**Adsorption of xanthate from aqueous solution by multilayer graphene oxide: an experimental and molecular dynamics simulation study**

**Objective**

In this paper, MGO rich in oxygen-containing functional groups and a typical two-dimensional fold structure was prepared, and the adsorption performance and mechanism for xanthate in wastewater were studied.

**Methodology**

The Forcite module of Materials Studio 8.0 was used for molecular dynamics simulations. The sp2 hybridized carbon was treated as uncharged Lennard-Jones spheres. A rectangular simulation cell of MGO with three-dimensional perimeter conditions of 39.5 × 29 × 100 Å (*X* × *Y* × *Z*) was built using an amorphous cell module containing 4 xanthate and 1000 water molecules (SPC model). The optimization and simulation were performed in two stages. During the first stage, constant pressure–temperature (NPT) time integration was performed using a Berendsen barostat and a Nosé–Hoover thermostat for 1 ns. Subsequently, a vacuum slab was added to the top of the system and ensuing molecular dynamics simulations were performed using the Nosé–Hoover thermostat in the canonical (NVT) ensemble. The temperature was 298.15 K, the simulation time was 10 ns, the van der Waals interaction cut-off was 12.5 Å, and the time step was 1.0 fs. The simulation of 5 ns after the balance period was the foundation of the ultimate calculation results. The polymer consistent force field (PCFF) of the Forcite module was used in the MD simulations.

**Findings**

It was demonstrated that the head group of the xanthate molecule was adsorbed on to the  
surface of MGO and the tail group faces the water, which meant that the electrostatic interaction between the head base of xanthate and MGO is greater than the van der Waals force interaction between the tail base and MGO. The maxima of head and tail groups appeared at 15.4 Å and 16.1 Å, respectively, indicating that the hydrophilic head group is more proximal to the MGO surface than its hydrophobic tail group. This signifies that the van der Waals force is stronger between the xanthogen group and the hydrophilic site of the MGO surface. The deformability of xanthate increased as the adsorption progressed, leading to an increase in the dispersion force between the head group and MGO. An implication of this is that the dispersion force is the dominant force affecting the process of xanthate adsorption by MGO.