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://vscentrum.be/.

Title of the application:

Structural transformations during dehydroxylation reactions of UiO-66 type metal-organic frameworks

Name and first name of the applicant:

Vandichel Matthias

Institution:

Ghent University

Research group / department:

EA17, Center for Molecular Modeling

Title / position:

FWO postdoc

e-mail address:

Matthias.Vandichle@Ugent.be

Total computing time that is needed, in node days:

4720

Total disk storage that is applied for:

2.140 TB

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

Increasing the catalytic activity of metal-organic frameworks by tailor-made modifications (FWO postdoc mandate Matthias Vandichel)

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)

2. Short description of the research project within the framework of which computing time is applied for (max. 1 A4 in Arial 12):

Metal-Organic Frameworks (MOFs) are crystalline nanoporous materials composed from both inorganic metal(oxide)s and organic linkers, with possible applications in gas separation/adsorption, catalysis, etc. This project aims at understanding the dehydroxylation behaviour of the MOF UiO-66 (Zirconium terephthalate), with structural formula $Zr_6O_4(OH)_4$[terephthalate]$_6$. When placed in vacuum at high temperatures, this material loses its hydroxyl (OH) groups (**Figure 1**).

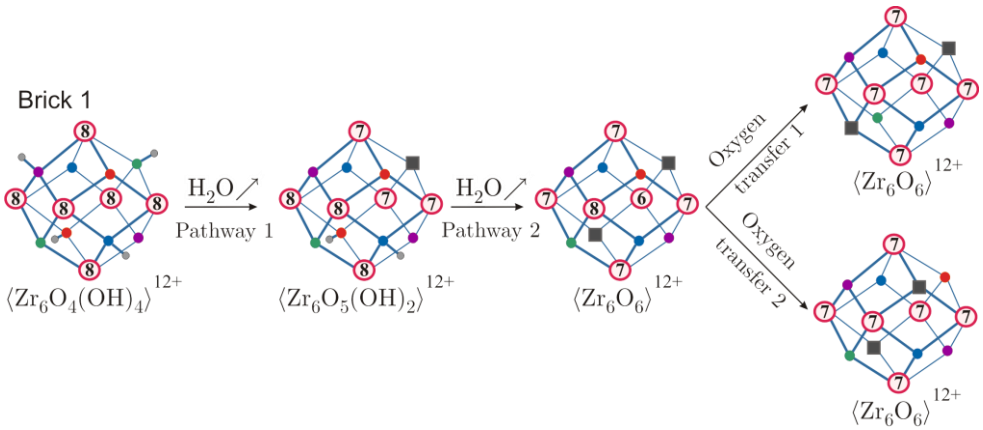

***Figure 1**: Dehydroxylation processes can start from $\{Zr_6O_4(OH)_4\}^{12+}$. Coordination numbers of the different Zr-atoms are given (encircled).*

Terephthalate defects result in catalytical activity of the UiO-66 materials (F.Vermoortele, M.Vandichel et al. *Angewandte Chemie Int. Ed.*, 51(20), 4887-4890, **2012** and *JACS* 135 (31), 11465–11468, **2013**). In the case of

such structural defects (missing terephthalates), the inorganic bricks have a different formula, for example $[Zr_6O_5(OH)_3]^{11+}$ or, $[Zr_6O_6(OH)_2]^{10+}$, and their dehydroxylation behaviour will be different. For the $[Zr_6O_6(OH)_2]^{10+}$ brick, there exist even 3 different isomeric possibilities, dependent on where the two terephthalate defects are located. It is highly important to investigate dehydroxylation processes, as these lead to more catalytically active UiO-66 type materials. We will obtain detailed insight into the active sites after such a dehydroxylation treatment and their energetic relevance. Furthermore, this active site information – highly relevant for the Zr-MOF community – can then be used for further computational studies.

To study the dehydroxylation pathways, we will use climbing image Nudged-Elastic Band (cNEB) simulations making use of the periodic code VASP. This will enable us to find the reaction pathways as well as good initial guesses for transition state structures.

3. 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).

Personal FWO postdoc fellowship of Matthias Vandichel, confirmation letter can be found at the end of the file.

FWO project 3G048612, confirmation letter can be found at the end of the file.

