# Enclosure 1b. Category 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-tier1

Title of the application:

Investigating active sites in hydroxylated and dehydroxylated UiO-66 for catalysis of Oppenauer-type oxidation

Name and first name of the applicant:

Chiara Caratelli

Institution:

Ghent University

Research group / department:

EA17, Center for Molecular Modeling

Title / position:

PhD Fellow

e-mail address:

*chiara.caratelli@ugent.be*

Total computing time that is needed, in node days:

2110

Total disk storage that is applied for (in GiB):

334 GiB

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

Combined experimental and computational study of electronically modulated metal-organic framework (MOF) catalysts, FWO project 3G048612 between COK (Prof. Dirk De Vos) and CMM (Prof. Veronique Van Speybroeck)

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)

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 new class of porous materials that can be exploited for a wide range of industrial applications, of which an important one is heterogeneous catalysis. UiO-66, a Zr terephthalate based MOF, is characterized by an exceptional stability (Cavka et al. 2008), which makes it a highly appealing catalyst. Catalytic activity is achieved when Zr atoms are not fully coordinated and Lewis acid sites are exposed. These active sites can emerge upon removal of an organic linker or dehydroxylation (Figure 1).

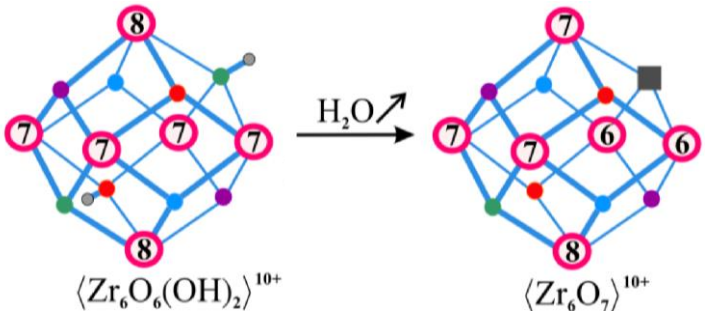


Figure 1: Zr brick with one missing linker, in hydroxylated (left) and dehydroxylated (right) form.

In this project we intend to explore available active sites for catalysis on hydroxylated and dehydroxylated UiO-66 for Oppenauer-type oxidation of prenol with furfural (Figure 2). Oppenauer oxidation (Boronat et al. 2006) is a reaction where an alcohol group is oxidized to a carbonyl and is essential in organic synthesis and in pharmaceutical chemistry.

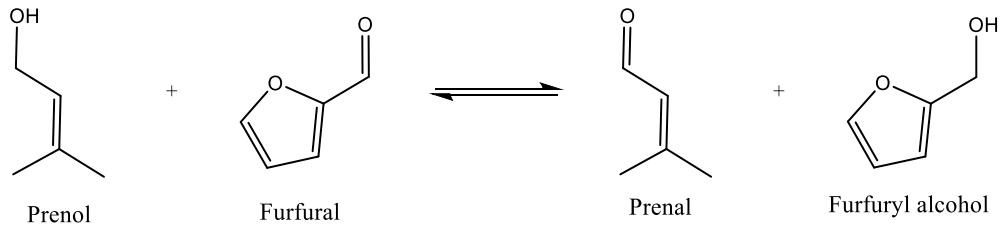


Figure 2: Scheme of the Oppenauer-type oxidation of prenol with furfural.

The use of catalytic reactions in oxidation is of importance in industrial processes from both an economic and an environmental point of view, and UiO-66 has been recognized by the scientific community as having a large potential as a catalyst (Chavan et al. 2010). This reaction has not yet been modeled on UiO-66, and since it can be catalyzed by this system it represents a good opportunity to study the active sites on this material.

In this work we will perform ab initio Molecular Dynamics (AIMD) simulations to find the most probable initial configurations. The reactions will then be modeled with high level static calculations. All the calculations will be periodic, which is necessary for an accurate study that takes into account environmental effects. The study of this reaction will bring insights into the behavior of this MOF, which needs to be fully understood in order to exploit its catalytic potential in large scale practical applications.

3. Provide an abstract (10 lines) for scientific communication on the website in layman's terms. See also item 12 of this application form.

