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Theoretical Investigation of Hetero–Diels–Alder Functionalizations on SWCNT and Their Reaction Properties

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ABSTRACT

Two–layered ONIOM method at the ONIOM(B3LYP/6–31G(d,p):AM1) theoretical level was applied to investigate the hetero Diels-Alder reaction functionalization of various nitrosoalkenes (NAs) and thionitrosoalkenes (TNAs) onto side–wall (5,5) armchair SWCNT. The results indicated that SWCNT can be functionalized with NAs and TNAs. The energy barriers of TNAs funtionalized SWCNT were lower than those of NAs. This implied that TNAs are easier to react with SWCNT than those of NAs. In addition, electronic properties and density of states of SWCNT were modified by the Diels-Alder functionalizations of NAs and TNAs.

1 Introduction

During the last decade, many researches have been focused on functionalizations of single–walled carbon nanotube (SWCNT) to make fascinating new physical and chemical properties for practical applications (Meyyappan, 2005). Generally, chemical functionalizations to SWCNT were achieved by covalent functionlizations onto the sidewall of tube at the sp^2 carbon system. The experimental functionlizations using fluorine (Chamssedine

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et al., 2011), diazonium salt (Bahr *et al*., 2001), and fuming nitric acid (Kitamura *et al*., 2011), and theoretical functionalizations using azomethine ylides (Cho *et al*., 2008), nitrene (Zhang *et al*., 2006), ozone (Yim & Johnson, 2009), ethene (Lawson & Walker, 2012), alanine and alanine radical (Rajarajeswari *et al*., 2012), and diazomethyl aromatic compound (Raksaparm *et al*., 2012), pyrazinamide (Saikia & Deka, 2010) on SWCNTs were successful studied and reported. Chemical cycloaddition on buckminsterfullerene (C_{60}) was reviewed by Yurovskaya and Trushhov (Yurovskaya, & Trushkov, 2002).

Diels–Alder reaction is well known to occur between a conjugated diene and a dieneophile and is particularly useful chemical modification to construct cyclic compounds. This reaction has also been explored on the functionalizations of the C_{60} (Ohno *et al*., 1993; Ohno *et al*., 1995; Yang *et al*., 2006; Nakahodo *et al*., 2008; Yang *et al*., 2009). Interestingly, the Diels–Alder cycloadditions on the sidewall SWNT were successful studied by experimental (Delgado *et al*., 2004; Ménard-Moyon *et al*., 2006) and theoretical (Lu *et al*., 2002) methods. Nitrosoalkenes (Tahdi *et al*., 2002; Gallos *et al*., 2003) and thionitrosoalkenes (Bryce *et al*., 1994; Reed & Zhang, 2001) are a class of hetero dienes. In principle, the SWCNTs should be traceable to these reactions with hetero compounds such as nitrosoalkenes (NAs) and thionitrosoalkenes (TNAs). However, experimental and theoretical studies of the side–wall addition of nitrosoalkene and thionitrosoalkene to SWCNT have not yet appeared to the best of our knowledge. In the present work, the hetero-Diels–Alder reactions of nitrosoalkene and thionitrosoalkene compounds on armchair (5,5) SWCNT have been investigated by using the quantum calculation.

2 Computational Details

Two-layered ONIOM method at the ONIOM(B3LYP/6–31G(d,p):AM1) theoretical level was applied to geometry optimizations of all species of cycloaddition functionalization onto side-wall (5,5) armchair SWCNT. The model of SWCNT ($C_{70}H_{20}$ model) was chosen with open ends and the hydrogen atoms were used to saturate the carbon atoms at the two terminated ends of the tube (Figure 1). The ball atoms of a pyrene (C_{16}) model cluster and those belonging to nitrosoalkene and thionitrosoalkene molecules were treated at the higher B3LYP/6–31G(d,p) level, and the remaining SWCNT atoms were treated with the AM1 method. Based on the two-layered ONIOM approach, a pyrene molecule shown as ball atoms of SWCNT was selected to be the high level layer. The hetero-Diels–Alder functionalizations were assigned to occur at the C1–C2 bond of SWCNT as shown in Figure 1. All of the structures of reactants, transition states and products were located by the ONIOM(B3LYP/6–31G(d,p):AM1) model achieved without any symmetry constraints. All transition states were characterized by single imaginary frequency.

The vibration frequency computations were performed at 298.15 K and the standard pressure as applied in our previous works (Wanno & Ruangpornvisuti, 2006). The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energy gaps and density of states (DOSs) were also been determined. All calculations were performed with the GAUSSIAN 03 program (Frisch *et al*., 2008). The molecular graphics of all related species were generated with the MOLEKEL 4.3 program (Flükiger *et al*., 2000).

