IV.E.4 Elucidation of Hydride Interaction Mechanisms with Carbon Nanostructures and the Formation of Novel Nanocomposites

Principal Investigator: Puru Jena

Organization: Virginia Commonwealth University

Program Scope

The objectives of this project are to provide, by working closely with experimentalists, a fundamental understanding of the structure-property relationships of a novel class of highly electronegative clusters in the gas phase, study their interaction with support and counter ions, and explore their potential as building blocks of materials with tailored properties. The project deals with four inter-related thematic areas of bare and supported clusters with rather uncommon properties. (1) Using first principles theory, we design new, highly electronegative clusters whose electron affinities far exceed that of chlorine and validate their properties by working closely with experimentalists. These species, called superhalogens and hyperhalogens, usually consist of a metal atom at the core surrounded by halogen or oxygen atoms. Our goal is to create superhalogens and hyperhalogens without a metal, halogen, or oxygen atom by tailoring their size and composition and to push their electron affinities to values even higher than that currently known. (2) By suitably identifying counter ions, we explore the ability of their corresponding salts to store hydrogen. (3) Superhalogens with magnetic moments are designed using transition metal atoms as key components. Their magnetic coupling is then studied by assembling them on graphene and noble metal substrates. (4) Using electronegative species as building blocks, we explore the potential of multifunctional nanoparticles with Janus anisotropy for application in light harvesting. The computations are carried out using multiscale theoretical approach based on density functional theory (DFT) with hybrid and generalized gradient approximation based exchange-correlation functionals. When needed, quantum chemical methods such as Moller-Plesset perturbation theory and coupled cluster CCSD(T) (coupled cluster single double [triple]) are used to test the accuracy of the DFT-based results.

FY 2014 Highlights

Publications

Thirty papers were published in peer reviewed journals. Space does not permit to list all. Following is a reduced list:

1. Chen, H., Kong, X., Zheng, W., Yao, J., Kandalam, A.K., and Jena, P.: "Anomalous Property of $Ag(BO_2)_2$ Hyperhalogen: Does Spin-Orbit Coupling Matter?" Chem. Phys. Chem. 14, 3303(2013).

2. Knight, D.A., Zidan, R., Lascola, R., Mohtadi, R., Ling, C., Sivasubramaniam, P.K., Kaduk, J.A., Hwang, S.-J., Samanta, D., and Jena, P.: "Stabilization of Hydrogen Rich, Yet Highly Pyrophoric $Al(BH_4)_3$ via the Synthesis of the Hypersalt $K[Al(BH_4)_4]$," J. Phys. Chem. C 117, 19905 (2013).

3. Kan, M., Zhou, J., Sun, Q., Kawazoe, Y., and Jena, P.: "Intrinsic Ferromagnetism in MnO_2 Monolayer," J. Phys. Chem. Letters 4, 3382 (2013).

4. Zhang, S., Wang, Q., Chen, X., and Jena, P.: "Stable Metallic 3D Metallic Phase of Carbon with Interlocking Hexagons," Proc. Nat. Acad. Sci. 110, 18809 (2013).

5. Zhang, S., Wang, Q., Kawazoe, Y., and Jena, P.: "Three Dimensional Metallic Boron Nitride," J. Am. Chem. Soc. 135, 18216 (2013).

6. Wang, H., Zhang, X., Jae Ko, Y., Grubisic, A., Li, X., Gantefoer, G., Schnoeckel, H., Eichhorn, B.W., Lee, M.S., Jena, P., Kandalam, A.K., Kiran, B., and Bowen, K.H.: "Aluminum Zintl Anion Moieties within Sodium Aluminum Clusters," J. Chem. Phys. 140, 054301 (2014).

7. Tao, K., Sun, Q., Wang, Q., Stepanyuk, V., and Jena, P.: "Self-consistent Determination of Hubbard U for Explaining the Anomalous Magnetism of Gd_{13} Cluster," Phys. Rev. B 89, 085103 (2014).

8. Child, B., Gronett, S., and Jena, P.: "Aromatic Superhalogens," Chemistry- A European Journal 20, 4736 (2014).

9. Giri, S., Moore, C.H., Mcleskey, J.T., and Jena, P.: "Origin of Red-shift in the Photo Absorption Peak in MEH-PPV Polymer," J. Phys. Chem. C 118, 13444 (2014).

10. Awnehss, A., Behera, S., El-Kaderi, H., and Jena, P.: "New Insights into Carbon Dioxide Interactions with Benzimidazole-linked Polymers," Chem. Comm. 50, 3571 (2014).

11. Eleven invited talks were delivered at conferences and academic institutes. One student was awarded a PhD.