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ABSTRACT BOOK

DEVELOPMENT OF RELIABLE CLASSICAL FORCE FIELDS FOR SIMULATIONS IN MICROPOROUS MATERIALS

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Microporous materials, such as zeolites [1], receive continuously strong attention from the scientific community, thanks to their widespread application in industrial processes (e.g., heterogeneous catalysis and gas separation, among many others).
In recent years, the increase of the computational power has made possible to study with *ab-initio* methods a wide number of systems. Despite that, as today, it is possible to perform a Born Oppenheimer Molecular Dynamics (BOMD) simulation only (without a supercomputer) for small systems (hundreds of atoms) and for short trajectory length (several ps).
For this reason the most common tool to investigate the diffusion of sorbed molecules inside these materials is the classical Molecular Dynamics technique, but, in order to perform reliable simulations one has to provide a full force field [2,3] to describe the system interactions.
The aim of this work is to obtain such force field starting from data obtained via DFT computations by means of a technique called force matching [4] which allows the automated search of the best parameters. The force matching procedure allows reproducing high quality results (DFT), by means of less expensive computations (classical MD).
The data are collected by performing short BOMD runs. The accuracy of the whole procedure is verified computing the Infra-Red (IR) spectra via both BOMD and classical MD, and comparing them with the experimental ones taken from the literature.

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