

Tier-1 Application form – English version

APPLICATIONS ARE PREFERABLY DRAWN UP IN ENGLISH. AN ENGLISH TRANSLATION HAS TO BE ENCLOSED WITH APPLICATIONS SUBMITTED IN DUTCH.

The application form is available in English on the website

<https://www.vscentrum.be/en/access-and-infrastructure/project-access-Tier-1>

Title of the application:

Investigating solvent effect in the acidity of UiO-66 metal organic framework for catalysis

Name and first name of the applicant:

Chiara Caratelli

Institution:

Ghent University

Research group / department:

Center for Molecular Modeling

Title / position:

PhD student

Email address:

chiara.caratelli@ugent.be

Total computing time that is needed, in node days:

4764

Total scratch disk storage that is applied for (in GiB) and number of files:

317.6 GiB + 12704 files

The total number of pages in this application should not exceed 18, excluding possible appendices (confirmation letter of financing institution, software license, etc.) which may be taken into account by the Tier-1 Allocation Board.

1. Title of the research project (with IWETO or FRIS link if available) within the framework of which computing time is applied for:

If this is a resubmission or continuation from an earlier Tier-1 proposal, mention the EasyChair code (e.g. 2018-XX).

“Characterization of active sites and catalysis in MOFs using first principle methods”, European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No: 641887 (H2020-MSCA-ITN “DEFNET”, Prof. Veronique Van Speybroeck)

Link: <https://researchportal.be/nl/project/defect-network-materials-science-and-engineering-0>

Continuation of project: 2017-43

2. Describe your research project in short. Explicitly mention the scientific questions that you are planning to address and the overall scientific goals of the project. (max. 1 A4 in Arial 12):

Metal organic frameworks (MOFs) are a recent class of nanoporous materials formed by metal or metal oxide clusters connected by organic linkers. Their true hybrid behavior, high metal content and porosity make them very appealing as catalysts. Among these, the Zr-based MOF denoted as UiO-66 [1] is characterized by an exceptional stability due to the high connectivity of its building blocks, Zr-oxide bricks and terephthalate linkers. The highly connected material allows for the presence of crystal defects such as missing linkers, which are responsible for its catalytic activity. Defects create active sites where metal atoms are not fully coordinated and can be exploited for catalysis. However extremely important, the study of these defects is a truly challenging task for which experiments and theory need to work in synergy. In particular, modeling of the material at true operating conditions is crucial in order to understand its properties during catalysis of reactions, and to engineer it for industrial applications. It is known [2] that on the defect sites not only the metal takes an active role as a catalyst, but also solvent molecules that are adsorbed in these sites. It has been seen that a methanol solvent [3] interacts with the active sites and can transfer protons and aid in reactions. The next step is probing the acidity of these sites in the presence of the solvent, to understand which Brønsted sites actually take part in the reactions. Umbrella sampling simulations will be performed to measure transfer of protons from the active sites to the solvent molecules, represented schematically in Figure 1. The collective variable chosen has been developed at the Van 't Hoff institute for molecular sciences at the University of Amsterdam, and is specifically designed to track protons in protic solvent, when atom labels can change because of atom transfers. These calculations will shed light on the acidic strength of the active sites which is something still unknown in these defective nanoporous materials.

