Design and Synthesis of a Hierarchical Nanocomposite for Selective Capture and Visible-Light-Driven Destruction of PFAS

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Per- and polyfluoroalkyl substances (PFAS) are anthropogenic contaminants used in superomniphobic products, due to the exceptional stability of their carbon–fluorine bonds, that allow them to persist in the environment for decades. PFAS have been detected in more than 99% of the population, and have been linked with major health problems, like immune dysfunction, carcinogenicity, and developmental disorders. Conventional remediation methods primarily rely on adsorption, which transfers PFAS into secondary waste streams. Moreover, destructive UV-based methods require high energy and have limited degradation rates. A multifunctional Beta-Cyclodextrin@Bismuth Ferrite/Reduced Graphene Oxide nanocomposite, synthesized using pulsed laser ablation in liquid (PLAL), was developed for the selective capture and degradation of PFAS. B-CD was selected for host–guest molecular recognition, $BiFeO_3$ for radical generation, and rGO for enhanced charge transfer. Before experimentation, density functional theory (DFT) and molecular dynamics (MD) were conducted to test adsorption mechanisms, stability, and interactions. To confirm successful synthesis, characterizations, including SEM, HRTEM, XRD, zeta potential, UV-Vis and DLS, were conducted. Performance testing showed destruction efficiencies of 99.6% for long-chain and 92.7% for short-chain PFAS ($p<0.001$, $d=1.41$, $R^2=0.963$, 95% CI), with high adsorption and defluorination rates under visible-light across different media. Also, the material showed a bandgap shift and an increase in structural stability compared to control samples. The nanocomposite was then integrated into capsule systems for practical use. "PEFMinC" achieved an eightfold increase in PFAS degradation, while remaining cost-effective and environmentally sustainable.

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