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Composite Mof/zr(oh)4-polymer Catalytic Filters For In-situ Removal And Destruction Of Chemical Warfare Agents

Nada Abdelaziz Missouri University of Science and Technology **Fateme Rezaei** Missouri University of science and Technology
Ali Rownaghi Missouri University of science and technology **Fateme Rezaei** Missouri University of science and Technology

Developing highly porous composite filters that possess both adsorptive and catalytic functionalities for in-situ capture and destruction of chemical warfare agents (CWAs) can dramatically advance the state-of-the-art military respiratory filters. Extensive research has been carried out over the past few years to improve the efficiency of the military filters, however, most of these laboratory efforts focus primarily on testing the materials under unrealistic conditions. Moreover, one of the main hurdles facing the development of catalytic filters is intradiffusional limitations which severely hamper their destruction performance. Introducing defects into filter materials and their surface functionalization appear to be two feasible approaches for addressing the low detoxification rate issues. In this research, we aim at developing novel composite materials based on metal-organic frameworks (MOFs) and their Zr(OH)4-incorporated polymers, and investigating their CWA detoxification performance under realistic conditions. This will be achieved by (i) defect engineering of the MOF filters via creating different types of defects such as mesopores, local defects, or linker vacancy into pore structure; and (ii) MOF functionalization with amines, bromide, amidoxime, or hydroxy groups. Low concentration of defects will lead to distribution of isolated defects, whereas a high concentration of large defects will lead to their aggregation and clustering, thereby creating mesopores. Moreover, since the presence of water is a necessity in the hydrolysis reaction of CWAs, the choice of a suitable functional group is necessary to boost the reaction rate. Additionally, introducing super acidity through a post synthetic method to increase the acidity of the active sites, can lead to the enhancement of the hydrolysis rate. Finally, the research will explore the effects of structure, composition, and surface chemistry of Zr(OH)4-incorporated polymers on the overall performance of the MOF/Zr(OH)4-polymer filters in capture and hydrolysis of type-G and type-X toxic nerve agent simulants. The outcome of this investigation will shed light on the structure-property-performance relations in advanced composite catalysts that exhibit high CWA removal and destruction efficiency for use in military filters.

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