International Journal of New Chemistry, 2014, 1 (4), 160-165.

Published online 2014 in http://www.ijnc.ir/.

Original Article

ISSN: 2383-188X

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Radial Distribution Function of H_2 Adsorption on Coronene and its Si Substituted at 298 K by Molecular Mechanic method

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Received 6 December 2014; Accepted 28 January 2015; Published 30 January 2015

Abstract

In this work, the radial distribution function (RDF) of H_2 adsorption on coronene (C_{24}) and its Si Substituted forms was investigated by Monte Carlo method. The effect of number and position of silicon substituent on the Coronene (C_{24}) was compared. The maximum value of RDF at 298 K and 0.1 MPa is 4.34 for 18 Si, A structure at 0.73 Å. On the basis of results, the Coronene with 18 Si can be suggested as a choice for hydrogen container.

Keywords: Coronene, Silicon, Radial Distribution Functions, Hydrogen, Monte Carlo.

1. Introduction

The use of hydrogen gas as fuel for cars in the future is discussed. In this context, finding carrier of hydrogen gas is important. The compactness and light weight are important features for hydrogen containers. One of the candidate as Hydrogen container is coronene. The three types of Carbon shows at fig1.

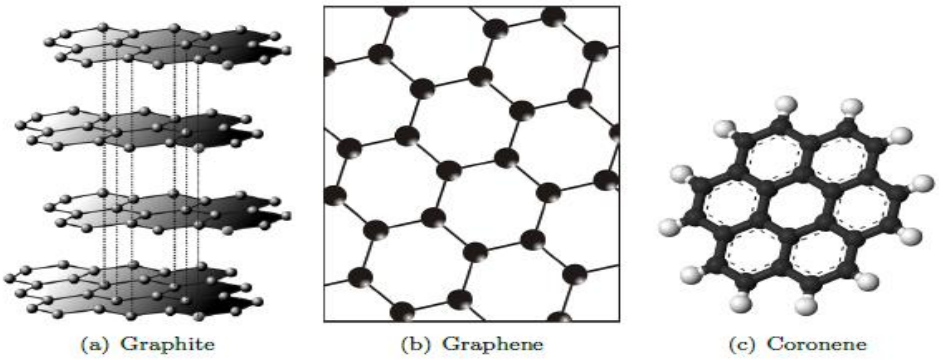

Fig1. Three types of Carbon: (a): Graphite, (b): Graphene, (c): Coronene

Coronene (also known as super Benzene) is a polycyclic aromatic hydrocarbon (PAH) comprising six peri-fused benzene rings [1]. Its chemical formula is C_{24}. It is a yellow material that dissolves in such solvents as benzene, toluene, and dichloromethane. It occurs naturally as the mineral carpathite, which is characterized by flakes of pure coronene embedded in sedimentary rock. Estimations show that physical adsorption of hydrogen on carbon is imposed vertically with 74 meV energy. The adsorbed Hydrogen is set in the middle of a carbon ring of coronene indicates 39.7 meV adsorption energy in 2.9 Å space. The study of Hydrogen adsorption was done by Froudakis and psofogiannak in 2009 with a semi empirical method. The Graphite surface forms a coronene that shows an appropriate site for hydrogen adsorption on hollow coronene sites with 30.4 meV energy in the space of 1.1 Å from coronene surface [2, 3, 4]. The physical adsorption of hydrogen was studied on Graphene and Carbon Nanotubes [5]. An experimental study shows that hydrogen can be stored in atmospheric pressure and room temperature [6]. The other studies show that the storage of hydrogen are happens in high pressures and low temperatures. Okamoto and Miyamoto show that the hydrogen adsorption with parallel navigation with graphene is much more stable [7,8]. The adsorption of hydrogen on single-walled nanotubes was studied by molecular dynamic method, and shows that this adsorption was happened at 600 K and 300 meV bond energy [9].

