

Advances in Fundamental Materials Research

Chemical Warfare Agent Decomposition on Zr(OH)₄ Powdered Materials: In the Presence and Absence of Contaminant SO₂

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The threat of chemical warfare agents (CWAs) has become increasingly apparent in the last decade. Additionally, ambient contaminants such as SO₂ and NO₂ also are a potential risk due to exposure both to the catalyst materials found in air filtration media, which could deactivate, and to civilians and military personnel when used as a weapon by terrorist organizations or individuals. Materials used today for decontamination of these toxic contaminants and agents are often corrosive, difficult to transfer, and only react with select chemicals. Zirconium hydroxide (Zr(OH)₄) has recently emerged as a possible alternative material for chemical decontamination for a wide range of chemicals,^{1,2} and the material is scalable. Other benefits of this material include its elemental abundance, low cost to manufacture, and low toxicity to humans and the environment.

Zirconium hydroxide materials have been shown recently to exhibit enhanced chemical warfare agent (CWA) adsorption and reactivity;^{1,2} however, there are many questions left to be answered involving what the mechanism is for this enhancement and how do contaminants (SO₂, NO₂, etc.) hinder or enhance CWA reactivity on these materials. Here we report the in-situ adsorption of two nerve surrogates (dimethyl methyl phosphonate, DMMP, and diisopropyl fluorophosphate, DIFP) and two nerve agents (sarin, GB, and soman, GD) on "clean" Zr(OH)₄ materials. We found decomposition of all these compounds on the clean surface. Interestingly, once the contaminant, sulfur dioxide, SO₂, was first introduced to the Zr(OH)₄ material, then the simulants and CWAs were subsequently introduced, a new CWA reaction mechanism was observed. Diffuse reflection infrared Fourier transform spectroscopy (DRIFTS) was used to measure the in-situ adsorption and reactivity of these complex molecules on Zr(OH)₄.

References:

1. Peterson, G. W.; Rossin, J. A.; DeCoste, J. B.; Killops, K. L.; Browe, M.; Valdes, E.; Jones, P. *Industrial & Engineering Chemistry Research* 2013, 52, 5462-5469.
2. Badosz, T. J.; Laskoski, M.; Mahle, J.; Mogilevsky, G.; Peterson, G. W.; Rossin, J. A.; Wagner, G. W. *The Journal of Physical Chemistry C* 2012, 116, 11606-11614.

This research was supported in part by an appointment for Monica McEntee to the Postgraduate Research Participation at the U.S. Edgewood Chemical Biological Center administered by the Oak Ridge Institute for Science and Education through interagency agreement between the U.S. Department of Energy and USAECBC. Greg Peterson, Wesley Gordon, and Alex Balboa also thank the Joint Science and Technology Office for Chemical Biological Defense for funding under project number CB10123.