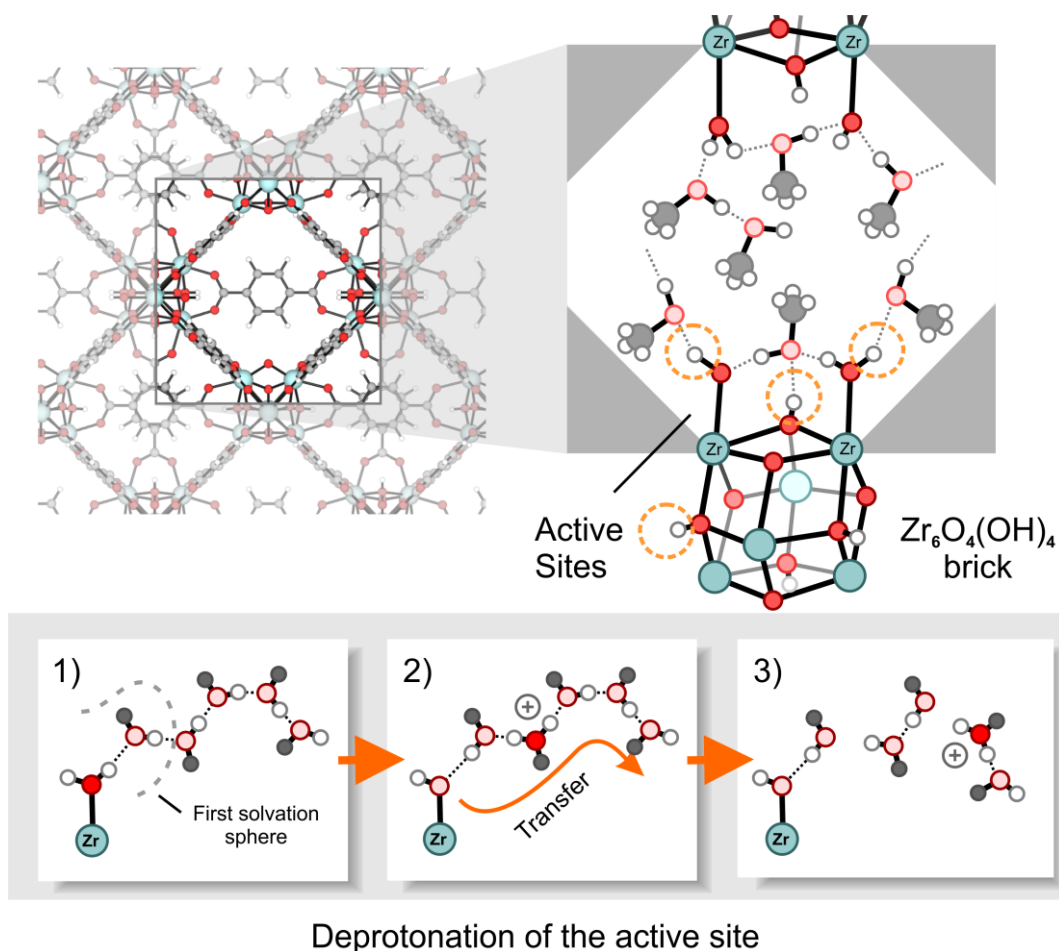


Figure 1 Scheme of the active sites on defective UiO-66

References:

- [1] J.H. Cavka, *et al.*, *J Am Chem Soc*, 130 (2008) 13850-13851.
- [2] C. Caratelli *et al.*, *J. Catal.*, 352 (2017) 401-414
- [3] C. Caratelli, *et al.* *Chemphyschem.* 19(4) (2018) 420-429

3. Provide an engaging abstract (10 lines) for scientific communication on the website in layman's terms. Should this application be bound by a confidentiality agreement (see also item 12 of this application form), provide more details about the specific nature of the confidentiality and indicate why an abstract may not be published.

UiO-66, composed of Zr-oxide bricks and terephthalate linkers, is currently one of the most studied metal-organic frameworks due to its exceptional stability. On this material, defects in the crystal structure, such as missing linkers, are responsible for catalytic activity. On these sites, the solvent can interact, facilitating transfer of protons and giving extra stabilization to charged configurations via hydrogen bonding, which could be crucial in stabilizing reactive intermediates. Therefore, investigating to what extent protons can be donated and how this dynamically occurs is of outmost

importance. The project investigates the acidity of these active sites to understand their role in catalytic applications.

