**Removal of Heavy Metal Ions Using Functionalized Graphene Membranes: A Molecular Dynamics Study**

**Objective**

In this study classical molecular dynamics (MD) simulations and density functional theory (DFT) calculations was used to investigate the desalination performance of nanoporous graphene (NPG) membranes for different pore sizes and chemical functionalization (hydroxyl, nitrogen and fluorine) of the pore.

**Methodology**

The functionalized NPG sheet is prepared by drilling off the carbon atoms from a GS of size 20  
Å x 20 Å. In order to perform MD simulations, they have replicated the DFT optimized 20 Å functionalized graphene sheet to create the GS membrane of size 110.55 Å × 106.36 Å having 25 pores. This is placed parallel to the *xy* plane in the center of the simulation box. The pores are functionalized using functional groups: hydroxyl (NPG-OH), nitrogen (NPG-N) and fluorine (NPG-F). All MD simulations are carried out with LAMMPS software. These simulations are performed for systems with various aqueous solutions of Cd(NO3)2, Cu(NO3)2, Pb(NO3)2, Co(NO3)2 and Zn(NO3)2 ionic salts. TIP3P model is used to represents the water molecules, and OPLS (optimized potential for liquid simulation) parameters are used for metal ions, GS and functional  
groups. The long-range electrostatic interaction is accounted using particle**-**particle particle**-**mesh (PPPM) technique. The carbon atoms in GS are modeled as uncharged and kept rigid. On the other hand, the functional groups on the GS pores are kept flexible.

**Findings**

This study shows that the NPG functionalized with N (NPG-N) shows higher salt rejection with  
intermediate permeability compared NPG functionalized with F (NPG-F) and OH (NPG-OH).  
NPG-OH shows higher water permeability with lower salt rejection compared to NPG-N and  
NPG-F. However, NPG-F shows lowest permeability compared to other two NPGs considered in  
this study. Even at high pressures like 500 MPa the salt rejection percentage is not less than 90%  
and the minimum permeability is 270 L/cm2-hr-bar.