourly rate for direct personnel declared by the [*Beneficiary*] [*Linked Third Party*] and recalculated by the Auditor for each staff member included in the sample (the names do not need to be reported);
6. A comparative table summarising for each person selected in the sample a) the time claimed by the [*Beneficiary*] [*Linked Third Party*] in the Financial Statement(s) and b) the time according to the time record verified by the Auditor;
7. A copy of the letter of representation provided to the Auditor.

Use of this Report

This Report has been drawn up solely for the purpose given under Point 1.1 Reasons for the engagement.

The Report:

- is confidential and is intended to be submitted to the Commission by the [*Beneficiary*] [*Linked Third Party*] in connection with Article 18.1.2 of the Agreement;
- may not be used by the [*Beneficiary*] [*Linked Third Party*] or by the Commission for any other purpose, nor distributed to any other parties;
- may be disclosed by the Commission only to authorised parties, in particular the European Anti-Fraud Office (OLAF) and the European Court of Auditors.
- relates only to the usual cost accounting practices specified above and does not constitute a report on the Financial Statements of the [*Beneficiary*] [*Linked Third Party*].

No conflict of interest[3] exists between the Auditor and the Beneficiary *[and the Linked Third Party*] that could have a bearing on the Report. The total fee paid to the Auditor for producing the Report was EUR _____ (including EUR _____ of deductible VAT).

[3] A conflict of interest arises when the Auditor's objectivity to establish the certificate is compromised in fact or in appearance when the Auditor for instance:

- was involved in the preparation of the Financial Statements;

We look forward to discussing our Report with you and would be pleased to provide any further information or assistance which may be required.

Yours sincerely

[legal name of the Auditor]

[name and title of the authorised representative]

[dd Month yyyy]

Signature of the Auditor

- stands to benefit directly should the certificate be accepted;

- has a close relationship with any person representing the beneficiary;

- is a director, trustee or partner of the beneficiary; or

- is in any other situation that compromises his or her independence or ability to establish the certificate impartially.

Statements to be made by the Beneficiary/Linked Third Party ('the Statements') and Procedures to be carried out by the Auditor ('the Procedures') and standard factual findings ('the Findings') to be confirmed by the Auditor

The Commission reserves the right to provide the auditor with guidance regarding the Statements to be made, the Procedures to be carried out or the Findings to be ascertained and the way in which to present them. The Commission reserves the right to vary the Statements, Procedures or Findings by written notification to the Beneficiary/Linked Third Party to adapt the procedures to changes in the grant agreement(s) or to any other circumstances.

If this methodology certificate relates to the Linked Third Party's usual accounting practices for calculating and claiming direct personnel costs declared as unit costs any reference here below to 'the Beneficiary' is to be considered as a reference to 'the Linked Third Party'.

Please explain any discrepancies in the body of the Report.	
Statements to be made by Beneficiary	**Procedures to be carried out and Findings to be confirmed by the Auditor**
A. Use of the Methodology I. The cost accounting practice described below has been in use since *[*dd Month yyyy*]*. II. The next planned alteration to the methodology used by the Beneficiary will be from [dd Month yyyy*]*.	**Procedure:** ✓ The Auditor checked these dates against the documentation the Beneficiary has provided. **Factual finding:** 1. The dates provided by the Beneficiary were consistent with the documentation.
B. Description of the Methodology III. The methodology to calculate unit costs is being used in a consistent manner and is reflected in the relevant procedures. *[Please describe the methodology your entity uses to calculate personnel costs, productive hours and hourly rates, present your description to the Auditor and annex it to this certificate]* *[If the statement of section "B. Description of the methodology" cannot be endorsed by the Beneficiary or there is no written methodology to calculate unit costs it should be listed here below and reported as exception by the Auditor in the main Report of*	**Procedure:** ✓ The Auditor reviewed the description, the relevant manuals and/or internal guidance documents describing the methodology. **Factual finding:** 2. The brief description was consistent with the relevant manuals, internal guidance and/or other documentary evidence the Auditor has reviewed. 3. The methodology was generally applied by the Beneficiary as part of its usual costs accounting practices.

