21. Grand Canonical -Molecular Dynamics simulations of sorption isotherms in Nanopores

Matias Factorovich and Damián Scherlis

Universidad de Buenos Aires, Argentina

We focus on the development and implementation of a hybrid, Grand Canonical Monte Carlo - Molecular Dynamics, method for a variety of potentials in Mesoporous materials to obtain adsorption isotherms which can reproduce the hysteresis commonly seen in these systems. With this approach we can sample the dynamical properties of the system (Molecular Dynamics), without loosing the Grand Canonical properties (Monte Carlo). We use LAMMPS as our main tool, a versatile program to perform molecular dynamics, to which we have added a Grand Canonical Monte Carlo subroutine in the main input script. We validate our implementation against previous Monte Carlo results in a simple system consisting of a fluid in a slit pore interacting via Lennard-Jones potentials. The main feature to be adjusted in this scheme is the ratio between the Monte Carlo and the Molecular Dynamics steps: we present how such ratio influence the outcome of the simulations, and the resulting isotherm for the optimized ratio. We also present results of this method to obtain sorption isotherms of water in pores of different geometries.