Int. J. New. Chem., 2020, Vol. 7, Issue 2, pp. 87-100.

International Journal of New Chemistry

Published online April 2020 in http://www.ijnc.ir/.

Open Access

Print ISSN: 2645-7236

Online ISSN: 2383-188x

Original Research Article

Quetiapine Adsorption on the Surface of Boron Nitride Nanocage ($B_{12}N_{12}$): A Computational Study

Mohammad Reza Jalali Sarvestani[1*], Maryam Gholizadeh Arashti[2], Betty Mohasseb[3]

[1*] Young Researchers and Elite Club, Yadegar-e-Imam Khomeini (RAH) Shahr-e-Rey Branch, Islamic Azad University, Tehran, Iran

[2]Department of Physics, Yadegar-e-Imam Khomeini (RAH) Shahre Rey Branch, Islamic Azad University, Tehran, Iran

[3]Department of Chemistry, Osmania University, Hyderabad- 500007, India

Received: 2020-01-07 *Accepted: 2020-02-20* *Published: 2020-04-01*

ABSTRACT

In this research, IR and frontier molecular orbital (FMO) computations were employed for investigating the performance of $B_{12}N_{12}$ as a novel recognition element for fabrication of quetiapine thermal and electrochemical sensors. All of the computations were done by density functional theory method in the B3LYP/6-31G(d) level of theory and in the aqueous phase. The obtained enthalpy changes (ΔH_{ad}), Gibbs free energy variations (ΔG_{ad}) and thermodynamic equilibrium constants (K_{th}) indicated that quetiapine interaction with boron nitride nanocage is exothermic, spontaneous, irreversible and experimentally feasible. The bond lengths between the adsorbent and the adsorbate and adsorption energy values showed quetiapine interaction with $B_{12}N_{12}$ is a chemisorption. The temperature was also optimized and the findings revealed 298.15 K is the best temperature for quetiapine adsorption on the $B_{12}N_{12}$ surface. The DOS spectrums showed $B_{12}N_{12}$ is an appropriate electroactive recognition for fabrication of new quetiapine electrochemical sensors. The specific heat capacity values (C_V) proved the thermal conductivity of quetiapine has improved after its interaction with the nanostructure. Some structural parameters including energy gap, chemical hardness, chemical potential, electrophilicity, maximum transferred charge, zero-point energy and dipole moment were also calculated and discussed in details.

Keywords: Quetiapine, Density functional Theory, Boron nitride nanocage ($B_{12}N_{12}$), Adsorption, Sensor.

***Corresponding author Tel.: +989102125066**
***E-mail: Rezajalali93@yahoo.com**