Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Colloquium

Boron Chemistry: What can theory contribute new and what to pay attention to for accurate calculations

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Boron chemistry has made tremendous progress in recent decades, leading to the isolation of a variety of compounds with remarkable electronic structures and properties. To stabilise such compounds, Lewis bases are of tremendous importance. Cyclic (alkyl) (amino) carbons (CAACs) and N-heterocyclic carbons (NHCs) are widely used, leading to compounds with closed shells but also with biradicaloid electronic structures. In this talk, we explore the underlying effects that determine the electronic structures of each species and show how UV-Vis spectra can be used to accurately characterise the electronic structure of biradicaloid electronic structures.[1-4]

In addition, we focus on anionic boron and carbon-based hetero-biradicaloids to uncover the reasons for their small singlet-triplet gaps.[5,6] For the various examples, we always highlight potential pitfalls in the calculations.

References:

[1] Welz et al. *JACS* **2018** DOI: 10.1021/jacs.8b07644
[2] Schmid, et al. *CHEM EJ* **2021** DOI: 10.1002/chem.202004619
[3] Legare et al. *Science* **2018** DOI: 10.1126/science.aaq1684
[4] Fantuzzi et al. *Chem. Sci.* **2022** DOI: 10.1039/d1sc05988b
[5] Maiti et al. JACS **2021** DOI: 10.1021/jacs.0c12624
[6] Jia et al. *Chem. Sci.* **2021** DOI: 10.1039/d1sc02409d

Wednesday, Sep 28th 2022

4:00 PM (Tea/Coffee at 3:45 PM)

Auditorium, TIFR-H