4. Financing institution or channel, financing the research project in full or in part (FWO, BOF, IWT, EU, etc.): Please attach the confirmation letter as enclosure. In case the project has not gone through a scientific approval process attach a letter of approval of your own institute.
 - European Research Council under the European Union's Horizon 2020 research and innovation programme (consolidator ERC grant agreement No 647755 – DYNPOR (2015-2020))
 - European H2020 research and innovation programme, MSCA grant agreement No: 641887
- Confirmation letters can be found at the end of the file

5. Name and email address of the promoter(s) of the research project:

Prof. Dr. ir. Veronique Van Speybroeck
veronique.vanspeybroeck@ugent.be

6. Persons mandated by the Applicant to compute on the Tier-1 within the framework of the present project: Please provide for every person:
 - name and first name
 - institution
 - research group / department
 - title / position
 - experience of using HPC resources (Tier-0/Tier-1/Tier-2 infrastructure in Belgium and abroad) in the past (specify names and when)

Chiara Caratelli

Ghent University

EA17, Center for Molecular Modeling

PhD fellow

vsc41771

2½ years experience with Tier-2 infrastructure of UGent

1 year experience with Tier-1 infrastructure (Muk)

1½ year experience with Tier-1 infrastructure (BrENIAC)

½ year of experience with Tier-1 and Tier-2 infrastructure of the Netherlands / University of Amsterdam

½ year experience with Tier-0 infrastructure (Fermi) of CINECA (Italy)

Pilot user for BrENIAC and Tier-2 cluster Swalot (UGent)

Julianna Hajek

Ghent University

EA17, Center for Molecular Modeling

Postdoc

vsc40880

4½ years experience with Tier-2 infrastructure of UGent

2 years experience with Tier-1 infrastructure (Muk)

1½ year experience with Tier-1 infrastructure (BrENIAC)

Pilot user for BrENIAC and Tier-2 cluster Swalot (UGent)

7. Explain why this project needs to run on a Tier-1 system, why the machine you have requested is suitable for the project and how the use of the system will enable the science proposed (max. ½ A4 in Arial 12).

The total number of tasks included in this research project is estimated to be 52, however to obtain accurate results, the simulations need to be well equilibrated and long simulation times are required to achieve statistically relevant data. 48 umbrella sampling simulations, each on 2 nodes will run in parallel as much as possible during the project. The system size (414 atoms, unit cell parameters of $15 \times 21 \times 15 \text{ \AA}^3$), and time that is required for the calculations (4764 node days) to describe the deprotonation reactions of UiO-66 in a solvent are beyond the reach of day-to-day calculations on Tier-2 infrastructure, providing a strong justification for the need of Tier-1. The Center for Molecular Modeling plays a leading role in the application of advanced molecular dynamics simulations in nanoporous environments. While the CMM published quite some papers with this application in zeolites, so far there are only two pioneering top publications reporting first principles molecular dynamics (MD) of MOFs for which calculations have been performed on BrENIAC. [J. Hajek et al., *Chemical Science*, 2018; C. Caratelli et al., *ChemPhysChem*, 2018] To maintain this leading role and to take this research line to the next level, it is of utmost importance that we have access to the most efficient computing infrastructure such as Tier-1.

8. Justify the number of node days requested. This should include information such as: number and nature of computing tasks, software used, and the sequence in which they will be performed.

Indicate for each typical computing task the required resources:

- wall clock time (note that 3 days is the maximal wall clock time for any job;)
- memory (maximum 128 GiB/node; 256 GiB/node is available upon motivated request)
- number of nodes (could be fractional)
- number of CPU cores
- disk space (estimated volume in GiB and the total number of files); make a clear distinction between usage of Tier-2 DATA/HOME partitions and the Tier-1 SCRATCH partition

- number of tasks, and an indication of how many such tasks would be submitted concurrently.

This information should take the form of a table (an example is provided as Table 1 on the next page). Provide additional descriptions of the computing tasks and comments as needed and clearly relate the described tasks to the tasks in the table. Resource estimates should be preferably based on the results of actual calculations on Tier-1 (via, e.g., a Starting Grant) for system/problem sizes that are on par with those of the intended computing tasks (e.g., same mesh sizes, actual molecular system, ...). If not, provide the name, architecture, #cores, memory, etc. of the machine that was used to obtain these results and explain how you have calculated/rescaled the wall clock times, number of cores, etc.

Please do take into account that after half of the allocation time has passed, the applicant loses 30% of the initially granted node days, if that 30% has not been used. (cf. regulations, § 9)

(typically, up to 2 A4 Arial 12).

