Molecular Simulations in Porous Materials: Environmental and Technological Applications

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With the increasing demand for efficient, environmentally friendly, and energy saving procedures, porous materials with tailored structures and tuneable surface properties are of wide spread use and this is only expected to intensify in the future. Knowledge of the adsorption and diffusion behaviour as a function of molecular composition and morphology is essential for an informed choice of material for a given application. Molecular Simulations are ideally suited to identify improved structures for adsorption applications and to guide the design of new materials. Efficient simulation methodology and accurate force field potentials are essential to reach this goal. Much progress has been made in the search of fast and efficient simulation and screening methods, but the development of good, transferable force fields, and accurate models for flexible structures is still a formidable challenge. We perform molecular simulations to study the adsorption and diffusion behaviour of a variety of molecules on metal-organic frameworks. These are a relative new class of porous materials with potential applications in molecular adsorption, gas separation, and storage/release applications due to their good stability, large void volumes, and well-defined cavities of uniform size. As an example, we can study structural deformation upon adsorption, identify the preferential adsorption sites as a function of pressure, temperature and humidity, study the effect of functionalization of open metal site find non-accessible places by comparing our results with experimental data, analyse molecular diffusion inside the pores, or study the framework composition and the mechanisms behind the instability of MOFs in humid environments.

Using simulations, we can evaluate the potential of existing (and even hypothetical) zeolites and metal-organic frameworks and possibly provide guidelines for next-generation adsorption materials. The knowledge provided by the simulations may guide the prediction of adsorption properties of a given material, to fine-tune this material for an application and also to steer the experimental effort in successful directions.