

See discussions, stats, and author profiles for this publication at: <https://www.researchgate.net/publication/265909109>

Structural and electronic properties of endohedral doped SWCNTs: A DFT study

ARTICLE *in* PHYSICA E LOW-DIMENSIONAL SYSTEMS AND NANOSTRUCTURES · JANUARY 2015

Impact Factor: 2 · DOI: 10.1016/j.physe.2014.08.009

READS

178

4 AUTHORS, INCLUDING:



Nibras Mossa Umran

Faculty of Science, Kerbala University , kar...

13 PUBLICATIONS 8 CITATIONS

[SEE PROFILE](#)



Vaneeta Bala

Punjab Technical University

11 PUBLICATIONS 4 CITATIONS

[SEE PROFILE](#)



Structural and electronic properties of endohedral doped SWCNTs: A DFT study



Nibras Mossa Umran ^{a,b}, Vaneeta Bala ^a, K. Seema ^a, Ranjan Kumar ^{a,*}

^a Department of Physics, Panjab University, Sector 14, Chandigarh 160014, India

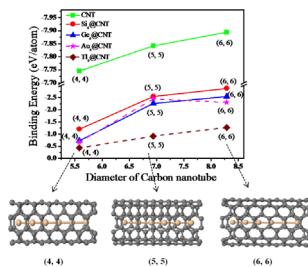
^b Department of Physics, Science College, Karbala University, Karbala, Iraq

HIGHLIGHTS

- We have studied electronic properties of pure and doped armchair and zigzag CNTs.
- On doping metallic character of the armchair CNTs increases.
- For zigzag CNTs, semiconducting character increases on doping.
- IP and EA for doped zigzag CNTs are independent of tube diameter and dopant type.
- For doped armchair CNTs, maximum IP and EA are observed for (5, 5) tube.

GRAPHICAL ABSTRACT

Structural and electronic properties of some semiconductors and metal atoms doped armchair (n, n) and zigzag ($n, 0$); $n=4–6$, carbon nanotubes have been studied using DFT.



ARTICLE INFO

Article history:

Received 13 May 2014

Received in revised form

9 August 2014

Accepted 14 August 2014

Available online 27 August 2014

Keywords:

Density functional theory

Endohedral doping

Carbon nanotubes

Electronic structure

ABSTRACT

The structural and electronic properties of semiconductors (Si and Ge) and metal (Au and Ti) atoms doped armchair (n, n) and zigzag ($n, 0$); $n=4–6$, single wall carbon nanotubes (SWCNTs) have been studied using an *ab-initio* method. We have considered a linear chain of dopant atoms inside CNTs of different diameters but of same length. We have studied variation of B.E./atom, ionization potential, electron affinity and HOMO–LUMO gap of doped armchair and zigzag CNTs with diameter and dopant type. For armchair undoped CNTs, the B.E./atom increases with the increase in diameter of the tubes. For Si, Ge and Ti doped CNTs, B.E./atom is maximum for (6, 6) CNT whereas for Au doped CNTs, it is maximum for (5, 5) CNTs. For pure CNTs, IP decreases slightly with increasing diameter whereas EA increases with diameter. The study of HOMO–LUMO gap shows that on doping metallic character of the armchair CNTs increases whereas for zigzag CNTs semiconducting character increases. In case of zigzag tubes only Si doped (5, 0), (6, 0) and Ge doped (6, 0) CNTs are stable. The IP and EA for doped zigzag CNTs remain almost independent of tube diameter and dopant type whereas for doped armchair CNTs, maximum IP and EA are observed for (5, 5) tube for all dopants.

© 2014 Elsevier B.V. All rights reserved.

1. Introduction

Carbon nanotubes (CNTs) have exceptionally high tensile strength, high resilience, metallic and semiconducting behavior, high current carrying capacity and high thermal conductivity [1–3]. CNTs

can be classified with respect to its structure by means of the rollup or the chirality vector. The chirality vector defines the rollup angle and the circumference of the CNTs. On the basis of classification based on chirality vector there exists three kind of CNTs: armchair (n, n), chiral (n, m) $0 < |m| < n$ and zigzag ($n, 0$) [4–6]. Due to unique mechanical and electronic properties, CNTs have been proved to be a very promising material for nano, medical and electronics applications. There are three main doping strategies employed for CNTs: endohedral doping, in-plane doping, and exohedral doping. Doping a

* Corresponding author. Tel.: +91 172 2534457.

E-mail address: ranjan@pu.ac.in (R. Kumar).

