Nanoseparation of Solvent Mixtures induced by Diffusion in Mesoporous Carbon Materials

Sofia Kolin[1], Moritz Marquardt[1], Stefan Naumann[2], Kristyna Pluhackova[1]

[1]) University of Stuttgart, SC SimTech, Universitätsstraße 32, 70569 Stuttgart, Germany
sofia.kolin@simtech.uni-stuttgart.de
[2]) University of Stuttgart, Institute of Polymer Chemistry, Pfaffenwaldring 55, 70569 Stuttgart, Germany

Mesoporous carbon is of interest in many applications due to its high surface area and physicochemical properties, including a high pore volume and good thermal and mechanical stabilities. It provides interconnected channels for the diffusion of organic solvents, which can be used for "flow-through" applications such as purification of drinking water or nanoseparation of proteins. The objectives of this work are to evaluate the impact of pore size, shape and polarity on the permeability of mesoporous carbon materials in comparison to experimental data. Using coarse-grained molecular dynamics we have established molecular models of two 3D structures of carbonaceous materials: (i) hexagonally ordered cylindric pores and a (ii) bicontinuous double primitive structure with two independent cylindrical pore channels. Moreover, variation of the pore diameter or percentage of oxidized species of these porous materials enables us to systematically evaluate the impact of the individual material properties on diffusion of e.g. hydrocarbons or alcohols. Simulations of the diffusion of mixtures of (i) differently sized solvents, (ii) polar and apolar solvents and (iii) solvents with different geometries allow us to unveil details about solvent competition and nanoseparation.