Molecular simulation of separation of C60 and coronene in silica nanopores

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Abstract

Classical liquid chromatography is one of the most used techniques in the field of nanoparticle separation. This is achieved by driving the nanoparticle containing liquid through a column densely packed with meso- and nanoporous particles. Separation efficiency can be improved through optimizing the interactions between the particles, the solvent and the pore surface using directed surface modifications or adjusting the solvent composition. Finding the best combination of solvents and functionalized surfaces is a complex optimization problem, which is often aided with molecular dynamics (MD) simulations. In this study, the diffusive transport of model nanonparticles, C_{60} fullerene and coronene was studied in nanoconfinement using molecular modeling. The MD simulations were carried out in a slit nanopore of fixed width made of crystalline, fully hydroxylated silica. As solvents, n-hexane and toluene mixtures of different compositions were used. Nanoparticle diffusivities computed both in the bulk and at the surface were used in our 2-state diffusion model to determine the solvent-dependent effective diffusivities of nanoparticles[1]. Our results help to rationalize the observed experimental retention time trends measured for C60 and coronene.

1.Andreas Baer, Paolo Malgaretti, Malte Kaspereit, Jens Harting, Ana-Sunčana Smith, Modelling diffusive transport of particles interacting with slit nanopore walls: The case of fullerenes in toluene filled alumina pores, vol 368, 2022, 0167-7322