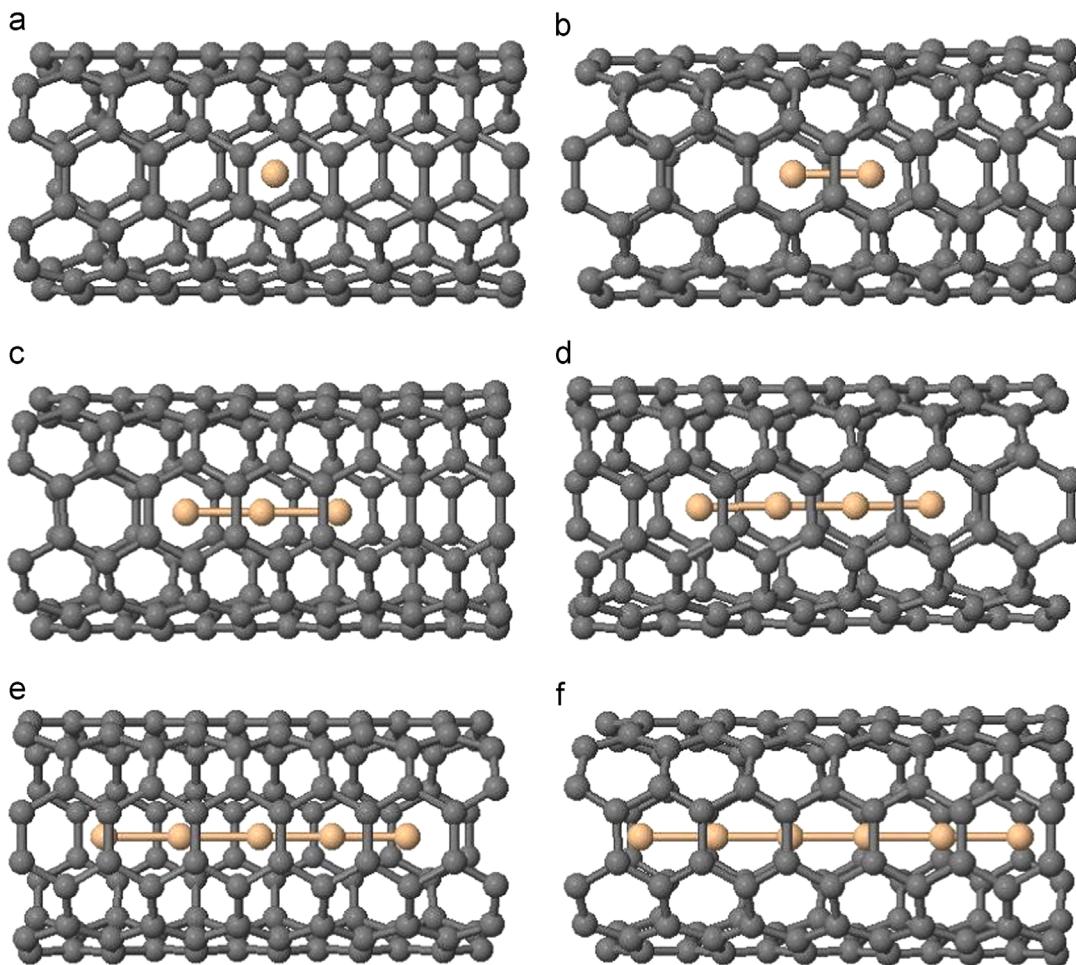
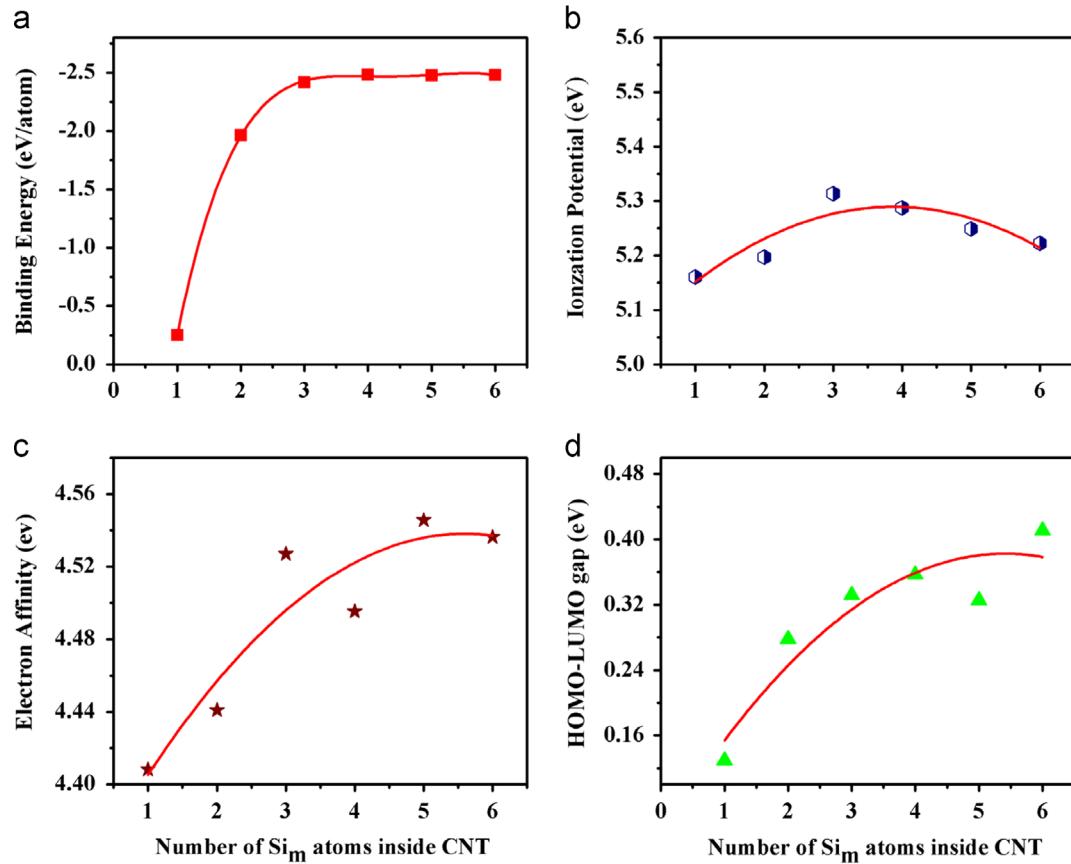
Fig. 1. The optimized structures of (5, 5) $\text{Si}_m\text{@CNT}$ ($m=1, 6$).