The workflow for this project consists in three types of simulations which will all be performed using the CP2K software package in a periodic unit cell of UiO-66 (414 atoms) containing one missing linker and which has been fully loaded with 32 molecules of methanol solvent. The computational requirements have been carefully considered based on the amount of seconds per MD step in test simulations run on this system on two full nodes in the NPT and NVT ensemble.

The following calculation workflow (2 nodes at a time) will be used to model the reactions:

1. Equilibration:

Before the different windows in the umbrella sampling (US) can be created, the system is equilibrated for about **4 ps** (8000 steps) using an NPT ensemble at 330 K and 1 atm. This first simulation will take **12 node days**.

2. Creation of umbrella windows:

The crucial step in the US methodology is the selection of the various windows on the reaction path along the collective variable (CV) and determination of the initial structures in each of these windows. We will apply an innovative method in the form of a moving umbrella which during the whole duration of the molecular dynamics (MD) crosses the entire range of CV with a constant velocity. In this constrained MD concept, a bias

potential is moved along a reaction coordinate to drive the system from the reactant to the product state at the same conditions. The deprotonation of each of the three different protons in the material will be modeled this way in the NVT ensemble. This creation of the windows will take about **16 ps** to ensure the sampling of all crucial configurations. It is expected that each of the three simulations will require about **48 node days**.

3. Umbrella sampling simulations:

For each of the three reactions, 16 equidistant snapshots will be extracted from the moving umbrella simulation and in each of those an MD simulation in the NVT ensemble with a static harmonic bias will be performed. The total number of MD jobs is thus 16 for each deprotonation reaction. Each of these tasks will run for approximately **32 ps**, requiring **96 node days**. All these simulations are independent and can easily run in parallel with each other.

This workflow has been successfully followed and validated in previous projects describing reactive processes and structural rearrangements in nanoporous materials, leading to publications in high impact journals.

Table 1 summarizes the estimated node and core days required for each simulation type and the requirements for scratch space and long-term storage for each simulation type. Because of the long simulation times, a complete MD trajectory cannot be obtained within the wall time limit of 72 hours, but requires several restarts.

Table 1

Computational task	Node day calculation				# CPU cores per task	Memory usage (GiB) / node per task	OpenMP / MPI / hybrid	Storage volume estimate	
	# of such tasks	Wall clock time (days) per task	# Tier-1 nodes per task	# total node days task				Tier-2 DATA/HOME volume (GiB) + number of files	Tier-1 SCRATCH volume (GiB) + number of files
Equilibration	1	6	2	12	56	25	MPI	0.8 GiB + 32 files	0.8 GiB + 32 files
Restrained MD	3	24	2	144	56	25	MPI	9.6 GiB + 384 files	9.6 GiB + 384 files
US	48	48	2	4608	56	25	MPI	307 GiB + 12288 files	307 GiB + 12288 files
TOTAL	52			4764				317.6 GiB + 12704 files	317.6 GiB + 12704 files

9. Describe the software required to perform the computing task(s). Please clearly provide the following per item in this regard:

- a reference to the software's web page
- the software license system (open source, GPL, etc.)
- if there is no free academic use of the software, state which license makes the installation and the use valid on the Tier-1 by the Applicant (+ add a copy of the signed license)
- if need be, which license server will be used (name + IP address)
- whether the software is already available on the Tier-1 and, if this is not the case, compilation and installation instructions (possibly with reference to existing Tier-2 installation)

Molecular dynamics simulations will be performed using the CP2K software package (<http://www.cp2k.org/>) with the PLUMED code (<http://www.plumed.org>), which are freely available under the GPL license. A patch for PLUMED (with license LGPL) is required to handle the used collective variable for these calculations, which can be installed with Easybuild. The installation of this PLUMED version on Tier-1 is necessary for the success of this project. A local version of PLUMED (versions 2.4.0) which contains this patch has been already successfully compiled by the applicant using Easybuild and tested on both haswell-ib and sandybridge architectures of the Tier-2 of UGent.

The Easybuild easyconfig files where all the dependencies are indicated, along with the used installation script, are located in the following folder:
/user/data/gent/vsc417/vsc41771/myapps/installation-CP2K-5.1-intel-2018a-PLUMED-2.4.0-PathCV

If the project is awarded, we will ask the KULeuven ICTS staff to make the software available as a module.

