عنوان مقاله:

Quetiapine Adsorption on the Surface of Boron Nitride Nanocage (B12N12): A Computational Study

محل انتشار:

فصلنامه شیمی نوین, دوره 7, شماره 2 (سال: 1399)

تعداد صفحات اصل مقاله: 14

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خلاصه مقاله:

In this research, IR and frontier molecular orbital (FMO) computations were employed for investigating the performance of B12N12 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 (ΔHad), Gibbs free energy variations (ΔGad) and thermodynamic equilibrium constants (Kth) 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 B12N12 is a chemisorption. The temperature was also optimized and the findings revealed 298.15 K is the best temperature for quetiapine adsorption on the B12N12 surface. The DOS spectrums showed B12N12 is an appropriate electroactive recognition for fabrication of new quetiapine electrochemical sensors. The specific heat capacity values (CV) 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

کلمات کلیدی:

Quetiapine, density functional theory, Boron nitride nanocage (B12N12), Adsorption, sensor