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Structure and electronic properties of Graphene-Triazine bilayered complexes: A computational investigation

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In the recent decades graphene immersed into the technology and industry with its various derivatives including with its immense functionality by making a complex, combination with other organic molecules, atoms and the combination of the both. Noncovalent functionalization creates scope of wide range of application of graphene complexes. Our intention is to characterize the stacking-like two-layered graphene nanoparticles. We selected the triazin and its substituted derivatives having donor-acceptor properties to layer on the graphene surface. We conducted the cluster and crystal model of the graphene surface to sketch the electronic and structural properties. We verified the stability of the complex using Density Functional Theory (DFT) by measure the interaction energy and charge transfer. On the other hand the macrostructural character was contemplated by the meta-dynamics simulation in material studio platform.

Biography:

Dr. Adhikary has completed his PhD from Inha University, Incheon, South Korea, in 2003 and 3 years postdoctoral studies from the department of chemisrery of the same university. He was an Associate Professor of the department of chemistry, Inha University upto the end of 2019. After Ph.D., he serves his academic role in the university of development alternative, Dhaka, Bangladesh for two years and currently academic faculty of the center for Green Chemistry and Environmental Biotechnology (GREAT) at Ghent University Global Campus (GUGC), Incheon, Korea. He has published several papers in the various reputed journals and has been serving as a guest editor of multiple journals.