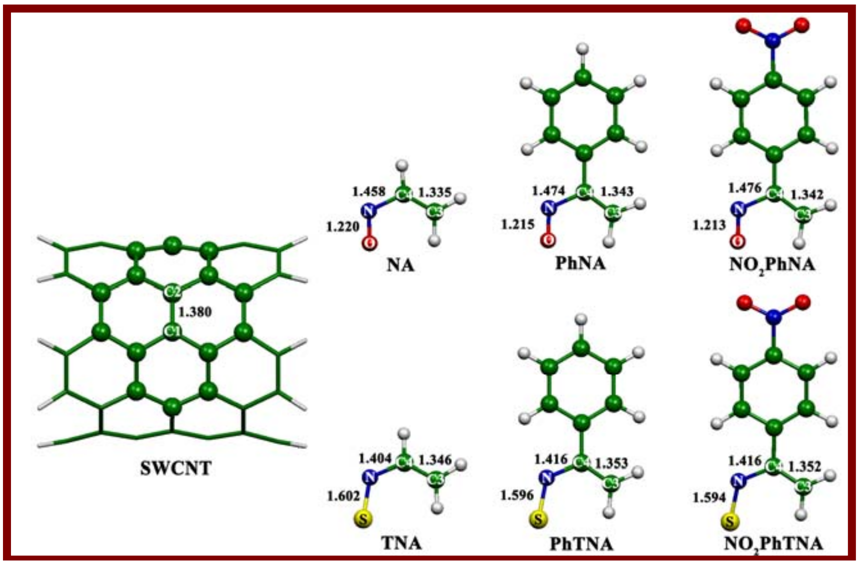


Figure 1: The optimized structures of single walled carbon nanotube (SWCNT), nitrosoalkene (NA) and thionitrosoalkene (TNA) reactants.

3 Results and discussion

The structural optimizations of (5,5) armchair SWCNT, nitrosoalkene and thionitrosoalkene, their product and transition state structures were carried out at the ONIOM(B3LYP/6–31G(d,p):AM1) level of theory. The optimized structures of SWCNT, nitrosoalkenes, and thionitrosoalkenes are displayed in Figure 1. The selected bond distances and bond angles of the optimized structures are considered and discussed. The average C1–C2 bond distance of SWCNT was 1.380 Å which is in good agreement with the previous reports (Raksaparm *et al*., 2012). For the nitrosoalkene reactants, the C3–C4 bond distances were

1.335, 1.343, and 1.342 Å, respectively whereas the N–O bond distances are 1.220, 1.215, and 1.213 Å. The C3–C4–N bond angles were 123.7, 119.0, and 119.3°, respectively whereas the C4–N–O bond angles were 114.5, 115.5, and 115.3° for NA, PhNA, and NO_2PhNA, respectively. The C3–C4 bond distances were 1.346, 1.353, and 1.352 Å, respectively whereas the N–S bond distances were 1.602, 1.596, and 1.594 Å. Moreover, the C3–C4–N bond angles were 128.2, 122.8, and 123.2°, respectively whereas the C4–N–S bond angle were 121.8, 123.8, and 123.6° for TNA, PhTNA, and NO_2PhTNA, respectively.