Fig. 2. The variation of (a) B.E. per atom, (b) IP, (c) EA, and (d) HOMO–LUMO gap with number of Si atoms in (5, 5) armchair SWCNT.

material is a novel technique to tailor the materials for specific requirement. Electronic properties of single carbon nanotubes (SWCNTs) depend upon their diameter, chirality, length and dopant atoms [7]. It has been observed that Nimesulide molecule adsorbed more strongly on Si doped SWCNT compared with pristine SWCNT [8]. It has been shown that Si-doped (10, 0) CNT and pristine CNT interact differently with H, F, Cl, CH₃, and SiH₃ molecules. Since doping and substitution modify electronic properties of CNT, therefore endohedral doping may be used to control optical properties, quantum dots engineering, and other applications [9]. Baierle et. al [10] have observed that Si impurity introduces a resonating level close to 0.7 eV above the Fermi level for the metallic nanotube. It is expected that the Si substitutional impurity will be highly reactive, serving as a binding center to other atoms or molecules. In another study it has been shown that the presence of Si or Ge atoms in CNTs increases their reactivity toward thiophene and benzothiophene [11]. The adsorption of these species on pristine CNTs seems very unlikely to occur, while the addition products involving doped CNTs were found to be very stable, with respect to the isolated reactants, in terms of Gibbs free energy. It suggests that Si and Ge defects on CNTs increase their reactivity toward unsaturated species, and could make them useful in the removal processes of aromatic sulfur compounds from oil-hydrocarbons [11]. Apart from certain important aspects related to the formation of dipoles at the interface, it is well known that the electronic structure alignment of the two materials near the

Fermi level is largely determined by the mismatch between the Fermi level of the substrate and the electron affinity/ionization potential of the adsorbed material, and their electrical properties can be modified by doping [12–16]. To modify the electronic structures of CNTs, numerous studies on the doping of CNTs have been performed. The elements Si and Ge are the abundant element on earth and the most important semiconductor materials in the microelectronic industry. These materials have already illustrated the unique potential offered by them. Apart from this, Si and Ge are the nearest neighbors of carbon in group IV, and therefore special candidates for designing novel nanostructures out of carbon [17–20]. It is important to mention that experimental realizations of Si and Ge doping in fullerenes [21,22] have been reported, which suggests that it is quite possible to dope CNTs with Si and Ge. The calculation of electron affinity and ionization energy of doping materials can be used to control the doping level in SWCNTs [23,24]. Electron affinity is the energy released to add an electron to form singly charged negative ion whereas ionization potential is defined as energy needed to remove one electron from a neutral atom to form a positively charged ion. Ionization potential is also closely related to the oxidation potential [25]. DFT calculations to investigate the interactions of small Au_n ($n=1–5$) clusters with SWCNTs and H₂ dissociation on the CNT supported clusters have also been reported [26]. Encapsulated Au clusters interact more strongly with the metallic CNTs than with the semiconducting ones,

