SOFT MATERIALS RESEARCH CENTER

SPECIAL SEMINAR SERIES

Atomistic molecular simulations of lyotropic liquid crystal nanopores

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We design and characterize new materials at the nanoscale through the use of theory and atomistic molecular simulation. We have been using these methods to study the atomistic details of the structure of lyotropic liquid crystals (LLC) membranes. As explored by the Gin and Noble groups, LLC's can form nanostructured materials that can be modified, assembled and crosslinked into stable membranes with uniform straight pores. Pore diameters on the order of 1 nm make LLC membranes well-suited for aqueous separations such as desalination and biorefinement. In theory, these LLC pores can perform solute specific separations and offer the ability to control pore architecture at the atomic length scale. However, a lack of understanding of the molecular details of these nanoporous materials have meant that that it is impossible to systematically improve them.

We have created an atomistically detailed molecular model which is maximally consistent with experimentally measured structural features and material properties. We have developed methods to simulate the crosslinking mechanism, simulate X-ray diffraction (XRD) patterns and measure ionic conductivity from atomistic simulations. Having characterized the atomistic details of the nanopores, we will next study the atomistic details of diffusion of solutes through these pores to better understand their differential transport behavior.

Wednesday, November 15th at 1:30 p.m. in Duane Physics G126

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