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Tunable Adsorbents For Hazardous Chemicals By Post-synthetic Modification Of Zirconium Metal-organic Frameworks

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A series of adsorbents based on the zirconium metal-organic framework (MOF) have been developed to target different classes of hazardous chemicals. For initial investigations, the UiO-66 family was selected for its thermal and chemical stability as well as ease of post-synthetic modification. The MOF UiO-66-NH₂ was modified to introduce phenolic sorbent groups with tunable electronics to modulate MOF binding affinity and selectivity for organophosphate chemicals. Upon investigation of adsorbent performance, these added functional groups were found to benefit DMMP adsorption in some cases. However, they also lowered the surface area of the adsorbent MOF, limiting the benefit of these added groups. In ongoing work, we aim to address these limitations by modifying MOFs with larger surface areas and pores such as MOF-808. Moreover, additional functional groups are being investigated to tune the adsorbent MOF's selectivity for different hazardous chemical classes, such as organophosphates, acids, and bases.

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