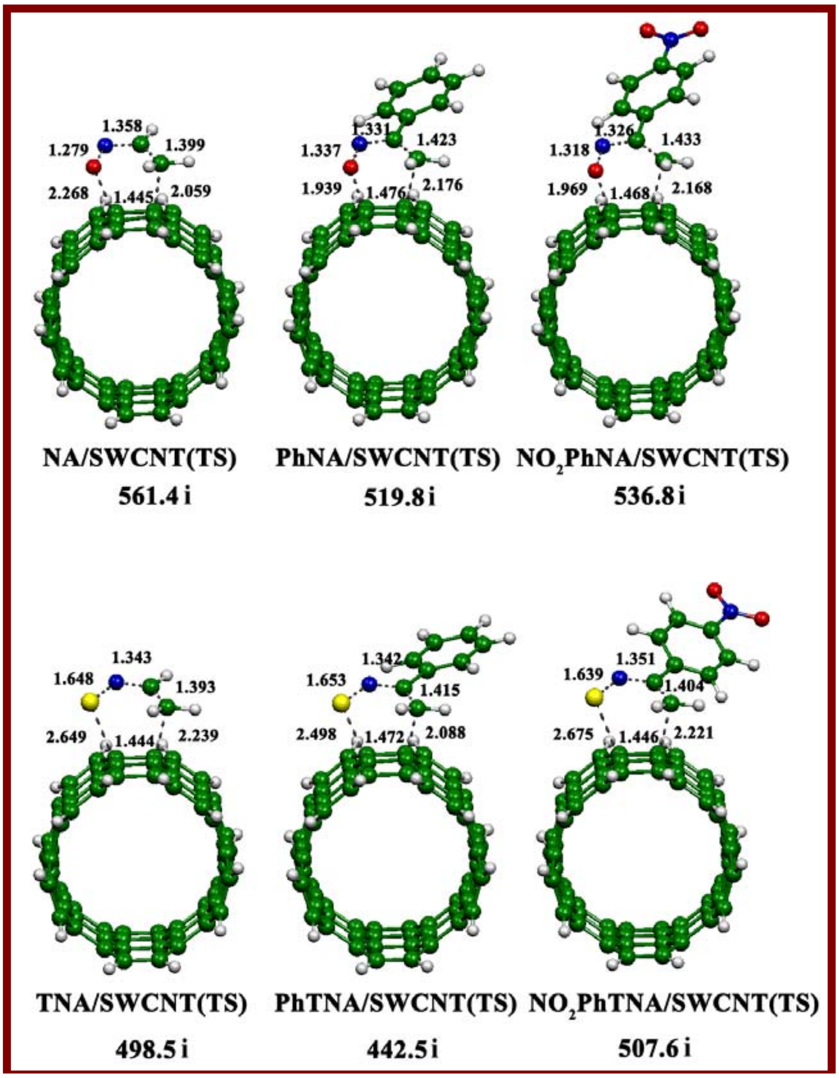
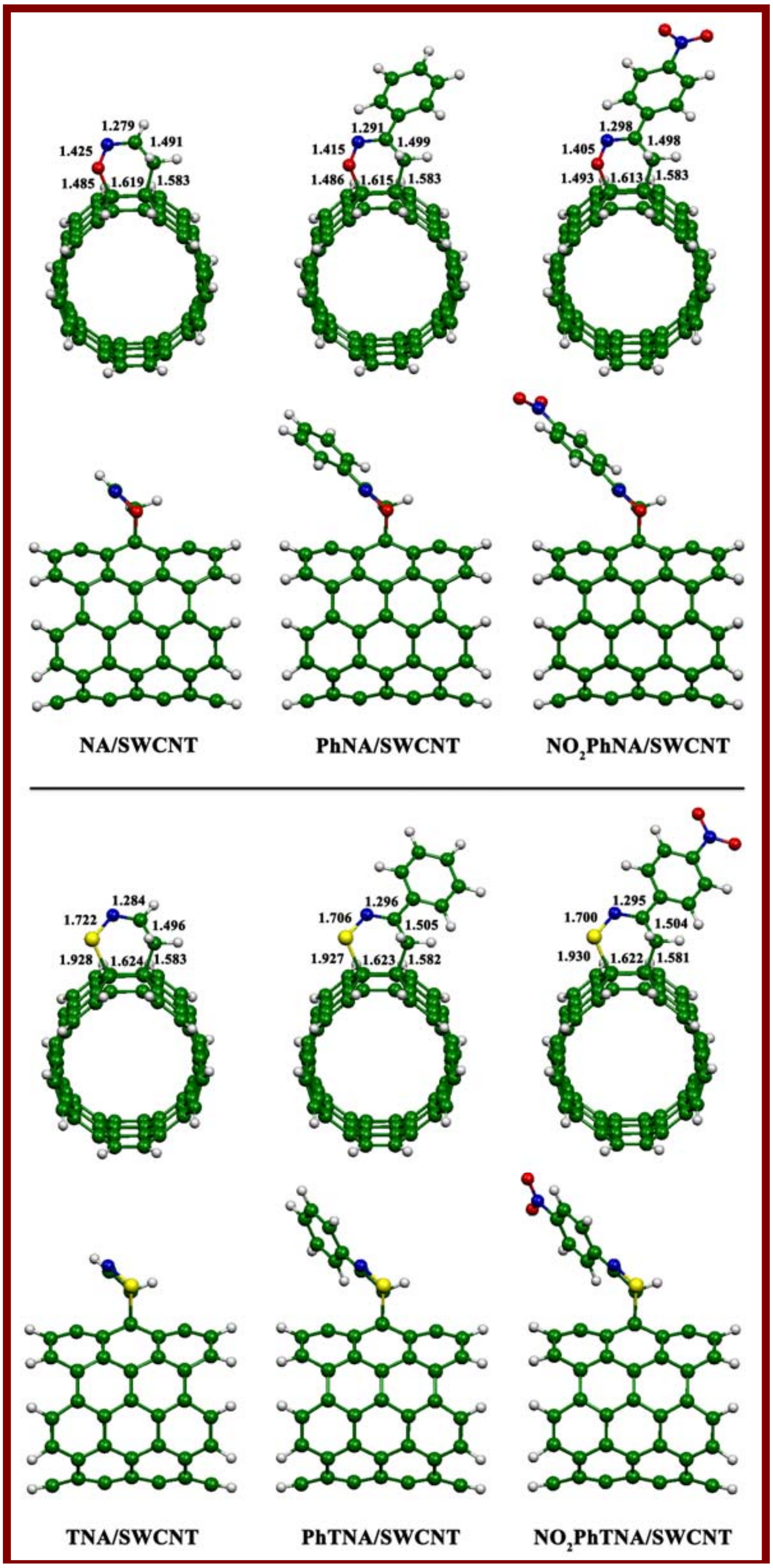


Figure 2: The ONIOM(B3LYP/6–31G(d,p):AM1)–optimized transition state structures for nitrosoalkenes (above) and thionitrosoalkenes (bottom).
Imaginary frequencies (in cm^{-1}) are also presented.