Please explain any discrepancies in the body of the Report.	
Statements to be made by Beneficiary	**Procedures to be carried out and Findings to be confirmed by the Auditor**
Factual Findings: - *…]*	
C. **Personnel costs** <u>General</u> IV. The unit costs (hourly rates) are limited to salaries including during parental leave, social security contributions, taxes and other costs included in the remuneration required under national law and the employment contract or equivalent appointing act; V. Employees are hired directly by the Beneficiary in accordance with national law, and work under its sole supervision and responsibility; VI. The Beneficiary remunerates its employees in accordance with its usual practices. This means that personnel costs are charged in line with the Beneficiary's usual payroll policy (e.g. salary policy, overtime policy, variable pay) and no special conditions exist for employees assigned to tasks relating to the European Union or Euratom, unless explicitly provided for in the grant agreement(s); VII. The Beneficiary allocates its employees to the relevant group/category/cost centre for the purpose of the unit cost calculation in line with the usual cost accounting practice; VIII. Personnel costs are based on the payroll system and accounting system. IX. Any exceptional adjustments of actual personnel costs resulted from relevant budgeted or estimated elements and were based on objective and verifiable information. *[Please describe the 'budgeted or estimated elements' and their relevance to personnel costs, and explain how they were reasonable and based on objective and verifiable information, present your explanation to the Auditor and annex it to this certificate].* X. Personnel costs claimed do not contain any of the following ineligible costs: costs related to return on capital; debt and debt service charges; provisions for future losses	**Procedure:** *The Auditor draws a sample of employees to carry out the procedures indicated in this section C and the following sections D to F.* *[The Auditor has drawn a random sample of 10 full-time equivalents made up of employees assigned to the action(s). If fewer than 10 full-time equivalents are assigned to the action(s), the Auditor has selected a sample of 10 full-time equivalents consisting of all employees assigned to the action(s), complemented by other employees irrespective of their assignments.].* For this sample: ✓ the Auditor reviewed all documents relating to personnel costs such as employment contracts, payslips, payroll policy (e.g. salary policy, overtime policy, variable pay policy), accounting and payroll records, applicable national tax , labour and social security law and any other documents corroborating the personnel costs claimed; ✓ in particular, the Auditor reviewed the employment contracts of the employees in the sample to verify that: i. they were employed directly by the Beneficiary in accordance with applicable national legislation; ii. they were working under the sole technical supervision and responsibility of the latter; iii. they were remunerated in accordance with the Beneficiary's usual practices; iv. they were allocated to the correct group/category/cost centre for the purposes of calculating the unit cost in line with the Beneficiary's usual cost accounting practices; ✓ the Auditor verified that any ineligible items or any costs claimed under other costs categories or costs covered by other types of grant or by other grants financed from the European Union budget have not been taken

