Publications

Journal Articles

1. Hossain, M. R. et al. DFT and QTAIM investigations of the adsorption of chlormethine anticancer drug on the exterior surface of pristine and transition metal functionalized boron nitride fullerene. J. Mol. Liq. 323, 114627 (2021).
2. Hossain, M. R. et al. Adsorption behaviour of metronidazole drug molecule on the surface of hydrogenated graphene, boron nitride and boron carbide nanosheets in gaseous and aqueous medium: A comparative DFT and QTAIM insight. Phys. E Low-dimensional Syst. Nanostructures 126, 114483 (2021).
3. Rahman, H., Hossain, M. R. & Ferdous, T. The recent advancement of low-dimensional nanostructured materials for drug delivery and drug sensing application: A brief review. J. Mol. Liq. 320-A, 114427 (2020).
4. Miah, M. H., Hossain, M. R., Islam, M. S., Ferdous, T. & Ahmed, F. A theoretical study of allopurinol drug sensing by carbon and boron nitride nanostructures: DFT, QTAIM, RDG, NBO and PCM insights. *RSC Adv.* **11**, 38457–38472 (2021).
5. Shamim, S. U. D. *et al.* Theoretical investigation of emodin conjugated doped B12N12 nanocage by means of DFT, QTAIM and PCM analysis. *Phys. E Low-dimensional Syst. Nanostructures* **136**, 115027 (2022).
6. Hasan, M. M. *et al.* The computational quantum mechanical investigation of the functionalized boron nitride nanocage as the smart carriers for favipiravir drug delivery: a DFT and QTAIM analysis. *J. Biomol. Struct. Dyn.* 1–17 (2021) doi:10.1080/07391102.2021.1982776.
7. Hossain, M. A. *et al.* An ab-initio Study of the B35 Boron Nanocluster for Application as Atmospheric Gas (NO,NO2,N2O,NH3) Sensor. *Chem. Phys. Lett.* **754**, 137701 (2020).
8. Shamim, S. U. D. *et al.* A DFT study on the geometrical structures, electronic, and spectroscopic properties of inverse sandwich monocyclic boron nanoclusters ConBm (n = 1.2; m = 6–8). *J. Mol. Model.* **26**, 1–17 (2020).
9. Rakib Hossain, M. *et al.* First-principles study of the adsorption of chlormethine anticancer drug on C24, B12N12 and B12C6N6 nanocages. *Comput. Theor. Chem.* **1197**, 113156 (2021).