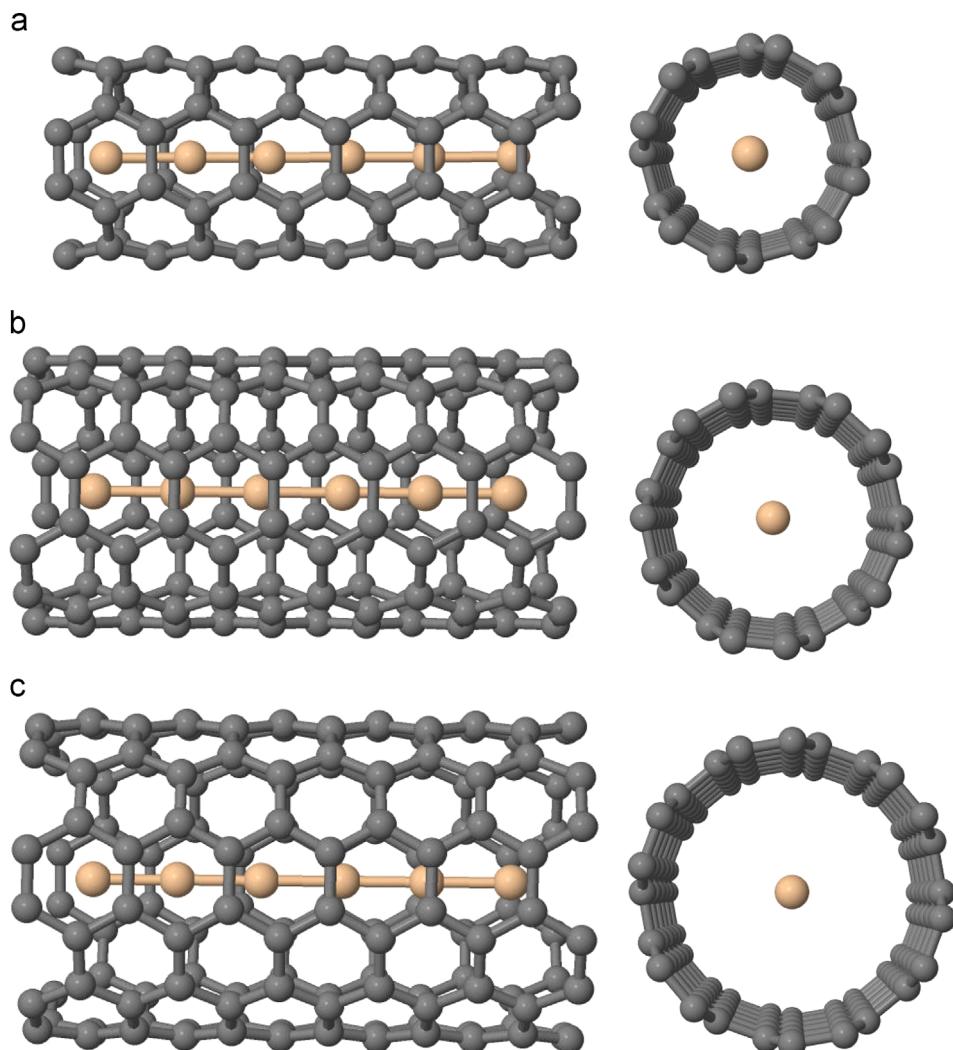


Fig. 3. The optimized structures of Si₆@CNTs (a) (4, 4), (b) (5, 5), and (c) (6, 6).

where charge transfers from CNTs to the clusters play an important role. Also H₂ dissociation becomes more favorable thermodynamically, especially on the encapsulated clusters [26]. Keeping in view importance of doping SWCNTs, in the present work we report the effect of endohedral impurities in armchair and zigzag SWCNTs. We have performed *ab-initio* calculations to understand the role of semiconducting and metal dopants atoms in modifying the electronic properties of SWCNTs. We have studied the stability, geometries, binding energy per atom, ionization potential, electron affinity and HOMO–LUMO gap of Si, Ge, Au and Tl doped CNTs.

2. Computational details

The calculations have been performed using DFT framework as implemented in the Spanish Initiative for Electronic Simulations with Thousands of Atoms (SIESTA) code [27]. It is based on the standard Kohn–Sham self-consistent DFT. Standard norm-conserving pseudo-potentials are constructed using Trouiller–Martins scheme [28] to describe the interaction of valence electrons with the atomic cores. The exchange-correlation potential of Perdew–Burke–Ernzerhof (PBE) for generalized gradient approximation (GGA) is adopted [29]. The Hamiltonian matrix elements are calculated by the charge density projection on a real-space grid with an equivalent plane-wave cutoff energy of 200 Ry. The conjugate gradient algorithm was

adopted for the relaxation of the doped CNTs. A double-zeta plus polarization (DZP) basis set is used for C, Si and Ge atoms. Previous studies with these bases have shown that they satisfactorily reproduce the energies of C [30,31], Si and Ge [32] systems.

