OPEN TALK ANNOUNCEMENT

2 March 2017 4:00 p.m Fermion

Speaker:

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(VASP Short Term Visitor to Dr. Sugata Mukherjee)

Affiliation:

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Title:

Many Faces of Carbon

Abstract:

Carbon is one of the most fascinating elements in the periodic table. It not only forms the basis of all life on the Earth but also it is important to technology. The unique properties of carbon emerge from its ability to form diverse sp^n ($1 < n < 3$) bonds. Until 1960's graphite with sp^2 and diamond with sp^3 bonding were the most common forms of carbon known. The discovery of one-dimensional (1D) chain-like polymer called "carbyne" in 1960 and later zero-dimensional (0D) carbon fullerenes, 1D carbon nanotube, and two-dimensional (2D) graphene, all with novel properties characteristic of their reduced dimensionality and size, has ushered a new era in carbon science. In recent years many new meta-stable forms of carbon exhibiting a mixture sp^1, sp^2 and/or sp^3 bonding pattern have also emerged. In this talk I will focus on the carbon allotropes that have been studied in our group[1-6]. These include functionalized C_{60} fullerenes for hydrogen storage[1, 2], semi-hydrogenated graphene for metal-free ferromagnet[3], metal-organic complexes with large electron affinity[4], 3D metallic carbon made of hybridized sp^2 and sp^3 bonded atoms[5], and a Cairo-tilling inspired quasi-2D penta-graphene made of only carbon pentagons[6]. All calculations have been carried out using gradient corrected density functional theory. Thermodynamic stability of the above carbon allotropes is confirmed by total energy calculations as well as quantum molecular dynamics. Potential applications of some of these carbon allotropes will be discussed.

1. Sun, Q., Jena, P., Wang, Q., and Marquez, M.: “First-principles study of hydrogen storage on $Li_{12}C_{60}$”, *J. Am. Chem. Soc.* **128**, 9741 (2006).

2. Berseth, P. A., Harter, A. G., Zidan, R., Blomqvist, A., Araujo, C. M., Scheicher, R. H., Ahuja, A., and Jena, P.: “Carbon Nanomaterials as Catalysts for Hydrogen Uptake and Release in $NaAlH_4$”, *Nano Letters.* **9**, 1501 (2009).

3. Zhou, J., Wang, Q., Sun, Q., Chen, X. S., Kawazoe, Y., and Jena, P.: “Ferromagnetism in semihydrogenated graphene”, *Nano Letters* **9**, 3867 (2009).

4. Giri, S., Child, B., Zhou, J., and Jena, P: “Unusual Stability of Multiply Charged Organo-metalic Complexes”, *RSC Advances* **5**, 44003 (2015).

5. 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).

6. Zhang, S., Zhou, J., Wang, Q., Chen, X., Kawazoe, Y., and Jena, P.: “Penta-graphene: A New Carbon Allotrope”, *Proc. Nat. Acad. Sci.* **112**, 2372 (2015).

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