

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

### MoS<sub>2</sub>/UiO-66-NH<sub>2</sub>/ Nanocomposites For Photocatalytic Degradation Of Chemical Warfare Agents

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UiO-66-NH<sub>2</sub> holds promise as a visible-light-driven catalyst for neutralizing chemical warfare agents (CWAs). However, its photocatalytic efficacy is hindered by rapid electron-hole pair recombination. In this investigation, we synthesized UiO-66-NH<sub>2</sub>/MoS<sub>2</sub> nanocomposites via a refined microwave synthesis approach, varying MoS<sub>2</sub> content. The resulting nanocomposites, featuring uniformly dispersed MoS<sub>2</sub>, demonstrated notable responsiveness to visible light and exhibited highly effective photocatalytic activity against a spectrum of CWAs, including soman, sulphur mustard, and the unconventional agent Novichok. The flower-like morphology of the nanocomposites facilitated greater exposure of active sites and promoted enhanced electronic charge transfer pathways, thereby augmenting their capacity for CWA decontamination. Additionally, density functional theory (DFT) calculations were employed to elucidate the fundamental mechanisms underlying CWA neutralization by MOF/MoS<sub>2</sub> composites. These findings underscore the significant potential of UiO-66-NH<sub>2</sub>/MoS<sub>2</sub> nanocomposites across diverse practical applications in CWA defense.