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Tunable water desalination across Graphene Oxide Frameworks
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"Water, water, everywhere, nor any drop to drink." wrote Samuel Taylor Coleridge in 1798. Today's scientific advances in water desalination promise to change the second part of the sentence into "and every drop to drink," by transforming sea water into fresh water and quench the thirst of 1.2B people facing shortages of water. To achieve this, the design of nanoporous materials with high water permeability and coupled with high salt rejection capacity is crucial. Graphene Oxide Frameworks (GOF) materials are a class of porous materials consisting of layers of graphene oxide sheets interconnected by linear boronic acid linkers. Water desalination across GOF is studied using classical Molecular Dynamics simulations. We used quantum mechanically obtained boron-related force field parameters to study the diffusion of water molecules inside bulk GOF. Properties, such as the self-diffusion coefficient of water molecules increases linearly with linker concentration n. Further, the desalination performance of GOF membranes reveals that the water permeability of GOF is several orders of magnitude higher than conventional membranes and an high water permeability can be coupled with a 100% efficiency of salt rejection by choosing the appropriate concentration n and thickness h.

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