Modeling nanoporous materials at the nanoscale

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Theoretical modeling has nowadays taken an indispensable role in many fields of science and engineering thanks to the availability of systematically stronger computing power and the steady development of new ingenious theoretical methods and numerical implementations. This lecture provides an introduction to the broad range of modeling tools adopted to understand the behavior of nanoporous materials at the nanoscale. Nowadays, this modeling toolbox contains a large range of methods, varying from purely quantum mechanical based methods to force field and coarse grained methods. The specific choice of methods suitable for a given problem depends on the typical length and time scale one wants to access during the simulation.

This lecture specifically focuses on modeling nanoporous materials, which are particularly tractable due their high surface area, porosity and chemical versatility. Specific case studies are selected from the fields of zeolites, metal-organic frameworks and covalent organic frameworks, with applications in catalysis, gas adsorption, sensing,… Experimentally, new nanoporous materials are being synthesized at a considerable pace, using the most advanced methods to tailor materials at the nanometer scale. To guide the experimentalists towards new applications and to optimize current processes to their full potential, model-guided design has become an essential part in this overall process. As a result, the field of theoretical modeling has evolved substantially and, nowadays, a variety of examples of this interplay between experiment and modeling are available, such as in high-throughput screening studies, in which a large database of hypothetical materials is screened theoretically for desirable properties.

In this lecture, various modeling tools within the field of heterogeneous catalysis will be highlighted. Within this respect, it is very important to study the catalyst at work, thus at operating conditions. This imposes a huge challenge for theory as this requires models that account for realistic process conditions involving actual reaction temperatures, pressures, loading of the guest species, and other degrees of freedom. One can imagine that in these circumstances the catalytic process becomes very complex and one can no longer resort to the textbook concept of a single transition state and a restricted number of configurations on the potential energy surface. Instead more advanced free energy sampling methods need to be used.

While the computational toolbox that is available nowadays is unprecedented in applicability, it can certainly not be used as a black box. Even though many programs are currently available for a large community, computationally modeling catalysis requires the knowledge of an advanced user, who masters the strengths and the weaknesses of current computational methods. Furthermore, modeling is ideally performed in close synergy with experimentalists. Within this respect, modeling is ideally suited to connect with findings obtained from various advanced spectroscopy and characterization tools. This interplay between experimentalists and computational scientists will be illustrated with some cases studies in this lecture.