

Enclosure 1b. Category 1 Application form 2015 – 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 Dutch on the website <https://vscentrum.be/>.

Title of the application: The electronic structure of functionalized luminescent Metal-Organic Frameworks.

Name and first name of the applicant: Vanpoucke Danny Eric Paul

Institution: Ghent University

Research group / department: Center for Molecular Modeling
/ Department of Applied Physics

Title / position: Dr. Dr. / Postdoctoral researcher

email address: Danny.Vanpoucke@UGent.be

Total computing time that is needed, in node days: 2905

Total disk storage that is applied for (in GiB): 105 GiB

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

Elucidating the role of 1-dimensional metal-oxide chains in the physical and chemical properties of porous metal organic frameworks by means of density functional theory calculations
(FWO project: 12S3415N)

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 and important class of porous materials with a wide range of possible industrial applications. Due to their large pore volume, they present materials with enormous “surface-area to volume” ratio, making them of great interest for catalysis, gas-storage, and also sensing applications. The tunability and easy interchangeability of their building blocks, on the other hand, makes them of interest for chemical engineering purposes. The application we are interested in this project is photoluminescence. Through the variation of functional groups, the luminescent wavelength can be tuned in experiment. To obtain a fundamental understanding of the mechanisms involved, we propose to perform high quality *ab initio* electronic structure calculations.

This project will be performed in close collaboration with an experimental partner who is currently synthesizing the functionalized MOFs: UiO-66-X (X=H, OH, SH, 2,5-OH, 2,5-SH).

In a first step, the band gaps are calculated using the HSE hybrid-functional, which is known to accurately predict the experimentally observed band gap.

The influence of the functional groups on the electronic structure (e.g. the formation of gap-states, changes in the shape of the valence/conduction band edges, ...) is investigated through the electronic band structure along lines of high symmetry. Bands pertaining to features of interest will be projected out, to present the (molecular) orbitals involved. This provides insight into the chemistry involved in the luminescence of the functionalized UiO-66 MOFs. In addition, calculated Hirshfeld-I charges will elucidate any charge-transfer mechanisms involved.

By investigating the modifications as function of the functional group and the number of functional groups per linker, it becomes possible to predict the luminescent behaviour of specific other functional groups for the UiO-66 MOF.

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

This project is part of a combined theoretical and experimental study. In this study, the role of linker functional groups on the photo-absorption properties of UiO-66 type materials is investigated. We aim at getting a more complete picture on the choice of functionalization, beyond the currently studied $-NH_2$ and $-NO_2$ groups. Both single and doubly functionalized linkers (with $X=-OH,-NH_2,-SH$) will be used. Periodic density functional calculations will be used to obtain an in depth understanding of the evolution of the electronic structure with different functionalization of the linker. The most simple aspects being the band-gap size and the formation of gap states.

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 4 "EasyChair proposals submission procedure").

FWO project: 12S3415N

5. Name and email address of the promoter(s) of the research project:
Dr. Dr. D. E.P. Vanpoucke (Danny.Vanpoucke@Ugent.be)

6. Billing address to which the payment invoice will be sent to:

Dr. Dr. Danny E. P. Vanpoucke
Center for Molecular Modeling (CMM)
Room: 60.03.120.024
Ghent University
Technologiepark 903
9052 Zwijnaarde
Belgium

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 of using HPC resources in the past (Tier0/Tier1/Tier2 infrastructure in Belgium and abroad)

name and first name: Vanpoucke Danny Eric Paul

institution: Ghent University

research group / department: Center for Molecular Modeling /
Department of Applied Physics

title / position: Dr. Dr. / Postdoctoral researcher

experience with TIER1/TIER2 infrastructure in Belgium and abroad

- Local cluster of the CMS group (University of Twente, The Netherlands)
- Huygens Supercomputer (SARA computing Center, The Netherlands)
- Ghent STEVIN TIER2 infrastructure (user & pilot user)
- Ghent MUK TIER1 infrastructure (pilot user + projects granted for 13000 node days)

7. Explain why this project needs to run on a Tier1 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 required CPU-time for this project is very hard to almost impossible to acquire on existing TIER2 facilities within a reasonable timeframe. The queuing times for such large jobs (14 nodes or more) can easily go up to one week, and this project requires over 70 of this type of calculations. Calculations requiring 30-56 nodes on the other hand are for all practical purposes impossible. In addition, the presence of MPI parallelism on the TIER1 machine, and K-point parallelisation of the VASP program, makes this infrastructure ideally suited. At the Ghent university, only the gulpin and delcatty clusters are suited for such calculation, and the former is known to be up to a factor two less efficient than the muk-cluster (TIER1).

