Abstract

This paper discusses the adsorption and dissociation of the hydrogen sulfide (H_2S) molecule on the titanium dioxide surface. They were studied by density function theory (DFT). The GGA + *U*approach was used to analyze the adsorption behavior of the H_2S molecule on the TiO_2 anatase (100) surface. The results presented include adsorption energies, structural and electronic properties, charge transfer and work function. Different adsorption configurations are considered with coordination of H_2S at the surface (Ti_{5c}, $(Ti_{5c})_2$, O_{2c} and O_{3c} sites). The calculated adsorption energies are −0.31, −0.28, −1.14 and −5.66 eV. The most favorable adsorption sites lead to the dissociation of H_2S into HS and H, where the S atom of HS binds to Ti_{5c} or O_{2c} atoms, leaving a dissociated H atom bonded to another O_{2c} site. Analysis of Bader's charges reveals a significant charge transfer between the molecule and the surface of the TiO_2 anatase. The adsorption process reduces the work function and bandgap of the system, which improves the photocatalytic properties of TiO_2.