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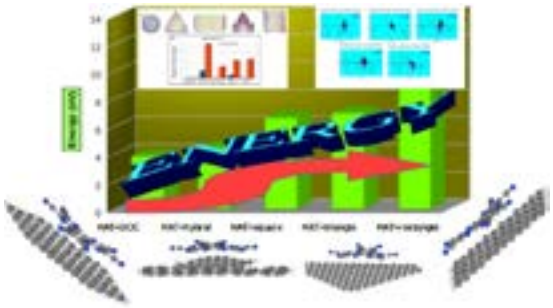
Understanding the non-covalent interaction mediated modulations to the electronic structure of quasi-zero-dimensional graphene nanoflakes

Amrit Sarmah[1,2] and **Pavel Hobza**[1,2]
[1]Institute of Organic Chemistry and Biochemistry - CAS, Czech Republic
[2]Palacky University, Czech Republic

In the contemporary years, the magnetic or electric field induced modulations to the electronic environment of single molecular systems are a common practice. In this particular study, we have instigated the possibility of controlling the electronic and spin-dependent properties of hydrogen-terminated graphene fragments, so-called graphene nanoflakes (GNF) using weak non-covalent interaction as the external stimuli. The topological frustration in the graphene fragment appreciated the compelling electronic behavior of the system. This leads to some unorthodox spin-distribution in the system and it is possible to synchronize this electronic perturbation switching through a non-covalent interaction. These findings institute new avenue to sculpting such donor-acceptor composite as a self-regulated spintronic device in the next generation electronics.



Recent Publications

1. Bruno de la Torre et al. (2018) Non-covalent control of spin-state in metal-organic complex by positioning on n-doped graphene. Nat. Comm. 9:2831.
2. Amrit Sarmah and Pavel Hobza (2018) Sequential BN-doping induced tuning of electronic properties in zigzag-edged graphene nanoribbons: a computational approach. RSC Adv. 8(20):10964-10974.
3. Amrit Sarmah and Pavel Hobza (2017) Understanding the spin-dependent electronic properties of symmetrically far-edge doped zigzag graphene nanoribbon from a first principles study. RSC Adv. 7(74):46604-46614.
4. Prasenjit Sarkar et al. (2017) An iminosemiquinone-coordinated oxidovanadium(v) complex: a combined experimental and computational study. Inorg. Chem. 56(14):8068-8077.

Biography

Amrit Sarmah pursued his PhD from the BITS Pilani, India. He is working in the field of theoretical and computational chemistry. After completing his PhD he had several international exposures in the field of theoretical chemistry and carried on his scientific endeavors at different places such as King Abdullah University of Science and Technology (KSA) Ben-Gurion University (Israel), JNCSR and IOCB (Czech Republic). His current research interest included computational design and fabrication of hybrid carbon nanomaterials and extensive theoretical investigation to tune their electronic and transport properties, modeling charge carrier mobility in 2D and quasi-2D semiconductors and non-covalent interaction mediated modulations to the spin-dependent properties of nanomaterials.

amrit.sarmah@uochb.cas.cz