Considering the transition state as show in Figure 2, the reaction started from nitrosoalkene or thionitrosoalkene molecules reacted to C=C bond of SWCNT via the transition state to form the functionalized SWCNT products. For the transition state structures of nitrosoalkenes, the



NA/SWCNT PhNA/SWCNT NO_2PhNA/SWCNT

TNA/SWCNT PhTNA/SWCNT NO_2PhTNA/SWCNT

Figure 3: The ONIOM(B3LYP/6–31G(d,p):AM1) – optimized product structures for nitrosoalkene (above) and thionitrosoalkene (bottom) functionalizations.

C1–O and C2–C3 bonds were formed at the sidewall of SWCNT, the C3–C4 and N–O bond distances were then elongated when comparing with its corresponding reactant structures. The

C1–O bond distances were 2.268, 1.939, and 1.969 Å for NA, PhNA, and NO_2PhNA, respectively, whereas the C2–C3 bond distances were 2.059, 2.176 and 2.168 Å for NA, PhNA, and NO_2PhNA, respectively. For the transition state structures of thionitrosoalkenes, when the C1–S and C2–C3 bonds were formed at the sidewall of SWCNT which the C3–C4 and N–S bond distances were also elongated. The C1–S bond distances were found to be 2.649, 2.498, and 2.675 Å for TNA, PhTNA, and NO_2PhTNA respectively, whereas the C2–C3 bond distances were 2.239, 2.088, and 2.221 Å for TNA, PhTNA, and NO_2PhTNA, respectively.

Geometrical structures of products are displayed in Figure 3 in which the products were represented the formation of the newly six-member ring of functionalized SWCNTs. The C1–O bond distances were 1.485, 1.486, and 1.493 Å for NA, PhNA, and NO_2PhNA, respectively, while the C2–C3 bond distances were 1.583, 1.583, and 1.583 Å for NA, PhNA, and NO_2PhNA, respectively, and C1–S bond distances were 1.928, 1.927, and 1.930 Å for TNA, PhTNA, and NO_2PhTNA, respectively, while the C2–C3 bond distances were 1.583, 1.582, and 1.581 Å for TNA, PhTNA, and NO_2PhTNA, respectively. After the functionalization completed each of C1 and C2 atoms formed 4 chemical bonds with neighboring atoms. This indicated that hybridizations of C1 and C2 atoms were completely changed from sp^2 to sp^3.

3.1 Reaction Energies and Energy Profiles

Energy profiles based on the ONIOM(B3LYP/6–31G(d,p):AM1) computation for the hetero-Diels-Alder functionalizations of nitrosoalkenes and thionitrosoalkenes onto SWCNT are displayed in Figure 4 and the reaction energies, reaction energy barriers, and imaginary frequencies of the functionalizations are listed in Table 1. The reaction profiles with initial reactants (R), transition state and reaction products (P) are also represented in Figure 4. The relative energy profiles showed that the energy barriers for nitrosoalkene functionalizations were 21.88, 24.76, and 27.64 kcal/mol for the NA, PhNA, and NO_2PhNA, respectively. It should be noted here that the NA addition showed the lowest in the activation barrier. In addition, the energy barriers of the thionitrosoalkene functionalizations were 15.01, 13.16, and 12.32 kcal/mol for the TNA, PhTNA, and NO_2PhTNA, respectively, in which the NO_2PhTNA addition showed the lowest in the activation barrier. Clearly, all of functionalizations were occurred via exothermic process. In both system, these energy barriers are strongly dependent on the nature of the heteroatoms and the molecular geometries presented on the reaction.

