

Accepted Manuscript

A Computational Study on Interactions of Ni- and Pt-Doped Boron nitride nano tubes with NH_3 in Presence and Absence of Electric Fields

Mohsen Mohsennia, Mahdi Rakhshi, Hossein Rasa

PII: S2210-271X(18)30179-8
DOI: <https://doi.org/10.1016/j.comptc.2018.05.013>
Reference: COMPTC 2799

To appear in: *Computational & Theoretical Chemistry*

Received Date: 8 February 2018
Revised Date: 18 May 2018
Accepted Date: 20 May 2018



Please cite this article as: M. Mohsennia, M. Rakhshi, H. Rasa, A Computational Study on Interactions of Ni- and Pt-Doped Boron nitride nano tubes with NH_3 in Presence and Absence of Electric Fields, *Computational & Theoretical Chemistry* (2018), doi: <https://doi.org/10.1016/j.comptc.2018.05.013>

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 Computational Study on Interactions of Ni- and Pt-Doped Boron nitride nano tubes with NH₃ in Presence and Absence of Electric Fields

Mohsen Mohsennia^{a, b, *}, Mahdi Rakhshi^a, Hossein Rasa^a

^a*Department of Chemistry, University of Kashan, Kashan, Iran*

^b*Institute of Nano science and Nanotechnology, University of Kashan, Kashan, Iran*

*Corresponding author: Tel: +98 31 55913065; Fax: +98 31 55912397

E-mail address: m.mohsennia@kashanu.ac.ir (M.Mohsennia)

Abstract

The density functional theory (DFT) has been used to study the surface interactions of pristine, Ni- and Pt-doped (4,4), (5,5), (7,7) and (8,8) boron nitride nanotubes (BNNTs) with ammonia (NH₃) molecules. To verify the impact of external electric field (EF) on the surface interactions between the nanotubes and adsorbed NH₃ molecules, in this work, the NH₃/(4,4) BNNTs adsorbed complex system under an applied EF with strength of 3×10^{-2} a.u. and 4×10^{-2} a.u., along the z axis (perpendicular to the tube axis) has been investigated. It was shown that after doping of Ni and Pt atoms, the primary symmetry of BNNTs was decreased, enhancing the chemical activity of BNNTs towards NH₃ molecules and subsequent resulting in dramatic changes of their electronic properties. Our overall results indicated that, in addition to the Ni and Pt doping, the applied external EF could enhance the sensitivity of BNNTs toward NH₃ molecule, which can be considered as a new strategy of sensor fabrication.

Keywords: Boron nitride nanotube, Density functional theory, Electric field, Surface interactions

1. Introduction

Boron nitride nanotubes (BNNTs), a polymorph of boron nitride with the structure analogous to carbon nanotubes (CNTs), have attracted considerable research effort over recent years [1-2]. In comparison with CNTs, BNNTs with uniform electronic properties show semiconductor behavior with wide band gaps, relative chemical inertness and decent heat resistance [3]. In addition to numerous applications in nano electronic devices, BNNTs with high chemical and

Download English Version:

<https://daneshyari.com/en/article/7838770>

Download Persian Version:

<https://daneshyari.com/article/7838770>

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