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Computational Studies of Formation Silicon Nanotubes-Propylthiouracil Hybrids to Investigate its Role in Confining Propylthiouracil Drug

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ABSTRACT

In order to search for the interaction between Propythiouracil(ptu) and infinitely long armchair single-walled silicon nanotubes (SiNTs) is investigated using density functional theory (DFT). The structures of individual counterparts and hybrids have been optimized and the molecular properties have been evaluated. The Nuclear magnetic resonance spectroscopy (NMR) are witness to the substantial changes in the electronic properties of the SiNTs systems following the attachment of the ptu with the tube surface.

Key words: Silicon Nanotubes, Propythiouracil, Density Functional Theory, NMR.

INTRODUCTION

The Propylthiouracil was synthesized by George W. Anderson and et al[1], with propylthiouracil (ptu) is among the most commonly employed antithyroidal drugs in use, for the treatment of hyperthyroidism[2]. the FDA published an alert "notifying healthcare professionals of the risk of serious liver injury, including liver failure and death, with the use of ptu[3]. As a result, ptu is no longer recommended in non-pregnant adults and in children as the front line antithyroid medication[4]. In this study, we performed first-principles simulation to study the interaction between Silicon Nanotubes and ptu.

Carbon nanotube research has been an extremely active field since their discovery by Iijima and structural identification[5,6]. They possess fascinating electronic, structural, and mechanical properties, and they could be used in a wide range of electromechanical devices as well as in the fabrication of robust and/or highly conducting composites[7,8]. Due to their unique and diverse physical properties, quasi-onedimensional Nanotubes show great promise to serve as active components in various nanoscale devices including sensitive chemical and biological detectors, electronic properties have been demonstrated to be effective gas chemical sensors for detecting many

molecules, such as NH_3,[9] O_2,[10] NO_2,[11] and etc. In recent years, CNTs, BNNTs, AlNNTs, SiNTs have been proposed to detect different molecules using density functional theory (DFT) calculation[12].

Computational details

The SiNTs models considered here are (5,5) armchair with their ends hydrogen atoms. The (5,5) model consists of 100 Si and 20 H atoms. Interaction of Propylthiouracil molecule with the SiNTs systems has been studied in the gas. This reduces the computational cost in comparison to treating each molecule separately. All the structures were optimized at 6-31+G*/B3LYP level of theory[13].

RESULT AND DISCUSSION

The adsorption energy of the adsorb ate ptu with the SiNTs is calculated according to the formula:

$$\Delta E_{ads} = E_{ptu\text{-}SiNTs} - (E_{SiNTs} + E_{ptu}) \quad ...(1)$$

The molecular systems include the individual SiNTs, the individual ptu and hybrid SiNTs-ptu (Fig. 1).

Fig. 1. Individual SiNTs and ptu model. The connecting atomic sites are Si7 and N1 atoms in the SiNTs-ptu hybrids.

Vibration frequencies have been also calculated at the same level to confirm that all the stationary points correspond to true minima on the potential energy surface.

The molecular systems include the individual SiNTs, the individual Ptu and hybrid SiNTs -Ptu (Fig. 1).

This work is to investigate the influence of SiNTs, as a representative nanostructure, on the optimized structures and properties of Ptu. To this aim, molecular and atomic properties (Tables 1) have been computationally evaluated for the investigated systems.

The resulting approaches for chemical shielding (CS) calculations in the principal axis system (PAS) with the order of $\sigma_{33} > \sigma_{22} > \sigma_{11}$[13] are converted into measurable NMR parameters (the chemical shielding isotropic CS (CS^I) and the chemical shielding anisotropic CS (CS^A) parameters) using Eq_s. (2) and (3)[14] and the NMR parameters of ^{29}Si and ^{13}C atoms for the investigated models of the SiNTs and SiNTs-Ptu are summarized in Table 2.

