عنوان مقاله:

A theoretical study on the adsorption behaviors of Ammonia molecule on N-doped TiO۲ anatase nanoparticles: Applications to gas sensor devices

محل انتشار:

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خلاصه مقاله:

We have performed density functional theory investigations on the adsorption properties of ammonia molecule on the undoped and N-doped TiO۲ anatase nanoparticles. We have geometrically optimized the constructed undoped and N-doped nanoparticles in order to fully understand the adsorption behaviors of ammonia molecule. For TiO۲ anatase nanoparticles, the binding site is preferentially located on the fivefold coordinated titanium sites. However, we have mainly studied the interaction of NH۳ molecule over the fivefold coordinated titanium sites including the bond lengths, bond angles, adsorption energies, density of states (DOSs) and molecular orbitals. The results indicated that the adsorption of NH۳ molecule on the N-doped nanoparticles is energetically more favorable than the adsorption on the undoped one, suggesting the strong adsorption of NH۳ molecule on the N-doped nanoparticles. Adsorption on the N-doped nanoparticles leads to the more stable and favorable complexes. Our theoretical work represents that the N-doped nanoparticles have higher sensing capability than the pristine ones to remove the hazardous NH۳ molecules from the environment.

کلمات کلیدی:

Adsorption, Density Functional Theory (DFT), Density of states, TiO۲, NH۳