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RESEARCH ARTICLE

Sugeno fuzzy inference system modeling and DFT calculations for the treatment of pesticide-laden water by newly developed arginine functionalized magnetic Mn-based metal organic framework

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Abstract

The uncontrolled utilization of pesticides poses a significant risk to the environment and human health, making its management essential. In this regard, a new arginine functionalized magnetic Mn-based metal–organic framework (Arg@m-Mn-MOF) was fabricated and assessed for the removal of cypermethrin (CYP) and chlorpyrifos (CHL) from aqueous system. The Arg@m-Mn-MOF was characterized by scanning electron microscopy, energy dispersive X-ray, Fourier transform infrared spectroscopy, X-ray diffraction, and Brunauer–Emmett–Teller analysis. Various parameters were optimized in a series of batch experiments and the following conditions were found optimal: pH: 4 and 5, contact time: 20 min, adsorbent dosage: 0.6 and 0.8 g L^{-1} with initial concentration: 10 mg L^{-1} and temperature: 298 K for CYP and CHL, respectively. The composite attained a maximum removal capacity of 44.84 and 71.42 mg g^{-1} for CYP and CHL, respectively. The elucidated data was strongly fitted to the pseudo-second-order model of kinetics ($R^2 > 0.98$) and Langmuir isotherm ($R^2 > 0.98$). Based upon 350 experimental datasets obtained from batch studies and interpolated data, the adsorption capacity of the adsorbent was elucidated with $R^2 > 0.97$ (CHL) and > 0.91 (CYP). The adsorption energy (− 11.67 kcal mol^{-1}) calculated by Gaussian software suggests a good interaction between arginine and CHL through H-bonding. The present study's findings suggested the prepared Arg@m-Mn-MOF as a promising adsorbent for the efficient removal of pesticides from agriculture runoff.

Keywords ANFIS · Adsorption · Arg@m-Mn-MOF · Chlorpyrifos · Cypermethrin · DFT modeling · Genotoxicity · m-Mn-MOF

Introduction

Increasing urbanization and efforts to meet the requirements of a constantly growing population has resulted in the utilization of significant amount of pesticides (Kansal et al. 2023). Pesticides are being introduced into the aquatic system more often through spraying, surface runoff from farms, and engineered drains. Chlorpyrifos (CHL) (O,O-diethyl O-3,5,6-trichloro-2-pyridyl phosphorothioate) which belongs to organophosphorus category is accounted to control bugs, worms, and lice in crops such as corn, citrus, and peanuts. Due to the strong holding capacity towards the soil, it can enter the water through runoff and leaching processes resulting in water pollution. Cypermethrin (CYP) [(RS) − αcyano-3-phenoxybenzyl (1S)-cis-3-(2,2-dichlorovinyl)-2,2-dimethylcyclopropanecarboxylate] is also a commonly used pyrethroid pesticide, effective against a wide range of crops like vegetables, cereals, and maize (Table 1) (Kansal et al. 2023). The extensive utilization of these pesticides has resulted in their accumulation and contamination of the environmental soil, water, and crops leading to severe health hazards. A fatality rate of 0.4 to 1.9% occurs yearly due to acute pesticide toxicity. Human exposure to pesticides has been linked to health issues such as prostate and lung malignancies and miscarriages, even

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