3. Results and discussion

First of all we have performed structural optimization of undoped (*n*, *n*) armchair and (*n*, 0) zigzag SWCNTs, *n*=4–6. We have optimized the structures using SIESTA. The structures have been allowed to relax until the forces are smaller than 0.04 eV/Å. The obtained C–C bond lengths for (4, 4), (5, 5), and (6, 6) armchair CNTs are 1.44 Å, 1.44 Å and 1.43 Å respectively. For zigzag CNTs obtained C–C bond lengths are 1.47 Å, 1.48 Å, 1.47 Å for (4, 0), (5, 0) and (6, 0) CNTs respectively. The calculated bond length values agrees well with previously reported values of 1.43 Å for (4, 4), (5, 5), (6, 6), (5, 0) CNTs [32,33] and 1.447 Å for (6, 0) CNTs [34].

In the next step we have considered an endohedral system by placing a chain of dopant atoms inside armchair or zigzag CNT. The chain of dopant atoms was formed by placing these atoms at a distance of about their bond length as experimentally reported [35]. The simulation procedure used was same as used for Si and Ge doped C₆₀ molecule [36]. This whole system was allowed to relax with respect to all degrees of freedom without additional

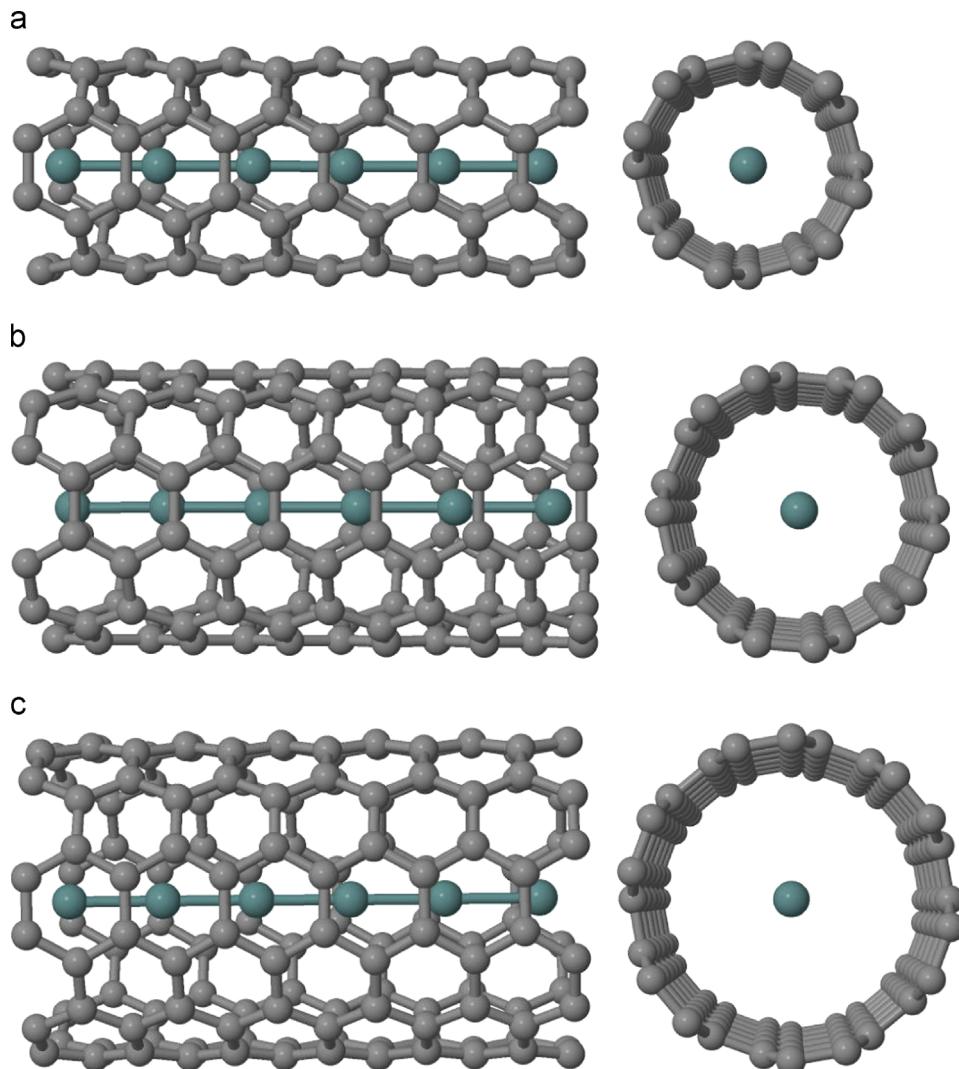


Fig. 4. The optimized structures of Ge₆@CNTs (a) (4, 4), (b) (5, 5), and (c) (6, 6).

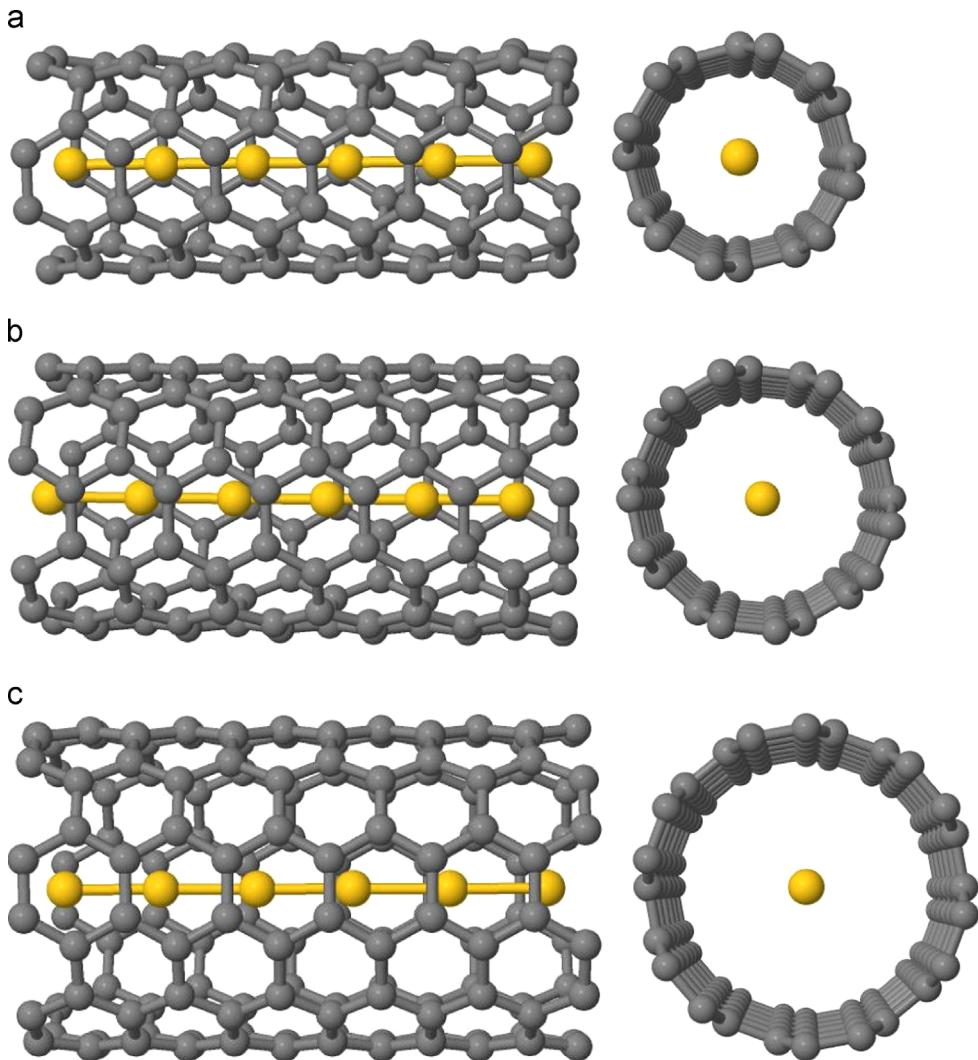


Fig. 5. The optimized structures of $\text{Au}_6@\text{CNTs}$ (a) (4, 4), (b) (5, 5), and (c) (6, 6).