Please explain any discrepancies in the body of the Report.	
Statements to be made by Beneficiary	**Procedures to be carried out and Findings to be confirmed by the Auditor**
or debts; interest owed; doubtful debts; currency exchange losses; bank costs charged by the Beneficiary's bank for transfers from the Commission/Agency; excessive or reckless expenditure; deductible VAT or costs incurred during suspension of the implementation of the action. XI. Personnel costs were not declared under another EU or Euratom grant (including grants awarded by a Member State and financed by the EU budget and grants awarded by bodies other than the Commission/Agency for the purpose of implementing the EU budget). <u>If additional remuneration as referred to in the grant agreement(s) is paid</u> XII. The Beneficiary is a non-profit legal entity; XIII. The additional remuneration is part of the beneficiary's usual remuneration practices and paid consistently whenever the relevant work or expertise is required; XIV. The criteria used to calculate the additional remuneration are objective and generally applied regardless of the source of funding; XV. The additional remuneration included in the personnel costs used to calculate the hourly rates for the grant agreement(s) is capped at EUR 8 000 per full-time equivalent (reduced proportionately if the employee is not assigned exclusively to the action). *[If certain statement(s) of section "C. Personnel costs" cannot be endorsed by the Beneficiary they should be listed here below and reported as exception by the Auditor in the main Report of*	into account when calculating the personnel costs; ✓ the Auditor numerically reconciled the total amount of personnel costs used to calculate the unit cost with the total amount of personnel costs recorded in the statutory accounts and the payroll system. ✓ to the extent that actual personnel costs were adjusted on the basis of budgeted or estimated elements, the Auditor carefully examined those elements and checked the information source to confirm that they correspond to objective and verifiable information; ✓ if additional remuneration has been claimed, the Auditor verified that the Beneficiary was a non-profit legal entity, that the amount was capped at EUR 8 000 per full-time equivalent and that it was reduced proportionately for employees not assigned exclusively to the action(s). ✓ the Auditor recalculated the personnel costs for the employees in the sample. **Factual finding:** 4. All the components of the remuneration that have been claimed as personnel costs are supported by underlying documentation. 5. The employees in the sample were employed directly by the Beneficiary in accordance with applicable national law and were working under its sole supervision and responsibility. 6. Their employment contracts were in line with the Beneficiary's usual policy; 7. Personnel costs were duly documented and consisted solely of salaries, social security contributions (pension contributions, health insurance, unemployment fund contributions, etc.), taxes and other statutory costs included in the remuneration (holiday pay, thirteenth month's pay, etc.); 8. The totals used to calculate the personnel unit costs are consistent with those registered in the payroll and accounting records; 9. To the extent that actual personnel costs were adjusted on the basis of budgeted or estimated elements, those elements were

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Statements to be made by Beneficiary	**Procedures to be carried out and Findings to be confirmed by the Auditor**
Factual Findings: - *…]*	relevant for calculating the personnel costs and correspond to objective and verifiable information. The budgeted or estimated elements used are: — (indicate the elements and their values). 10. Personnel costs contained no ineligible elements; 11. Specific conditions for eligibility were fulfilled when additional remuneration was paid: a) the Beneficiary is registered in the grant agreements as a non-profit legal entity; b) it was paid according to objective criteria generally applied regardless of the source of funding used and c) remuneration was capped at EUR 8000 per full-time equivalent (or up to up to the equivalent pro-rata amount if the person did not work on the action full-time during the year or did not work exclusively on the action).
D. Productive hours XVI. The number of productive hours per full-time employee applied is *[delete as appropriate]*: A. 1720 productive hours per year for a person working full-time (corresponding pro-rata for persons not working full time). B. the total number of hours worked in the year by a person for the Beneficiary C. the standard number of annual hours generally applied by the beneficiary for its personnel in accordance with its usual cost accounting practices. This number must be at least 90% of the standard annual workable hours. <u>If method B is applied</u> XVII. The calculation of the total number of hours worked was done as follows: annual workable hours of the person according to the employment contract, applicable labour agreement or national law plus overtime worked minus absences (such as sick leave and special leave). XVIII. 'Annual workable hours' are hours	**Procedure (same sample basis as for Section C: Personnel costs):** ✓ The Auditor verified that the number of productive hours applied is in accordance with method A, B or C. ✓ The Auditor checked that the number of productive hours per full-time employee is correct and that it is reduced proportionately for employees not exclusively assigned to the action(s). ✓ If method B is applied the Auditor verified i) the manner in which the total number of hours worked was done and ii) that the contract specified the annual workable hours by inspecting all the relevant documents, national legislation, labour agreements and contracts. ✓ If method C is applied the Auditor reviewed the manner in which the standard number of working hours per year has been calculated by inspecting all the relevant documents, national legislation, labour agreements and contracts and verified that the number of productive hours per year used for these calculations was at least 90% of the standard number of working hours per year.

