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Engineering Scaffolds For Chemical Warfare Agent Uptake And Destruction

Amanda Morris Virginia Tech **Eric Johnson** Virginia Tech **Bradley Gibbons** Virginia Tech **Naveen Kumar** Virginia Tech

Through previous pioneering DTRA work, zirconium-based metal-organic frameworks (ZrMOFs) have become one of the most promising materials for adsorption and hydrolytic destruction of chemical warfare agents (CWAs). Numerous studies have optimized reactivity through manipulation of MOF three-dimensional structure, missing linker or missing cluster defects, and molecular post-synthetic additives.1-3 Indeed, the Morris group has extensively studied the role of defects on the uptake and catalytic turnover of nerve agent simulants in UiO-66.1 While the results are promising, the transition of MOFs to applications would benefit from (1) better performance in gas-phase reactivity, (2) the extension of reactivity beyond hydrolysis, and (3) the development of functional forms for deployment in masks, clothing, etc. The Morris group has recently demonstrated the hydrolysis of an organophosphate simulant at Cu single-atom-catalyst-(SAC)-modified MOF powders.4 We have extended these results to many other SAC on UiO-66 and MOF-808. The materials have transitioned to the Chemical and Biological Center (CBC) and have shown promise for reactivity. In addition to the SAC work, we have explored the use of MOF gels for organophosphate simulant degradation. Xerogel forms of UiO-66 and NU-1000 outperform their powdered counterpoints, indicating that modification of macromorphology may also provide optimized catalysis.

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