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Computational Design and Functionalization of 2D Materials and their Heterostructures

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The discovery of Graphene in the beginning of this century, apart from all its superlative properties, marked the beginning of a new class of 2D materials that have been emerging with far reaching potential applications. In spite of all its superlative physical properties, pure Graphene has some serious drawbacks, such as absence of band gap, that limits its usage in devices. 2D nanosheets analogous to graphene, such as h-BN, III-IV-V nanosheets phosphorene, layered transition metal dichalcogenide (MX_2, M=TM, X=S, Se, Te) etc. exhibit band gaps that can be tailored by varying the number of layers, by cutting nanoribbons along Zigzag or Armchair edges, by heterostructuring or by chemical functionalization. For example, there is an interesting manifestation of quantum size effect on the electronic behavior of layered VX_2 as a function of the number of layers. Many of these quasi-2D TMDC's, grown epitaxially on metallic or semiconducting substrates, result in lattice matched / mismatched heterostructures with different kinds of bonding ranging from weak Van der Waals bonding to relatively stronger ionic/covalent bonding. Physical and chemical properties of such overlayers often get modulated by the sub-surface layers of the corresponding substrates, leading to manifestation of new properties. In this talk, I shall discuss how density functional theory (DFT) based first principles simulation can be used in designing different classes of 2D materials and also to functionalize these for various applications in materials science, catalysis and device physics. Finally, I shall highlight the increasing relevance of combining machine learning and combinatorial techniques with DFT data base on 2D and quasi-2D materials.

Biography:

Dr. G.P. Das is a condensed matter physicist and a materials scientist working as a senior professor in the Indian Association for the Cultivation of Science in Kolkata, India. His research interests span a wide cross-section encompassing electronic structure and properties of various kinds of alloys, interfaces, clusters, and nanostructured materials. He has been working on spintronics materials, hydrogen storage materials, two dimensional nanostructures beyond graphene, and various quantum structures. He served as visiting scientist in several institutes abroad viz. Max Planck Institute Stuttgart (Germany), Virginia Commonwealth University, Richmond (USA), Institute of Materials Research, Sendai (Japan), University of New South Wales (Australia).