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Effects of surface group deprotonation on the water desalination by graphene oxide membranes CHAO FANG, ZHOU YU, RUI QIAO, Department of Mechanical Engineering, Virginia Tech — Graphene-based membranes have shown great potential in enabling highly efficient water desalination from salty water. Effectively engineering these membranes necessitates a fundamental understanding of how the molecular structure and chemical details of the nanopores in these membranes govern the transport of water and ions through them. Here, we use molecular dynamics simulations to investigate how deprotonation of the carboxyl groups along the perimeter of the nanopores in single-layer graphene oxide membranes affects the water transport and salt leakage through these pores. Modest deprotonation lowers the energy barrier for water translocation through the pores and thus enhances the water flux; too strong a deprotonation, however, reduces the water flux by slowing down the dynamics of water molecules inside the pores. These effects are pronounced for pores with a diameter of 0.68nm but is weak for pores with a diameter of 1.12nm. Deprotonation only modestly increases the ion leakage through the nanopores. These results suggest that the deprotonation of the surface groups in graphene oxide membranes may be tailored to improve the performance of these membranes.

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