

Accepted Manuscript

A novel strategy for SO_x removal by N-doped TiO₂/WSe₂ nanocomposite as a highly efficient molecule sensor investigated by van der Waals corrected DFT

Amirali Abbasi, Jaber Jahanbin Sardroodi

PII: S2210-271X(17)30252-9

DOI: <http://dx.doi.org/10.1016/j.comptc.2017.05.020>

Reference: COMPTC 2515

To appear in: *Computational & Theoretical Chemistry*

Received Date: 16 April 2017

Revised Date: 12 May 2017

Accepted Date: 16 May 2017



Please cite this article as: A. Abbasi, J.J. Sardroodi, A novel strategy for SO_x removal by N-doped TiO₂/WSe₂ nanocomposite as a highly efficient molecule sensor investigated by van der Waals corrected DFT, *Computational & Theoretical Chemistry* (2017), doi: <http://dx.doi.org/10.1016/j.comptc.2017.05.020>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

A novel strategy for SO_x removal by N-doped TiO₂/WSe₂ nanocomposite as a highly efficient molecule sensor investigated by van der Waals corrected DFT

Amirali Abbasi^{a,b,c*}, Jaber Jahanbin Sardroodi^{a,b,c}

a. Molecular Simulation laboratory (MSL), Azarbaijan Shahid Madani University, Tabriz, Iran

b. Computational Nanomaterials Research Group (CNRG), Azarbaijan Shahid Madani University, Tabriz, Iran

c. Department of Chemistry, Faculty of Basic Sciences, Azarbaijan Shahid Madani University, Tabriz, Iran

* Corresponding Author, Tel: +98-412-432-7541; Email: a_abbasi@azaruniv.edu

Abstract

On the basis of density functional theory (DFT) calculations, we demonstrate the potential applicability of TiO₂/WSe₂ nanocomposite as a highly sensitive molecule sensor for SO₂ and SO₃ molecules. SO_x molecules chemically adsorb on TiO₂/WSe₂ 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 TiO₂/WSe₂ nanocomposites. The fivefold coordinated titanium atoms in the TiO₂ act as the binding sites. On the N-doped TiO₂/WSe₂ 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 TiO₂/WSe₂ with adsorbed SO_x molecules. Over the TiO₂/WSe₂ nanocomposites, SO₃ molecule dissociates into SO₂ and detached oxygen atom. The results present a great potential of TiO₂/WSe₂ nanocomposites for application as a highly efficient molecule sensor for SO_x detection.

Keywords: Adsorption; Density functional theory; DOS; SO_x; TiO₂/WSe₂ nanocomposite

Download English Version:

<https://daneshyari.com/en/article/5392383>

Download Persian Version:

<https://daneshyari.com/article/5392383>

[Daneshyari.com](https://daneshyari.com)