**REVIEW PAPER 01**

**TITLE**

**Salt separation from water using graphene oxide nanochannels: A molecular dynamics simulation study**

**OVERVIEW**

One of the greatest concerns of the twenty-first century is the increasing shortage of freshwater, which is a result of the fast industrialization, climate change, and global environmental contamination. This increased interest in creating new, affordable desalination techniques for supplying companies and communities with fresh water. Numerous nano-structured materials have been shown to be more effective against RO-membranes in recent years. This includes graphene, carbon nanotubes (CNTs), carbon nanowires, nanoparticle-embedded-thin film nanocomposites and covalent triazine frameworks (CTFs), as well as novel zeolitic frameworks. Graphene, on the other hand, has far greater salt rejection than CTFs and its characteristics can be readily modified by functionalization, making it one of the most promising options for the next generation of desalination membranes. In addition to single-layer graphene uses, multilayer stacked graphene oxide (GO) membranes have been discovered to achieve ion separation from saline water. This is an especially appealing technique since GO membranes are simple to manufacture on a big scale and can be simply assembled into stacked layers.

**MATERIALS AND METHODS**

The molecular structure of GO contains hydroxyl, epoxy formyl and carboxyl groups randomly distributed on both sides of the graphene sheet. The GO model use in this work consists of randomly distributed hydroxyl groups on both sides of the 3 nm × 3 nm pristine graphene sheet. All simulations are carried out using the LAMMPS molecular dynamics simulation package. The all atom optimized potentials for liquid simulations (OPLS–AA) force field was used for both the GO as well as for the Na+, and Cl− ions. The OPLS force field is optimized for TIP3P and TIP4P water models and the latter water model is computationally expensive.

**RESULTS AND DISCUSSION**

The dynamic stability of hydrogen bonds between water and OH groups by calculating continuous hydrogen bond correlation function, and intermittent hydrogen bond correlation. The results presented in this work highlight a trade-off between the high separation efficiency found in narrower channels and a greater water permeance observed for the wider ones. Moreover, the higher oxidation of the graphene oxide channels also bears a negative effect on the water permeance. The results are given in the hope to improve the understanding of the behavior of GO membranes in the context of desalination, with the long-term goal of aiding the development of novel and much needed technologies for facing the growing need of fresh water.

**CONCLUSION**

In this work, molecular dynamics simulation techniques were employed to investigate the ion separation efficiency and water structure in pristine graphene and graphene oxide nanochannels of varying interlayer spacing and oxidation degree. Among the systems tested, the graphene oxide nanochannel with 10% or lower oxidation and a 0.8 nm interlayer spacing show the best ion separation efficiency while retaining a high enough water permeance, making it an interesting choice for the development of future water desalination membranes. Furthermore, the water structure inside the nanochannels is strongly affected by the interlayer spacing and oxidation degree, which can greatly affect the desalination performance of these systems. The results from this work also show that water molecules prefer flowing through the unoxidized regions of the narrower channels, suggesting the existence of capillary channels. Nevertheless, water flow was observed through both oxidized and unoxidized regions of the larger channels.