constraints. The reason for choosing a chain of dopant atoms owe to the cylindrical cavity available inside CNT. We have considered endohedral doping in armchair and zigzag SWCNTs of different diameters. The length of SWCNTs was fixed to 12.47 \AA . Initially we have placed one Si atom inside CNT. The dopant was placed at different positions inside CNT. We found that Si atom at the center give rise to most stable structure. Then we have gradually increased number of Si atoms to six. The structures obtained after relaxation are shown in Fig. 1(a)–(f). The binding energy (B.E.) per doped atom (U_M) of the endohedral CNT was calculated as follows:

$$U_M = [E_{Mm@\text{CNT}} - E_{\text{CNT}} - mE_M]/m \quad (1)$$

where E_{CNT} is the total energy of undoped CNT and E_M is the total energy of one dopant atom. $E_{Mm@\text{CNT}}$ is the total energy of endohedral complex and m the number of dopant atoms in CNT. The variation of B.E./Si atom is shown in Fig. 2(a). Clearly B.E./Si atom increases with increase in number of silicon atoms and saturate up to $m=6$. The variation of ionization potential (IP), electron affinity (EA) and HOMO-LUMO gap with number of Si atoms in CNT is shown in Fig. 2(b)–(d). Clearly EA and HOMO-LUMO gap increase with number of dopants in CNT and seems to saturate at $m=5, 6$. IP remains almost constant with change in number of dopants. So we conclude that various properties get saturated at $m=6$. Therefore we will discuss the results corresponding to doping of chain of six atoms in armchair and zigzag CNTs.

3.1. Armchair SWCNTs

We have considered (4, 4), (5, 5) and (6, 6) armchair SWCNTs for endohedral doping of Si, Ge, Au and Tl. Figs. 3–6 illustrate the optimized structures after doping the chain consisting of six atoms of Si, Ge, Au, and Tl in armchair CNTs. The variation of B.E./atom with diameter for pure and doped CNTs is shown in Fig. 7. Clearly from Fig. 7, the B.E./atom changes with change in diameter. The values of the B.E./atom for pure CNTs were found to be in the range -7.745 eV to -7.893 eV as shown in Fig. 7. The minimum value of B.E./atom is -1.204 eV and -0.725 eV for Si and Ge doped (4, 4) CNTs with diameter 5.686 \AA respectively. The maximum value of the B.E./atom is -2.880 eV and -2.540 eV for Si and Ge doped (6, 6) CNT with diameter 8.283 \AA respectively. We found that B.E./dopant atom increases while going from (4, 4) to (6, 6) tube. Our calculations show that (6, 6) tube is most suited for Si/Ge doping as binding energy is maximum for the same. The effect of the tube diameter on the stability of the tube is interesting. In a finite nanotube, quantum confinement may induce a strong dependence of the electronic properties on the nanotube diameter. For Au and Tl doped (4, 4) CNT (diameter = 5.686 \AA), the B.E./atom is -0.666 eV and -0.436 eV respectively. For doped (5, 5) CNTs, the value of B.E./atom increases to -2.445 eV and -0.915 eV for Au and Tl doping respectively. With further increase in diameter to 8.283 \AA , the value of B.E./atom decreases to -2.304 eV for Au doping whereas for Tl

