**ABSTRACT**

Adsorption of methylene blue (MB, cationic) and methyl orange (MO, anionic) dyes by [graphene oxide](https://www.sciencedirect.com/topics/physics-and-astronomy/graphene-oxide" \o "Learn more about graphene oxide from ScienceDirect's AI-generated Topic Pages) (GO) and [reduced graphene oxide](https://www.sciencedirect.com/topics/physics-and-astronomy/reduced-graphene-oxide) (rGO) were investigated experimentally. To understand the adsorption properties of rGO with dyes, dye-rGO interaction was analysed by [density functional theory](https://www.sciencedirect.com/topics/physics-and-astronomy/density-functional-theory) (DFT). The GO was predominantly decorated by oxygen functional groups and rGO was characterised by both oxygen functional groups and [vacancy defects](https://www.sciencedirect.com/topics/physics-and-astronomy/vacancy-defect). Fast and efficient adsorption of both MB and MO dyes was observed by rGO while GO showed higher adsorption of MB compared to MO. Studies reveal that the interaction of cationic dye with GO was found to be facilitated by oxygen functional groups via [electrostatic](https://www.sciencedirect.com/topics/physics-and-astronomy/electrostatics) interaction whereas interaction of cationic and anionic dyes with rGO was found to be facilitated by oxygen functional groups and [vacancy defects](https://www.sciencedirect.com/topics/physics-and-astronomy/vacancy-defect), via [electrostatic](https://www.sciencedirect.com/topics/physics-and-astronomy/electrostatics) and [π](https://www.sciencedirect.com/topics/materials-science/polyimide) – [π](https://www.sciencedirect.com/topics/materials-science/polyimide) interactions. The results could be useful for the designing and understanding of adsorbents capable of removing cationic and anionic dyes (mixed dye) from waste water.