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

**Objective**

The heavy metal ions (lead, Pb) adsorption process was studied using an artificial intelligence simulation based model for prediction of the adsorption process by using magnetic ash/graphene  
oxide (GO) nanocomposite. Also, the adsorption mechanism of Pb ions on the adsorbent were investigated using molecular dynamics (MD) calculations in aqueous solution.

**Methodology**

Simulation of data about the lead ion removal using magnetic nanocomposite was performed through a machine learning model using artificial neural network (ANN) method. The JMP software was used for ANN calculations that can predict the output parameter and provide the relation of the input and output parameters. The structure of ANN model was optimized by trial and error via changing the type of  
network, activation functions, and node. The model was established with two hidden layers which include linear and non-linear activation functions for predicting the Eq. concentration as output. The validation technique was performed using KFOLD and in all models K was 3.

**Findings**

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. The results showed that the adsorption process between M+ and the GO/G complex surface is mutual attraction. The GO/G complex structure has a greater adsorption activity for M+ with a larger radius. The larger the hydration ion radius of M+, the stronger the diffusion of M+ during adsorption with GO/G. The obtained model was assessed in  
prediction of equilibrium concentration, and revealed that increasing the initial concentration of heavy metal ions had a significant effect on the equilibrium concentration and Pb ion removal, while the initial temperature of solution does not change the equilibrium concentration significantly.