Provide the results of efficiency tests that were conducted with this software, preferably on the current VSC Tier-1 (using, e.g., a Starting Grant) for system/problem sizes that are on par with those of the intended computing tasks (e.g., same mesh sizes, actual molecular system, ...). If not run on the current VSC Tier-1, provide the name, architecture, #cores, memory, etc. of the machine that was used to obtain these results and how you think this compares to the current

VSC Tier-1. If a different system/problem size is used provide some guidance how it relates to the problem size in the application.

Provide both a table and efficiency plot such as Table 2 and Plot 1 below (log scale X-axis) (typically up to 3 A4 in Arial 12).

Important: the baseline configuration (first line in the table) should be the *minimal* configuration on which your computation could be carried out, where the number of cores for this baseline configuration could be 1, 2, ..., 28, 56, Please start the scaling of your code within one node (1, 2, ... cores), or explicitly mention why this is not possible. *Table and plot should be created w.r.t. the baseline configuration.*

Discuss the plot and table (explain any anomalies). Explain why you make a specific choice for a given number of nodes (in case of multi node jobs).

In case your tasks are single node jobs (HTC), describe how you will manage your jobs, e.g. will you make use of the Worker Framework¹ or something similar?

If the simulation contains a significant amount of I/O, then mention its impact on the calculations.

Scaling of the CP2K software (version CP2K/3.0-intel-2016a) on BrENIAC has been tested for the system under study (UiO-66 reduced cell with one defect site and 32 molecules of methanol solvent, 414 atoms in total). Short NVT MD runs (20 steps) have been performed on from 1 to 448 cores on the BrENIAC cluster and the average time per step in second was extracted, for which the results are summarized in Table 2.

Table 2: Results of CP2K scaling test performed on Tier-1 for UiO-66

# nodes	# cores	Wall clock time per step (s)	Speedup (with respect to 1 core)	Efficiency (with respect to 7 cores)
1	1	2489.22	1	1.000

¹ <https://www.vscentrum.be/cluster-doc/running-jobs/worker-framework>

1	4	667.17	3.73	0.933
1	8	357.32	6.97	0.871
1	16	184.30	13.51	0.844
1	28	110.73	22.48	0.803
2	56	60.20	41.35	0.738
4	112	34.59	71.96	0.642
8	224	21.44	116.10	0.518
16	448	14.82	167.97	0.375

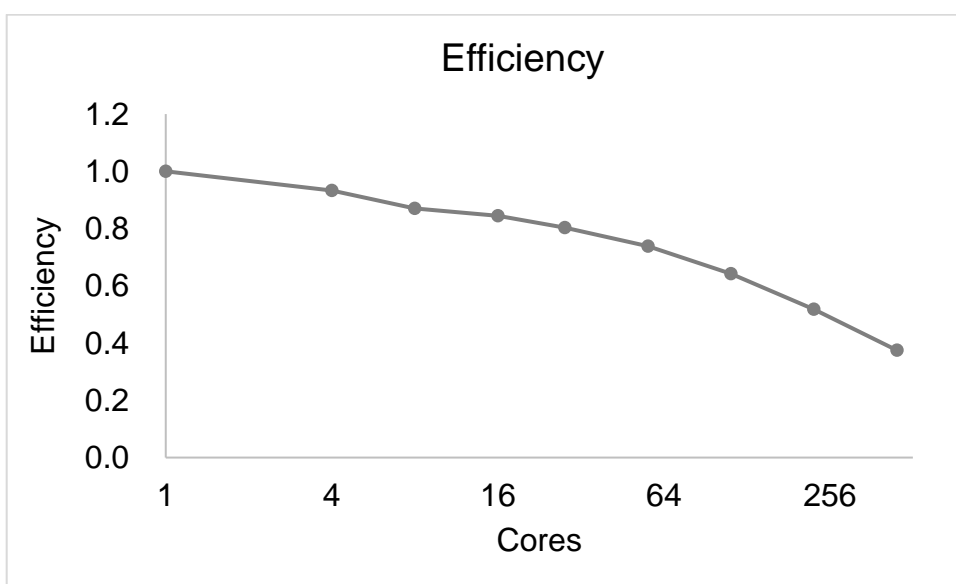


Figure 2 efficiency of CP2K for the system under study from 1 to 448 cores

Figure 2 shows the efficiency for CP2K. We find that the optimum number of cores to run MD calculations on UiO-66 is 56 (**2 nodes**) with efficiency of **73.8%**, as any larger count gives a parallel efficiency of less than 70%, whereas 2 nodes maximize throughput time.

