COMP: Division of Computers in Chemistry

562 - Diffusion in nanoporous materials: Assessing the long time scale from short molecular dynamics trajectories

View Session Detail

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Abstract:The mobility of guest molecules that adsorb in nanoporous crystals, such as zeolites, metal-organic frameworks, or molecular sieving membranes, has a direct effect on the overall dynamical behavior of the adsorption process. For instance, in gas separation, carbon capture, and catalysis in zeolitic materials, the overall selectivity in the observed retention times depends on the inter- and intracrystal diffusion. Simulations at the atomic level are required to gain insight in the diffusive process in case of tight-fitting cages or tight-fitting rings connecting these cages. Unfortunately, the timescale that can be currently reached with molecular dynamics simulations is often too short to assess the diffusion process accurately. In this contribution, a methodology is presented that replaces a single long trajectory by a set of shorter trajectories that are fit together after rebiasing. Nevertheless the long scale diffusivity can still be extracted. The error on the methodology is assessed with a textbook example, and the methodology is validated with the test case of the SAPO-34 material, which is a industrial catalyst in the methanol-to-olefin process. This methodology will be particular useful for extracting diffusivities from ab initio molecular dynamics trajectories, which are necessarily much shorter than the classical force field simulations because of their computational cost.