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Study of surfactant adsorption on graphene nanosheets by molecular dynamic simulation

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Abstract
Graphene is used in various fields such as energy, composite, biotechnology, electronics, and so on due to its two-dimensional structure, high surface area and unique mechanical, thermal, optical and electrical properties. However, these applications depend on the mass production of high quality and low cost graphene. Direct graphene exfoliation from graphite parts in aqueous solution of surfactants is considered as one of the graphene production techniques. This method is limited to the accumulation of exfoliated hydrophobic graphene sheets in aqueous solution, leading to a decrease in the concentration of monolayer graphene. Physical adsorption of surfactants on graphene surfaces plays a major role in dispersing graphene nanosheets in aqueous medium. Understanding the adsorption mechanism and self-aggregation of surfactants on the graphene surface is of great importance for better optimization of the graphene dispersion process. This study aims to analyze the adsorption of a mixture of cation-rich and anion-rich surfactants on graphene nanosheets using molecular dynamics simulations, followed by the effect of temperature, the presence of electrolytes and alcohol in aqueous solution of surfactants on the adsorption phenomenon. The results showed that by adding an electrolyte to the aqueous solution of surfactants, the surfactant adsorption on the graphene surface was improved.
Keywords: Graphene, Adsorption, Surfactant, Molecular dynamic simulation.