- Describe how you will manage the resources requested in the period during which the task is to be performed. What usage pattern do you anticipate (similar usage on monthly basis, bursts, ...)?

In case the disk storage or the number of files that is applied for exceed the defaults of 2 TiB and 200.000 files (cf. regulations §4, (5)), describe how the transfer of files to/from Tier-1 will be managed, if data reduction and/or compression of files will be performed, and if you can provide information about IOPS.

We estimate to perform the calculations over a time period of approximately 8 months, preferably starting in July 2018. In a first phase of equilibration of the structures, less computational time will be needed. When starting the umbrella simulations afterwards, it is our intention to proceed with constant monthly usage. This estimated timeframe takes into account the actual runtime of the simulations, as well as intermediate data analysis tasks and frequent job restarts. At the beginning of each run, only three small text files are required (input file, coordinate file and submit script). The simulations run with a constant computational cost per step, as each step takes the approximately the same amount of seconds to be computed. Most of the simulations cannot be completed within the wall time limit of 72 hours, therefore job restarts are required. This can be easily done using small automatically generated restart files, which take the last computed quantities as input, as the simulations are not history dependent. Each run will consist therefore of a 72 hours (wall time) simulation whose output will be generated in a separate folder. The folder will be copied upon completion to the Tier-2 data storage, where the whole simulation is stored, for analysis. Therefore, data transfer will be spread over the duration of the project. At the end of the project the data will be removed from the Tier-1 scratch.

11. List the granted computing time allocations to the promoter(s) of this research project, on the Flemish Tier-1 systems, as well as other Tier-1 and Tier-0 systems. Also, describe the scientific output obtained within the framework of computing time that was granted during the past two years on the Flemish Tier-1 systems or on other Tier-1 or Tier-0 supercomputers. DOI links are sufficient.

List of the research projects granted to C. Caratelli or J. Hajek on the Flemish Tier-1 system:

BrENIAC:

- 2017-43: “Probing the strength of basic sites on UiO-66 using pKa calculations” (C. Caratelli, node days: 4450)
- 2016-62: “Ab initio umbrella sampling simulations of dehydration of UiO-66” (J. Hajek, node days: 3972)

Muk:

- 2016-7: “Investigating active sites in hydroxylated and dehydroxylated UiO-66 for catalysis of Oppenauer-type oxidation” (C. Caratelli, node days: 2110)
- 2015-21: “Unraveling dehydroxylation pathways on UiO-66 type systems with metadynamics” (J. Hajek, node days: 3304)
- 2015-5: “Structural transformations during dehydroxylation reactions of UiO-66 type metal-organic frameworks; an extension with normal mode analysis” (M. Vandichel, node days: 2726)
- 2014-43: “Structural transformations during dehydroxylation reactions of UiO-66 type metal-organic frameworks” (M. Vandichel, node days: 4720)
- 2014-25: “Modeling aldol condensations in metal-organic frameworks with hybrid functional calculations” (J. Hajek, node days: 2304)
- 2013: “Unraveling reaction pathways on UiO-66 type systems with metadynamics” (M. Vandichel, node days: 4432)

The abovementioned Tier-1 projects have resulted in publications in major journals:

<http://dx.doi.org/10.1039/C7SC04947A>
<http://dx.doi.org/10.1002/cphc.201701109>
<http://dx.doi.org/10.1016/j.jcat.2017.06.014>
<http://dx.doi.org/10.1002/cctc.201601689>
<http://dx.doi.org/10.1039/C4RA16800C>
<http://dx.doi.org/10.1039/C4CE01672F>
<http://dx.doi.org/10.1016/j.jcat.2015.08.015>
<http://dx.doi.org/10.1016/j.jcat.2016.05.018>
<http://dx.doi.org/10.1039/C6CE01027J>
<http://dx.doi.org/10.1039/C6SC00987E>

