# 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:**

Shape tuning of CdSe nanostructures by ab initio determination of the anisotropic growth mechanism.

**Name and first name of the applicant:**

Sluydts Michael

**Institution:**

Ghent University

**Research group / department:**

Center for Molecular Modeling

**Title / position:**

PhD fellow

**e-mail address:**

michael.sluydts@ugent.be

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

4752

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

602.1

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

   $I-III-VI_2$ Semiconductor Nanocrystals, from a fundamental understanding of the hot injection synthesis to a novel colloidal quantum dot material family

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):

   CdSe nanocrystals are the prototype system for the hot injection synthesis of colloidal quantum dots, desired for their tunable optical behavior. The procedure involves injection of precursor molecules into a heated coordinating solvent. This leads to a nucleation phase followed by growth of the nuclei until the synthesis is stopped or the precursors are depleted. During the entire process the growing nanocrystals are encapsulated by a ligand shell composed of coordinating solvent molecules. The growth rate of the nanocrystals is determined by the adsorption strength and kinetics of these ligands to the nanocrystal surface. The surface itself is composed of distinct facets with a morphology according to the crystal symmetry. By choosing ligand molecules to prefer specific facets not only the size but also the shape of the nanocrystal can be tuned. This has led to the synthesis of structures such as nanorods and even tetrapods which translate their shape into anisotropic optical properties. In recent years it has become apparent that the nanocrystal surface is not merely the same as a bulk surface but is enriched by excess metal ions. This has greatly changed the prevalent view of the chemical processes taking place on these facets. While attempts have been previously made to explain the mechanism of anisotropic growth through simulation, none have taken into account this updated picture of the surface interactions. The goal of this project is to determine the correct interactions between the relevant ligands and metal-enriched surfaces. Understanding the true anisotropic growth mechanism will enable more finely tuned shape control. To study this we will use the framework of ligand addition energies which we have previously developed to study the interactions between different ligands and materials. Ab initio calculations are used to determine the energetic cost or gain of stepwise ligand addition to the excess surface from a ligand reservoir. By studying when this process becomes endothermic the surface stoichiometry and morphology in presence of the ligand is deduced. This procedure is performed on the common (0001), (000-1) and (11-20) surfaces of a CdSe nanocrystal, and will for instance determine the selectivity between the top, bottom and side of a nanorod.

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

   The optical properties of colloidal quantum dots are tuneable: the color of their emitted light can be varied upon changing the size and shape of the dot.This is interesting for applications such as LEDs and LASERs where the color of the light is normally fixed for a specific material. In this project we investigate the anisotropic growth of CdSe nanorods. In solution these nanorods are surrounded by a shell of molecules. Depending on which facets of the crystal these ligand molecules prefer their growth rate will vary and with them the shape of the nanocrystal. We examine how to optimize this shape control by simulating and determining the specific mechanism of adsorption.

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 G.0760.12, confirmation letter attached at the end of the file.

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

   Zeger Hens – zeger.hens@ugent.be

   Stefaan Cottenier – stefaan.cottenier@ugent.be

   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)

ir. Michael Sluydts (vsc40479)
Ghent University
Center for Molecular Modeling
PhD Fellow
Four years of experience using VASP on both TIER2 and TIER1.

Prof. Dr. ir. Veronique Van Speybroeck (vsc40021)
Ghent University
Center for Molecular Modeling
Professor
Experience with a wide variety of DFT packages since the opening of the Ghent VSC on both TIER2 and TIER1.

Prof. Dr. Stefaan Cottenier (vsc40026)
Ghent University
Center for Molecular Modeling
Assistant Professor
Experience with a wide variety of DFT packages since the opening of the Ghent VSC on both TIER2 and TIER1.

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).

This project combines a screening aspect in its initial phase with resource-intensive calculations in the secondary phase (see section 8). In both cases the workload requires a high availability of computational resources typically not available on TIER2. The type of calculations performed will be highly similar to those previously run in our pilot project, but with more degrees of freedom. Additionally we will make use of our self-developed high-throughput management software to facilitate the screening procedure and enable an automatic transition to the secondary phase. This software was tested on TIER1 during our previous project and enables advanced tracking of consumed resources as well as a gradual increase of accuracy settings to limit unnecessary resource consumption, combined with automatic checkpointing.

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).

   Within this project six ligand species (three main species + deprotonated variants) will be simulated on each of the three surfaces. In each case four addition steps will be performed representing an increase of the surface ligand density. This leads to a total of 6*3*4 = 72 identical calculation workflows which need to be traversed. In the initial stage a screening of 4 positions in 2 ligand orientations will be performed in each case, for a total of 8 positions per ligand. This screening will be performed at lower accuracy (‘soft’ settings) to reduce calculation time. The 'hard' relaxation and frequency calculation continue with the best result from the screening phase, in both cases at higher accuracy. All parallelization is performed using VASP's MPI-driven k-point parallelism which leads to minimal communication between nodes, scaling is illustrated in section 9. Average resource consumption per task is given in Table 1.

