22nd Iranian Chemistry Conference, 23-25 August, 2023
University of Kurdistan

# The computational study of the interaction of Hydroxycarbamide molecule with pristine, Ni-doped $C_{20}$ nanocage: AIM, NBO, DFT, and TD-DFT

**A. Bagheri, M. Talaei, Z. Zand, M. Rezeai Sameti***
***Department of Applied Chemistry, Faculty of Science, Malayer University, Malayer, 65174, Iran***
*E-mail: mrsameti@malayeru.ac.ir*

**Abstract:**

After the discovery of carbon nanoparticles, great attention focused on other nanoparticles and nanocages such as $C_{20}$ nanocage due to thermal stability, high conductivity, high hardness, gas sensing, hydrogen storage, electronic devices [1], and other adsorption properties[2–3]. This study aims to investigate the adsorption of hydroxy carbamide (HCA) drugs on the surfaces of the pristine and Ni-doped $C_{20}$ nanocage. For this purpose, at the first step, we consider different configurations for adsorbing HCA on the surface of nanocage, and then all considered structures are optimized at the cam-B3LYP / LanL2DZ level of DFT theory by using Gaussian software (09). The quantum parameters, thermodynamic parameters, molecular electrostatic potential, TD-DFT parameters, UV-visible spectrum, the density of state (DOS), and MEP graphs are calculated and all calculated results are analyzed. The Uv-visible results demonstrate that with adsorbing HCA drug and functionalizing Ni atom, the adsorption frequency increased significantly from the original state. The HOMO-LUMO and MEP results show that the charge density transferred from the HCA drug towered nanocage surface and so the nucleophilic properties of nanocage surface increase. The quantum parameters show that the gap energy of the system after adsorbing HCA alters silently from the original state, and so the $C_{20}$ nanocage is not a good sensor for detecting drugs. On the other than the values of thermodynamic parameters such as enthalpy and Gibbs free energy for all adsorption models are negative and favorable in the thermodynamic approach. These results confirm that the pristine and Ni-doped $C_{20}$ nanocage can be used as adsorbed for HCA molecules.

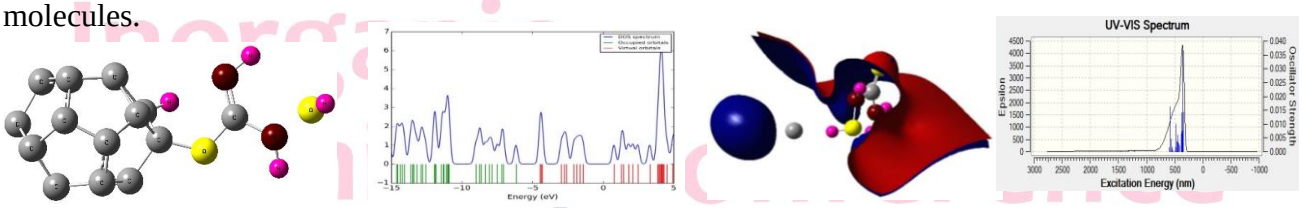



**Figure 1:** The optimized structure, DOS, MEP, and UV-visible plot of $C_{20}$ nanocage with HCA drug complex.

***Keywords:*** $C_{20}$ nanocage, Hydroxycarbamide, Ni, NBO, DOS

**References**

[1] R. Rahimi, R., H. Solimannejad, M., *Str. Chem*. **2020**, 31, 133.
[2] P. Fallahi, H. Jouypazadeh, H. Farrokhpour, *J. Mol. Liq*. **2018**, 260, 138–148.
[3] M. Rezaei-Sameti, H. J. Behbahani, *Phys Chem Res*. **2018**, 6(1), 31–43.