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Comparing graphene and graphene oxide nanosheets in dye adsorption: Molecular dynamics simulation study

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Abstract

Adsorption is one of the most effective methods in water purification processes such as dye removal from aqueous medium. Various adsorbents are applied; at present, the use of graphene nanoplates and its derivatives such as graphene oxide nanosheets has been highly regarded due to their unique properties at the atomic level. In this paper, molecular dynamics simulation at temperature 298 K is applied to compute and compare some properties including zdensity, potential of mean force, mean square displacement analysis and adsorption capacity of the aqueous medium on the graphene and graphene oxide nanosheets. According to the current results, the graphene oxide nanoplate is appropriate for dye adsorption. Interestingly, this observation is comparable with experiment.

Keywords: ***Adsorption- Dye- Graphene oxide nanosheet- Molecular dynamics simulation.***