**Removal of Pb (II) Ion Using PAMAM Dendrimer Grafted Graphene and Graphene Oxide Surfaces: A Molecular Dynamics Study**

**Objective**

The main objective of this research was to investigate the molecular mechanisms involved in the adsorption of metal ions on the graphene, graphene oxide, and polyamidoamine (PAMAM) dendrimers with different terminal group grafted graphene and graphene oxide surfaces.

**Methodology**

Using VMD software, GS of 71Å×71Å sheet was built. For the atomistic GO model,   
hydroxyl and epoxy groups functionalized on the basal plane. The epoxy and hydroxyl groups are randomly grafted to the carbon atoms on a 71 Å × 71 Å graphene basal plane. The carboxyl groups are also attached to the carbon atoms on the edges randomly. A covalent bond was made between the GS/GO and the dendrimer by using the AMBER LEAP module. The electrostatic potential (ESP) method was used for charge calculation during optimization. The TIP3P model was used to model water-water interaction, and OPLS (optimized potential for liquid simulation) parameters are used for metal ions, and graphene, and different terminal groups of the PAMAM dendrimer. All MD simulations were carried out using the LAMMPS package.

**Findings**

Increasing the salt concentration in the ionic solutions will affect the density profiles of metal ions near the bare GO and dendrimer grafted GO surfaces. The maximum adsorption capacity of Pb2+ ion on the GO-PAMAM-COO- surface, calculated from this work, is ∼62% higher than that from the experimental work. diffusion coefficient for Pb2+ ions near the different surfaces decreases with increasing metal ion concentration. The results show that adsorption capacity of the Pb2+ ion is improved significantly using carboxyl terminal groups of dendrimer grafted on a graphene oxide surface.