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Structure and Properties of Stacking-type Complexes of Triazin at Graphene Surface: A Theoretical Assessment

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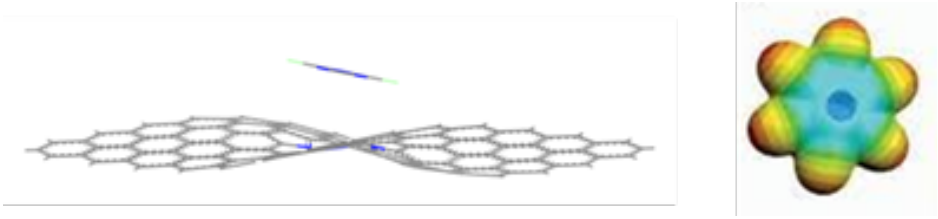
In recent decades graphene immersed into the technology and industry with its various derivatives including with its immense functionality by making a complex, combination with other organic molecules, atoms and the combination of the both. Noncovalent functionalization creates a wide range of applications for these graphene complexes. Our intention was to characterize the stacking-like two-layered graphene nanoparticles. We selected triazin and its substituted derivatives ((1) 2,4,6-tris(dimethylamine)-1,3,5-triazine (TDA); (2) 2,4,6-triamino-1,3,5-triazine (TAM); (3) 2,4,6-trihydroxy-1,3,5-triazine (THO); (4) 1,3,5-triazine (TZN); (5) 2,4,6-trithiol-1,3,5-triazine (TTH); (6) 2,4,6-trichloro-1,3,5-triazine (TCL); and (7) 2,4,6-trifluoromethyl-1,3,5-triazine (TFM).) having donor-acceptor properties of the stacked layer on the graphene surface. We conducted cluster and crystal model calculations for the graphene surface to sketch the electronic and structural properties. We verified the stability of the formed complexes using Density Functional Theory (DFT) by quantification of the interaction energy and charge transfer.

Keywords: Cluster and Crystal model, Electron acceptors and Electron donors, Electrostatic potentials, Partial electron density, Band-gap, Electron holes.



The electrostatic potential including the magnitude of the π-hole, Vs.max, of the acceptors on a defective graphene surface.

Biography:

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