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ARTICLE

Experimental and DFT Modeling Studies for the Adsorptive Removal of Reactive Dyes from Wastewater

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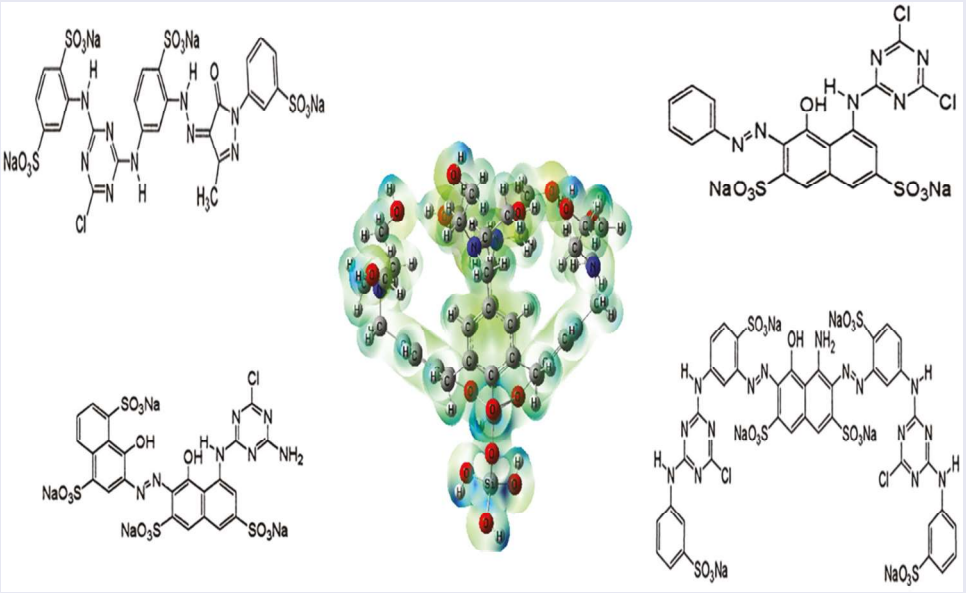
ABSTRACT

The current research demonstrates the adsorptive removal of RY-18, RR-2, RB-13, and RB-171 dyes from wastewater samples using *p*-diethylaminomethylcalix[4]arene silica appended (DSA) resin. The DSA resin shows high adsorption capacity for reactive dyes during the batch adsorption experiments under the optimized parameters such as DSA resin dosage, pH, and temperature. The adsorption equilibrium results were defined by Irving-Langmuir and Freundlich-isotherm models and it was found that the Freundlich model is the best fit with good multilayer adsorption capacity along with good correlation coefficient value (R^2 0.9991) for reactive dyes, while the energy calculated by D-R model describes the adsorption mechanism that is physisorption in nature. Moreover, a thermodynamic study was also performed, which shows that the adsorption of reactive dyes is endothermic and spontaneous in nature. From the kinetic study, it has been revealed that the adsorption takes place by following a pseudo-second-order kinetic model. Besides this, the adsorption phenomenon is explained by density functional theory DFT calculations. The DSA resin was applied onto industrial wastewater samples and it has been observed that above 98% reactive dyes were adsorbed successfully. After washing for regeneration, the DSA resin has above 98% adsorption capacity, which proves that the DSA is a regenerable adsorbent.



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KEYWORDS
Adsorption Modeling Studies; calix[4]arene based adsorbent; reactive dyes; removal of dyes

Introduction

Textile, rubber, paper, and plastic industries release toxic dyes in freshwater springs about 280,000 tons per year. The dyes are also known as water-polluting toxicants because of their adverse effect on humans, which are commonly utilized in daily life activities like

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