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Applications of molecular modelling in environmental chemistry

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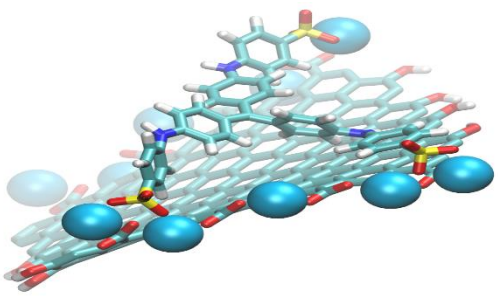
Abstract

Recently the presence of micro-pollutants such as pharmaceuticals, hormones, herbicides, insecticides, pesticides and industrial chemical products such as perfluorinated compounds and flame retardants become crucial problem in aquatic environments. Concentration of some micro-pollutants is under the detection limit of analytical chemical methods thus special separation and techniques are needed for their quantitative measurements. As they are bioactive materials, therefor understanding their interaction with components of aquatic system is needed.

Classical molecular dynamics (MD) simulation, based on solving the Newton equation of motion, is one of the computational methods, which can give very useful information about such interactions. As many micro-pollutants have hydrophobic groups, thus they can show surface propensity to the air/water interface thus influence the bulk and surface properties of water. Understanding the interfacial properties of dissolved micro-pollutants with soil components can provide useful information on dissolution, aggregations or precipitation of them in aqueous solutions.

In this talk briefly, the machinery of MD simulation will be introduced then the properties of electrolyte solutions will be discussed. After introduction of MD, some applications of MD simulation for prediction of properties of electrolyte solutions will be presented then some applications of MD simulations in environmental chemistry applications such as the interaction of micro-pollutants with models of humic acid and fulvic acid will be presented.

The results of MD simulation to reveal the interaction of ions and micro-pollutants with nano-particles such as graphene oxide will be discussed. Interactions, dynamical and structural properties from MD simulations for nano-materials such as graphene oxide revealed that it is potential material for removal of micro-pollutants such as drugs, pharmaceutical and personal care products from aquatic environments.



Interaction of graphene oxide with methyl blue.