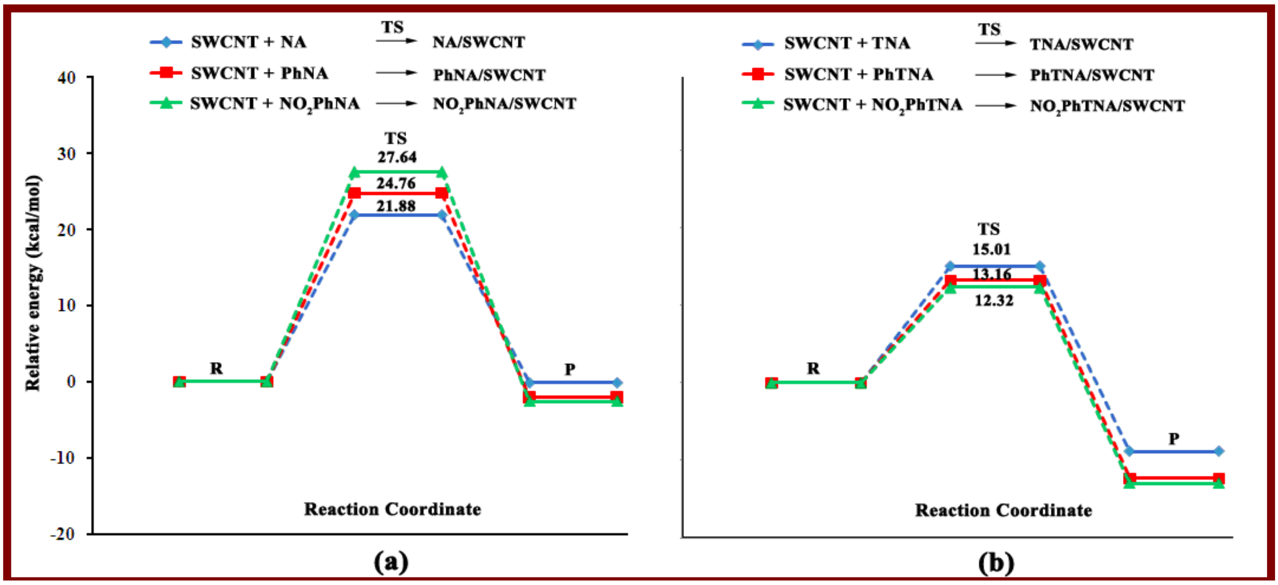


Figure 4: The reaction profiles and relative energy profiles (in kcal/mol) of (a) nitrosoalkene and (b) thionitrosoalkene functionalizations. Where R is reactants, TS is transition state and P is reaction products.

Table 1: Reaction energies (ΔE), reaction barriers ($\Delta E^{\neq}$) and the imaginary frequencies (ν_i) for the transition state of hetero Diels-Alder functionalizations computed at the ONIOM(B3LYP/6–31G(d,p):AM1) level of theory.

Reactions	ΔE^{a}	$\Delta E^{\neq,a}$	ν_i^{b}
Nitrosoalkene addition			
SWCNT+NA → NA/SWCNT	-0.11	21.88	561.4i
SWCNT+PhNA → PhNA/SWCNT	-2.05	24.76	519.8i
SWCNT+NO_2PhNA → NO_2PhNA/SWCNT	-2.60	27.64	536.8i
Thionitrosoalkene addition			
SWCNT+TNA → TNA/SWCNT	-8.55	15.01	498.5i
SWCNT+PhTNA → PhTNA/SWCNT	-12.34	13.59	450.5i
SWCNT+NO_2PhTNA → NO_2PhTNA/SWCNT	-12.95	12.32	507.6i

[a] In kcal/mol. [b] Imaginary frequencies (cm^{-1}).

Table 2: The E_{LUMO} and E_{HOMO} energies and E_{gap} of tube and its adduct complexes computed at the ONIOM(B3LYP/6–31G(d,p):AM1) level of theory

Species	$E_{\mathrm{LUMO}}{}^{a}$	$E_{\mathrm{HOMO}}{}^{a}$	$E_{\mathrm{gap}}{}^{a,\,b}$
SWCNT	–2.28	–4.45	2.17 [2.20] [c]
NA/SWCNT	–2.31	–4.47	2.16
PhNA/SWCNT	–2.29	–4.45	2.16
NO_2PhNA/SWCNT	–2.61	–4.60	1.99
TNA/SWCNT	–2.35	–4.48	2.13
PhTNA/SWCNT	–2.33	–4.45	2.12
NO_2PhTNA/SWCNT	–2.58	–4.61	2.03

[a] In eV. [b] $E_{\mathrm{gap}} = E_{\mathrm{LUMO}} - E_{\mathrm{HOMO}}$.
[c] Computed at B3LYP/6–31G* level (reported by Zhou *et al*. 2004)