**Table 1: Calculation of required node days and storage**

| | Node day calculation | | | | | | Storage volume estimate | |
|---|---|---|---|---|---|---|---|---|
| **Computation task** | **# of tasks** | **Walltime/task (days)** | **# nodes / task** | **# node days/ task** | **# cores / task** | **Memory (GiB) / task** | **Tier-2 storage (GiB) + inodes** | **Tier-1 storage (GiB) + inodes** |
| **Soft relax (screening)** | 72*8<br>= 576 | 3 | 2 | 3456 | 32 | 12 | 567*0.2 GiB<br>= 113.4 GiB<br>567*1 inodes (archive) | 567*1.5 GiB *0.2<br>= 170.1 GiB (only running tasks)<br>72* (52 files+1 folder)<br>= 3 816 inodes |
| **Hard relax** | 72 | 3 | 3 | 648 | 48 | 32 | 72*0.5 GiB<br>= 36 GiB<br>72*1 inodes (archive) | 72*3GiB = 216 GiB<br>72* (52 files+1 folder)<br>= 3816 inodes |
| **Frequency** | 72 | 3 | 3 | 648 | 48 | 64 | 72*0.5 GiB<br>= 36 GiB<br>72*1 inodes (archive) | 72*3GiB = 216 GiB<br>72* (52 files+1 folder)<br>= 3816 inodes |
| **Total** | | | | **4752** | | | **185.4 GiB + 711 inodes** | **602.1 GiB+ 11448 inodes** |

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).

Used software:

VASP 5.4.1
- http://www.vasp.at
- License: attached at the end of the document
- The software is already available on the TIER1 infrastructure.

Scaling behavior was tested for the CdSe surface without adsorbed ligands. This subsystem largely defines the total system size and thus the scaling behavior within a single iteration of the program. Upon addition of ligands the cell size will remain fixed resulting in similar grid sizes. Ligand addition will lead to similar scaling, but more total iterations due to the added degrees of freedom (the surface is partially fixed). Calculation time was was summed over 20 electronic iterations in each case to negate the effect of random variations. Results are shown in Tables 2, 3 and 4 for the soft relaxation, hard relaxation and frequency calculation respectively, combined in Figure 1. Parallelization over 1, 3 and 9 nodes was chosen for optimal division of irreducible k points of the system over the computing resources.

**Table 2: Scaling test for the soft relaxation (screening) task**

| # nodes | # cores | absolute timing (s) | speedup | # cores x timing |
|---|---|---|---|---|
| 1 | 16 | 1556.867 | 1 | 24909.87 |
| 3 | 48 | 617.973 | 2.519312 | 29662.71 |
| 9 | 144 | 321.898 | 4.836517 | 46353.37 |

**Table 3: Scaling test for the hard relaxation task**

| # nodes | # cores | absolute timing (s) | speedup | # cores x timing |
|---|---|---|---|---|
| 1 | 16 | 3800.375 | 1 | 60806.00 |
| 3 | 48 | 1537.237 | 2.472211 | 73787.38 |
| 9 | 144 | 739.3956 | 5.139839 | 106473.00 |

**Table 4: Scaling test for the frequency task**

| # nodes | # cores | absolute timing (s) | speedup | # cores x timing |
|---|---|---|---|---|
| 1 | 16 | 3807.422 | 1 | 60918.75 |
| 3 | 48 | 1472.744 | 2.585257 | 70691.72 |
| 9 | 144 | 661.3761 | 5.756818 | 95238.16 |

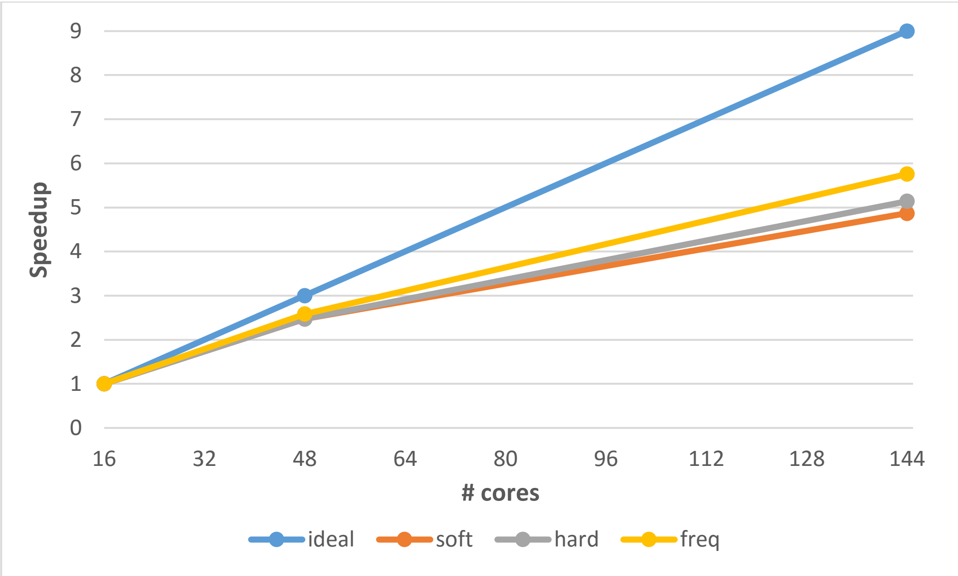


**Figure 1: Scaling behavior of a CdSe slab model in the ideal case, during a soft relaxation, hard relaxation and frequency calculation for 16, 48 and 144 cores**