4. Promoter of the research project:

Dr. ir. Matthias Vandichel

Prof. Dr. ir. Veronique Van Speybroeck

5. Persons mandated by the Applicant to compute on the TIER1 within the framework of the present project: Please provide for every person:

- name and first name
- institution
- research group / department
- title / position
- experience with TIER1/TIER2 infrastructure in Belgium and abroad

Matthias Vandichel

Ghent University
EA17, Center for Molecular Modeling
FWO-postdoc
vsc40048
Experience with Tier1 and Tier2 infrastructure of UGent

Julianna Hajek
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PhD fellow
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Experience with Tier1 and Tier2 infrastructure of UGent

Veronique Van Speybroeck
Ghent University
EA17, Center for Molecular Modeling
Professor
vsc40021
Experience with Tier2 infrastructure of UGent

6. Description of the computing task, justification for the computing time, disk storage and memory that are applied for, and description of the software tools required (max. 3 A4 in Arial 12). Please clearly provide the following in this regard:

- the number of nodes/cores that are applied for per computing task, with a subdivision of the computing time in sub-tasks indicating the sequence of the sub-tasks
- whether these tasks use diversification (OpenMP, MPI, hybrid OpenMP/MPI …)
- the estimated memory use of a computing task (maximum 64GiB/node)
- whether a vSMP system will be used
- the requirements for disk storage (estimated volume in GiB and the total number of files), more specifically for:
    - required input files (data set, parameter files, etc.)

- SCRATCH volume used during the performing of the computing tasks
- result files

We aim to simulate 59 climbing image Nudged Elastic Band (cNEB) runs each with 8 images.

For the intended dehydroxylation study, we investigated already the first water removal from an inorganic $[Zr_6O_4(OH)_4]^{12+}$–brick as benchmark. Therefore, we had to split up the water removal in 3 Nudged Elastic Band simulations, containing each 8 images, running each image on 32 cores (2 nodes). In total 240 node days (= 3 NEBs x 5 days x 8 images/NEB x 2 nodes/image) are thus required to have for 3 NEB runs. Based on this initial simulation, we obtained insight into the scaling behaviour and could make a realistic estimation of the total required computational time.

The required time per optimization step (time/step) for one image in a NEB run, is for the first step similar to time/step needed a standard geometry optimization (this was tested with automatic real space projection). After the first step, the following optimization steps of an image within a NEB simulation become much faster; as due to the fixation of the outer two images less intermediate Self-Consistent-Field steps are required.

Extensive scaling tests have been previously performed with the VASP software package [1,2]. Optimal scaling can be obtained by combining intranode MPI parallelization and internode k-point parallelization. This k-point parallelization divides the job into near-serial subprocesses over points on a discrete grid. While our cNEB calculations are Γ- point simulations, we expect cNEB to scale equal or even better than k-point parallelization. A typical relaxation can be seen as two nested loops: the inner loop calculates electronic energies, the outer then uses these results for the ionic energies. With k-point parallelization communication takes place for each step of the inner loop. For cNEB calculations the individual images can be calculated independently, with only limited interaction to exchange forces for each step of the outer loop. Since this data is very limited and occurs an order of magnitude less than the interactions in k-point parallelization scaling should be nearly perfect.

Based on this info and initial VASP-benchmark calculations from our previous TIER1 project, we could make a fair estimate of the computational time needed (Table 1) and the memory use (Table 2).

Table 1: Estimated node and core days for the project.

Unit cell – formula	#cNEBs/H_2O-removal x **#H_2O removals**	#cNEBs O-transfer	#days x #nodes /cNEB	Total computational time (total node days)
Ideal structure (no terephthalate defect)				
$<Zr_6O_4(OH)_4(OOCCC_4H_4CCOO)_6>_2$ ()	3 x **4**	1 x 2	5 days x (8 images x 2 nodes/image)	1120
Defect structures (1 terephthalate defect)				
$<Zr_6O_4(OH)_4(OOCCC_4H_4CCOO)_6>$ $<Zr_6O_6(OH)_2(OOCCC_4H_4CCOO)_5>$	3 x **3**	2 x 2	5 days x (8 images x 2 nodes/image)	1040
$<Zr_6O_5(OH)_3(OOCCC_4H_4CCOO)_{11/2}>$ $<Zr_6O_5(OH)_3(OOCCC_4H_4CCOO)_{11/2}>$	3 x **2**	1 x 2	5 days x (8 images x 2 nodes/image)	640
Defect structures (2 terephthalate defects)				
$<Zr_6O_6(OH)_2(OOCCC_4H_4CCOO)_{10/2}>$ $<Zr_6O_6(OH)_2(OOCCC_4H_4CCOO)_{10/2}>$ Structural isomer 1	3 x **2**	1 x 2	5 days x (8 images x 2 nodes/image)	640
$<Zr_6O_6(OH)_2(OOCCC_4H_4CCOO)_{10/2}>$ $<Zr_6O_6(OH)_2(OOCCC_4H_4CCOO)_{10/2}>$ Structural isomer 2	3 x **2**	1 x 2	5 days x (8 images x 2 nodes/image)	640
$<Zr_6O_6(OH)_2(OOCCC_4H_4CCOO)_{10/2}>$ $<Zr_6O_6(OH)_2(OOCCC_4H_4CCOO)_{10/2}>$ Structural isomer 3	3 x **2**	1 x 2	5 days x (8 images x 2 nodes/image)	640
				4720

