Adsorption and Chromatographic Separation of Chain Molecules on Nanoporous Substrates

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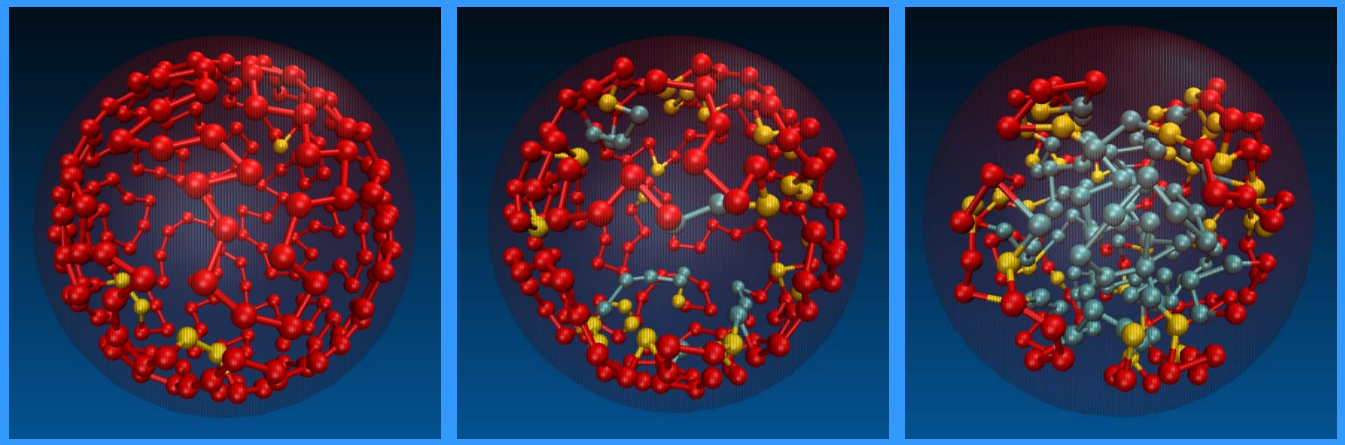
Polymer simulation: We aim at a fundamental understanding of the physico-chemical mechanisms of polymer adsorption in nanopores. To that end, we have implemented a novel Monte Carlo algorithm that can ascertain the free energy of a given polymer chain, leading to accurate predictions of separations and conformations.



(Left) Snapshots of a 200 monomer chain adsorbing in a spherical pore. Left, temperature of T^* = 1, center 2, and right 8. Color indicates layering: red is monolayer, yellow is second layer. Strong adsorption is noted at low temperatures, while entropic effects dominate at higher temps.

(Bottom) Relative efficiency of our new method versus the traditional method, in number of MC steps for identical accuracy. The new method is about an order of magnitude more efficient.

To predict the partitioning of polymers, accurate values for the free energy of adsorbed molecules must be calculated. We have implemented a polymer extension to the gauge cell mesoscopic ensemble Monte Carlo method, which allows one to "measure" the chemical potential of chain molecules faster than currently available methods.

The results of this project served a foundation on the full-scale NSF-GOALI grant proposal awarded to the PI in 2011.