$$CS^I = 1/3(\sigma_{11} + \sigma_{22} + \sigma_{33}) \quad ...(2)$$

$$CS^A = \sigma_{33} - ½(\sigma_{22} + \sigma_{11}) \quad ...(3)$$

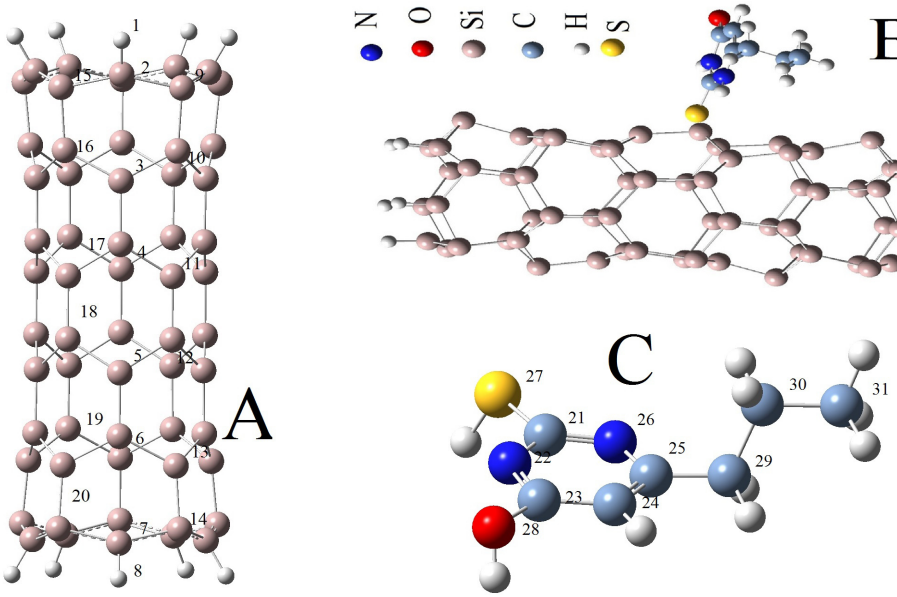

Fig. 1: The optimized structure of SNTs and Ptu model a) SNTs b) Ptu, c) SNTs-Ptu complex

Table 1: properties atomic and physical SiNTs(modelA), Ptu-SiNTs, Ptu

Model A bond lengths(A^0)	6-31+G*	Model B bond lengths(A^0)	6-31+G*	Model C bond lengths(A^0)	6-31+G*
Si-H 1-2	1.43	Si-H 1-2	1.43	C=O 23-28	1.43
Si-Si 2-9	2.17	Si-Si 2-9	2.21	C=S 21-27	1.78
Si-Si 2-15	2.17	C=O 23-28	1.43	C-N 21-26	1.39
Si-Si 9-10	2.22	C=S 21-27	1.78	C-N 21-22	1.39
Angel		Angel		Angel	
Si-H-Si 1-2-9	104.58	Si-H-Si 1-2-9	122.76	S-C-N 27-21-22	120.01
Si-H-Si 1-2-15	104.58	Si-H-Si 1-2-15	122.76	0-C-N 28-23-22	119.99
Si-Si-Si 2-9-10	118.54	Si-Si-Si 2-9-10	119.71	N-C-N 26-21-22	119.99
tip diameter(A0)	17.54	tip diameter(A0)	17.54	tip diameter(A0)	8.11
DM(Debye)	0.016	DM(Debye)	7.51	DM(Debye)	6.21
E(kev) -472.8	E(kev)	-496.11	E(kev)	-23.28	
∆Eads(eV)	0	∆Eads(eV)	-30	∆Eads(eV)	0

Table 2: NMR parameters SiNTs, SiNNTs-Ptu

SiNNTs		SiNNTs-Ptu		
CS	**CA**	**CS**	**CA**	**Si2**
378.0077	145.2369	408.8515	87.9639	Si4
363.7112	181.1276	364.4184	118.0616	si9
198.3024	210.4733	188.2051	134.0988	Si10
358.9619	111.5763	364.9487	2.359	Si14
224.079	182.861	-	-	Si15
396.1703	198.2104	409.5577	123.0493	

Three sets of optimization processes have been performed to generate the stabilize structures. The first set of optimizations has been performed for the free Ptu structures and the second set have has been performed for the free SiNTs. At the third set, the hybrid models including the SiNTs and Ptu together (Fig. 1) have been optimized to see the relaxation of each Ptu model on the surface of SiNTs.

CONCLUSION

In this paper, we performed the DFT calculations to study the interaction between SiNTs and ptu molecules, it is found that ptu can be chemically adsorbed on SiNTs with appreciable adsorption energies. The ptu molecule uses its O, S, H and C atoms to bond with Si atom, respectively, of the tube, forming a four-membered ring. Significant charges are transferred from SiNTs to ptu molecules, which lead to changes of conductance of SiNTs and render this kind of nanotubes suitable for ptu detection.

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