

PROTECTION - SCIENCE AND TECHNOLOGY ADVANCES FOR CHEMICAL AND BIOLOGICAL PROTECTION

Single Atoms Modification Of MoF-808 For Nerve Agent And Simulant Degradation

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Through previous pioneering DTRA work, zirconium-based metal-organic frameworks (Zr-MOFs) have become one of the most promising materials for adsorption and hydrolytic destruction of chemical warfare agents (CWAs). Among them, MOF-808 has demonstrated remarkable catalytic activity in accelerating the degradation of G-series nerve agents in aqueous environments.¹ However, its effectiveness is hampered in the gas phase due to catalytic poisoning caused by the tightly bound hydrolyzed product.² The Morris group has recently demonstrated the hydrolysis of an organophosphate simulant at Cu single-atom-catalyst-(SAC)-modified MOF powders.³ By introducing single atoms onto these Zr-MOFs, we aim to alter the binding mode of the hydrolyzed product to a weaker monodentate configuration, thereby reducing desorption energies and mitigating catalyst poisoning. Our current research focuses on synthesizing single atom-modified MOF-808 catalysts to investigate the hydrolytic degradation of nerve agents. Preliminary results suggest that the incorporation of metal single atoms into MOF-808 leads to the rapid desorption of the hydrolyzed product in the gas phase.

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