Adsorption in Nanoporous Materials: High-Throughput Screening, Machine Learning, and First Principles Simulations

J. Ilja Siepmann [C, S]
Department of Chemistry and Chemical Theory Center,
and Department of Chemical Engineering and Materials Science, University of Minnesota,
Minneapolis, Minnesota, U.S.A.
siepmann@umn.edu

Nanoporous materials, such as zeolites and metal-organic frameworks, play numerous important roles in modern oil and gas refineries and have the potential to advance the production of fuels and chemical feedstocks from renewable resources. The performance of a nanoporous material as separation medium depends on its framework structure and specific adsorption sites. Hierarchical high-throughput computational screening allows for the discovery of promising nanoporous materials for a given application from the large pool of candidate structures is attractive for accelerating the pace of materials discovery. The large data sets from high-throughput simulations can be utilized to develop and train machine learning models that, in turn, can make continuous predictions of loading surfaces to enable selection of optimal process conditions for a given nanoporous adsorbent or of optimal adsorbents for a given set of process conditions. First principles Monte Carlo simulations with the potential energy calculated on-the-fly using Kohn-Sham density functional theory allow for the prediction of highly selective adsorption of gas molecules in metal-organic frameworks with under-coordinated metal nodes and of reaction equilibria in cation-exchanged zeolites.