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Water Purification across MoS_2 Nano-porous Membranes MOHAMMAD HEIRANIAN, AMIR BARATI FARIMANI, NARAYANA R. ALURU, Univ of Illinois - Urbana — A 2D material, molybdenum disulfide (MoS_2), is proposed as a nano-porous membrane for water desalination. By performing detailed molecular dynamics simulations, we find that salt ions are rejected efficiently across a single-layer MoS_2 while water permeates at high rates. Depending on the pore area, which ranges from 20 to 60 $Å^2$, the nanopore allows less than 12% of ions to pass through even at theoretically high pressures of 350 MPa. Water permeation across the MoS_2 membrane is found to be as high as 12 $L/cm^2/day/MPa$ which is at least two orders of magnitude higher than that of other existing nano-porous membranes. Pore chemistry is shown to be one of the important factors leading to large water fluxes. MoS_2 pore edges terminated with only molybdenum atoms result in higher fluxes which are about 70% higher than that of graphene nanopores. These findings are explained and supported by the permeation coefficients, energy barriers, water density and velocity distributions in the pores.

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