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 Tier2 DATA/HOME partitions and the Tier1 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 Tier1 (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).

| Computational task | Node day calculation | | | | # CPU cores per task | Memory usage (GiB) / node per task | OpenMP / MPI / hybrid / vSMP | Storage volume estimate | |
|---------------------|----------------------|---------------------------------|------------------------|----------------------|----------------------|------------------------------------|------------------------------|--|--|
| | # of such tasks | Wall clock time (days) per task | # Tier1 nodes per task | # node days per task | | | | Tier2 DATA/HOME volume (GiB) + number of files | Tier1 SCRATCH volume (GiB) + number of files |
| Struc. optimization | 70 | 2.5 (1) | 14 | = 35 | 224 | 2 | Hybrid OpenMP/MPI | 2 GiB + 50 | 2 GiB + 50 |
| Density of States | 7 | 0.5 | 21 | = 10 | 336 | 2 | Hybrid OpenMP/MPI | 2 GiB + 10 | 2 GiB + 10 |
| Band structure | 7 | 0.17 | 30 | =5 | 480 | 5 | Hybrid OpenMP/MPI | 5 GiB + 10 | 5 GiB + 10 |
| HSEo6-DOS | 7 | 0.9 | 56 | = 50 | 896 | 5 | Hybrid OpenMP/MPI | 5 GiB + 10 | 5 GiB + 10 |
| Total | 91 | | | 2905 | | | | 105 GiB (2) | |

(1) This is an average, some of these tasks will require multiple runs (2) upon reduction after the structural optimization is terminated

Calculation flow:

- 1) **Geometric optimization** : Using an fit to an equation of state, requiring 10 fixed volume relaxations.[1]
- 2) Qualitative electronic structure calculations:
 - a. **Density of states**
 - b. **Band structure**
- 3) High quality **quantitative electronic structure**: HSE06-Density of states

[1] *Accuracy of structure optimizations, phonons and elasticity of metal-organic frameworks*. An Ghysels, Danny E. P. Vanpoucke, Kurt Lejaeghere, and Veronique Van Speybroeck (in preparation)

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 Tier1 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 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)

Provide the results of scaling tests that were conducted with this software, preferably on Tier1 (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).

Software:

- a) VASP 5.3.3 +DFT D3
 - i. <http://www.vasp.at/>
 - ii. Licence: cf. Appendix
 - iii. Software is available for users (linked to the licence in appendix)
- b) Intel compilers, FFTW, blas, (sca)lapack
 - i. Part of the basic installation of the infrastructure

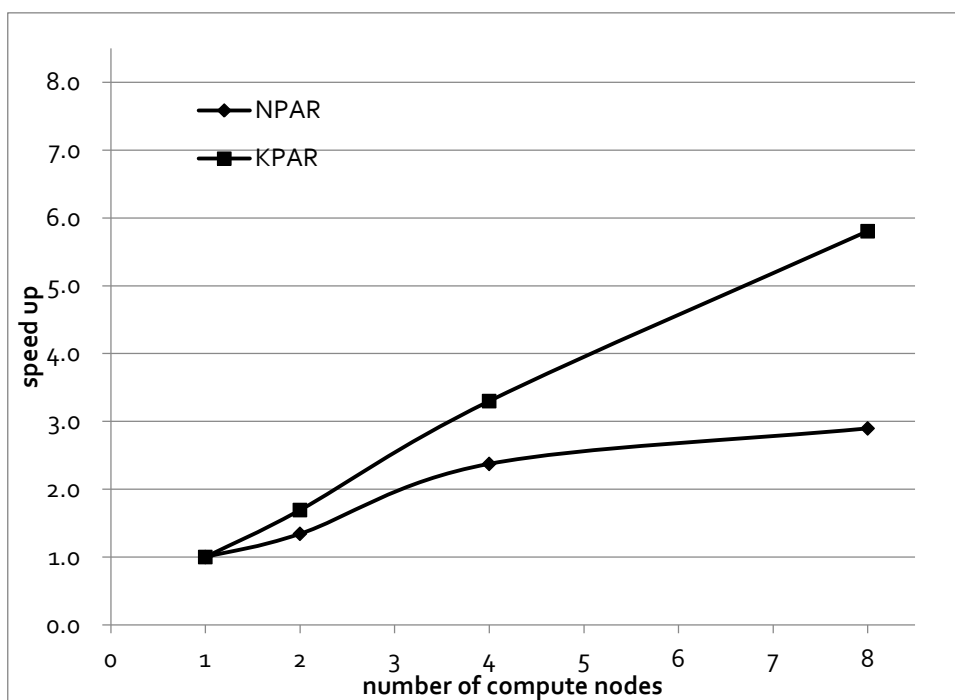
All software is already installed on the TIER-1 infrastructure.

