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Study of Evaporation Rate of Water in Hydrophobic Confinement using Forward Flux Sampling SUMIT SHARMA, PABLO G. DEBENEDETTI, Princeton University — Drying of hydrophobic cavities is of interest in understanding biological self assembly, protein stability and opening and closing of ion channels. Liquid-to-vapor transition of water in confinement is associated with large kinetic barriers which preclude its study using conventional simulation techniques. Using forward flux sampling to study the kinetics of the transition between two hydrophobic surfaces, we show that a) the free energy barriers to evaporation scale linearly with the distance between the two surfaces, d; b) the evaporation rates increase as the lateral size of the surfaces, L increases, and c) the transition state to evaporation for sufficiently large L is a cylindrical vapor cavity connecting the two hydrophobic surfaces. Finally, we decouple the effects of confinement geometry and surface chemistry on the evaporation rates.

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