Together, this yields 4720 node days. This approach is truthfully of high-throughput nature: the requirements for a single calculation are not that intensive, but the images are interdependent, and so good efficiency is achieved based on multi-node parallelization available on TIER1 cluster. For this reason we will use 16 full nodes for relaxation per one cNEB.

Table 2: Estimated memory storage

	SCRATCH storage (GB)
1 cNEB-optimization (8x2x16 cores)	36
Total (59 cNEBs)	**2140**

As one cNEB-job requires approximately 36 GB of temporary storage, we estimate to need at maximum around 2.140 TB of temporary storage on the gpilot scratch. However, once a cNEB run is finished, we will remove temporary files (WAVECAR, CHGCAR) to reduce the size of one folder below 1.25 GB. In total (for the 59 cNEB runs) 74 GB of more permanent storage will be needed for the (data).

We will not use a vSMP scheme.

7. Please indicate why the TIER1 is the appropriate machine to perform the computing task (max. 1/2 A4 in Arial 12):

In this work, climbing image Nudged Elastic Band simulations are needed (1) to unravel reaction pathways of dehydroxylation and (2) to obtain accurate insight in the active sites after dehydroxylation. Due to the size of the systems and the fact that several images are running in parallel, the amount of calculations that need to be performed goes beyond what can comfortably be done (within a reasonable timeframe) on a TIER2 cluster. The queuing times for such large jobs (16 nodes) can easily go up to one week, and this project requires 59 of this type of calculations.

8. Summary of the software required to perform the computing task, and possible installation and compilation instructions (max. 2 A4 in Arial 12). Please clearly provide the following per item in this regard:

- a reference to the software's web page

- the software licence system (open source, GPL, etc.)
- if there is no free academic use of the software, state which licence makes the installation and the use valid on the TIER1 by the Applicant (+ add a copy of the signed licence)
- if need be, which licence server will be used (name + IP address)
- whether the software is already available on the TIER1 (see https://vscentrum.be/nl/tier1-rekenen) and, if this is not the case, compilation and installation instructions (possibly with reference to existing TIER2 installation)

VASP 5.3.3

- http://www.vasp.at

- License: see at the end of the file

- The software is already available on the TIER1 infrastructure.

We require a new VASP-compilation in which both the dftd3 patch and the vtst-patch are included, to use the more advanced climbing Nudged Elastic Band method.

Nowadays, a VASP version exist to perform climbing image Nudged Elastic band simulations (VASP/5.3.3-ictce-4.1.3-vtst-3.0c-20130327-mt), however, in this version no dftd3 dispersion corrections are included.

9. Period during which the task is to be performed:

The calculations are intended to be performed in the timeslot: November 2014 - April 2015.

10. Describe the results that were obtained within the framework of computing time that was attributed during the past two years on the TIER1 or on other TIER1 or TIER0 supercomputers (max. 2 A4 in Arial 12):

During the previous two Tier1-projects and the pilot usage, several aspects of UiO-66 type MOFs have been investigated:

1. Strategies to increase the catalytic activity via synthesis modulators
   status: published online [3]

   As MOFs contain many metal sites, which might be catalytically active, they have the potential to replace homogenous catalysts in important

industrial applications. Within the family of Zr-benzenedicarboxylate (Zr-BDC or UiO-66) type MOFs, missing linkers were found to be responsible for the catalytic activity. Experimental procedures were developed to create more of such active Zr-sites by adding an excess of modulator (MDL) to the synthesis mixture (F. Vermoortele, et al., M. Vandichel, et al., *JACS*, 135 (2013) 11465-11468.). Subsequently, the incorporated modulators can be removed by a post-synthesis treatment at elevated temperature, thereby creating new active Zr-sites. We managed to explain experimental observations with computational insights focusing on modulating species trifluoroacetic acid (TFA), HCl and H_2O [1]. At synthesis conditions, the coordination strength of these species predicts the stability (from high to low): BDC > TFA > HCl > H_2O. High MDL:BDC ratios are thus required to achieve incorporation. Post-synthesis removal of the defect-coordinating species follows, as expected, the opposite trend: H_2O > HCl > TFA > BDC. {~ 1000 node days used }

