GHENT UNIVERSITY

CENTER FOR MOLECULAR MODELING

Several PhD / postdoc positions available in the field of zeolite catalysis within the research group of V. Van Speybroeck 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 several FWO projects together with national and international partners, various research positions within **the field of zeolite catalysis** are available for prospective PhD and postdoctoral researchers at the Center for Molecular Modeling (CMM, http://molmod.ugent.be) of Ghent University under the supervision of Prof. V. Van Speybroeck.

The **Center for Molecular Modeling (CMM)** is a multidisciplinary research center of about 40 researchers from the Faculties of Sciences and Engineering and Architecture of Ghent University. The CMM, which is led by Prof. V. Van Speybroeck, is composed of an interdisciplinary research team which consists of chemists, chemical engineers, physicists, engineers in physics, chemical technology and bio-engineers. The Center focuses on frontier research in six major areas: nanoporous materials, modeling of solid-state physics, spectroscopy, many-particle physics, model development and bio- and organic chemistry.

The research team of Prof. V. Van Speybroeck focuses on modeling 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 in and phase transformations of these nanoporous materials at operating conditions. This research fits into a large-scale investment we have started since 2015 within the framework of an ERC Consolidator grant to use first principle molecular dynamics methods within the field of catalysis and nanoporous materials. To this end, we employ a complementary set of modeling techniques, either based on first principle methods such as density functional theory or on first-principle derived force fields, in combination with advanced sampling methods to unravel the governing free energy profile 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. The research group is internationally regarded to be at the forefront in its field.

In the framework of the various research programs we would like to enforce our team **in zeolite catalysis**. Within this area we not only have a solid research track record in the field of the methanol to olefins process and olefin cracking, but we are also working towards new topical areas such as the CO_2 to hydrocarbons process and the conversion of biomass-related feedstocks to chemicals. All work is performed in close collaboration with prominent experimental partners at the national and international level. For all these processes we aim to describe reactions and intermediates at operating conditions, thus at realistic working temperatures, loadings within the pores… To pursue these goals, we have developed a branch of first principle molecular dynamics methods that is recognized at the international level.

Profile of potential PhD candidates:

- Master degree in Chemistry, Chemical Engineering, 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 2019 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 vacancy.
- 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.
- Motivation to collaborate within a larger team of researchers

It is the intention to fill these 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 international research teams 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

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