You shall (not) pass! Molecular selectivity in nanoporous carbon

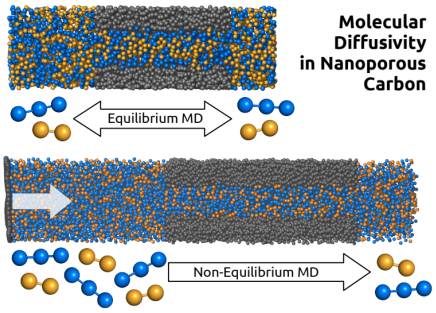
Kristyna Pluhackova

SC SimTech, University of Stuttgart, Germany

Nanoporous carbon materials combine high surface area, chemical stability, tunable surface chemistry, and interconnected pore networks, making them versatile platforms for applications ranging from nanoseparation and purification to catalysis and energy technologies.

In this work, we developed coarse-grained molecular models of nanoporous carbon structures to investigate solvent diffusion and nanoseparation. Systematic variation of pore diameter, geometry, surface roughness, and degree of oxidation enabled a detailed assessment of how structural and chemical material properties govern molecular transport.

Coarse-grained molecular dynamics simulations reveal that separation performance is maximized at pore diameters just above the size-exclusion limit, while surface oxidation strongly modulates the diffusivity of polar molecules. Molecular shape and pore geometry were also identified as important determinants. By employing Markov state modeling, the probability of molecules following distinct transport pathways was quantified, offering a robust framework for predicting separation efficiency in nanoporous systems under equilibrium and non-equilibrium conditions. [1]



[1] S. Kolin, M. G. Marquardt, G. Fläschner, M. Kessler, S. Naumann, K. Pluhackova, *ACS Materials. Lett.*, **2025**, 7, 11, 3714-3723