عنوان مقاله:

Density functional theory study of the adsorption of NO۲ molecule on Nitrogen-doped TiO۲ anatase nanoparticles

محل انتشار:

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خلاصه مقاله:

Adsorption of NO۲ molecule on pristine and N-doped TiO۲ anatase nanoparticles have been studied using the density functional theory (DFT) technique. The structural properties (such as bond lengths and bond angles) and the electronic properties (such as density of states, band structures and atomic partial charges) have been computed for considered nanoparticles. The results show that, the adsorption of NO۲ molecule on N-doped nanoparticles is more energetically favorable than the adsorption of NO۲ molecule on the pure TiO۲ nanoparticles. However, on the base of .the obtained results, the N-doped TiO۲ nanoparticles can be used in NO۲ sensing and removing applications

کلمات کلیدی:

Density Functional Theory (DFT), Titanium dioxide, Nitrogen dioxide, Mulliken analysis, Density of states, Band Structure