عنوان مقاله:

The investigation of adsorption of drug anticancer Ceritinib on surfaces Nanotubes Boron Nitride: A DFT study

محل انتشار:

هجدهمین همایش شیمی فیزیک ایران (سال: 1394)

تعداد صفحات اصل مقاله: 2

نویسندگان:

Sh Mehrafza - *Department of Chemistry, Pharmaceutical Sciences Branch, Islamic Azad University, Tehran, Iran*

A Shameli - *Department of Chemistry, Omidiyeh Branch ,Islamic Azad University , Omidiyeh, Iran*

E Balali - *Department of Chemistry, Pharmaceutical Sciences Branch, Islamic Azad University, Tehran, Iran*

R Khadivei - *Department of Chemistry, Pharmaceutical Sciences Branch, Islamic Azad University, Tehran, Iran*

خلاصه مقاله:

Boron nitride nanotubes (BNNTs) were first theoretically predicted in1994 [1] and thenexperimentally synthesized in 1995. Because of their un usual mechanical properties,excellent chemical and thermal stabilities, the BNNTs have been promising potential forapplication sin nano electronic devices such as sensor and hydrogen storage media. Thefunctionalize dordoped BNNTs further en large the applications in nano molecular range. Inthe process of preparations or modifications, various types of defects on BNNTs can beformed, such as impurity atom doping. The doped BNNTs with low dimension and highsurface to volume ratio have been demonstrate das gas chemical sensors to detect manymolecules, such as CO, NO , CO2 , NH3, H2 and soon. Cu functionalized BNNT exhibitconsiderably improved ability to monitor CO2. Both aluminum and gallium doping cansignificantly enhance the adsorption energy of NH3/ BNNTs complexes [2,3]. In this paper,consisting of armchair cores BNNT are optimized by the density functional theory (DFT)method. The structural stability is investigated by analyzing the parametric variation in thetube radius, .energy, and deformation electron density

کلمات کلیدی: