BES002 Elucidation of Hydrogen Interaction Mechanisms with Metal-Doped Carbon Nanostructures

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Program Scope

This program supports the Office of Basic Energy Sciences (BES) mission through the development of a basic understanding of the formation and the physicochemical properties of carbon nanostructures, formed by the interaction of doped carbon nanomaterials with hydrides and/or hydrogen gas. For many years extensive work has been conducted on hydrogen interaction with metals and alloys forming hydrides. The research work on metal hydrides involved a significant number of studies and characterization efforts, where chemical, electronic, optical, and magnetic properties were determined. Our work continues to focus on a unique class of materials—metal-doped carbon nanostructures—and the interaction of these materials with hydrogen. Our work will continue to focus on understanding the formation of these materials and on investigating their chemical, electronic, optical, and magnetic properties when reacted with hydrogen. Previous work in our group through BES programs has led to advances in control over a material's properties at the electronic, molecular, and atomic level, which serve as the foundation of new energy technologies and can support other aspects of DOE missions. Our group has observed related properties in the materials such as hydrogen storage and luminescence with potential applications in clean energy and energy storage. However, developing customizable functional materials requires relating the microstructure of the materials to their physical properties. Our research activities will be aimed at developing and characterizing a novel class of hydride materials based on metal-carbon nanostructures. The current work will investigate different carbon materials utilizing their structure as building blocks for achieving unique properties based on zero, one, and two dimension (0D, 1D, 2D) structures such as fullerenes, carbon nanotubes, and graphene, respectively.

FY 2014 Highlights

Theoretical calculations (Prof. Jena, Virginia Commonwealth University) reveal that a new class of highly electronegative species can be created when a central metal atom is surrounded by superhalogen moieties. Building on this knowledge, we were able to synthesize and characterize a stable hyperhalogen salt, $K[Al(BH_4)_4]$, whose anion, $Al(BH_4)_{4-}$, has an extremely high electron affinity. Unlike the few hypersalts synthesized so far, this new salt is stable at temperatures of up to 154°C. Besides providing a new functional material, the work validates the use of computational studies for rational design of new compounds based on superhalogens and hyperhalogens. Building on our previous study of ionic mobility in a $LiBH_4$-C_{60} system, a series of electrochemical measurements was performed to quantify the lithium ionic mobility in the material under various conditions. This study also demonstrated that the material can be used as a solid electrolyte in an all solid-state lithium ion battery. Theoretical calculations by Prof. Jena's group indicated that the $Li+BH_{4-}$ bonding is perturbed in the presence of C_{60} resulting in a highly mobile Li ion due to the C_{60}-BH_{4-} interaction. This suggests a nanoionic mechanism is responsible for the enhanced Li ion mobility due to the formation of new interfaces at the nanoscale favoring the production of charge carriers. Further Laser-Desorption/Ionization Time-of-Flight Mass Spectrometry (LDI-TOF-MS) analysis of a sodium intercalated fullerene (Na_xC_{60}) in the hydrogenated state provided the first spectroscopic evidence for the formation of $C_{60}H_{60}$ among other highly hydrogenated fullerenes ($C_{60}H_{>36}$). This finding was also confirmed through deuteration of the same material to form $C_{60}D_{60}$. Current efforts in this system are focusing on the isolation of the $C_{60}H_{60}$ from the other fullerenes for further analysis and characterization. Our current work is aimed at understanding how hydrogen interaction with C_{60} and other carbon nanomaterials can potentially lend itself to other energy storage systems and energy conversion devices.