CBD SOT CONFERENCE TODAY'S INNOVATION, TOMORROW'S WARFIGHTER CAPABILITIES

Advances in Fundamental Materials Research

Design and Synthesis of Stratified and Gradient MOFs for Selective Capture of CWAs and TICs

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Metal-organic frameworks (MOFs), with their large porosity and internal surface area, are promising adsorbent materials that can selectively concentrate, accommodate, and convert various guest species, including chemical warfare agents (CWAs) and toxic industrial chemicals (TICs). We are developing multi-functional hybrid materials that combine the desirable properties of different component MOFs to capture and concentrate target molecules. Arranging multiple functional MOF domains in a stratified fashion can benefit the selectivity and efficiency of CWA/TIC uptake in the overall material.

To realize such hybrid materials as advantageous CWA/TIC adsorbents, we first investigate how different functional groups affect the uptake of CWA/TIC molecules using a series of isoreticular MOFs with different target functional groups, which have been identified through first-principles modeling. Secondly, we report a unique MOF stratification approach, which achieves porosity and functional gradients, instead of abrupt interfaces, in between adjacent MOF domains within individual MOF crystals. We propose that these gradient MOFs can retain the combined merits of stratified MOFs, and remove the potential interface barrier that may inhibit guest diffusion and transport. Using Temperature Programmed Desorption (TPD) measurements, we determine the binding energies of different CWA/TIC simulants adsorbed in stratified MOFs and compare these with modeling results. The identification of the desorbed products combined with spectroscopic observations will allow us to propose a mechanism of binding of target molecules.

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