BOSE COLLOQUIUM

Friday, 20 June 2014 **4:00 p.m.** **Fermion**

Speaker:

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Title:

All-metal aromaticity and conceptual DFT

Abstract:

Several metal clusters exhibit aromatic behaviour. Conceptual density functional theory has been found to be useful in analyzing the behaviour of all- metal aromatic compounds like Al_4^{2-} and all-metal antiaromatic compounds like Al_4^{4-} and their complexes in terms of different global and local reactivity descriptors as well as the nucleus independent chemical shift. Aromaticity and antiaromaticity in cyclic alkali clusters like Na_6 and K_6, polyacene analogues of inorganic ring compounds, multivalent superatoms, trigonal cyclic π - bonded dianions like Be_3^{2-} and Mg_3^{2-} as well as their different sandwich and multi- decker complexes are analyzed in terms of those reactivity descriptors and the associated electronic structure principles. The hydrogen storage ability of these clusters has been explored.

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