THESIS

SURFACE MODIFIED GRAPHENE-BASED NANOCOMPOSITE FOR SELECTIVE MOLECULAR SIEVING AND ADSORPTION OF AQUEOUS IONS

Submitted by

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Abstract

Even if, granular media filtration demonstrates efficacy in diminishing water turbidity, its constrained surface functionalities and inherent physical attributes limit its capacity to efficiently adsorptive removal of contaminants from aqueous environments. Concurrently, graphene oxide (GO), employed across various adsorptive removal endeavors targeting toxic metals and molecules, presents challenges in recovery following dispersion within aqueous matrices. Addressing this shortfall, we have engineered a GO/sand composite (M-GO/S) via coating GO on purified sand without using a binding agent to optimize contaminant removal efficacy in aqueous systems. This innovation not only reduces water turbidity but also enhances the mechanical integrity of GO and activates the sand's surface. When graphene oxide (GO) is applied to the surface of sand, it perturbates the local hydrogen-bonded structure of the sand, exposing the Si-OH sites for chemisorption. M-GO/S achieves fluoride removal efficiency exceeding 70% at a pH of approximately 6.30, as per the Hill adsorption model. In tests using simulated water samples, the M-GO/S composite significantly reduced solution turbidity by 87%, lowering it from 0.08 to 0.01 NTU. These findings suggest that M-GO/S is an effective material for simultaneously reducing both fluoride levels and turbidity in water. M-GO/S outperformed commercial coal powdered activated carbon by removing 75% of calcium ions from simulated hard water (pH 8), indicating superior efficacy. The detection of (-O-Ca-O-) chemical bonds on the nanocomposite's surface post-calcium ion equilibration reveals chemical interactions. This highlights the M-GO/S nanocomposite as a promising option for hard water treatment. The M-GO/S nanocomposite effectively adsorbed toxic metals such as Pb (52 mg/g), Cr (37 mg/g), Cd (40 mg/g), and Ni (21 mg/g) and silanol groups acting as

active sites for ion exchange. Graphene oxide's adsorption mechanism is driven by its oxygen-rich functional groups (hydroxyl, epoxide, and carboxyl), which boost its affinity for metal ions via complexation, electrostatic attraction, and cation exchange. The M-GO/S composite, leveraging the synergistic surface properties of sand and GO, effectively removes not just cations and anions but also cationic and anionic molecules. Its notable adsorption capacity for substances like Methylene Blue (259.5 mg/g) and MCPA (47.3 mg/g) indicates that this composite may serve as a promising material for molecular sieving. Developing a chemical-free synthesis method for GO is essential for the large-scale production of M-GO/S, aimed at extensive water purification applications.

Keywords: Adsorptive removal, Contaminants, Graphene oxide, Sand, Water purification