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Advances in Fundamental Materials Research

In Situ Probes of Capture and Decomposition of Chemical Warfare Agent Simulants by Zr-Based Metal Organic Frameworks

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Zr-based metal organic frameworks (MOFs) have been recently shown to be among the fastest catalysts of nerve-agent hydrolysis in solution. We report a detailed study of the adsorption and decomposition of a nerve-agent simulant, dimethyl methylphosphonate (DMMP), on UiO-66, UiO-67, MOF-808, and NU-1000 using synchrotron-based X-ray powder diffraction, X-ray absorption, and infrared spectroscopy, which reveals key aspects of the reaction mechanism. The diffraction measurements indicate that all four MOFs adsorb DMMP (introduced at atmospheric pressures through a flow of helium or air) within the pore space. In addition, the combination of X-ray absorption and infrared spectra suggests direct coordination of DMMP to the Zr6 cores of all MOFs, which ultimately leads to decomposition to phosphonate products. These experimental probes into the mechanism of adsorption and decomposition of chemical warfare agent simulants on Zr-based MOFs open new opportunities in rational design of new and superior decontamination materials.

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