UiO-66 is a Zr based metal organic framework that is considered a new catalyst with promising industrial applications. Among the reactions that can be catalyzed by this material, Oppenauer type oxidation has an industrial and pharmaceutical interest. Unravelling the mechanism of this reaction on UiO-66 will help to understand its behavior, which is an essential step in further development of the catalyst. For this purpose, ab initio Molecular Dynamics is a suitable tool that we will use to obtain the most probable configuration for the system. Static calculations will also be done to compare the possible paths and unravel the reaction mechanism.

4. Financing institution or channel, financing the research project in full or in part (FWO, BOF, IWT, EU, ...): Please attach the confirmation letter as enclosure (see instructions in enclosure 3 "EasyChair proposals submission procedure").

- FWO project 3G048612
- 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 in the past (Tier-0/Tier-1/Tier-2 infrastructure in Belgium and abroad)

Chiara Caratelli
Ghent University
EA17, Center for Molecular Modeling
PhD fellow
vsc41771
3 months experience with TIER2 infrastructure of UGent
½ year experience with TIER0 infrastructure of CINECA (Italy)

Julianna Hajek
Ghent University
EA17, Center for Molecular Modeling
PhD fellow
vsc40880
1 ½ year experience with TIER1 infrastructure of UGent
2 ½ year experience with TIER2 infrastructure of UGent

Veronique Van Speybroeck
Ghent University
EA17, Center for Molecular Modeling
Professor
vsc40021
2 year experience with TIER1 infrastructure of UGent
6 ½ year experience with TIER2 infrastructure of 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).

Due to the large size of the systems, between 210 and 220 atoms, even periodic static calculations would require more than 200 node days before convergence, which cannot be acquired on the TIER2 machines. In order

to obtain results in a reasonable timeframe we face the necessity to run highly efficient multinode jobs. Moreover, since the calculations on the different molecular clusters are independent, they can be run in parallel. The Center for Molecular Modeling was one of the first research groups to model catalysis on UiO-66, and nowadays the potential of this material is well known, even if the role of active sites on this MOF is not yet clear. This work will bring us one step forward towards a full understanding of its catalytic behavior, which is essential for future practical applications.

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; checkpointing should be used for longer run times)
   - memory (maximum 64 GiB/node)
   - number of nodes
   - 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 2 in the appendix). Provide additional descriptions of the computing tasks and comments as needed. 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.

   (max. 1 A4 Arial 12).

The following calculation workflow will be used to model the reactions. AIMD simulations (points 1 and 2) will be performed with the CP2K package, while static periodic calculations (points 3 and 4) will be run with VASP.

1. **Cell optimization at constant pressure and temperature (NPT)**:

NPT simulations at 363 K and 1 atm will be performed on hydroxylated and dehydroxylated unit cells (for a total of 2), in order to obtain the fully converged cell parameters (required MD time 30 ps) to be used in the following periodic calculations.

2. **AIMD simulations of adsorption states**:
   In order to find the most probable configurations for the adsorbed reactants, a total of 9 AIMD simulations will be performed (each of the two reactants can be adsorbed on 3 different sites, separately and jointly). A long sampling (100 ps) is needed to have a good statistics, since these calculations are done to extract a probability distribution of the visited geometries, which are used as initial guesses for the static calculations.

3. **Periodic static calculations:**
   Periodic static calculations will be performed to model the stages of the reaction mechanism (reactants, transition states, intermediates and products) on the possible active sites, starting from the configurations obtained in the previous step. Each cell must first be optimized (2 optimizations) with fixed cell parameters determined by MD simulations at given temperature (363 K). Then, on each of the 3 active sites the reaction proceeds in 8 steps (3 transition states and 5 minima), for a total of 26 optimizations.

4. **Frequency calculations**:
   Frequency calculations on periodic systems with full Hessian matrix approach will be performed to test the quality of the optimization and to obtain free energies differences that account for thermal correction. Based on our previous TIER1 projects and the experience with the system, we know that the procedure to optimize transition states can be quite cumbersome, and involves typically an initial frequency computation to find the normal mode corresponding to the transition state, followed by the transition state optimization. Frequency computations need to be performed on 6 nodes in order to finish before the wall time limit (72 hours).

