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Charged nanoporous graphene membrane for enhancing reverse osmosis water desalination performance. CHINH NGUYEN, ALI BESKOK, Southern Methodist University — Positively and negatively charged single-layer nanoporous graphene membranes are investigated for applications in water desalination using molecular dynamics (MD) simulations. Pressure-driven flows are induced by moving specular reflection boundaries with a constant speed. Simulations are performed for hydraulic pore diameter membrane as large as 14.40 Å with four different electric charges distributed on the pore edges. Salt rejection efficiencies and the resulting pressure drops are compared with the obtained base-line case of 9.9 Å diameter uncharged nanoporous graphene membrane, which exhibits 100% salt rejection with 35.02 MPa pressure drop at the same flow rate. For the positively charged membranes, q = 9e shows 100% and 98% rejection for Na^+ and Cl^- ions respectively, with 35% lower pressure drop than the reference. For the negatively charged membranes, optimum rejection efficiencies of 94% and 93% are obtained for Na^+ and Cl^- ions with q = -6e, which requires 60.6% less pressure drop than the reference. The results indicate the high potential of using charged nanoporous in reverse osmosis (RO) desalination systems with significantly enhanced performance.

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