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Counterintuitive flow from low-pressure bulk to high-pressure nanopore[1] AN ZOU, MANISH GUPTA, SHALABH MAROO, Syracuse University — In a typical pipe or tube, liquid always flows from high pressure to low pressure. Here, we present a counterintuitive phenomenon observed in molecular dynamics (MD) simulations: a passive evaporation-induced liquid flow from low-pressure bulk to high-pressure nanopore. In our simulations, the nanopore is formed between two parallel hydrophilic surfaces, and is connected to a conventional bulk liquid. At equilibrium (without any evaporation/flow), the pore pressure is an order magnitude high than that in bulk due to the strong solid-liquid interaction. Evaporation was achieved by removing atoms at the liquid-vapor interface, while the same amount of atoms were added in the bulk. A steady-evaporation state was reached associated with a constant liquid flow from bulk to nanopore. The bulk pressure maintained similar to that at equilibrium; while the pore pressure was reduced by around 25 atm, but still an order higher than that in bulk. This reduced pressure, from thermodynamically equilibrium state, drives liquid flow from low-pressure bulk to high-pressure nanopore. The work presented here has been published in J. of Phys. Chem. Lett., 11: 3637-3641 (2020).

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