عنوان مقاله:

Van der Waals corrected DFT study on the adsorption behaviors of TiO2 anatase nanoparticles as potential molecule sensor for thiophene detection

محل انتشار:

مجله بین المللی فناوری نانو در آب و محیط زیست, دوره 2, شماره 1 (سال: 1395)

تعداد صفحات اصل مقاله: 14

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خلاصه مقاله:

Density functional theory investigations were conducted in order to study the effects of the adsorption of thiophene on the structural and electronic properties of TiO2 anatase nanoparticles. The ability of pristine and N-doped TiO2 anatase nanoparticles to recognize toxic thiophene was surveyed in detail. It was found that thiophene molecule is chemisorbed on the N-doped anatase nanoparticles in S site geometries with large adsorption energy and small distance. By including van der Waals (vdW) interactions between thiophene molecule and TiO2, we found that the adsorption on the N-doped TiO2 is energetically more favorable than the adsorption on the pristine one, suggesting that the nitrogen doping can energetically facilitate the thiophene adsorption on the N-doped nanoparticle. The order of adsorption energy is Parallel(S site)> Perpendicular(S site)> Perpendicular (H site). The interaction between thiophene and N-doped TiO2 can induce substantial variations in the HOMO/LUMO molecular orbitals of the nanoparticle, changing its electrical conductivity, which is helpful for designing the novel sensor and remover devices. Charge analysis based on Mulliken charges reveals that charge is transferred from thiophene molecule to TiO2 nanoparticle

کلمات کلیدی:

Thiophene; TiO2; Electronic properties; Density functional theory