Scaling tests were performed on a 100 atom periodic system, with a kpoint-set which reduces to 8 irreducible k-points. Two modes of parallelization are shown: NPAR: parallelization over bands, KPAR: parallelization over K-points. In this project Parallelization over K-points will be used by default, with additional parallelization over bands when the

amount of RAM memory is insufficient or when a single static calculation may not be finished with the allotted wall time limit of 3 days.

Since the scaling tests were performed during a full-TIER-1 project, explicit permission should be obtained from the applicant for use or redistribution of the data presented below.

| # nodes | # cores | absolute timing (s) | | speedup | |
|---------|---------|---------------------|---------|---------|------|
| | | NPAR | KPAR | NPAR | KPAR |
| 1 | 16 | 1707.43 | 1707.43 | 1.00 | 1.00 |
| 2 | 32 | 1150.96 | 1016.29 | 1.34 | 1.69 |
| 4 | 64 | 730.75 | 535.93 | 2.37 | 3.30 |
| 8 | 128 | 603.43 | 314.85 | 2.90 | 5.80 |



Further scaling information on the VASP code can be found here:

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

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, ...)?

Continuous monthly usage.

11. List the granted computing time allocations to the promoter(s) of this research project, on the Flemish Tier1 system, as well as other Tier1 and Tier0 systems. Also, describe the scientific output obtained within the framework of computing time that was granted during the past two years on the Flemish Tier1 or on other Tier1 or Tier0 supercomputers. DOI links are sufficient.

2009 Granted 20 000 hours CPU time by the Stichting Nationale Computer Faciliteiten (NCF) on the Dutch Huygens supercomputer, for the project: “Ab initio modeling of metallic monatomic nanowire arrays on Ge(001)”

2013 Granted 8000 node days on the Flemish Tier-1 supercomputer, for the project: “Structural and atomic charge evolution in the breathing behavior of Metal Organic Frameworks”

2014 Granted 4700 node days on the Flemish Tier-1 supercomputer, for the project: “The electronic and magnetic structure of Breathing Metal-Organic Frameworks”

During the previous projects and the pilot period, several aspects of MIL-47/53 type MOFs have been investigated:

- I.) Accurate ab-initio calculation of the thermal, electronic and mechanical properties of MOFs

For high quality atomic scale results in solid state physics, quantum mechanical calculations within the density functional (DFT) approximations present the current state of the art. In this work we have studied how the properties of a MOF vary under different numerical settings (real-space and reciprocal space integration grids, the presence of symmetry...). It shows that dense integration grids are required to reduce egg-box effects to manageable levels. In addition, Pulay stresses are shown to artificially push breathing MOFs into a narrow pore configuration. [1] {~700 node days}

II.) Functionalized MOFs

In this work, the influence of functional groups on the geometric and electronic structure of MOFs is investigated. It shows the functional group introduces a gap-state and a rotation of the linker molecule. Using the calculated charges of the functionalized MOF frameworks, a force-field is constructed to calculate Henry-coefficients for CO₂ adsorption in these frameworks. [3] **{~1000 node days}**

III.) Electronic structure of MOFs

In this work, the geometric and electronic structure of the MIL-47(V) metal-organic framework (MOF) is investigated, placing special focus on the relation between the spin configuration and the properties of the MOF. The ground state is found to be anti-ferromagnetic, with an equilibrium volume of 1554.70 Å³. The transition pressure of the pressure-induced large-pore-to-narrow-pore phase transition is calculated to be 82 MPa and 124 MPa for systems with ferromagnetic and anti-ferromagnetic chains, respectively. Mapping DFT energies onto a spin-Hamiltonian shows both the intra- and inter-chain coupling to be anti-ferromagnetic, with the latter coupling constant being two orders of magnitude smaller than the former, suggesting the MIL-47(V) to present quasi-1D behavior. The electronic structure of the different spin configurations is investigated and it shows that the band gap position varies strongly with the spin configuration.[2] **{~600 node days}**