MD simulations in our system take between 48 and 96 node days. An optimization of a local minimum takes typically 10-12 node days (dependent on system size), while a transition state search and optimization costs on average at least 34-36 node days. The frequency computations will cost between 16-18 node days. With this information we can estimate the total node days needed.

| | Node day calculation | | | | | | | Storage volume estimate | |
|---|---|---|---|---|---|---|---|---|---|
| Computational task | # of such tasks | Wall clock time (days) per task | # Tier-1 nodes per task | # node days per task | # CPU cores per task | Memory usage (GiB) / node per task | OpenMP / MPI / hybrid / vSMP | Tier-2 DATA/HOME volume (GiB) + number of files | Tier-1 SCRATCH volume (GiB) + number of files |
| NPT MD | 2 | 24 | 2 | 96 | 1536 | 20 | Intranode OpenMP/ Internode MPI | 8 GiB + 20 files x 2 | 8 GiB + 20 files x 2 |
| Ads (NVT) MD | 9 | 48 | 2 | 864 | 13824 | 40 | Intranode OpenMP/ Internode MPI | 16 GiB + 20 files x 9 | 16 GiB + 20 files x 9 |
| Static (TS) | 9 | 18 | 2 | 324 | 5184 | 6 | Intranode OpenMP/ Internode MPI | 4 GiB + 12 files x 9 | 4 GiB + 12 files x 9 |
| Static (Minima) | 17 | 6 | 2 | 204 | 3264 | 2 | Intranode OpenMP/ Internode MPI | 2 GiB + 12 files x 17 | 2 GiB + 12 files x 17 |
| Frequency | 26 | 3 | 6 | 468 + 33%* | 7488 + 33%* | 8 | Intranode OpenMP/ Internode MPI | 4 GiB + 12 files x 26 | 4 GiB + 12 files x 26 |
| | | | | = **2110** | | **76** | | **334 GiB** | **334 GiB** |

*In 33% of the calculations, there are small residual imaginary frequencies and therefore we need some additional computational time to get rid of them in another subsequent frequency computation.

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 (see https://www.vscentrum.be/cluster-doc/software/tier1-muk) and, if this is not the case, compilation and installation instructions (possibly with reference to existing Tier-2 installation)

   Provide the results of scaling tests that were conducted with this software, preferably on 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, provide the name, architecture, #cores, memory, etc. of the machine that was used to obtain these results.
   Provide both a table and scaling plot such as table 1 and plot 1 in the appendix (max. 2 A4 in Arial 12).

AIMD simulations will be done using the CP2K software package (www.cp2k.org). CP2K is freely available under the GPL license and is already available on the TIER1 infrastructure.

In a previous TIER1-project, a scaling MD test of 100 steps on the system under investigation (UiO-66 without defects, 228 atoms) has been performed with the following results.

| # nodes | # cores | Absolute timing (s) | Speedup | # cores*timing |
|---|---|---|---|---|
| 1 | 16 | 2211 | 1.000 | 35376 |
| 2 | 32 | 1377 | 1.605 | 44064 |
| 4 | 64 | 993 | 2.227 | 63552 |
| 8 | 128 | 778 | 2.841 | 99584 |

