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Advances in Fundamental Materials Research

"MOF-Fabric" Prepared via Directed Supramolecular Assembly of UiO-66-NH2 Crystals on ALD-coated Cloths for Rapid Catalytic Destruction of Chemical Warfare Agent Simulants

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Chemical warfare agents (CWAs) are a serious concern, particularly following publicity of attacks using sarin (GB) in Syria. In addition to sarin, other organophosphorus nerve agents, such as VX and soman (GD), also continue to pose a significant potential threat to warfighters and civilians. Porous metal-organic frameworks (MOFs) composed of metal-containing clusters and organic linkers are promising catalysts for decontamination of toxic compounds, in part because of the chemical flexibility of both the metal sites and the organic linkers within the MOF structure. A key problem, however, is that MOFs synthesized in powder form are not amenable to handling, rapid deployment, and utilization. To overcome the difficulties, researchers are exploring a range of techniques to integrate MOFs into different form factors, including membranes and functional polymer textiles.

In this study, we describe a facile route to uniformly coat polypropylene (PP) fibrous mats with as-synthesized Zr-based UiO-66-NH_2 MOF crystals at room temperature. We chose UiO-66-NH_2 MOF because it is highly stable and catalytically reactive against CWAs. ZnO thin films (~15 nm thickness) were coated onto polypropylene fibers via atomic layer deposition (ALD) to impart hydroxyl groups. Then we assembled as-prepared UiO-66-NH_2 nanocrystals onto the ALD ZnO surface by means of assembly agents, β-cyclodextrin (β-CD) and cetyltrimethylammonium bromide (CTAB). Around 30 wt.% mass fraction of dense MOF coatings was obtained on the ALD-pretreated fiber scaffolds via the assembly method. We confirmed that the void space of MOF-coated fiber networks was also filled with MOF crystals, leading to high MOF mass loading. Moreover, N_2 isotherm analysis exhibits high BET surface area (more than 200 $m^2/g_{(MOF+Fiber)}$) of the MOF-coated fiber mats. The functional textiles present fast catalytic destruction of dimethyl 4-nitrophenyl phosphate (DMNP), a GD simulant, with the half-life of DMNP less than 5 minutes.

We believe that this room-temperature MOF assembly approach can be extended to a wide range of MOFs and polymeric fibrous materials and that it holds promise as a scalable integration method to produce large fabrics, for example for mask filters and military garments, to enable hazardous chemical detoxification and product capture.