CBD S&T CONFERENCE TODAY'S INNOVATION, TOMORROW'S WARFIGHTER CAPABILITIES

Advances in Fundamental Materials Research

Design of Metal-Organic Framework-based Catalysts for Rapid Partial Oxidation of a Mustard Gas Simulant

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First used during World War I, mustard gas (HD) continues to exist in stockpiles around the world. HD causes irreversible damage to exposed skin or tissues by alkylating DNA. Despite an international ban, evidence of HD's use on civilians and military forces has been found in the Middle East over the past few years. Thus, there is still need to safely handle and detoxify this chemical agent.

The partial oxidation of HD is a promising degradation pathway for obtaining a non-toxic product. Ideal catalysts for the oxidation of HD and similar chemical warfare agents (CWAs) would perform under ambient conditions and be capable of using environmentally accessible reagents, such as dioxygen. Metal–organic frameworks (MOFs) are promising catalysts and catalyst supports because they are highly tunable and can be designed to have permanent porosity and high thermal/chemical stability which is important for a heterogeneous catalyst/support.

This presentation will discuss the installation of a representative polyoxometalate (POM), for the first time, in a channel-type MOF. By using a hierarchical channel-type MOF, the POM was installed without compromising the stability or porosity of the composite, unlike previous POM@MOF examples. The composite material showed enhanced reactivity compared to either component alone in a simple sulfide oxidation reaction using hydrogen peroxide. Further, the nodes of the MOF remained accessible as potential active sites for other CWA detoxification, for example nerve agent hydrolysis. Current efforts on creating a champion catalyst for accomplishing the detoxification of 2-chloroethyl ethyl sulfide (CEES), a mustard gas simulant, using air as the oxidant will be discussed. While beyond the scope of this work, the findings may improve our capabilities for decontaminating and protecting against chemical weapons.