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Tracking nerve-agent simulant decomposition in UiO-67 using in situ total scattering pair distribution function analysis

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The ability to selectively take up and store gases is one of the promising properties of metal–organic frameworks (MOFs) already implemented for industrial applications. Judicious choice of secondary building units can allow for further catalyzing reactions with stored content; for example, much research is currently pursuing their use for filtration of chemical warfare agents. Recently, the Zr-based MOF UiO-67 was shown to effectively adsorb and decompose the nerve-agent simulant, dimethyl methylphosphonate (DMMP).

Various methods are available for probing the gas sorption and reaction pathway, but quantitative structural information on the localized binding is difficult to obtain. A better understanding of the binding behavior is necessary to improve the performance of these MOFs for chemical agent neutralization. Here, we demonstrate the quantitative tracking of both framework and binding component structures using in situ X-ray total scattering measurements of UiO-67 under DMMP exposure, pair distribution function analysis, and theoretical calculations. The adsorption and desorption of DMMP within the pores, association with linker-deficient Zr6 cores, and decomposition to irreversibly bound methyl methylphosphonate were directly observed and analyzed with atomic resolution.

Going forward, wider access to powerful synchrotron beamlines and robust in situ capabilities will allow for comprehensive investigations into the structural implications of the full processing procedure from activation to adsorption, reaction, and re-activation. The procedures developed in this study could help guide further investigations into processes in other MOF/functional systems.

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