12. Are the applicants of this application bound by a confidentiality agreement? If so, the abstract of this application will not be published on the website of the FWO / Flemish Supercomputer Center, only the title.

no

Should you have any questions or encounter any difficulties during the electronic submission of an Application, please contact by email:
Associatie KU Leuven: hpcinfo@kuleuven.be
Associatie Universiteit Gent: hpc@ugent.be
Associatie Universiteit Hogescholen Antwerpen: hpc@uantwerpen.be
Associatie Universiteit Hogescholen Limburg: geertjan.bex@uhasselt.be
Universitaire Associatie Brussel: hpc@vub.ac.be
For the other institutions: caroline.volckaert@fwo.be

ACCESSION FORM FOR BENEFICIARIES

UNIVERSITEIT GENT (UGent), 248015142, established in SINT PIETERSNIEUWSTRAAT 25, GENT 9000, Belgium, BE0248015142, ('the beneficiary'), represented for the purpose of signing this Accession Form by Anne DE PAEPE, Rector,

hereby agrees

to become beneficiary ('6')

in Agreement No 641887 ('the Agreement')

between RUHR-UNIVERSITAT BOCHUM **and** *the Research Executive Agency (REA) ('the Agency')*, under the power delegated by the European Commission ('the Commission'),

for the action entitled 'DEFect NETwork materials science and engineering (DEFNET)'.

and mandates

the coordinator to submit and sign in its name and on its behalf any **amendments** to the Agreement, in accordance with Article 55.

By signing this Accession Form, the beneficiary accepts the grant and agrees to implement the action in accordance with the Agreement, with all the obligations and conditions it sets out.

SIGNATURE

For the beneficiary

Anne DE PAEPE with ECAS id npaeanne signed in the Participant Portal on 22/12/2014 at 16:37:25 (transaction id SigId-27420-d6uyZcxc41Bc44BDyB4mjm3PcnyOziEntAZqs3UBeyuwZKL9mo23867rtmIRVRLct9QPVIyszRpDU4jgo0HteV-PHslUMVSYCYcXZAW3OHozsk-bMbbtkGtcng8sJSi6EP6aUltrKzQnKaWezZ1xmXpI2i0). Timestamp by third party at Mon Dec 22 16:37:31 CET 2014



European Research Council
Executive Agency

Established by the European Commission

Brussels,

Veronique VAN SPEYBROECK
UNIVERSITEIT GENT
Technologiepark 903
9052 ZWIJNAARDE
BELGIUM

Subject: Invitation to grant preparation
H2020 - ERC-2014-CoG
647755 - DYNPOR

Dear **Veronique VAN SPEYBROECK**,

We are pleased to inform you that the European Research Council Executive Agency (ERCEA) is now in a position to initiate the preparation of the grant agreement for your abovementioned proposal.

The ERCEA intends to follow the Evaluation Report advice which has been already transmitted to you and consequently, it is estimated that the maximum EU financial contribution to your project could be up to 1 993 750.00 Euro for a period of up to 60 months.

With reference to the submitted proposal and its evaluation, the grant preparation shall be based on the following:

The deadline for the submission of the data required for the grant agreement, including any additional documents, as detailed in the Annex attached is 02/03/2015.

Failure to respect the deadline indicated above will be considered as a wish not to enter into the grant preparation and, therefore, to withdraw your proposal. In such a case, the ERCEA will initiate the procedures to reject your proposal, unless alternative arrangements have been accepted by the ERCEA.

Considering the above, we expect the granting process to be completed as soon as possible, and within 4 weeks of the date of this letter.

The grant preparation process, including communication with the **ERCEA**, and the subsequent signature of the Grant Agreement, shall be carried out through the Research **Participant Portal Grant Management Service (PP GMS)**. By logging into your individual account in the Participant Portal and selecting the project under the Grant Management Service section, each step of the grant preparation process can be followed, and all relevant documents consulted, at any time.

Please see however in the Annex of this letter the additional documents required which you will have to submit by email to the officer in charge of your project (see: “Additional Information for the grant preparation attached to this invitation”).

