Theoretical investigation of methane adsorption onto boron nitride and carbon nanotubes

Author Masoud Darvish Ganji, Amir Mirnejad and Ali Najafi

Affiliations Department of Chemistry, Islamic Azad University, Ghaemshahr Branch , Mazandaran, Iran

E-mail ganji_md@yahoo.com

Journal Science and Technology of Advanced Materials Create an alert RSS this journal

Issue Volume 11, Number 4

Citation Masoud Darvish Ganji *et al* 2010 *Sci. Technol. Adv. Mater.* **11** 045001

doi: 10.1088/1468-6996/11/4/045001

Article | References

Tag this article Full text PDF (3.20 MB)

Abstract Methane adsorption onto single-wall boron nitride nanotubes (BNNTs) and carbon nanotubes (CNTs) was studied using the density functional theory within the generalized gradient approximation. The structural optimization of several bonding configurations for a CH_4 molecule approaching the outer surface of the (8,0) BNNT and (8,0) CNT shows that the CH_4 molecule is preferentially adsorbed onto the CNT with a binding energy of −2.84 kcal mol^{-1}. A comparative study of nanotubes with different diameters (curvatures) reveals that the methane adsorptive capability for the exterior surface increases for wider CNTs and decreases for wider BNNTs. The introduction of defects in the BNNT significantly enhances methane adsorption. We also examined the possibility of binding a bilayer or a single layer of methane molecules and found that methane molecules preferentially adsorb as a single layer onto either BNNTs or CNTs. However, bilayer adsorption is feasible for CNTs and defective BNNTs and requires binding energies of −3.00 and −1.44 kcal mol^{-1} per adsorbed CH_4 molecule, respectively. Our *first-principles* findings indicate that BNNTs might be an unsuitable material for natural gas storage.

PACS 68.43.Mn Adsorption kinetics
71.15.Mb Density functional theory, local density approximation, gradient and other corrections
61.46.Fg Nanotubes
71.15.Nc Total energy and cohesive energy calculations

Subjects Condensed matter: electrical, magnetic and optical
Surfaces, interfaces and thin films
Nanoscale science and low-D systems

Dates Issue 4 (August 2010)
Received 24 十一月 2009 , accepted for publication 21 七月 2010
Published 10 九月 2010

Your last 10 viewed

1. Theoretical investigation of methane adsorption onto boron nitride and carbon nanotubes
Masoud Darvish Ganji *et al* 2010 *Sci. Technol. Adv. Mater.* **11** 045001
2. Present status of amorphous In–Ga–Zn–O thin-film transistors
Toshio Kamiya *et al* 2010 *Sci. Technol. Adv. Mater.* **11** 044305

Users also read What's this?

1. A method for the extraction of the voltage-dependent quantum capacitance of carbon nanotubes using *ab initio* simulations
2. A methodology to investigate the intrinsic effect of the pulsed electric current during the spark plasma sintering of electrically conductive powders
3. High-frequency micromechanical columnar resonators

More

Related review articles What's this?

1. Advances in principal factors influencing carbon dioxide adsorption on zeolites
2. Competing interactions in molecular adsorption: NH_3 on Si(001)
3. Understanding voltage-induced localization of nanoparticles at a liquid–liquid interface

More

Article links

Post to CiteUlike
Post to Connotea
Post to Bibsonomy

View by subject

All Subjects
All Dates
All journals | This journal only
Search

Export

BibTeX format (bib)
Abstract | References
Export Results