Title:	Self-passivated nanoporous phosphorene as a membrane for water desalination.
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Abstract:	Using molecular dynamics simulations, we investigated the mechanism of water transport and ions movement across nanoporous phosphorene for water desalination performance. Phosphorene nanopore areas ranged from 4 Å2 to 41 Å2. The self-passivated phosphorene nanopores showed 100% ability to reject salt ions (Na+ and Cl−) for all pore areas even at higher pressures. Water flux through narrow pores exhibits a slow increase while sharper increase and linear dependence is observed for wider pores i.e. D16 and D18. The increase in water flux is attributed to broadened cross-sectional area and dense water layering in the vicinity of pores. The desalination performance is strongly influenced by structure of nanopore such as size, shape; water-membrane interaction and applied pressure. Further, oxygen density maps reveal the hydrophilic nature of phosphorene nanopores hence, it effects the water flux. Our results also indicate that during the entire simulation, pore atoms of the membrane retained their atomic arrangement implying the stability of phosphorene as a membrane. Findings of this work establish molecular insight into phosphorene desalination performance, which helps in systematic design of water treatment plants.
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