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Ozark Nanopore: Highly efficient and selective Graphene Nanopore designed by Artificial Intelligence for water desalination YUYANG WANG, ZHONGLIN CAO, AMIR BARATI FARIMANI, Carnegie Mellon University — Nanoporous Graphene has been proven to be a strong candidate for water desalination applications. Its ultrathin-thickness makes energy-efficient water desalination possible. The geometry of the pore on Graphene membrane plays a significant role in its water desalination performance. In this work, we proposed a nanopore geometry optimization method for Graphene membrane using Deep Reinforcement Learning (DRL). The nanopore designed using DRL looks similar to Ozark lake fractal shape located in Missouri, enabling significant ion rejection while allowing maximum permeation. The Ozark-shaped pore designed by DRL is shown to have 10% higher ion rejection rate compared with circular pores while allowing the same level of water flux. We further discovered that the reason behind high ion rejection of Ozark-shaped Graphene nanopores is that its shape limited the passage of hydrated ions in some regions inside of the pore.

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