Table 1: Results of CP2K scaling test performed on TIER1 for UiO-66

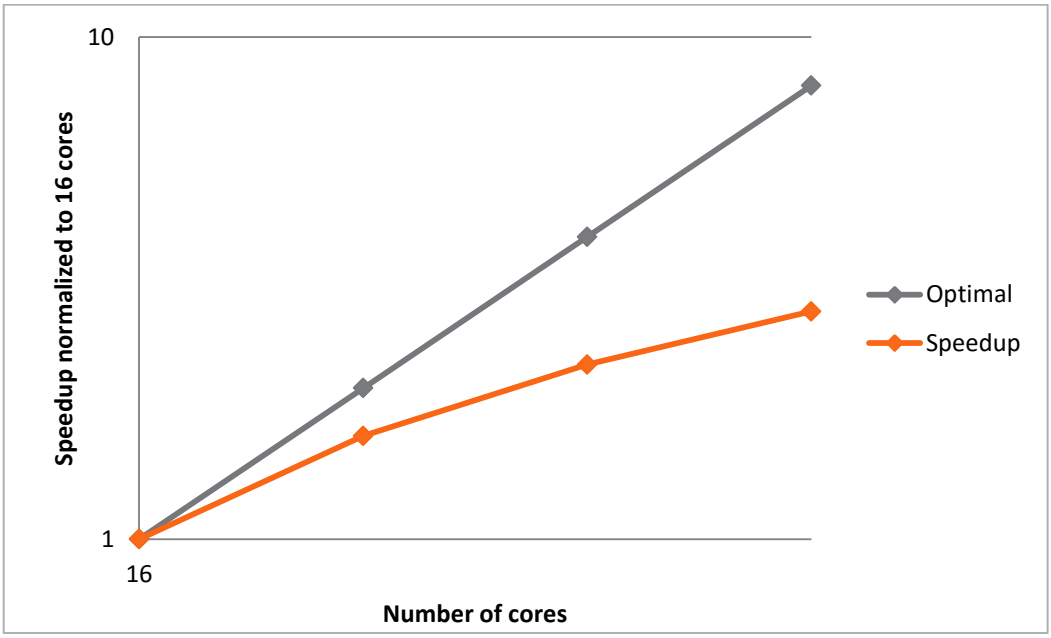


Figure 3: CP2K scaling tests performed on TIER1 for UiO-66

Periodic static calculations will be performed with VASP 5.4.1 (www.vasp.at). License is attached at the end of file and the software is already available on the TIER1 infrastructure.

Scaling of VASP has been tested in the framework of previous TIER1 projects of our group. For this project, a scaling test was made by Julianna Hajek on the system under investigation (UiO-66 with one defect site, 210 atoms). The results are reported in the following table and figure, and show a good parallelization for 2 nodes.

| # nodes | # cores | Absolute timing (s) | Speedup | # cores*timing |
|---|---|---|---|---|
| 1 | 16 | 3213 | 1.000 | 51408 |
| 2 | 32 | 1938 | 1.658 | 62016 |
| 4 | 64 | 1149 | 2.796 | 73536 |
| 8 | 128 | 936 | 3.433 | 119808 |

Table 2: Results of VASP scaling test performed on TIER1 for UiO-66

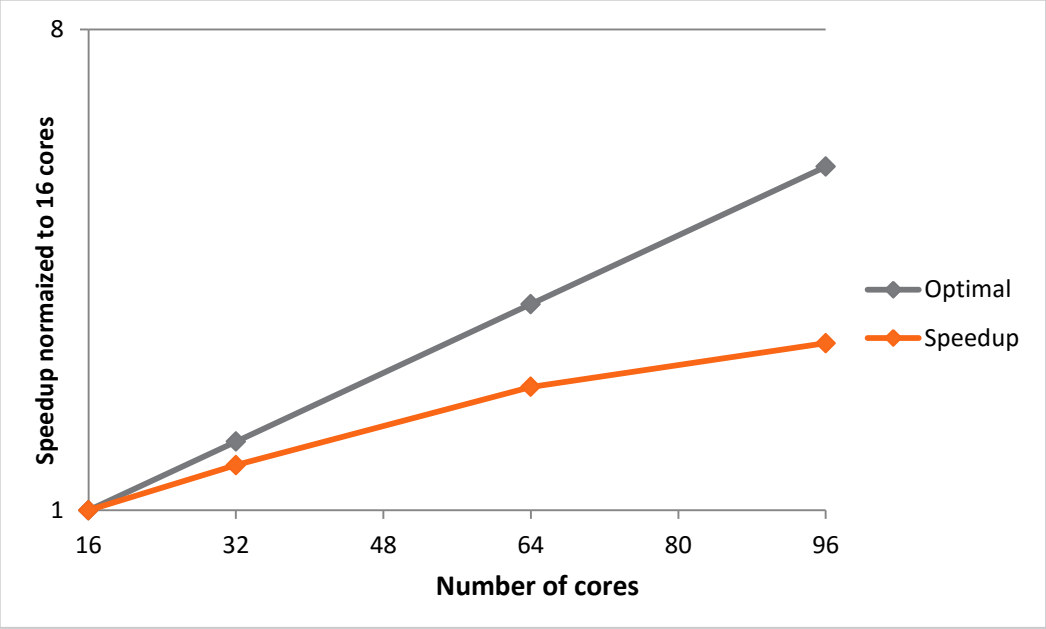


Table 3: VASP scaling tests performed on TIER1 for UiO-66

10. 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, …)?

We estimate to perform the calculations over a time period of approximately six months starting from March 2016. It is our intention to proceed with constant monthly usage.

11. List the granted computing time allocations to the promoter(s) of this research project, on the Flemish Tier-1 system, 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 or on other Tier-1 or Tier-0 supercomputers. DOI links are sufficient.

