**Molecular dynamic simulation and artificial intelligence of lead ions removal from aqueous solution using magnetic-ash-graphene oxide nanocomposite**

**Objective**

The objective of this paper was to study adsorption process of metal ions (lead). An artificial neural network (ANN) model was used to predict the adsorption process by using a nanocomposite material of ash/graphene oxide. Adsorption mechanism was investigated using molecular dynamics simulations in the aqueous solutions.

**Methodology**

The experiments of Pb ions removal from aquatic media were performed in batch mode. In each experiments the effect of different operating parameters including temperature and the initial  
concentration of Pb ion in the solution on the removal process were studied.

The Materials Studio software was employed to analyze the molecular quantum calculations through DFTB+ module. The Hyperchem software was used for initial geometry optimization  
of different structure. In every calculation, a mixture of 12 molecules of heavy metals, five molecules of water and one molecule of adsorbent were simulated, and the low energy configurations and energy distribution of the mixture were calculated. Simulation of data about the lead ion removal using magnetic nanocomposite was performed through a machine learning model using artificial neural network (ANN) method.

**Findings**

The initial concentration of lead had a great effect on Eq. concentration and increasing the initial concentration led to an increment in Eq. concentration. On the other hand, temperature had a lower effect on the Eq. concentration. Increasing the temperature changed the Eq. concentration negligible. The temperature increasing adversely affected the rate of the ion removal which is  
in agreement with the exothermic nature of the process. It can be concluded that the Pb  
ions adsorption on the GO in composite structure is occurred easier due to high reactivity of GO molecule instead of ash. 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.