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Water Desalination with Two-dimensional Metal Organic Framework Membranes ZHONGLIN CAO, VINCENT LIU, AMIR FARIMANI, Carnegie Mellon University — Providing fresh and drinkable water is a grand challenge the world is facing today. Development in nano-materials can create possibilities of using energy-efficient nanoporous materials for water desalination. In this work, we demonstrated that ultrathin Metal Organic Framework (MOF) is capable of efficiently rejecting ions while giving access to high water flux. Through molecular dynamic simulation, we discovered perfect ion rejection rate by two-dimensional multi-layer MOF. The naturally porous structure of 2D MOF enables significantly 3 to 6 orders of magnitude higher water permeation compared to that of traditional membranes. Few layers MOF membranes show one order of magnitude higher water flux compared to single layer nanoporous graphene or molybdenum disulfide without the requirement of drilling pores. The excellent performance of 2D MOF membranes is supported by water permeation calculations, water density/velocity profiles at the pore and the water interfacial diffusion near the pore. Water desalination performance of MOF offers a potential solution for energy-efficient water desalination.

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