

Several PhD / postdoc positions available at the Center for Molecular Modeling Ghent University, Belgium

Within the framework of various large-scale research projects such as an ERC Consolidator Grant (**DYNPOR**) entitled "*First principle molecular dynamics simulations for complex chemical transformations in nanoporous materials*" and a concerted research action of the Ghent University on *covalent organic frameworks*, various research positions are available for prospective PhD and postdoctoral researchers at the Center for Molecular Modeling (CMM, <http://molmod.ugent.be>) of the Ghent University under the supervision of Prof. V. Van Speybroeck.

The **Center for Molecular Modeling (CMM)** is a multidisciplinary research center of about 35 researchers consisting of one full professor, one associate professor, two assistant professors and one part-time associate professor, 7 postdocs and 20 PhD students belonging to the Faculties of Engineering and Science. The Center focuses on frontier research in the following areas: chemical kinetics in nanoporous materials, computational design of nanostructured materials, spectroscopy, many-body techniques and bio- and organic chemistry. The success of the CMM builds on its interdisciplinary research team consisting of chemists, chemical engineers, physicist, physical engineers and bioengineers.

The research team of Prof. V. Van Speybroeck focuses on modelling complex transformations in nanoporous materials such as zeolites, metal-organic frameworks and covalent organic frameworks. Our aim is to obtain physical and chemical insight into chemical reactions, phase transformations at realistic conditions of temperature, pressure, loading of guest molecules,... To this end we are using a complementary set of modelling techniques, either based on first principle methods such as Density Functional theory or first-principle derived force fields, in combination with advanced sampling methods to obtain free energies of various complex transformations. The research team consists of various junior and senior researchers with various backgrounds which enables us to give a proper intellectual environment for the conducted research. We stimulate interaction between researchers with various backgrounds to enable groundbreaking research at the interface of physics, chemistry and materials science. The research is conducted in close collaboration with excellent experimental groups to guide the design towards new and promising functional materials.

Within the framework of the various research programs we would like to enforce our team on following topics :

- **Adsorption of guest molecules in nanoporous materials at realistic operating conditions** of temperature, pressure,... for important catalytic processes such as the conversion of alcohols towards olefins.
- **Advanced computational spectroscopy on oligoatomic metal clusters encapsulated in zeolitic materials** that are promising materials for application in different fields encompassing catalysis, photonics and electronics.
- **Computational screening of existing and hypothetical COFs** to assess their flexibility, stability and adsorption properties
- **Advanced electronic structure characterization of COF materials** and metal complexes towards effective **photoredox catalysts** using state-of-the-art first-principles methods
- **Advanced sampling methods to study complex chemical and physical transformations** in zeolites and metal-organic frameworks

Profile of potential PhD candidates:

- Master degree in Chemistry or Chemical Engineering.
- Master degree in Physics, Engineering Physics or Physical Chemistry
- Experience with using molecular simulation codes and programming (Python, bash, C ...) is an asset.
- Excellent study results are an asset.
- Fluent in English.
- Strong motivation to work in a highly ambitious research team.
- Students who expect to obtain their Master degree before July 2017 can also apply.

Profile of the potential postdoc candidates:

- PhD in Physics, Chemistry, Chemical Engineering, Physical Engineering or a related field.
- Proven track record in conducting excellent research.
- Proven track record related to the topic of the vacancies.
- Proven track record in using various molecular simulation codes.
- Programming skills are an asset.
- Fluent in English.
- Strong motivation to work in a highly ambitious research team.

It is the intention to fill in the positions as soon as possible. The selected candidate(s) will have the ability to attend various international conferences and to include research stays abroad in the most prominent research teams of the world in this field within the framework of his/her PhD or postdoc. Selected postdoc candidates will get the ability to strengthen their CV within the context of a multidisciplinary team.

Further information can be obtained with Prof. Veronique Van Speybroeck.
Interested candidates should mail their CV and a letter of motivation to

Prof. Dr. V. Van Speybroeck – Head of the Center for Molecular Modeling

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