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Statements to be made by Beneficiary	**Procedures to be carried out and Findings to be confirmed by the Auditor**
during which the personnel must be working, at the employer's disposal and carrying out his/her activity or duties under the employment contract, applicable collective labour agreement or national working time legislation. XIX. The contract (applicable collective labour agreement or national working time legislation) do specify the working time enabling to calculate the annual workable hours. <u>If method C is applied</u> XX. The standard number of productive hours per year is that of a full-time equivalent; for employees not assigned exclusively to the action(s) this number is reduced proportionately. XXI. The number of productive hours per year on which the hourly rate is based i) corresponds to the Beneficiary's usual accounting practices; ii) is at least 90% of the standard number of workable (working) hours per year. XXII. Standard workable (working) hours are hours during which personnel are at the Beneficiary's disposal preforming the duties described in the relevant employment contract, collective labour agreement or national labour legislation. The number of standard annual workable (working) hours that the Beneficiary claims is supported by labour contracts, national legislation and other documentary evidence. *[If certain statement(s) of section "D. Productive hours" cannot be endorsed by the Beneficiary they should be listed here below and reported as exception by the Auditor:* - *…]*	**Factual finding:** <u>General</u> 12. The Beneficiary applied a number of productive hours consistent with method A, B or C detailed in the left-hand column. 13. The number of productive hours per year per full-time employee was accurate and was proportionately reduced for employees not working full-time or exclusively for the action. <u>If method B is applied</u> 14. The number of 'annual workable hours', overtime and absences was verifiable based on the documents provided by the Beneficiary and the calculation of the total number of hours worked was accurate. 15. The contract specified the working time enabling to calculate the annual workable hours. <u>If method C is applied</u> 16. The calculation of the number of productive hours per year corresponded to the usual costs accounting practice of the Beneficiary. 17. The calculation of the standard number of workable (working) hours per year was corroborated by the documents presented by the Beneficiary. 18. The number of productive hours per year used for the calculation of the hourly rate was at least 90% of the number of workable (working) hours per year.
E. Hourly rates The hourly rates are correct because: XXIII. Hourly rates are correctly calculated since they result from dividing annual personnel	**Procedure** ✓ The Auditor has obtained a list of all personnel rates calculated by the Beneficiary in accordance with the methodology used. ✓ The Auditor has obtained a list of all the relevant employees, based on which the

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Statements to be made by Beneficiary	**Procedures to be carried out and Findings to be confirmed by the Auditor**
costs by the productive hours of a given year and group (e.g. staff category or department or cost centre depending on the methodology applied) and they are in line with the statements made in section C. and D. above. *[If the statement of section 'E. Hourly rates' cannot be endorsed by the Beneficiary they should be listed here below and reported as exception by the Auditor:* - *…]*	personnel rate(s) are calculated. For 10 full-time equivalent employees selected at random (same sample basis as Section C: Personnel costs): ✓ The Auditor recalculated the hourly rates. ✓ The Auditor verified that the methodology applied corresponds to the usual accounting practices of the organisation and is applied consistently for all activities of the organisation on the basis of objective criteria irrespective of the source of funding. **Factual finding:** 19. No differences arose from the recalculation of the hourly rate for the employees included in the sample.
F. Time recording XXIV. Time recording is in place for all persons with no exclusive dedication to one Horizon 2020 action. At least all hours worked in connection with the grant agreement(s) are registered on a **daily/weekly/monthly** basis *[delete as appropriate]* using a **paper/computer-based system** *[delete as appropriate]*; XXV. For persons exclusively assigned to one Horizon 2020 activity the Beneficiary has either signed a declaration to that effect or has put arrangements in place to record their working time; XXVI. Records of time worked have been signed by the person concerned (on paper or electronically) and approved by the action manager or line manager at least monthly; XXVII. Measures are in place to prevent staff from: i. recording the same hours twice, ii. recording working hours during absence periods (e.g. holidays, sick leave), iii. recording more than the number of productive hours per year used to calculate the hourly rates, and	**Procedure** ✓ The Auditor reviewed the brief description, all relevant manuals and/or internal guidance describing the methodology used to record time. The Auditor reviewed the time records of the random sample of 10 full-time equivalents referred to under Section C: Personnel costs, and verified in particular: ✓ that time records were available for all persons with not exclusive assignment to the action; ✓ that time records were available for persons working exclusively for a Horizon 2020 action, or, alternatively, that a declaration signed by the Beneficiary was available for them certifying that they were working exclusively for a Horizon 2020 action; ✓ that time records were signed and approved in due time and that all minimum requirements were fulfilled; ✓ that the persons worked for the action in the periods claimed; ✓ that no more hours were claimed than the productive hours used to calculate the hourly

