# Center for Dynamics and Control of Materials: *MRSEC Seminar*

## *Few and Far In-between: Probing The Structure-Selectivity Relationship In Membranes Using Path Sampling Techniques*

## Monday, November 7th, 1.30 pm-2.30 pm

**utexas.zoom.us/j/98071041801**

The ability of semipermeable membranes to selectively impede the transport of undesirable ions and molecules is key to many applications, from desalination and gas separation to biological membrane transport. For instance, membranes that are only permeable to water and reject most other ions and molecules are used in water desalination. Designing more selective membranes requires characterizing the kinetics and mechanism of the transport of the species rejected by the membrane. The timescales associated with such processes, however, can be too long to be accessible to conventional MD simulations. Moreover, the non-equilibrium nature of the underlying separation processes excludes the utilization of advanced sampling techniques that require microscopic reversibility. Finally, the separation of timescales between the transport of desirable species (such as water) and undesirable species (such as salts) will result in considerable changes in reservoir concentration throughout an MD trajectory, which can skew the kinetics and mechanism of transport in ways that are difficult to quantify and correct. Recently, we utilized jumpy forward flux sampling (jFFS), a path sampling technique developed in my group, and non-equilibrium MD to study pressure-driven ion transport through nanoporous graphitic membranes. Our approach addresses all these challenges. It not only allows us to accurately and efficiently estimate arbitrarily long mean first passage times in pressure- and field-driven filtration processes, but also to compute fluxes and permeabilities within a pseudo-equilibrium ensemble in which both reservoirs are at different- but almost constant- chemical potentials.

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