



**March 13, 2017, 12:00 pm**

**Seaver Science Library, Room 150**

*SSC Auditorium next to the library*

## **Professor Joel Eaves**

*Department of Chemistry and Biochemistry*

*University of Colorado Boulder*

# **Aqueous Flow Through Two-Dimensional Crystals**

### **Abstract:**

In this talk, I will describe our recent work on the dynamics of water moving through porous two-dimensional crystals, like perforated graphene. These systems are promising candidates for the next generation of reverse osmosis membranes because they are atomically thin. But they also remain challenging to model because the motions of individual water molecules moving through the pores of the membrane bottleneck the macroscopic current across it. I will briefly describe the method that we have developed to perform atomistic simulations for this class of systems and then use it to establish a connection between fast water passage and the types and strength of intermolecular interactions accessible in the burgeoning library of two-dimensional crystals. The out-of-equilibrium hydrophobic effect is subtle, with competing static and dynamical aspects that have analogs to capillary action and hydrodynamic friction. Using a random walk model, we find a surprising connection between the transport of individual water molecules and the clogging dynamics of granular flows.

Hosted by Professor Anna Krylov

*The scientific community is invited*

**USC Department of Chemistry**

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