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High-Capacity Mesoporous Metal Oxides for Toxic Gas Adsorption and Degradation

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Chemical Warfare Agents (CWAs) have long existed as a threat to civilians and the military. Gas masks equipped with filters containing activated carbon and metal oxides have been used as a means of protection against these toxic agents. To ensure the effectiveness of these masks, materials must be developed to degrade and adsorb these CWAs. This research focuses on the synthesis of mesoporous Titanium and Magnesium metal oxides that will most efficiently degrade Sarin (GB). Sarin is a highly toxic inhibitor of the acetylcholinesterase enzyme, which is essential to the function of the nervous system. Due to the high toxicity of Sarin, Dimethyl Methylphosphonate (DMMP, a common sarin simulant) will be used for safety and experimental purposes. Techniques used include soft-templating or cooperative self-assembly and hard templating (nanocasting) to increase surface area and overall reactivity of mesoporous metal oxides. X-ray diffraction (XRD), nitrogen adsorption, and diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) will be used to analyze how pore size and structure affect reactivity of mesoporous metal oxides with DMMP. Through the DRIFTS study, we observed that DMMP appears to be decomposing on the surface of mesoporous TiO_2 but not on TiO_2 nanoparticles. This observation provides justification for the synthesis of mesoporous materials which have not been as extensively researched as nanoparticles. We will utilize several techniques to further our investigations. Ambient pressure x-ray photoelectron spectroscopy (APXPS) will help us to understand the nature of binding in our specialized system. Fixed feed temperature program modulation (FFTPM) will be used to measure thermodynamic properties to help understand how tightly DMMP binds to surfaces. Finally, we will work with a computational team to create models on how DMMP decomposes and reacts with TiO_2 surfaces.