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A theoretical survey on the chlorine dioxide (ClO2) and its decomposed species detection by the AlN nanotube in presence of environmental gases

Z. Rahmani, Saeed Fosshat, +3 authors A. Ebadi • Published 8 December 2021 • Monatshefte für Chemie - Chemical Monthly

The adsorption of N2, O2, H2O, hydrogen chloride (HCl), Cl2, hypochlorous acid (HClO), and ClO2 gases was explored onto an AlN nanotube (AlNNT) through density functional theory computations. As N2, O2, H2O, HCl, Cl2, and HClO approach the AlNNT, their adsorption releases 7.1, 12.6, 22.3, 26.5, 30.2, and 41.2 kJ/mol of energy, respectively, indicating a physisorption. In addition, the electronic properties of the nanotube do not change significantly. As chlorine dioxide (ClO2) approaches the… Expand

Figures and Tables from this paper

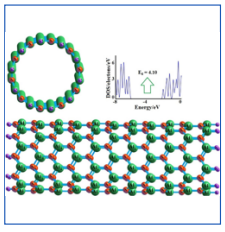

Figure 1

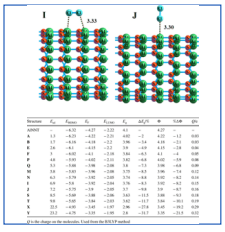

Table 1

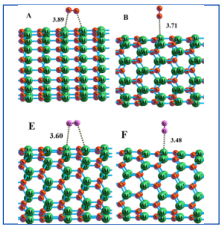

Figure 3

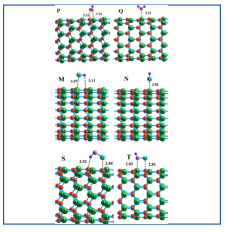

Figure 5

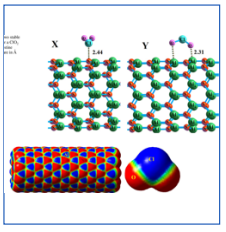

Figure 8

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Theoretical study of aluminum nitride nanotubes for chemical sensing of formaldehyde

A. Ahmadi, N. Hadipour, Mohammad Kamfiroozi, Z. Bagheri • Materials Science • 2012

Abstract Semiconductive carbon nanotubes (CNTs) have demonstrated great sensitivity toward molecules such as NH3, NO, and NO2. Nevertheless, pristine CNTs cannot be used for detection of some highly… Expand

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F−, Cl−, Li+ and Na+ adsorption on AlN nanotube surface: A DFT study

M. Samadizadeh, Somayeh F. Rastegar, A. A. Peyghan • Materials Science • 2015

Abstract Adsorption of two anions (F − and Cl −) and two cations (Li + and Na +) on the surface of aluminum nitride nanotubes (AlNNTs) is investigated by density functional theory. The reactions… Expand

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DFT study on the adsorption behavior and electronic response of AlN nanotube and nanocage toward toxic halothane gas

R. Mohammadi, A. Hosseinian, E. S. Khosroshahi, L. Edjlali, E. Vessally • Materials Science • 2018

Abstract We have investigated the adsorption of a halothane molecule on the AlN nanotube, and nanocage using density functional theory calculations. We predicted that the halothane molecule tends to… Expand

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Associative vs. dissociative mechanism: Electrocatalysis of nitric oxide to ammonia

Chaozheng He, Jia Wang, Ling Fu, Chenxu Zhao, Jin-Rong Huo • Chemistry • Chinese Chemical Letters • 2021

ABSTRACT Nitric oxide reduction to ammonia by electrocatalysis is the potential application in the elimination of smog and energy conversion. In this work, the feasibility of the application of… Expand

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Fluorination of the exterior surface of AlN nanotube: A DFT study

M. T. Baei, A. A. Peyghan, Z. Bagheri • Materials Science • 2013

Abstract Fluorination of a zigzag AlN nanotube (AlNNT) with one to four F atom(s) has been investigated using density functional theory in terms of energetic, geometric, and electronic properties.… Expand

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Effect of electrostatic interaction on the methylene blue and methyl orange adsorption by the pristine and functionalized carbon nanotubes

D. Robati, S. Bagheriyan, M. Rajabi, O. Moradi, A. A. Peyghan • Chemistry • 2016

Abstract Multi-walled carbon nanotubes (MWCNTs) were functionalized with cysteamine groups by several percentage of mass as adsorbents, then kinetics adsorption capacity was investigated for… Expand

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Nitrous oxide adsorption on pristine and Si-doped AlN nanotubes

J. Beheshtian, M. T. Baei, A. A. Peyghan, Z. Bagheri • Materials Science, Medicine • Journal of Molecular Modeling • 2012

Using density functional theory, we studied the adsorption of an N2O molecule onto pristine and Si-doped AlN nanotubes in terms of energetic, geometric, and electronic properties. The N2O is weakly… Expand

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DFT study of the dissociative adsorption of HF on an AlN nanotube

M. Noei, A. Salari, Nastaran Ahmadaghaei, Z. Bagheri, A. A. Peyghan • Chemistry, Materials Science • 2013

Abstract We have investigated the adsorption of hydrogen fluoride (HF) on the AlN nanotube surface using density functional theory in terms of energetic, structural and electronic properties. By… Expand

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The effect of surface curvature of aluminum nitride nanotubes on the adsorption of NH3

A. Ahmadi, Mohammad Kamfiroozi, J. Beheshtian, N. Hadipour • Chemistry • 2011

Our main objectives are to address the following fundamental issues: (1) A density functional theory study on the structural and electronic properties of the zigzag single-walled aluminum nitride… Expand

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B-doping makes the carbon nanocones sensitive towards NO molecules

M. T. Baei, A. A. Peyghan, Z. Bagheri, M. B. Tabar • Physics • 2012

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