Functionalized Graphene Nanosheets as Filtration Membranes for the Removal of Cd$^{2+}$ from Wastewater

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ABSTRACT

Toxic metals such as Pb, Cu, Cd, Zn, Ag, and Hg can be seen in industrial wastewater. The existence of these heavy metals in environment can cause liver and kidney disease, and thus is extremely harmful. Filtration-based membranes, such as reverse osmosis and nanofiltration membranes, can help to remove heavy metals from contaminated water by physical separation. The membrane acts as a barrier that allows only water molecules to pass through, while blocking pollutants, e.g., heavy metal ions. The process can effectively reduce the concentration of heavy metals in water, making it safer for consumption and other uses. In this study, the performance of nonporous graphene (NPG), which is functionalized by hydrogen (NPG-H) and hydroxyl (NPG-OH) as a nanostructure membrane, has been investigated by molecular dynamics techniques. These membranes had two different pore sizes, for which the radius is 5 and 10 Å, respectively, leading to 4 different types of membranes. An external pressure was applied to the system to mimic pressure-driven filtrations. It was found that with a small pore (5 Å), both NPG-H and NPG-OH totally rejected Cd$^{2+}$ and Cl$^{-}$, while with a large pore (10 Å), Cd$^{2+}$ gradually passed through NPG-H and NPG-OH membranes. In terms of water molecules filtered, membranes with large pores have a larger permeability compared to those with small pores. For the effects of functional groups, compared to NPG-OH, NPG-H can allow more water molecules to permeate the pore, regardless of pore sizes. On the other hand, the rejection rates of functional groups for Cd$^{2+}$ and Cl$^{-}$ show dependences on pore sizes. The underlying mechanisms for these observations will be explored. The results obtained shed lights on the effects of pore sizes and functional groups on water permeability and Cd$^{2+}$ rejection rate for graphene-based filtration membranes.