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The Removal of a Textile Dye from an Aqueous Solution Using a Biocomposite Adsorbent

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Abstract: The adsorption mechanisms of methylene blue (MB) onto olive waste (residue) treated with KOH (OR-KOH) and onto an OR-KOH and PEG–silica gel composite (OR-KOH/PEG-SG) at various temperatures were investigated using a combination of experimental analysis and Monte Carlo ab-initio simulations. The effects of adsorption process variables such as pH, temperature, and starting adsorbate concentration were investigated. The experimental data were fitted to Langmuir and Freundlich models. The maximum adsorption capacities of MB onto OR-KOH and OR-KOH/PEG-SG adsorbents reached values of 504.9 mg/g and 161.44 mg/g, respectively. The experimental FT-IR spectra indicated that electrostatic attraction and hydrogen bond formation were critical for MB adsorption onto the adsorbents generated from olive waste. The energetic analyses performed using Monte Carlo atomistic simulations explained the experimental results of a differential affinity for the investigated adsorbents and confirmed the nature of the interactions between methylene blue and the adsorbents to be van der Waals electrostatic forces.

Keywords: adsorption; DFT; Monte Carlo simulations; Langmuir–Freundlich

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1. Introduction

To the best of our knowledge, the first use of natural dyes was reported as far back as 2600 BC but only in 1856, when William Henry Perkin attempted to synthesize artificial quinine from allyltoluidine to treat malaria, was the first dye material synthesized which he called "mauve" (aniline, a basic dye). After that, the synthetic dye industry was born [1].

Nowadays, synthetic dyes represent a relatively large group of organic chemical compounds used in our daily life [2,3]. Global production is estimated to be about 700,000 tons/year, of which 140,000 tons are released into effluents during various applications and manufacturing stages because of wrong or negligent discharges [4,5]. If not