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Statements to be made by Beneficiary	**Procedures to be carried out and Findings to be confirmed by the Auditor**
iv. recording hours worked outside the action period. XXVIII. No working time was recorded outside the action period; XXIX. No more hours were claimed than the productive hours used to calculate the hourly personnel rates. *[Please provide a brief description of the time recording system in place together with the measures applied to ensure its reliability to the Auditor and annex it to the present certificate[4]].* *[If certain statement(s) of section "F. Time recording" cannot be endorsed by the Beneficiary they should be listed here below and reported as exception by the Auditor:* *- …]*	personnel rates; ✓ that internal controls were in place to prevent that time is recorded twice, during absences for holidays or sick leave; that more hours are claimed per person per year for Horizon 2020 actions than the number of productive hours per year used to calculate the hourly rates; that working time is recorded outside the action period; ✓ the Auditor cross-checked the information with human-resources records to verify consistency and to ensure that the internal controls have been effective. In addition, the Auditor has verified that no more hours were charged to Horizon 2020 actions per person per year than the number of productive hours per year used to calculate the hourly rates, and verified that no time worked outside the action period was charged to the action. **Factual finding:** 20. The brief description, manuals and/or internal guidance on time recording provided by the Beneficiary were consistent with management reports/records and other documents reviewed and were generally applied by the Beneficiary to produce the financial statements. 21. For the random sample time was recorded or, in the case of employees working exclusively for the action, either a signed declaration or time records were available; 22. For the random sample the time records were signed by the employee and the action manager/line manager, at least monthly. 23. Working time claimed for the action occurred in the periods claimed; 24. No more hours were claimed than the number productive hours used to calculate the hourly

[4] The description of the time recording system must state among others information on the content of the time records, its coverage (full or action time-recording, for all personnel or only for personnel involved in H2020 actions), its degree of detail (whether there is a reference to the particular tasks accomplished), its form, periodicity of the time registration and authorisation (paper or a computer-based system; on a daily, weekly or monthly basis; signed and countersigned by whom), controls applied to prevent double-charging of time or ensure consistency with HR-records such as absences and travels as well as it information flow up to its use for the preparation of the Financial Statements.

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Statements to be made by Beneficiary	**Procedures to be carried out and Findings to be confirmed by the Auditor**
	personnel rates; 25. There is proof that the Beneficiary has checked that working time has not been claimed twice, that it is consistent with absence records and the number of productive hours per year, and that no working time has been claimed outside the action period. 26. Working time claimed is consistent with that on record at the human-resources department.

[official name of the** [Beneficiary] [Linked Third Party]**]	***[official name of the Auditor]***
[name and title of authorised representative]	***[name and title of authorised representative]***
[dd Month yyyy]	***[dd Month yyyy]***
<Signature of the** [Beneficiary] [Linked Third Party]**>	***<Signature** of the Auditor**>***

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