SAND2013-7986P

From Sarin Micro-Hydration to Graphene/Liquid Crystal Nanocomposites: Recent Efforts in my Lab

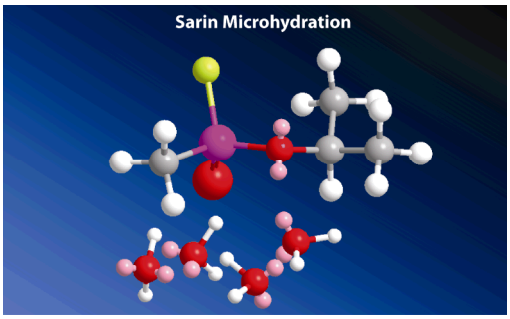
Dr. Todd M. Alam

Dept. of Electrical, Optical and Nanostructured Materials
Sandia National Laboratories, Albuquerque, NM 87185

In this seminar I will present an overview of two very different research efforts the NMR laboratory has been involved with in the last few years.

The interaction of water chemical warfare agents (CWA) is known to impact the performance of filtration devices, the efficiency of decontamination procedures, and the environmental persistence of CWA. The first portion of this presentation involves *ab initio* computational efforts predict the impact of micro-hydration the relative energies, conformations and surface adsorption energies on Sarin (GB) and the simulant dimethoxymethyl phosphonate (DMMP). The calculations involved both small silicate clusters, as well as larger amorphous silica glass surfaces. The impact of hydration on the IR frequencies will also been discussed. Experimental examples of monitoring the performance of different decontaminations foams using NMR spectroscopy will also be presented.

The final portion of the presentation will describe recent deuterium (^{2}H) NMR experiments to look at the orientational order of graphene/liquid crystal nanocomposites. NMR provides an excellent tool to directly measure the orientational order, and allows molecular level details about the liquid crystal response to the addition of graphene to be realized. It is experimentally demonstrated that increasing graphene concentrations influence both the nematic to isotropic phase transition in these materials, and increases/decreases orientational order based on the makeup of the nanocomposite. Future efforts to incorporate these graphene/LC nanocomposites into polymer matrices will be discussed.



Sandia National Laboratories is a mulit-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin company, for the U.S. Department of Energy's National Nuclear Security administration under contract DE-AC04-94AL85000. This research was funded through DTRA JTSO and Sandia's LDRD program.

Invited Presentation
Department of Chemistry and Physics
West Texas A&M
Canyon, TX
Oct. 3, 2013