2. Hybrid functional calculations of aldol condensations pathways
   status: in preparation [4]

In this work, hybrid functional calculations on periodic models have been performed (1) to truthfully compare the periodic and cluster calculations; (2) to more accurately describe environmental effects. Due to the size of the systems and the amount of calculations that need to be performed, it is clear that these calculations go beyond what can comfortably be done (within a reasonable timeframe) on a TIER2 cluster. All calculations have finished; the obtained free energy profiles for both periodic and cluster computation compare well, and the stabilization effect the environment is more visible in some reaction steps. The paper will be submitted in October 2014. As not all computational time was granted in the previous Tier1 project, we decided to compute only a part of the intended calculations. {~ 1500 node days used}

3. Au@UiO-66: an oxidation catalyst
   status: in preparation [5]

In this work, a new UiO-66 MOF with embedded gold Nanoparticles was experimentally synthesized, characterized (via N_2 sorption, XRPD, UV-Vis, XRF, XPS and TEM analysis). The Au@UiO-66 was furthermore tested in several catalytic reaction, however, the mechanism remained unclear and spectroscopic efforts (IR, Raman) in

combination with molecular modelling were required to unravel possible reaction paths. We performed periodic MD-simulations (NVT/NPT) to unravel an experimentally obtained IR-spectrum. From our simulations, we constructed velocity power spectra to distinguish between adsorbed and chemisorbed pentanol species. All calculations have finished and the paper will be submitted in October 2014. {~ 800 node days used}

4. Unravelling reaction pathways systems with metadynamics
   status: in preparation

In our first TIER1 project, we successfully identified the right collective variables to model the citronellal cyclization within the metadynamics simulations on different UiO-67-X materials (NPT ensemble). We obtained good estimates for the reaction barriers, accounting for both framework and linker flexibility. This type of computations goes beyond the state of the art. We are finalizing the data-mining and writing a research paper and need to perform some NVT simulations to have a more solid benchmark for the obtained results from the NPT simulations. {~ 2000 node days used}

References:

[1] http://www.hector.ac.uk/cse/distributedcse/reports/vasp01/vasp01_kpoint.pdf

[2] http://www.hector.ac.uk/cse/distributedcse/reports/vasp02/vasp02.pdf

[3] Active site engineering in UiO-66 type Metal Organic Frameworks by intentional creation of defects: A theoretical rationalization, Matthias Vandichel, Julianna Hajek, Frederik Vermoortele, Michel Waroquier, Dirk E. De Vos, Veronique Van Speybroeck, *CrystEngComm*, 2014, **DOI:10.1039/C4CE01672F**

[4] Theoretical study of aldol condensations on UiO-66 and UiO-66-NH_2, Julianna Hajek, Matthias Vandichel, Dirk De Vos, Michel Waroquier, Veronique Van Speybroeck, to be submitted

[5] Au@UiO-66: an oxidation catalyst, Karen Leus, Patricia Concepcion, Maria Meledina, Matthias Vandichel, Abdessamad Grirrane, Dolores Esquivel, Stuart Turner, Dirk Poelman, Michel Waroquier, Veronique Van Speybroeck, Gustaaf Van Tendeloo, Hermenegildo García, Pascal Van Der Voort, to be submitted

Should you have any questions or encounter any difficulties during the electronic submission of an Application, please contact by e-mail:
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Betreft: **Toekenning Postdoctoraal Onderzoeker 2013-2016**

Geachte heer,

De Raad van Bestuur heeft u vandaag aangesteld als Postdoctoraal Onderzoeker met ingang van 1 oktober 2013 tot en met 30 september 2016. Het reglement vindt u als bijlage.

Graag wil ik u feliciteren met deze aanstelling als Postdoctoraal Onderzoeker van het FWO.

In het kader van de verdere administratieve opvolging van uw aanstelling zal het FWO u nog vóór 19 juli 2013 een arbeidsovereenkomst bezorgen.

Voor bijkomende inlichtingen kan u steeds terecht bij de dossierbeheerder van uw wetenschapsgebied op bovenvermeld e-mailadres.

Tenslotte vraag ik u met aandrang om op uw publicaties steeds uw titel Postdoctoraal Onderzoeker van het FWO te vermelden.

Ik wens u veel succes toe in uw verdere onderzoeksloopbaan.

Hoogachtend,

dr.ir. Elisabeth Monard
secretaris-generaal

Bijlage: 1

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

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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

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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

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(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.

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For the Universität Wien:

Jürgen Hafner
Fakultät für Physik, Universität Wien
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Date

For the UG

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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)