INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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SHORT ABSTRACT

The applicability of graphene oxide (GO) and graphene for separation and purification applications is investigated using non-equilibrium molecular dynamics (MD) simulations. The effect of internal structure of the layered GO membrane on its performance as a forward osmosis (FO) membrane for sea water desalination and dehydration of acetic acid is studied. GO membranes composed of nanosheets of smaller lateral dimensions found to have higher water permeance and lower salt rejection than GO membranes composed of nanosheets of larger lateral dimensions. The performance of layered GO membrane is also dependent on its interlayer distance. The water permeance increases and the draw solute rejection decreases as the interlayer spacing between the GO layers increases to an optimum value, after that, with further increase in the interlayer spacing the water permeance decreases and the salt rejection of the membrane increases.

The presence of the cations can also significantly influence the performance of layered GO membranes both in FO and reverse osmosis (RO) processes. For the same interlayer spacing, the cation intercalated layered GO membranes have higher water flux as compared to corresponding pristine layered GO membranes. On the other hand, the intercalation of the cations (K^+, Mg^{2+}) lead to higher rejection of Na^+ ions whereas the rejection of Cl^- ions slightly decreases.

In this present study, the electro-osmotic flow behavior through a graphene nanochannel with surfaces having striped charge distribution are also discussed in detail using non-equilibrium molecular dynamics simulations. The velocity of the water molecules and the water permeance through the nanochannel gradually increases with the increase in surface charge density from 0.005 Cm^{-2} to 0.025 Cm^{-2}. With further increase in the surface charge density beyond 0.025 Cm^{-2}, the velocity of the water molecules and the water permeance through the nanochannel gradually decreases. Here the thickness of the diffuse layer and the interaction between water molecules and the wall play significant roles in determining the flow behavior through the nanochannel.