National Technical University of Athens, School of Chemical Engineering

Department of Materials Science and Engineering

Computational Materials Science and Engineering Group (Co.M.S.E.)

"*Development of DFT-Based Force Fields for Atomistic Simulations in Microporous Materials*"

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Abstract

Sorption and diffusion of sorbates inside microporous materials are routinely studied by means of atomistic simulations like Molecular Dynamics (MD) and Grand Canonical Monte Carlo (GCMC). In order to be employed, these techniques require knowledge of all the interactions of the systems, specified through a force field. The quality of the computed properties, then, will rely on the given force field, so that its accuracy is of uttermost importance. Even though generic force fields are available from the literature, sometimes these are found to be unsatisfactory. In these cases it is important to develop a force field tailored to the specific system under investigation. This is a nontrivial task, requiring the optimization of dozens of parameters. A useful approach relies in the development of force fields based on accurate but computationally expensive Density Functional Theory (DFT) data. The bonded interactions are obtained by adjusting the force field parameters until the DFT forces for a set of system configurations are reproduced at best by the MD ones. On the other hand, partial charges are adjusted until the model system reproduces at best the DFT electrostatic potential computed on an opportune mesh of points inside the system. Finally, van der Waals interactions can be modelled through the 12-6 Lennard-Jones potential, with parameters found matching both the empirically corrected DFT dispersion energies and forces.