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Exploring of new Poly(Thiourea-Amide) as a prospective bismarck Brown Y dye adsorbent: Synthesis *via* ultrasound irradiation, isotherms, kinetic, thermodynamic, and DFT studies

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ABSTRACT

In this work, a facial ultrasound technique was employed to synthesize poly (N^1-((6-aminopyridin-2-yl)carbamothioyl)-N^3-carbamothioylisophthalamide) (PTUA) as a new polymer from a condensation reaction of isophthaloyl diisothiocyanate and 2, 6-diaminopyridine. Different techniques were utilized to identify the chemical structure of the synthesized polymer including FTIR spectra, ^{1}HNMR spectra, thermal gravimetric analysis (TGA), Brunauer-Emmett-Teller (BET), and field emission scanning electron microscopy (FESEM). The capability of the synthesized polymer to adsorb Bismarck brown Y (BBY) dye from an aqueous solution was analytically evaluated. Several effective parameters on the adsorption process including contact time, pH, dye concentration, adsorbent dose, and temperature were extensively investigated. The adsorption process was found to be completed with a contact time of 45 min. The results indicated that the optimal adsorption pH was 8 with removal efficiency of 85.331 % and the adsorbed amount of BBY dye increased when the temperature was increased. The adsorption isotherms analysis revealed that the Langmuir model with a correlation coefficient (R^2 = 0.9982) was the most relevant to describe the adsorption process compared with the Freundlich model (R^2 = 0.9863). By applying the Langmuir isotherm, the maximum adsorption capacity was obtained with a value of 132.39 mg/g. The study of adsorption kinetics showed that the adsorption model of BBY dye onto the polymer surface significantly correlated with a pseudo-second-order model. Based on the thermodynamic studies, the calculated ΔG was negative, ΔH was endothermic, and ΔS was positive, verifying the adsorption process is spontaneous. The desorption percentage of BBY dye was calculated with a value of 81.574 % utilizing methanol as an optimal solvent. The density functional theory (DFT) approach was applied to acquire good understanding for the adsorption process.

1. Introduction

Water pollution constitutes a widespread problem to humanity and it occurs when harmful or toxic materials contaminate any water sources. Rapid industrialization and the focal point of extensive research globally are the main sources of contaminated water [1]. Discharging of synthetic and organic dyes from various textile and dyeing industries is a major contributor to water pollution due to their non-biodegradable properties [2]. The textile industry releases many industrial organic dyes into water body and other aquatic resources leading to water quality degradation over time [3]. The majority of the synthesized dyes comprises intricate structures containing azo groups. Exposure to these dyes, mainly through the ingestion of water contaminated with dye poses serious health risks and can ultimately lead to the development of cancer in various regions of the human body [4]. One type of cationic basic diazo dye is Bismarck brown (BBY). It is usually used for staining process of paper, pulp, wool, leather and other materials. Both short and long dyes contact with the skin or eyes causes severe health problems such as irritation, redness, and etc. [5]. It is toxic to organisms found in water, therefore the discover or develop an innovative method for the removal of this type dye from wastewater is of great interest of many researchers [6].

Various methods have been reported in the literature focus on the removal of dyestuffs, including catalytic reduction [7], electrochemical

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