IV.) Breathing MOFs

In this work, breathing curves for different MIL47-like MOFs were constructed. Clear stability trends as function of the metal cluster are observed. Further processing of the obtained data is still required. **{~8000 node days}**

[1] *Accuracy of structure optimizations, phonons and elasticity of metal-organic frameworks*. An Ghysels, Danny E. P. Vanpoucke, Kurt Lejaeghere, and Veronique Van Speybroeck (in preparation)

[2] *Quasi-1D physics in metal-organic frameworks:*

MIL-47(V) from first principles. Danny E.P. Vanpoucke Jan W. Jaeken, Stijn De Baerdemacker, Kurt Lejaeghere and Veronique Van Speybroeck.

Beilstein J. Nanotechnol. 2014, 5, 1738–1748

DOI: 10.3762/bjnano.5.184

[3] *The Role of Functional groups in Metal-Organic frameworks*. Danny E.P. Vanpoucke, Toon Verstraelen, and Veronique Van Speybroeck (in preparation)

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 Hercules Foundation / Flemish Supercomputer Center.

no

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|---|
| 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 |
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| For the other institutions: marc.luwel@herculesstichting.be |

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 organisational 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.

¹Please 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.

²Please 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, proprietary 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)



**Fonds Wetenschappelijk Onderzoek
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Stichting van Openbaar Nut
Ondernemingsnummer 0880.212.840

Ik aanvaard mijn aanwerving als Postdoctoraal Onderzoeker van het Fonds Wetenschappelijk Onderzoek – Vlaanderen met ingang van 1/10/2014 tot en met 30/09/2017 met het oog op het doorvoeren van het wetenschappelijk onderzoek, vermeld in mijn mandaataanvraag, aan de Universiteit Gent.

Ik ben ervan op de hoogte dat ik administratief en juridisch onder de bevoegdheid kom van het Fonds Wetenschappelijk Onderzoek - Vlaanderen, vertegenwoordigd door zijn voorzitter en zijn secretaris-generaal, en dat ik disciplinair onder de bevoegdheid kom van de academische overheid van de universiteit en eventueel de wetenschappelijke instelling waaraan ik mijn werkzaamheden doorvoer.

Ik neem er nota van dat:

- a) deze arbeidsovereenkomst wordt geschorst gedurende langdurig ziekteverlof, ouderschapsverlof, zwangerschaps- en borstvoedingsverlof, palliatief verlof en verlof voor medische bijstand.
- b) het me niet is toegestaan, behoudens formele machtiging, mijn mandaat bij het FWO te cumuleren met welke andere toelage of bezoldiging ook;
- c) - de salarisschaal van postdoctoraal onderzoeker de salarisschaal doctorassistent is volgens het besluit van de Vlaamse Regering van 4 mei 2001 inzake de salarisschalen van toepassing op het assiterend personeel van de universiteiten in de Vlaamse Gemeenschap (BS 9 januari 2002);
- de bruto wedde per maand varieert tussen minimaal 3.896,31 euro (0 jaar geldelijke anciënniteit) en maximaal 6.074,02 euro (index 1,6084 op 1 januari 2013);
- de wedde wordt aangepast aan de toegekende geldelijke anciënniteit op basis van artikel 25 van het reglement inzake mandaat Postdoctoraal onderzoeker van het FWO;
- het vakantiegeld en de eindejaarstoelage overeenstemt met het vakantiegeld en de eindejaarstoelage dat ik zou ontvangen als doctorassistent aan een universiteit in de Vlaamse Gemeenschap.

Ik verbind me er toe strikt het reglement inzake het mandaat Postdoctoraal Onderzoeker van het FWO, waarvan ik verklaar een exemplaar ontvangen te hebben, en de voorschriften van mijn academische overheid na te leven.

Op al mijn publicaties en hun overdrukken, zal ik mijn hoedanigheid van Postdoctoraal Onderzoeker van het Fonds Wetenschappelijk Onderzoek - Vlaanderen vermelden.

Datum en handtekening voorafgegaan door de woorden: 'gelezen en goedgekeurd'

gelezen en goedgekeurd
03/08/2014

Danny Vanpoucke

PS: De keerzijde van dit document eveneens aanvullen.