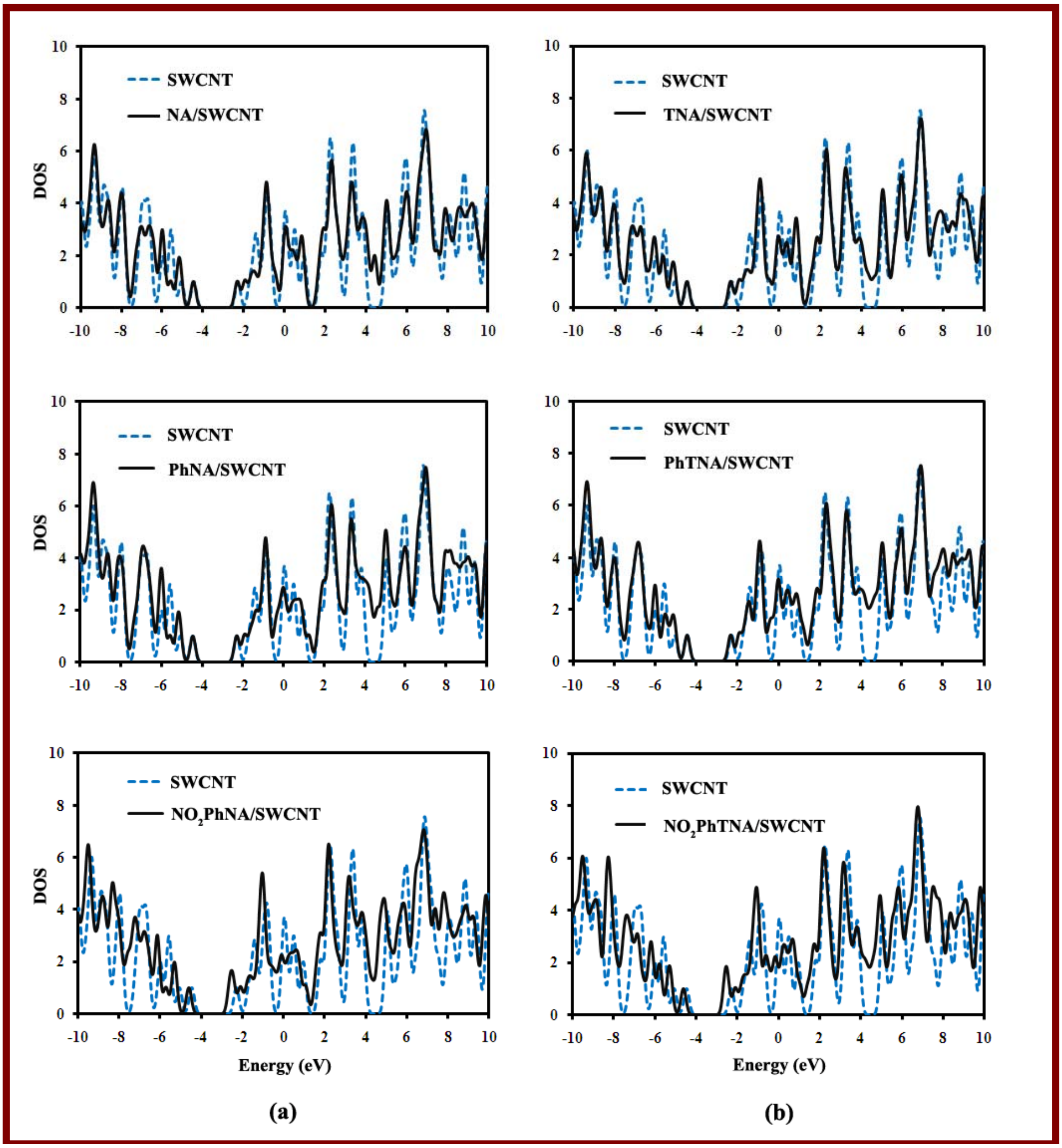


Figure 5: The density of states of the SWCNT,
compared with (a) nitrosoalkene and (b) thionitrosoalkene complexes.

3.2 Electronic properties and density of state

The E_{LUMO} and E_{HOMO} energies and frontier molecular orbital energy gaps (E_{gap}) of SWCNT and its adduct complexes computed at the ONIOM(B3LYP/6–31G(d,p):AM1) level are displayed in Table 2. The results showed that, E_{gap} for the pure SWCNT was 2.17 eV which is in good agreement with the previous results (2.20 eV) reported by Zhou *et al*. (2004). For NA, TNA, PhNA, and PhTNA complexes with SWCNT, the E_{gap} were slightly different from SWCNT. On the other hand, for the NO_2PhNA and NO_2PhTNA complexes with SWCNT, their E_{gap} values were 1.99 and 2.03 eV, respectively which was different from the other products.

Plots of the density of states of the NA, PhNA, and NO_2PhNA and TNA, PhTNA, and NO_2PhTNA functionalized SWCNTs, compared with the armchair (5,5) SWCNT are displayed in Figure 5. It was shown that electronic structure of the SWCNT was sensitive to the hetero Diels–Alder functionalizations. The band gaps of SWCNT near Fermi level become narrower, which suggested that the conductivity of SWCNT was modified by nitrosoalkene and thionitrosoalkene functionalizations.