List of the granted research projects on UiO-66 catalysis on the Flemish Tier 1 system:

- “Unraveling dehydroxylation pathways on UiO-66 type systems with metadynamics” (J. Hajek, M. Vandichel, V. Van Speybroeck, node days: 3304)

- “Structural transformations during dehydroxylation reactions of UiO-66 type metal-organic frameworks; an extension with normal mode analysis” (M. Vandichel, J. Hajek, node days: 2726)
- “Structural transformations during dehydroxylation reactions of UiO-66 type metal-organic frameworks” (M. Vandichel, J. Hajek, node days: 4720)
- “Modeling aldol condensations in metal-organic frameworks with hybrid functional calculations ” (J. Hajek, M. Vandichel, node days: 2304)
- “Unraveling reaction pathways on UiO-66 type systems with metadynamics” (M. Vandichel, node days: 4432)

The abovementioned TIER1-projects on UiO-66 systems have resulted in 3 publications in major journals.

- 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

Two papers that discuss our recent TIER1 calculations on UiO-66 are currently being prepared.

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

Yes

| |
|---|
| Should you have any questions or encounter any difficulties during the electronic submission of an Application, please contact by e-mail: |
| 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: rosette.vandenbroucke@vub.ac.be |
| For the other institutions: caroline.volckaert@FWO.be |

Fonds Wetenschappelijk Onderzoek
Research Foundation – Flanders

Prof. Dirk De Vos
Katholieke Universiteit Leuven
Oppervlaktechemie en Katalyse
Kasteelpark Arenberg 23
3001 LEUVEN

| uw kenmerk | ons kenmerk | contact | datum |
|---|---|---|---|
| | 05_05<br>G.0486.12 | bio@fwo.be<br>cult@fwo.be<br>wt@fwo.be<br>gm@fwo.be<br>med@fwo.be<br>interdisciplinair@fwo.be | 16 november 2011 |

Betreft: **Toekenning project G.0486.12**

Geachte professor,

De Raad van Bestuur van het FWO heeft uw bovenvermelde aanvraag voor een onderzoeksproject goedgekeurd. De bijgevoegde overeenkomst werd opgesteld volgens het reglement van de Onderzoeksprojecten van het FWO.

Graag wil ik u hierbij feliciteren met de toekenning van het door u aangevraagde onderzoeksproject.

Mag ik u vragen alle exemplaren te ondertekenen, één kopie voor u te bewaren en mij het origineel samen met de overige kopie(ën) per kerende post terug te sturen.

De toegekende toelage is beschikbaar voor zover de financierende overheden hiervoor de nodige middelen vrijmaken. Onderzoek waarvoor medisch ethisch advies noodzakelijk is, kan pas starten als de onthaalinstelling hierover positief advies uitbrengt.

Slechts uitzonderlijk kan, met akkoord van het FWO, de oorspronkelijke bestemming van dit krediet worden gewijzigd.

Tenslotte vraag ik u met aandrang om op uw publicaties steeds te vermelden dat ze tot stand kwamen met de financiële steun van het FWO. Vacatures gekoppeld aan onderzoeksprojecten kunnen bekend worden gemaakt via de FWO-website. U kan het vacaturebericht aan het FWO bezorgen via communicatie@fwo.be. Aanvullend kan het nuttig zijn om dergelijke berichten ook te publiceren via de Euraxess website van de Europese Commissie: http://ec.europa.eu/euraxess/ .

./..

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../..

Fonds Wetenschappelijk Onderzoek
Research Foundation – Flanders

Voor bijkomende inlichtingen kan u steeds terecht bij uw dossierbeheerder. De e-mailadressen zijn voor de Biologische Wetenschappen: bio@fwo.be, voor de Cultuurwetenschappen: cult@fwo.be, voor de Gedrags- en Maatschappijwetenschappen: gm@fwo.be, voor Wetenschap en Technologie: wt@fwo.be, voor de Medische Wetenschappen: med@fwo.be en voor het Interdisciplinair onderzoek: interdisciplinair@fwo.be.

