Physical Chemistry Seminar

Tuesday, March 1, 2016

11:00 am Room 1315 Chemistry Building

Atomistic Hydrodynamics and the Dynamical Hydrophobic Effect in Porous Two Dimensional Crystals

Professor Joel Eaves

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Host: Ned Sibert

Porous two dimensional crystals offer many promises for applications in water desalination, but for computer simulation to play a predictive role in this area, one needs to have reliable methods for simulating an atomistic system in hydrodynamic currents. In this talk I will describe our methodology and show how statistical mechanical models give microscopic insights into the collective and atomic interactions that control aqueous flows through atomically thin and narrow channels. The hydrophobic effect can both help and hinder water transport in these materials and has important manifestations at small and large lengthscales, in and out of thermal equilibrium.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students can meet with the speaker in Room 8305F at 1:00 pm