عنوان مقاله:

Theoretical investigation about the attachment of Bis-GMA molecule onto the surface of SiO2

محل انتشار:

چهارمین کنفرانس بین المللی یافته های نوین علوم و تکنولوژی (سال: 1396)

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خلاصه مقاله:

First-principle calculations based on density functional theory (DFT) have been carried out to investigate the adsorption of Bis-GMA onto the SiO2 monolayer. The obtained results demonstrated that the Bis-GMA molecule has been physically adsorbed onto the surface of SiO2 with the adsorption energy of about -0.83 eV. Moreover, exploring the electronic properties of the system upon the adsorption process have revealed that the SiO2 has preserved its intrinsic electronic properties as the Bis-GMA molecule bound to the surface. The results of the present work seem to be very useful in providing deep insight about interface interactions between biologically relevant molecules and inorganic nanostructures and are hoped to aid future experimental investigations in this topic.

کلمات کلیدی:

DFT, Adsorption, SiO2, Bis-GMA