OPEN TALK ANNOUNCEMENT

28 February 2017 4:00 p.m Fermion

Speaker:

Prof. Purusottam Jena

(VASP Short Term Visitor to Dr. Sugata Mukherjee)

Affiliation:

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Title:

Beyond the Periodic Table of Elements

Abstract:

The building blocks of all materials known to man are derived from the 90 naturally occurring elements in the periodic table. While some of these elements are abundant and cheap, several technologically important ones are either scarce or expensive. Ways to overcome this limitation was proposed a quarter century ago [1] when it was realized that atomic clusters with specific size and composition can be designed to mimic the chemistry of atoms. These clusters, known as super-atoms, can be used as building blocks of a new three-dimensional periodic table. Understanding the structure-property relationships of these super-atoms can then lead to a rational design of materials that nature did not intend. This talk will describe how simple electron counting rules developed over the past century can be used to design these super-atoms by focusing on Group I (alkalis) and Group 17 elements (halogens). I will show how complex clusters known as super-alkalis and super-halogens [2, 3] can be designed that not only mimic the chemistry of alkali and halogen atoms, but also can form super-salts with potential applications in energy storage (e.g. Li-ion batteries) and conversion (e.g. solar cells) [4,5].

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2. Gutsev, G.; Boldyrev, A. I. DVM-Xα Calculations on the Ionization Potentials of MX_{k+1}^- Complex Anions and the Electron Affinities of MX_{k+1} "Superhalogens". Chem. Phys. **56**, 277(1981)
3. Willis, M., Gotz, M., Kandalam, A. K., Gantefor, G, and Jena, P.: "Hyperhalogens: Discovery of a New Class of Electro-negative Species", Angew. Chem. Int. Ed. **49**, 8966 (2010)
4. Giri, S., Behera, S., and Jena, P.: "Superhalogens as Building Blocks of Halogen-free Electrolytes in Li-ion Batteries", Angew. Chem. Int. Ed. **53**, 13916 (2014); Zhao, H., Zhou, J., and Jena, P.: "Stability of $B_{12}(CN)_{12}^{2-}$: Implications for Lithium and Magnesium Ion Batteries", Angew. Chem. Int. Ed. (*VIP*) **55**, 3704 (2016)
5. Fang, H. and Jena, P.: "Super-ion Inspired Colorful Hybrid Perovskite Solar Cells", J. Mat. Chem. A **4**, 4728 (2016); Fang, H. and Jena, P.: "Molecular Origin of the properties of organic-inorganic hybrid perovskites: The Big Picture from Small Clusters", J. Phys. Chem. Lett. **7**, 1596−1603 (2016)

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