

Abstract Submitted
for the DFD20 Meeting of
The American Physical Society

Reasons behind superior water desalination performance of nanoporous MoS₂ ZHONGLIN CAO, VINCENT LIU, AMIR BARATI FARIMANI¹, Carnegie Mellon Univ — Water desalination is one of the most prevailing technologies to solve freshwater scarcity nowadays. Membranes made of two-dimensional (2D) materials such as single-layer MoS₂ and Graphene have been demonstrated to be able to significantly increase the water desalination performance. In this work, we made thorough comparison between popular 2D materials including MoS₂, MoSe₂, Graphene, Boron Nitride, and Phosphorene and conclude that MoS₂ constantly performs 20% - 38% better than the others. We further revealed the reasons of the superior performance of MoS₂ from the perspective of water dynamics and structure near the membrane/inside the pores, and the energy barrier for water molecules to transport through the pore.

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Date submitted: 03 Aug 2020

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