Masterthesis: Investigation of adsorption-induced strain in silica nanopores through hybrid Grand Canonical Monte Carlo and Molecular Dynamics simulations

Background

The effects of confinement on matter in nanoporous materials play an important role in natural processes such as clay swelling, frost heave or transport in biological tissues. In addition, applications based on porous media offer great potential for technological advances such as catalysis, sensing and energy storage/generation (see for example the EHAWEDRY project). To understand these natural processes and exploit the technological potential of nanoporous materials, a precise understanding of the effects resulting from the interaction of confined matter with the host material is essential. One of these effects, which is still the subject of scientific debate, is the deformation of nanoporous materials due to adsorption of liquids.

Project Task

The aim of this project is to study the asymmetric deformation of cylindrical silica nanopores with a pore diameter of 3 nm at different adsorption equilibrium states of water. Towards this goal Grand Canonical Monte Carlo (GCMC) computer simulations with complementary classical Molecular Dynamics (MD) computer simulations are to be performed and analysed. The simulations will be conducted with the software LAMMPS on High Performance Computing (HPC) clusters. You will be guided step by step to work with LAMMPS and how to use the HPC cluster for your simulation. Therefore, no previous knowledge but an interest in computational modelling and materials science is required for a successful and fun project. Many components that are important for an atomistic simulation, like suitable interaction models and an initial atomic configuration, are available from a previous water imbibition study and can be built upon in this project. Therefore, this investigation has a good chance of success and of generating scientifically relevant results.

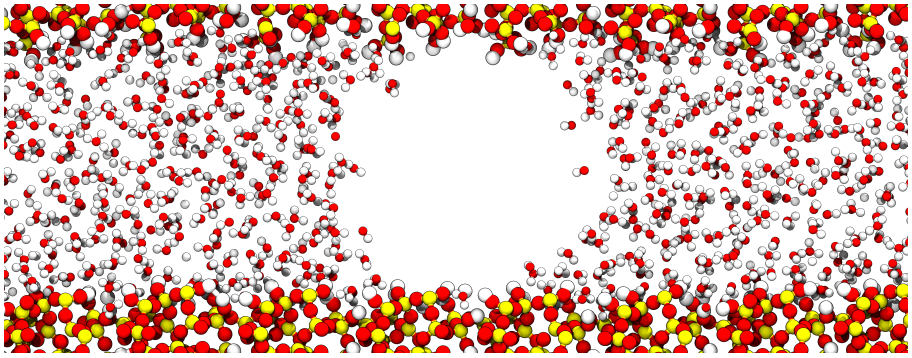

Figure 1: Molecular Dynamics simulation of water imbibition into 3 nm silica nanopore.

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