

Non-covalent interactions on Carbeneous Materials

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The study of the interaction of CNSs with metal ions and small molecules has gained extensive attention and potential applications in biology and materials. A hybrid QM/QM approach has been employed to quantify the strength of these interactions. The identification of factors which influence such interactions is an important basis for manipulating their properties for desired applications. The talk covers the interaction of various metals and metal ions, nucleobases, aminoacids and other small molecules with CNSs. The focus will be on the aspect to demonstrate how the various carbon based nanomaterials differ in their reactivity towards diverse systems. Chirality and curvature of the carbon nanostructures seem to play a major role in determining the structural, energetic and functional properties. In addition, the importance of the functionalization of CNSs and its effect on their physical properties will also be discussed. Apart from the fundamental aspects, how these studies can propel the understanding of the nano-bio interface will be highlighted.

Brief CV: G. Narahari Sastry obtained his B.Sc. and M.Sc. from Osmania University and Ph.D. from University of Hyderabad. After PDF stays in Israel and Switzerland, he started his independent research career in 1997 at Pondicherry University. In 2002, he moved to Indian Institute of Chemical Technology to establish and head Centre for Molecular Modeling. Prof. Sastry's research interests are computational chemistry and computer aided drug design. Several of his computational predictions have seen experimental realization. He has published over 230 papers which received about 4300 citations. He has been awarded with several awards including Shanthi Swarup Bhatnagar Prize in chemical sciences (2011), National Bioscience award (DBT) 2009, Swarnajayanthi Fellowship 2005 (DST), B.M. Birla Young scientist award for 2001, B.C. Deb memorial award (2008), CRSI Medal 2011, AvH fellowship, etc. He was a visiting professor at IMS, Japan (2011); LMU, Munich, Germany (2005-06); and Jackson State University, USA (2008). He was elected as a Fellow of National Academy of Sciences (FNASc), Fellow of the Indian Academy of Sciences (FASc), Fellow of Association of Biotechnology and Pharmacy (FABP) and Andhra Pradesh Academy of sciences (FAPAS). He is currently a visiting professor in Professor Yoshizawa's group, Kyushu university, Fukuoka, Japan for a period of two months (May to June 2014).

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