Job opening EU PhD - Computational Chemistry - understanding defects and disorder in MOFs

Job opening: PhD (Marie Skłodowska-Curie H2020) in Theoretical and Computational Chemistry - understanding defects and disorder in MOFs

PhD fellowship - summary

The Center for Molecular Modeling (CMM) is a multidisciplinary research center of Ghent University (Prof. Veronique Van Speybroeck). The CMM is participating in an EC-funded European Training Network called DEFNET, running from January 2015 until December 2018. This Marie Skłodowska-Curie H2020 scheme provides generous funding for an Early-Stage Researcher (ESR) with good salary and travel/mobility/family allowances. We’re looking for an outstanding postgraduate typically within 4 years of his/her MSc (see eligibility conditions below).

The successful candidate will use computational modeling as a tool to unravel various types of defects and structural disorder in Metal-Organic Frameworks (MOFs). MOFs are made up of both inorganic and organic moieties and have developed into an important new class of crystalline porous materials. Their unique structural characteristics open a range of possible application areas. MOFs have multiple uses such as gas adsorption, molecular storage, drug delivery and heterogeneous catalysis. Furthermore, linker defects can be present after the MOF synthesis or even be engineered within MOF-materials and these defects can influence required properties. For example, the catalytic activity can be increased by the creation of a larger number of defect sites (missing organic linkers), or due to modulating effects resulting from functionalization of the linkers. It has been demonstrated that UiO-66 materials synthesized from terephthalates substituted with electron withdrawing groups are significantly more active.

The research involves (1) the construction of defect models, going from non-periodic small models to fully periodic systems and (2) performing static calculations and proceed to ab initio molecular dynamics simulations. A broad variety of computational programs (VASP, CP2K, Gaussian, etc.) is available at the CMM to perform such type of simulations. More specifically, the computational focus will be laid on (i) quantifying free energy for creation of various defects and simulation protocol for reactive processes; (ii) infrared spectra and adsorption energies of small probe molecules; (iii)
unraveling of reaction pathways; (iv) material properties of defective MOFs; (v) comprehensive modelling of defects for targeted properties.

Day-to-day guidance in Ghent will be performed by the experienced scientific staff at CMM consisting of senior PhDs and postdocs focusing catalysis and defects in MOFs with typically more than 5 years’ experience in computational modeling.

The tentative start date is June 2015, though there is some degree of flexibility. Salary conditions, travel/mobility allowances, and benefits will follow the attractive EU amounts for Early Stage Researchers in program H2020-MSCA-ITN-2015.

As this PhD position is embedded in the DEFNET the European Training Network, strong interaction with experimental partners are foreseen. Furthermore the computational modeling work will be conducted in close collaboration with two other modeling partners of the DEFNET program: SCM, a scientific software company located in Amsterdam, The Netherlands, developing software packages in the area of computational quantum chemistry and materials science and the Computational Materials Chemistry group of Ruhr-University Bochum (RUB) (PD Dr. Rochus Schmid).

**Job requirements**

Requirements:

- Knowledge of computational chemistry methods.
- MSc degree in Chemistry, Materials Chemistry, Chemical engineering, Physics or Engineering Physics.
- Maximum of four full-time years research experience after MSc degree, and not being in possession of a PhD degree.
- Good written and verbal communication skills in the English language.
- Strong motivation to work in a highly ambitious research team.
- Strong communication skills to interact efficiently with experimental partners.

Desirable additional knowledge and experience:

- General programming skills (UNIX, scripting languages, debugging, etc.).
- Team player, with good two-way communication skills, highly self-motivated and able to work independently with excellent time management skills.

**What we offer**

The PhD fellowship will consist of an initial 3-year full-time position at the Ghent University with the possibility to prolong with a 4th year to complete his/her PhD. The position is available from June 2015 but there is (some) flexibility concerning the starting date. Salary and secondary benefits (including pension fund) will follow EU rules for salaries of Early Stage Researchers. Tax free
fellowship including full social security coverage (net monthly amount starting at ± 1.900 EUR/month + (if applicable) family allowance of 500 EUR. In addition, the EU provides funding for training and transfer of knowledge expenses to the institutes.

**Project details**

The project is part of the European Training Network ("DEFect NETwork materials science and engineering", DEFNET), led by Prof. Dr. R. A. Fischer (Ruhr-University Bochum). From the DEFNET abstract: "DEFNET focuses on porous coordination network compounds: Metal-organic Frameworks (MOFs) [...]. MOFs are just on their way to become widely applicable. Intense research is ongoing with intense global competition. DEFNET materials based on MOFs hold promise for innovative functionalities which cannot be achieved by other materials and benchmarking is done against zeolites, which are established porous materials in industry for catalysis and sorption applications."

**About the Center for Molecular Modeling (Ghent University)**

The CMM is a multidisciplinary research center that is currently composed of about 35 researchers from the Faculties of Sciences and Engineering and Architecture of Ghent University. The Center focuses on frontier research in six major areas: chemical kinetics in nanoporous materials, computational material research on the nanoscale, spectroscopy, many-particle physics, model development and bio- and organic chemistry. The whole team consists of one full professor, one associate professor, one part-time associate professor, two part-time assistant professors and one emeritus full professor, seven post-doctoral researchers, 21 PhD students, one administrative staff member and various master students on a yearly basis. The basis of the success of the CMM lies in the interdisciplinary composition of the research team which consists of chemists, chemical engineers, physicists, physical engineers and bio engineers. Since its foundation in 2000 it has acquired a prominent position in previous research fields.

**Eligibility**

We especially invite women to apply. EU mobility rules apply. For this position in Amsterdam, the selected candidate may not have lived in The Netherlands for more than 12 months in the three years preceding the recruitment date. In principle, applicants can have any nationality, and any current residence (although immigration rules apply, favoring EU applicants). Candidates who already have more than 4 years (full-time equivalent) of research experience after obtaining their MSc degree or who have already been awarded a PhD degree are not eligible according to the EU rules for this project: "Early-Stage Researchers (ESRs) shall, at the time of recruitment by the host organisation, be in the first four years (full-time equivalent research experience) of their research careers and not yet have been awarded a doctoral degree. Full-Time Equivalent Research Experience is measured from the date when a researcher obtained the degree which would formally entitle him/her to embark on a doctorate, either in the country in which the degree was obtained or in the country in which the researcher is recruited or seconded, irrespective of whether or not a doctorate is or was ever envisaged."
Further information, applying

Detailed information on CMM can be found at the CMM’s website. Those interested in this position are encouraged to contact CMM (Veronique.vanspeybroeck@ugent.be) for further information. Job applications can be sent by E-mail to the same address. Applications should contain a CV, data to support that you are an excellent young scientist, a letter explaining the detailed motivation for applying, a list of publications, and last but not least a clear and complete summary of your programming and method development experience (as opposed to using standard existing software) and your experience with computational molecular modeling. References may be requested at a later stage.