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Simulating and Modeling Transport Through Atomically Thin Membranes JOSEPH OSTROWSKI, JOEL EAVES, University of Colorado, Boulder — The world is running out of clean portable water. The efficacy of water desalination technologies using porous materials is a balance between membrane selectivity and solute throughput. These properties are just starting to be understood on the nanoscale, but in the limit of atomically thin membranes it is unclear whether one can apply typical continuous time random walk models. Depending on the size of the pore and thickness of the membrane, mass transport can range from single stochastic passage events to continuous flow describable by the usual hydrodynamic equations. We present a study of mass transport through membranes of various pore geometries using reverse nonequilibrium simulations, and analyze transport rates using stochastic master equations.

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