PhD position available in the field of "thermodynamic modeling of adsorption in flexible nanoporous materials" under the supervision of prof. L. Vanduyfhuys at the Center for Molecular Modeling, Ghent University, Belgium.

The multidisciplinary Center for Molecular Modeling (CMM, http://molmod.ugent.be), is looking for a highly motivated researcher to perform state-of-the-art research in the field of thermodynamic modeling of adsorption in nanoporous materials. We especially welcome highly motivated candidates with a strong track record who may become eligible to apply for a prestigious PhD fellowships at our national funding agency (FWO).

Thermodynamics may be regarded as one of the most widely applied branches of physics, interwoven in many aspects of life on our planet. Although it was originally developed mainly to increase the efficiency of steam engines, its applications have evolved greatly and now include a description of chemical reactions, physical and chemical equilibria. Statistical thermodynamics is a particularly interesting extension of thermodynamics, where one tries to understand the thermodynamics of macroscopic systems from a statistical description of the microscopically accessible states. The application of statistical physics can be used to make the bridge between the output of molecular simulations such as molecular dynamics and Monte Carlo on the one hand, and the thermodynamic observables we can measure macroscopically on the other hand. In this PhD, it is the intention to apply the principles from thermodynamics and statistical physics to investigate the behaviour of a new class of nanoporous materials, i.e. soft porous crystals (SPCs). Some metal organic frameworks (MOFs) are an example of such SPCs. These MOFs are hybrid materials made up from metal ions or metal clusters linked together by organic linkers. It was discovered that some MOFs show "flexible" behavior in the sense that they are capable of transforming between various phases accompanied by substantial changes in the unit cell volume (up to 40%) while retaining their structural integrity. Such transformations can be instigated by various triggers such as mechanical pressure, temperature as well as adsorption of guest molecules.

The goal of this PhD research is to develop mathematical models for the thermodynamic potential of guest-loaded nanoporous materials as function of temperature, pressure and chemical potential in various ensembles (eg. the canonical and the grand canonical ensemble). To obtain the required information for the construction of these models, the candidate will perform various molecular simulations such as molecular dynamics (MD), Monte Carlo (MC) and classical density functional theory (cDFT). Furthermore, it also intended to implement the resulting thermodynamic models in a user-friendly program package to allow for an easy application of the models.

The prospective candidate will join a strongly connected research team and will collaborate with national and international academic partners. He/she will benefit from the experience present in the Center for Molecular Modeling (CMM), specifically on performing advanced molecular simulations and the development of general procedures to model physical transformations in nanoporous materials, as well as its implementation in dedicated software packages. The CMM is an interfaculty research unit at Ghent University headed by Prof. Van Speybroeck, grouping about 40 scientists from the Faculty of Science and the Faculty of Engineering and Architecture. The research team consists of various junior and senior researchers with various backgrounds which enables us to provide a proper intellectual environment for the conducted research. The CMM performs interdisciplinary research at the crossroads between physics, chemistry and materials engineering with the aim to design molecules, materials, and processes at the nanoscale. To this end, the CMM consists of six synergetic research areas: "Nanoporous materials", "Solid-state physics", "Bio/organic chemistry",

“Model and software development”, “Spectroscopy”, and “Many-particle physics”. The research of this PhD situates mainly in the areas “Nanoporous materials” and “Model and software development”, but to enable groundbreaking research at the interface of physics, chemistry, and materials science, we strongly stimulate interactions between the various researchers of all areas as well as with the vast network of national and international partners. The CMM is internationally regarded to be at the forefront in its field.

Who are we looking for?
We are looking for a highly motivated and creative PhD candidate with:

- A master’s degree of a university or international equivalent in the field of Physics, Engineering Physics, Physical Chemistry or a related field;
- Perseverance and an independent, pro-active working style;
- The willingness to look beyond the borders of his/her own discipline and a strong motivation to work in a multidisciplinary team;
- Experience in coding (Python, C, ...) is an advantage. At the very least, the candidate must be willing to learn these skills during the first year of the PhD.
- Excellent collaboration and communication skills (written and verbally) in English.

What can we offer you?
The selected candidate will have the opportunity to attend various international conferences and to include research stays abroad in the some of the most prominent international research teams in this field within the framework of his/her PhD. He/she will get the ability to strengthen his/her CV within the context of a strongly motivated and multidisciplinary research team.

How to apply?
It is the intention to fill this position as soon as possible. Fill in the application form (in attachment) and send the form together with all required documents to prof. Louis Vanduyfhuys (louis.vanduyfhuys@ugent.be) and to cmm.vacancies@ugent.be, mentioning “Vacancy PhD position in the field of thermodynamic modeling of adsorption in nanoporous materials” in the subject of your e-mail.