The Grant Agreement preparation data provided through the Participant Portal (pre-filled with the information already available in the Beneficiary Register, and structured data from your proposal) are needed in order to prepare the grant agreement and provide programme-wide statistical information.

Kindly note that some information related to the legal and financial status of participants is read-only and may only be updated by the Legal Entity Appointed Representative (LEAR) of the organisations concerned through the Participant Portal <http://ec.europa.eu/research/participants/portal>. It is therefore important to ensure that all participants are aware of the need to appoint a **LEAR, within 2 weeks from the date of dispatch of this invitation letter**.

Further information providing practical details on grant preparation as well as technical guidance, are available in the [H2020 Online Manual](#) section of the Participant Portal.

This letter should not be regarded under any circumstances as a formal commitment by the ERCEA to provide financial support, as this depends on the satisfactory and timely conclusion of grant agreement preparation and on the satisfactory finalisation of the ethics review process (where applicable).

In case your project needs to undergo an ethics review and/or assessment by the ERCEA, you will, if not already the case, be soon contacted by our Scientific Department (Ethics team). We draw your attention to the fact that the granting process cannot be finalised and your project can not start until all ethical issues are either cleared or have been considered by the Ethics team as having to be cleared during the course of the project.

Should you need further details concerning the granting process, you are invited to contact the **officer in charge of your project** (Mr. Kris PIOT – functional e-mail address ERC-COG-GRANTING@ec.europa.eu)

Yours sincerely,

Marja HENNESSY
Head of Unit
ERC Executive Agency

Enclosure(s):

Annex: Additional Information for the grant preparation

cc: Nathalie Vandepitte

Annex: Additional Information for the grant preparation

Please remember that Horizon 2020 actions (i.e. projects) must be implemented in accordance with the assessed proposal. The Description of the Action must not differ from the proposal (see also below). This is without prejudice to any corrections needed:

- as a result of an ethical review,
- to ensure the project conforms to the applicable rules, e.g. legal and financial rules,
- to remove clerical errors or clear inconsistencies,
- when, under exceptional circumstances, a participant is removed during grant preparation.

In line with the above, the following should be taken into account for the ERC grant agreement preparation:

1. Description of the Action (DoA, Annex 1 to the grant agreement) and Estimated budget for the action (Annex 2)

The **Description of the Action** (DoA, Annex 1 to the grant agreement) should include the narrative description of the budget, as in the proposal. The budget table should only be shown in the **Estimated budget** for the action (Annex 2).

Therefore, when preparing it, please remember to **remove the budget table** from your proposal (Part B), before uploading the Description of the Action (DoA) in the Participant portal. However tables that provide additional information (e.g. more detailed breakdown of certain cost categories) compared to the budget table of Annex 2 can remain. **All eligible costs must be included in the narrative budget description of the DoA.** Please remember to use whole Euro values only.

Description of the Action (Annex 1) – **Part A:** please note that section 1.3. Workplan Tables - Detailed implementation does not have to be filled in for the ERC grant preparation.

2. Statement of Changes (SoC)

In addition to the submission of the data through the system please also provide a one page statement describing any changes that have been made in the Description of the Action compared to the original proposal.

Even in case there are no changes in the DoA from the original proposal, **please include a clear statement** ("Statement of changes", to be uploaded in the Participant portal).

3. Supplementary Agreement (SA)

Please use the model for H2020 ERC supplementary agreement found at the [ERC Documents website](#) (*to be sent by email to the officer in charge of your project*).

4. PI's passport

Only if the PI has **not** provided a copy of his/her identity document during the interview (evaluation of proposal) **or** this document has been modified or renewed, then the PI is requested to provide a copy of such a document (*to be sent by email to the officer in charge of your project*).

5. Links to other useful documents and guidelines:

[Participant Portal](#)

[Proposal Management and Grant Preparation](#)

[Grant Preparation](#)

[Grant signature](#)



Horizon 2020
European Union Funding
for Research & Innovation

ERC Executive Agency – Grant Management Department
BE-1049 Brussels, Belgium | <http://erc.europa.eu> | Email: ERC-COG-GRANTING@ec.europa.eu