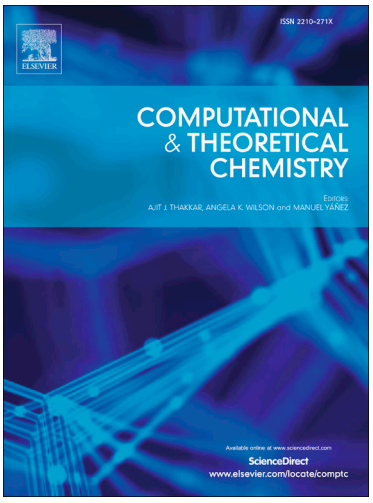

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A novel strategy for SO_x removal by N-doped TiO_2/WSe_2 nanocomposite as a highly efficient molecule sensor investigated by van der Waals corrected DFT

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Abstract

On the basis of density functional theory (DFT) calculations, we demonstrate the potential applicability of TiO_2/WSe_2 nanocomposite as a highly sensitive molecule sensor for SO_2 and SO_3 molecules. SO_x molecules chemically adsorb on TiO_2/WSe_2 nanocomposite via strong chemical bonds. With vdW interactions included, the adsorption energies were corrected for long range dispersion energy, indicating adsorption energetic and possible configurations of SO_x molecules towards TiO_2/WSe_2 nanocomposites. The fivefold coordinated titanium atoms in the TiO_2 act as the binding sites. On the N-doped TiO_2/WSe_2 nanocomposite, the adsorption process is found to be more favorable in energy than the adsorption on the intrinsic one, indicating that the N-doped nanocomposites have higher sensing capability than the undoped ones. The charge transfer based on NBO analysis reveals that the SO_x molecule behaves as an electron acceptor. The electronic properties of the system were also investigated in view of the projected density of states and molecular orbitals of the TiO_2/WSe_2 with adsorbed SO_x molecules. Over the TiO_2/WSe_2 nanocomposites, SO_3 molecule dissociates into SO_2 and detached oxygen atom. The results present a great potential of TiO_2/WSe_2 nanocomposites for application as a highly efficient molecule sensor for SO_x detection.

Keywords: Adsorption; Density functional theory; DOS; SO_x; TiO_2/WSe_2 nanocomposite