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Macromorphological Control Of Zr-based Metal-organic Frameworks For Hydrolysis Of A Nerve Agent Simulant

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Zirconium-based metal-organic frameworks (Zr-MOFs) have emerged as highly promising materials for the adsorption and destruction of chemical warfare agents (CWAs).1,2 While numerous studies have highlighted variations in reactivity based on MOF topology and post-synthetic modifications, the impact of modifying MOF macromorphology remains less explored.3 MOF xerogels exhibit altered defect levels and increased porosity compared to their powder counterparts, resulting in enhanced accessibility to potential active sites. Notably, UiO-66 and NU-901 xerogels demonstrate reaction rates 2 and 3 times higher, respectively, for the hydrolysis of DMNP relative to their powder forms. Furthermore, in recycling tests, MOF-808 xerogel surpasses its powdered counterpart, previously recognized as the fastest Zr-MOF for the hydrolysis of organophosphate nerve agents. This improvement in reactivity is primarily attributed to the higher external surface area and the introduction of mesoporosity to previously microporous materials. Our findings underscore the significant impact of macromorphological modifications on the reactivity of Zr-MOFs, offering valuable insights for the design and optimization of MOF-based materials for chemical defense applications.

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