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Adsorption of ACID-RED 88 on graphene nanosheet: A molecular dynamics simulation

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Abstract

Water is one of the most important compounds necessary to survive on the Earth, which directly affects the health of the community, industry and the economy. Therefore, water treatment and reuse of wastewater are important aspects of water resources management. Dyes are considered as water pollutants, which are found to be very high in the wastewater of textile, cosmetics and food industries. One of the effective ways to remove this pollutant is adsorption by an adsorbent. One of the proposed materials is the graphene's nanosheets. By investigating the radial distribution function, hydrogen bond interactions, combined distribution function and calculating the dye position relative to the adsorbent, the present molecular dynamics simulation at 298 K shows that graphene nanosheet has the acceptable ability to adsorb molecules of the dye from the water. Comparing with experiment confirms that graphene nanosheet can be applied at purification of wastewater in related industries.

Keywords: *Water- Adsorption- Graphene nanosheet- Purification- Molecular dynamics.*