**Molecular dynamics simulation of the adsorption properties of graphene oxide/graphene composite for alkali metal ions**

**Objective**

Materials Studio (MS) software was used to simulate the molecular dynamics of the interaction between graphene oxide/graphene (GO/G) composite and alkali metal ion (M+). Based on the calculation of the interaction energy, diffusion coefficient and radial distribution function (RDF), The adsorption law of GO/G on M+ was investigated and its mechanism was revealed.

**Methodology**

In this work Materials Studio was used to establish the interaction between M+ solution and GO/G and performed molecular dynamics simulations. First, a two-dimensional (2D) G and GO models were constructed. The condensed phase optimized molecular potential for atomistic simulation studies (COMPASS) Force Field was used in geometry optimization and dynamics calculation. The layered models of interaction between M+ solution and GO/G composite were constructed. MD simulations of the interactive layer models were performed in the NVT (constant number of particles, volume, and temperature) ensemble. To ensure accuracy of computing results in the shortest possible time, in this work, the time step, total simulation time and output per frame are set as 1 fs, 2000 ps and 5000 steps, respectively.

**Findings**

The calculated results show that the interaction energy between different M+ and GO/G is negative, indicating that the interaction between them is mutual attraction. The energy of GO/G composites and the total energy of M+-GO/G increase with the increase of M+ radius. The larger the hydrated ion radius of M+ is, the larger the diffusion coefficient is. According to RDF analysis, M+-GO and M+ - O (GO) both have bonding within 3.5 Å and nonbonding after 3.5 Å, and the non-bonding interaction of M+-GO is greater. However, the bonding interaction between M+-O(GO) is larger than the non-bonding interaction, indicating that there are bonding and nonbonding interactions in the system when GO/G composite adsorb M+. The interaction between M+ and GO surface is mainly provided by non-bonding interaction, while the interaction between M+ and O atoms of GO surface is mainly provided by bonding interaction.