4 Conclusion

The hetero-Diels-Alder functionalizations of various nitrosoalkenes (NAs) and thionitrosoalkenes (TNAs) onto side-wall (5,5) armchair SWCNT were investigated by using the two-layered ONIOM method at the ONIOM(B3LYP/6-31G(d.p):AM) theoretical level. The results indicated that SWCNT can be functionalized with NAs and TNAs. The energy barriers of TNAs funtionalized SWCNT were lower than those of NAs. This implied that TNAs are easier to react with SWCNT than those of NAs. In addition, hetero-Diels-Alder functionalizations affected to electronic properties and density of states of SWCNT.

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6 References

Bahr, J.L., Yang, J., Kosynkin, D.V., Bronikowski, M.J., Smalley, R.E. & Tour, J.M. (2001). Functionalization of carbon nanotubes by electrochemical reduction of aryl diazonium salts: A bucky paper electrode. *Journal of American Chemical Society*. 123, 6536-6542.

Bryce, M.R., Heaton, J.N., Taylor, P.C. & Anderson, M. (1994). Diels–Alder and ene reactions of new transient thionitrosoarenes (Ar-N=S) and thionitrosoheteroarenes (Het–N=S) generated from *N*-(arylaminosulfanyl) and *N*-(heteroarylaminosulfanyl)-phthalimides: synthesis of cyclic and acyclic sulfenamides. *Journal of the Chemical Society, Perkin Transactions 1*, 1935-1944.

Chamssedine, F., Guérin, K., Dubois, M., Disa, E., Petit, E., El Fawal, Z. & Hamwi, A. (2011). Fluorination of single walled carbon nanotubes at low temperature: Towards the reversible fluorine storage into carbon nanotubes. *Journal of Fluorine Chemistry*. 132, 1072-1078.

Cho, E., Shin, S. & Yoon, Y.G. (2008). First-principles studies on carbon nanotubes functionalized with azomethine ylides. *The Journal of Physical Chemistry C*. 112, 11667-11672.

Delgado, J.L., Cruz, P., Langa, F., Urbina, A., Casadoc, J. & Navarretec, J.T.L. (2004). Microwave-assisted sidewall functionalization of single-wall carbon nanotubes by Diels–Alder cycloaddition. *Chemical Communications*. 1734-1735.

Flükiger, P., Lüthi, H.P., Portmann, S. & Weber, J. (2000) Molekel 4.3. Swiss Center for Scientific Computing, Manno.

Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G.E., Robb, M.A., Cheeseman, J.R., Montgomery, J.A. Jr., Vreven, T., Kudin, K.N,, Burant, J.C., Millam, J.M., Iyengar, S.S., Tomasi, J., Barone, V., Mennucci, B., Cossi, M., Scalmani, G., Rega, N., Petersson, G.A., Nakatsuji, H., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Klene, M., Li, X., Knox, J.E., Hratchian, H.P., Cross, J.B., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R., Stratmann, R.E., Yazyev, O., Austin, A.J., Cammi, R., Pomelli, C., Ochterski, J.W., Ayala, P.Y., Morokuma, K., Voth, G.A., Salvador, P., Dannenberg, J.J., Zakrzewski, V.G., Dapprich, S., Daniels, A.D., Strain, M.C., Farkas, O., Malick, D.K., Rabuck, A.D., Raghavachari, K., Foresman, J.B., Ortiz, J.V., Cui, Q., Baboul, A.G., Clifford, S., Cioslowski, J., Stefanov, B.B., Liu, G., Liashenko, A., Piskorz, P., Komaromi, I., Martin, R.L., Fox, D.J., Keith, T., Al-Laham, M.A., Peng, C.Y., Nanayakkara, A., Challacombe, M., Gill, P.M.W., Johnson, B., Chen, W., Wong, M.W., Gonzalez, C. & Pople, J.A. (2008) Gaussian 03, Revision E.01. Gaussian, Inc, Wallingford.

Gallos, J.K., Sarli, V.C., Varvogli, A.C., Papadoyanni, C.Z., Papaspyrou, S.D. & Argyropoulos, N.G. (2003). The hetero-Diels-Alder addition of ethyl 2-nitrosoacrylate to electron rich alkenes as a route to unnatural α-amino acids. *Tetrahedron Letters*. 44, 3905-3909.

Kitamura, H., Sekido, M., Takeuchi, H. & Ohno, M. (2011). The method for surface functionalization of single-walled carbon nanotubes with fuming nitric acid. *Carbon*. 49, 3851-3856.

Lawson, D.B. & Walker, A. (2012). Cycloaddition of ethene on a series of single-walled carbon nanotubes. *Computational and Theoretical Chemistry*. 981, 31-37.

Lu, X., Tian, F., Wang, N. & Zhang, Q. (2002). Organic functionalization of the sidewalls of carbon nanotubes by Diels−Alder reactions: A theoretical prediction. *Organic Letters*. 4, 4313-4315.

