MITIGATION - SCIENCE AND TECHNOLOGY ADVANCES FOR CHEMICAL AND BIOLOGICAL HAZARD MITIGATION

CNF/UiO-66-NH2 Aerogel Nanocomposites For Photocatalytic Degradation Of Chemical Warfare Agents

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A novel MOF/CNF aerogel composite was synthesized via cross-linking and freeze-drying of a simple mixture comprising UiO-66-NH2 and CNF. The inclusion of CNF aerogel not only ameliorated MOF performance issues such as agglomeration and recycling challenges but also endowed the composite with a three-dimensional sponge-like structure, enhancing active site availability for photocatalytic reactions. These nanocomposites exhibited remarkable responsiveness to visible light and demonstrated highly efficient photocatalytic activity against a range of chemical warfare agents (CWAs), encompassing GD, HD, Novichok, and their simulants. Furthermore, density functional theory (DFT) calculations were conducted to elucidate the fundamental mechanisms underlying CWA neutralization by MOF/CNF aerosol composites. These findings underscore the considerable potential of MOF-CNF nanocomposites aerogel across a wide spectrum of practical applications in CWA defense.