For each of the three tasks parallel performance evolves in a nearly identical fashion. This is not entirely unexpected as the operations performed in each case are virtually identical. At 3 nodes approximately 85% of the expected speedup is obtained which decays to 55-65% for 9 nodes. Scaling performance appears to improve with higher accuracy settings. This suggests the workload for this system (size: 168 electrons) may be insufficient for large-scale parallelization. Scaling performance may actually slightly increase as ligands are added to the system. Keeping this in mind, we will aim to run calculations k-point parallel on 2-4 nodes depending on the number of irreducible k-points for the specific system. A system with more attached ligands, will have less symmetry, more irreducible k-points and should scale better. Should the optimal choice of k points lead to a calculation exceeding the walltime our automation software will end the calculation in a way it can be continued and resubmit it without user interference. This should ensure no resources are wasted.

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, …)?

    Similar continuous usage throughout the project period.

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.

    Projects:

    **Pilot** - Exploring surface doping and adsorption in semiconducting systems using a high throughput ab initio methodology for applications in nanoelectronics and photonics

    **2014-032** - High-throughput determination of vacancy trapping enthalpies for the improvement of electronic device production

    Output:

    http://dx.doi.org/10.1021/acsnano.5b06965

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.

    No

**Overview of attachments:**

1. VASP software license
2. FWO funding letter

| 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 |

# 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)

B/12578/01 UT
4BC2

FWO

FWO - Stichting van Openbaar Nut – Ondernemingsnummer 0880.212.840

# OVEREENKOMST FWO - ONDERZOEKSPROJECT

TUSSEN

Het Fonds Wetenschappelijk Onderzoek – Vlaanderen, Egmontstraat 5, 1000 Brussel, vertegenwoordigd door dr. ir. Elisabeth Monard, secretaris-generaal, hierna het FWO genoemd, enerzijds,

de onthaalinstelling(en)

Universiteit Gent

01000176300004
Prjdef: B/12578 Doctyp: Contract

EN

de verantwoordelijk woordvoerder van het onderzoeksproject van het FWO met dossiernummer **G.0760.12N**

Zeger Hens
Universiteit Gent

anderzijds,

WORDT HET VOLGENDE OVEREENGEKOMEN

**Artikel 1** - De volgende bijlagen maken integraal deel uit van deze overeenkomst:

Bijlage 1: Projectomschrijving – onderzoeksproject G.0760.12N
Bijlage 2: Het FWO - Reglement inzake de onderzoeksprojecten
Bijlage 3: Het FWO - Algemeen reglement

## UITVOERING

**Artikel 2** - De vermelde promotor en copromotoren verbinden er zich toe het onderzoeksproject, zoals omschreven in de oorspronkelijke kredietaanvraag, uit te voeren.

**Artikel 3** - het FWO verbindt er zich toe de subsidies vermeld in bijlage 1 voor de duur van de overeenkomst en overeenkomstig de modaliteiten van het FWO-reglement inzake onderzoeksprojecten, uit te betalen.

UNIVERSITEIT GENT

FACULTEIT **INGENIEURSWETENSCHAPPEN**

INGEKOMEN DOZA
09 MAART 2012
NR.: 1072 / DL

3 pag.
B/12578
1/46800 1/633
1/1433 1/262

**Barbara Lobert**
**Afdeling Onderzoekscoördinatie**
Sint-Pietersnieuwstraat 25
9000 GENT

| **uw kenmerk** | **ons kenmerk** | **datum** |
|---|---|---|
| | | 08 12 2011 |
| **contactpersoon** | **e-mail** | **tel.** |
| Veronique Van Speybroeck | Veronique.VanSpeybroeck@UGent.be | +32 9 264 65 58 |

**<u>Betreft</u>: Aanvraag tot financiële verdeling FWO-project 3G07[redacted]6012 (B/12578/*)**

Geachte Mevr. Lobert,

Het budget verbonden aan FWO-project 3G07[redacted]6012 staat onder het beheer van de hoofdpromotor van het project, Prof. Zeger Hens. Om praktische redenen is echter het opportuun dat Prof. Veronique Van Speybroeck als co-promotor over een eigen deel van het budget kan beschikken. Er wordt voorgesteld om 150000 euro / 50% van het budget te behouden op B/12578/01, met Prof. Zeger Hens als budgethouder, en een nieuw WBS-element aan te maken met 150000 euro / 50% waarover Prof. Van Speybroeck als budgethouder kan beschikken. Wij willen u dan ook vriendelijk vragen gevolg te geven aan dit verzoek.

Hoogachtend,

Prof. Zeger HENS

Prof. Veronique VAN SPEYBROECK

Prof. Stefaan COTTENIER

01000176300003
Prjdef: B/12578 Doctyp: Contract