Hoogachtend,

dr. ir. Elisabeth Monard
secretaris-generaal

Bijlagen: 2

Kopie: Prof. Veronique Van Speybroeck

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**ANNEX 3**

## 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-d6uyZcxc41Bc44BDyB4mjm3PcnyOziEntAZqs3UBeyuwZKL9mo23867rtmIRVRLct9QPViYszRpDU4jgo0HIeV-PHslUMVSXYCxZAW3OHozsk-bMbbtkGtcng8sJSl6EP6aUltfKzQnKaWezZ1xmxpI2i0). Timestamp by third party at Mon Dec 22 16:37:31 CET 2014

# SOFTWARE LICENSE AGREEMENT FOR THE USE OF VASP5.2 BY ACADEMIC INSTITUTIONS

The Universität Wien, Austria (UW in the following) and
Ghent University, Belgium (UG in the following) [1]
conclude the following agreement:

(1) The UG acquires a non-exclusive academic license for the use of the software-package VASP (Vienna ab-initio simulationprogram) for ab-initio local-density-functional total-energy and molecular-dynamics calculations, versions VASP5.2 and VASP4.6, by the research group Functional Nanomaterials (FUNNANO)[2]. Under this licence the use of the software is restricted to a maximum of six researchers or students, all belonging to this research group and to the same organisatorial unit and working at the same location. The licence does not cover the use of VASP by external collaborators working at other institutions.

(2) The license covers access to the source-code, the program documentation and to the data-base for ultrasoft pseudopotentials and PAW-potentials. UW reserves the exclusive property of the software. It declines any liability for the software and any responsibility for the results of calculations produced with the program. The license does not cover any maintenance service for the software or support for its implementation.

(3) The license is not transferable to another research group of UG without the written agreement of UW. UW reserves the right to refuse authorization of such a transfer. A transfer to a research group not belonging to UG is excluded.

(4)The UG guarantees that the software or parts thereof shall not be made accessible to third parties without the explicit written consent of UW. Access to the code and to the data-base shall be made available through an account of the UW. The UG guarantees that the password for this account will be known only to one contact-person and shall not be communicated to temporary co-workers or guests. All installations of the source code, the executable or the data-base must be copy-protected and accessible only to the authorized users.

[1] Please insert here the name of the institution concluding this agreement with UW. This institution must be a legal person and the agreement must be signed by an authorized representative of this institution. Define the acronym (replacing .....) under which this institution is referred to in the text of the agreement.

[2] Please insert here the name and affiliation research group for which the license is acquired

## SOFTWARE LICENSE AGREEMENT FOR THE USE OF VASP5.2 BY ACADEMIC INSTITUTIONS

(5) If VASP is used as the basis of further methodological or software-development, UG agrees to make these additions available to UW. UW will also be entitled to include these additions in further releases of VASP.

(6) In future publications of work performed using VASP, the use of the software shall be properly acknowledged, e.g. in the form
"The calculations have been performed using the ab-initio total-energy and molecular-dynamics program VASP (Vienna ab-initio simulation program) developed at the Institut für Materialphysik of the Universität Wien [1-3]."
[1] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11 169 (1996).
If the PAW-version is used, reference will be made to
[2] G. Kresse and D. Joubert, Phys. Rev. **59**, 1758 (1999).
If special features implemented in VASP will have been used, reference should be made to the relevant publications as listed on the VASP home-page.

(7) The UG accepts to pay to UW a licence fee Euro 4.000,- (fourthousand Euro). The licence fee is strongly discounted and applies only to academic institutions with undergraduate teaching.

(8) The licensee will use VASP exclusively for non-profit research. If VASP is used in contractual research in cooperation with or for industry or for military institutions, the financial conditions will have to be re-negotiated.

(9) UW declares that it has the full power and authority to grant the rights granted in this agreement without the consent of any other person, and that the license and use of the software by the licensee will not in any way constitute an infringement or other violation of any copyright, proprietory right or any other rights of any third party.

(10) Any disputes arising from the license agreement are subject to the laws of the Republic of Austria.

(11) The terms of this agreement shall prevail any terms or conditions of the licensee.

**SOFTWARE LICENSE AGREEMENT FOR THE USE OF VASP5.2 BY ACADEMIC INSTITUTIONS**

For the Universität Wien:

Jürgen Hafner
Fakultät für Physik, Universität Wien
Sensengasse 8/12, A-1090 Wien, Austria

Date

For the UG

Name (in print): Michel Waroquier
Institution: Faculty of Sciences, Ghent University

Address: Technologiepark 903, BE-9052 Zwijnaarde, Belgium

Date: 26 January 2010

For the research group entitled to use VASP5.2:

Name (in print): Veronique Van Speybroeck (FUNNANO)