2. Computational details

The effect of position substituted silicon on coronene (C_{24}) is important for radial distribution function (RDF) of hydrogen. In this study the RDF of hydrogen for silicon substituted structures of coronene C_{24}, $C_{24-n}Si_n$ (n=4-24) were compared at 298 K and 0.1 MPa by using MS modeling software by (NVT) molecular mechanics method. In this work, the radial distribution of hydrogen on coronene (C_{24}) and its Si substituted forms, C_{24}, $C_{24-n}Si_n$ (n=4-24), fig 2, have been investigated at 298 K and 0.1 MPa using (N, V, T) Monte Carlo simulation by Lennard- Jones (LJ) 12-6 potential ($\emptyset_{LJ(r)}$), Eq. 1 [10].

$$\emptyset_{LJ(r)} = 4\,\varepsilon_{gc}\,[(\frac{\sigma_{gc}}{r})^{12} - (\frac{\sigma_{gc}}{r})^{6}] \qquad (1)$$

Where r is the distance between gas molecules and surface atoms in the coronene structures, σ_{gc} denotes the LJ gas- coronene collision diameter, and ε_{gc} is the LJ gas- carbon potential well depth. The Lennard- Jones parameters for the interaction between the gas and coronene surfaces were calculated using the Eq. 2, 3 [11-13]. We are considered these parameters for Si-C, C-C, H_2-H_2, C-H_2 and Si-H_2 pairs [14-19].

Structure	RDF (max)	r(Å)	Structure	RDF (max)	r(Å)
C_{24}	3.24	0.73	$C_{14}Si_{10}$, isomer B	3.01	0.75

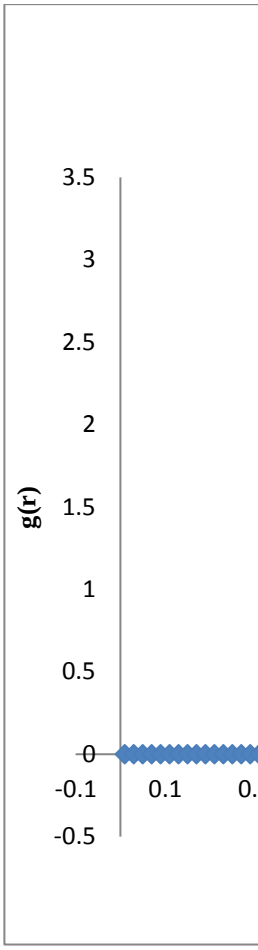

Fig 1. RDF of C_{24} Vs. r (Å)

3. Results and discussion

The aim of this

Tale1. RDF (max) of structures Vs, distance (Å)

$C_{20}Si_4$	3.10	0.73	$C_{14}Si_{10}$, isomer D	3.23	0.73
C_{18} Si_6 ,isomer A	3.44	0.75	$C_{12}Si_{12}$, isomer A	2.89	0.73
$C_{18}Si_6$, isomer B	2.84	0.73	$C_{12}Si_{12}$, isomer B	3.39	0.73
$C_{16}Si_8$, isomer A	2.70	0.71	$C_{12}Si_{12}$, isomer D	3.23	0.73
$C_{16}Si_8$, isomer B	3.12	0.73	$C_{10}Si_{14}$	3.06	0.73
$C_{16}Si_8$, isomer D	3.00	0.73	C_9Si_{15}	3.28	0.73
$C_{15}Si_9$, isomer zigzag A	3.06	0.71	C_8Si_{16}, isomer A	2.95	0.73
$C_{15}Si_9$, isomer zigzag B	3.00	0.73	C_6Si_{18}, isomer A	4.34	0.73
$C_{14}Si_{10}$, isomer A	2.61	0.73	C_6Si_{18}, isomer B	3.09	0.75
Si_{24}	3.55	1.01			

work is investigation of effect of number of substituted silicon and its position in RDF (max) of hydrogen at 298K. The Results show that the increasing of number of silicon doesn't create special magnificence of RDF, but the position of silicon is important at maximum of radial distribution function. The some of structures are show at figure 1(a- i), as sample.

The maximum of radial distribution function is equal to 4.34 at 0.73 Å for coronene structure with 18 silicon substituted at 298 k, (Table1).

4. Conclusion

The results show that the symmetric silicon substituted structures have more RDF than asymmetric types. The increase of number of silicon substitution doesn't have effect on the value of RDF. The maximum value of radial distribution is 4.34 for C_6Si_{18} isomer A (fig 2-u) structure at 0.73 Å.

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