Ménard-Moyon, C., Dumas, F., Doris, E. & Mioskowski, C. (2006). Functionalization of single-wall carbon nanotubes by tandem high-pressure/Cr(CO)6 activation of Diels-Alder cycloaddition. *Journal of the American Chemical Society*. 128, 14764-14765.

Meyyappan, M. (2005). Carbon nanotubes science and applications. CRC Press LLC, New York.

Nakahodo, T., Takahashi, K., Ishitsuka, M.O., Tsuchiya, T., Maeda, Y., Fujihara, H., Nagase, S. & Akasaka, T. (2008). Synthesis of selenylfullerene with selenium-containing dibenzo[*b,g*]cyclooctane moiety. *Tetrahedron Letters*. 49, 2302-2305.

Ohno, M., Azuma, T. & Eguchi, S. (1993). Buckminsterfullerene C60-*o*-quinone methide cycloadduct. *Chemistry Letters*. 22, 1833-1834.

Ohno, M., Kojima, S., Shirakawa, Y. & Eguchi S (1995). Hetero-diels-alder reaction of fullerene: Synthesis of thiochroman-fused C60 with *o*-thioquinone methide and oxidation to its S-oxides. *Tetrahedron Letters*. 36, 6899-6902.

Rajarajeswari, M., Iyakutti, K. & Kawazoe, Y. (2012). Noncovalent and covalent functionalization of a (5,0) single-walled carbon nanotube with alanine and alanine radicals. *Journal of Molecular Modeling*. 18, 771-781.

Reed, M.G. & Zhang, D.Y. (2001). Thionitroso or thiazyl? Density functional studies of relative stabilities between the two structural isomers. *Journal of Molecular Structure: THEOCHEM*. 548, 107-112.

Saikia, N. & Deka, R.C. (2010). Theoretical study on pyrazinamide adsorption onto covalently functionalized (5,5) metallic single-walled carbon nanotube. *Chemical Physics Letters*. 500, 65-70.

Tahdi, A., Titouani, S.L., Soufiaoui, M., Komiha, N., Kabbaj, O.K., Hegazi, S., Mazzah, A. & Eddaif, A. (2002). Réaction hétéro-Diels–Alder nitrosoalcènes avec le 2H-pyrrole approche expérimentale et théorique. *Tetrahedron*. 58, 1507-1512.

Raksaparm, U., Morakot, N. & Wanno, B. (2012). Functionalization of Diazomethyl Aromatic Compounds onto Single Wall Carbon Nanotubes: A DFT Study. *International Transaction Journal of Engineering, Management, & Applied Sciences & Technologies*. 3(4), 467-476.

Wanno, B. & Ruangpornvisuti, V. (2006). DFT investigation of structures of nitrosamine isomers and their transformations in gas phase. *Journal of Molecular Structure: THEOCHEM*. 766, 159- 164.

Wanno, B. & Ruangpornvisuti, V. (2006). Structures of gas-phase nitrosamine-dimer isomers, their interconversions and energetics: A DFT study. *Journal of Molecular Structure: THEOCHEM*. 775, 113- 120.

Yang, H., Ruan, X., Miao, C., Xi, H., Jiang, Y., Meng, Q. & Sun, X. (2009). Hetero-Diels–Alder reaction of [60]fullerene with nitrosoalkene. *Tetrahedron Letters*.

50, 7337-7339.

Yang, H.T., Wang, G.W., Xu, Y. & Huang, J.C. (2006). Heterocycloaddition of thermally generated 1,2-diaza-1,3-butadienes to [60]fullerene. *Tetrahedron Letters*. 47, 4129-4131.

Yim, W.L. & Johnson, J.K. (2009). Ozone oxidation of single walled carbon nanotubes from density functional theory. *The Journal of Physical Chemistry C*. 113, 17636-17642.

Yurovskaya, M.A. & Trushkov, I.V. (2002). Cycloaddition to buckminsterfullerene C_{60}: advancements and future prospects. *Russian Chemical Bulletin, International Edition*. 51, 367-443.

Zhang, C., Li, R., Liang, Y., Shang, Z., Wang, G., Xing, Y., Pan, Y., Cai, Z., Zhao, X. & Liu, C. (2006). The nitrene cycloaddition on the sidewall of armchair single-walled carbon nanotubes. *Journal of Molecular Structure: THEOCHEM*. 764, 33-40.

Zhou, Z., Steigerwald, M., Hybertsen, M., Brus, L. & Friesner, R.A. (2004). Electronic Structure of Tubular Aromatic Molecules derived from the Metallic (5,5) Armchair Single Wall Carbon Nanotube. *Journal of the American Chemical Society*. 126, 3597-3607.

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