Materials Advances

PAPER

View Article Online
View Journal | View Issue

Cite this: *Mater. Adv.*, 2025, **6**, 5648

Design and DFT-based optimization of a GO-containing guar gum hydrogel for dye removal†

Reyaz Ahmad Rather, Jan Mohammad Mir, Mushtaq Ahmad Bhat and Aabid Hussain Shalla*

Received 23rd April 2025,
Accepted 22nd June 2025

DOI: 10.1039/d5ma00389j

rsc.li/materials-advances

A superabsorbent hydrogel composed of graphene oxide (GO), guar Gum (GG), and resorcinol (Res), cross-linked by lanthanum nitrate trihydrate (La^{3+}) ions, was synthesized through the solvent rotation method. All the components involved in the formation of the hydrogel complex were optimized separately using the Gaussian16W/GaussView6.1 software package and density functional theory (DFT), followed by the optimization of the complex and the target dye crystal violet (CV). The Stuttgart–Dresden (SDD) basis set and the WB97XD functional were used for the GO–GG–Res–La(III) complex, and for the rest of the computations, the combination of B3LYP functional and 6-311G(d,p) basis set was used. To correlate the adsorption of CV with the designed hydrogel, the key electronic structures and the covalent and non-covalent factors responsible for the adsorbent behaviour were examined. Moreover, molecular orbital energies, electronegativity, ionization energy, electron affinity, and other global reactive descriptors were explained in the context of the aim of this study. Experimentally, the prepared hydrogel exhibited significant swelling behaviours in water across solutions of varying ionic strengths and pH environments for both GO and non-GO beads. The equilibrium elimination capacity of the crystal violet (CV) dye increased from 134.88 mg g^{-1} to 234.32 mg g^{-1} in deionized water and from 226.66 mg g^{-1} to 241.09 mg g^{-1} at pH 9, both with and without graphene oxide (GO), respectively. Various kinetic adsorption isotherms were also applied. The enhanced dye removal efficacy of CV supported by the DFT integrated experimental studies, indicates the potential of these hydrogel beads in wastewater treatment.

1. Introduction

Fast industrialization and population growth are the two primary aspects of the modern world that are primarily responsible for the increased release of hazardous pollutants, including pharmaceuticals, biomedicals, dyes, heavy metals, and pesticides, into the environment. The accelerated production and use of such hazardous materials have caused devastating environmental issues, which are primarily related to air, soil, and water. Water pollution is a major pollution caused by industries that frequently release dyes, heavy metals, and various other organic pollutants.[1,2] Dyes such as methylene blue (MB), methyl red (MR), and crystal violet (CV) are known for their carcinogenic nature.[3] The CV dye falls in the category of triarylmethane-based systems, and in aqueous solution, it transmits a violet color. All these organic dyes, including CV, have severe impacts on human health and marine life, even at low concentrations.[4] These dyes could induce hazardous effects on the eyes and skin, and inhaling them causes digestive tract irritation.[5] Among the vast number of such pollutants, synthetically prepared dyes produce toxic chemicals with carcinogenic nature *via* different processes, causing severe harm to the environment and to the overall health of humans and animals.[6,7] In the aquatic environment, these dye molecules inhibit photosynthetic activity due to a reduction in light transmittance.[8,9] In the water treatment, desalination and purification industries, hydrogels are the first choice of material. In most cases, they are made up of either synthetic or natural polymers and are suitable for the removal of a broad variety of pollutants, including dyes, agricultural wastes, pesticides, and heavy metal ions, which are particularly found in water.[29] For the removal of water pollutants, mainly dyes, numerous methods have been used for water treatment, including chemical deposition, ion exchange,[10] adsorption,[11–13] coagulation–flocculation,[11] photocatalytic degradation,[14]

Soft Chemistry Lab, School of Sciences, Islamic University of Science and Technology, IUST Awantipora, J&K, 192122, India. E-mail: Sheenf@gmail.com

† Electronic supplementary information (ESI) available. See DOI: https://doi.org/10.1039/d5ma00389j