Molecular Simulations Insights into the Performance of Hybrid Graphene Oxide Membranes for Water Treatment

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The scarcity of fresh water represents a serious global concern, which is predicted to worsen in the future [1]. Recently, nanoporous membranes have attracted considerable attention due to their remarkable potential for the removal of ions and pollutants immersed in water [2]. Graphene oxide (GO) can be regarded as an 'ultimate' membrane, because it is stronger, thinner and more chemically resistant than the amide layers [3]. Moreover, the characteristic nanochannels of GO nanosheets can be manipulated via intercalation of embedded organic molecules and/or polymeric structures, to form hybrid materials with enhanced desalination and water treatment properties. The confinement effects on the separation parameters such as adsorption and diffusion, is far from being straightforward. Hence, in this study, we have designed multilayer graphene oxide membranes embedded with organic molecules, and the effects of different parameters, such interlayer spacing, functionalization and the pressure have been examined by using equilibrium and non-equilibrium molecular dynamic simulations [4,5], in order to increase permeability and impurities rejection, while comparing with experimental results. Analysis of the simulation results suggests that upon adsorbing on the GO surface, the translational motion of some impurities in water would be suppressed. Nevertheless, hydrophilicity affects the permeability for membranes, owing to these strong hydrogen bonds.

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