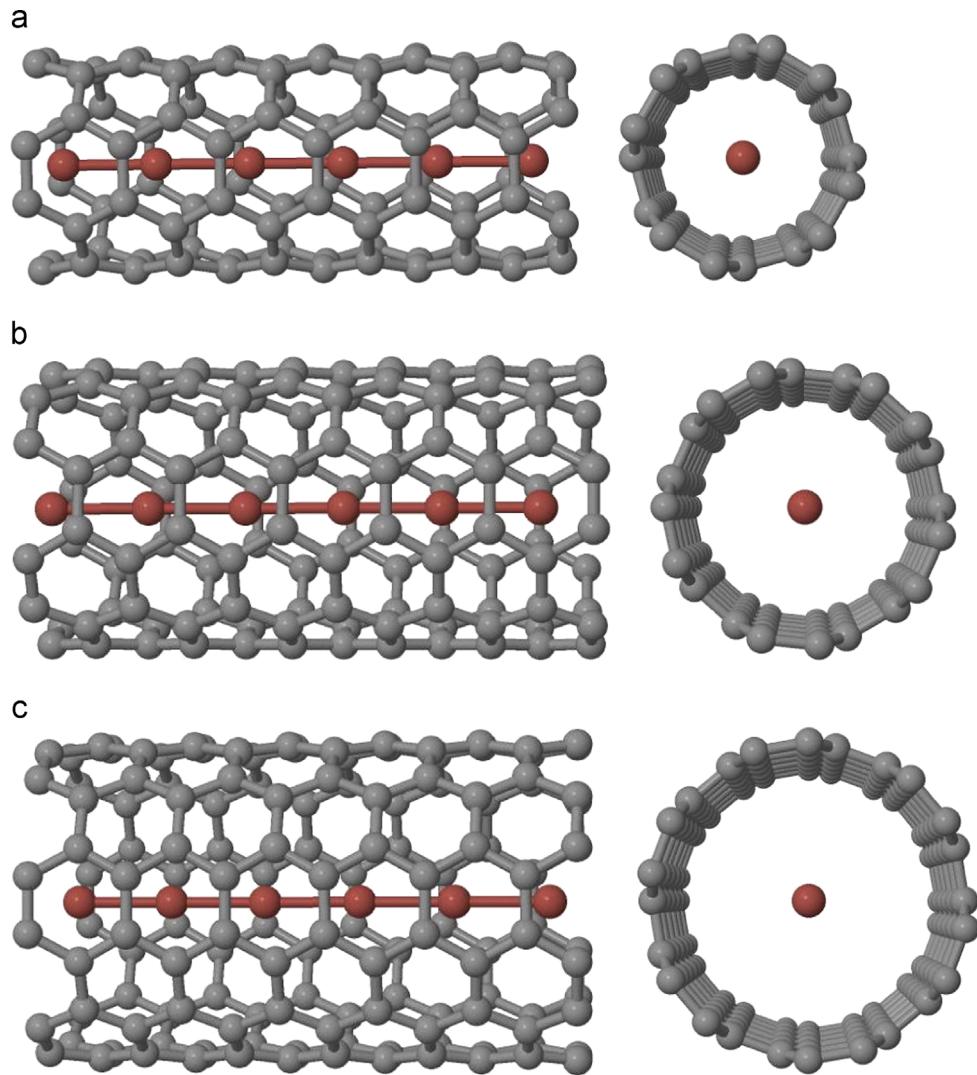


Fig. 6. The optimized structures of $\text{Tl}_6@\text{CNTs}$ (a) (4, 4), (b) (5, 5), and (c) (6, 6).

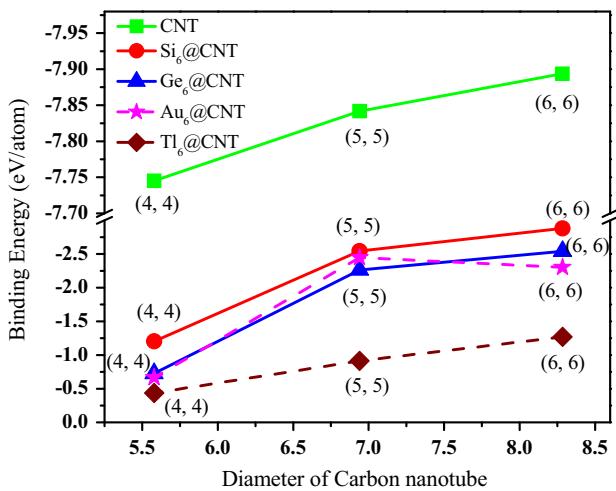


Fig. 7. The variation of binding energy per atom with diameter for Si, Ge, Au and Tl encapsulated armchair (n, n) , $n=4\text{--}6$ CNTs.

doped CNT the value increases to -1.269 eV. This shows that for $\text{Au}_6@\text{CNT}$, most stable CNT is (5, 5). B.E./atom increases monotonically with increase in diameter for $\text{Tl}_6@\text{CNT}$ and is maximum for (6, 6) CNT i.e. (6, 6) CNT is most stable.

In order to have a clear insight of electronic properties, we have studied IP and EA of the pure and doped CNTs. We put one extra electron on $\text{Si}_6@\text{CNT}$ molecule and compute the total energy. Subtracting the total energy obtained from the total energy of $\text{Si}_6@\text{CNT}$ yields electron affinity of $\text{Si}_6@\text{CNT}$. Similarly, we have computed IP by making $\text{Si}_6@\text{CNT}$ one electron deficit. These quantities give us an idea about the chemical reactivity of endohedral CNTs. The variation of IP and EA with tube diameter is shown in Figs. 8 and 9 respectively. We found that in pure CNTs the maximum value of IP is about 4.65 eV. IP for pure CNT decreases slightly with increasing diameter of armchair tube. For pure CNTs, EA increases with diameter but not monotonically.

The endohedral doping of linear atomic chain changes IP and EA significantly. We have found that for Si, Ge, Tl doped (4, 4) tube, IP and EA decrease as compared to pure (4, 4) CNT. IP of Au doped (4, 4) tube is very close to that of pure (4, 4) CNT whereas EA of this tube is greater as compared to corresponding pure CNT. The minimum value of IP and EA is observed for (4, 4) CNTs whereas maximum IP is observed for (5, 5) CNT. The value of IP for doped (5, 5) tube is greater than corresponding pure tube for Si, Au and Tl chains whereas for Ge doping, IP and EA are very close to pure CNT. Further increase in CNT diameter leads to decrease in IP and EA values for $\text{Si}_6@\text{CNT}$. For $\text{Ge}_6@\text{CNT}$, maximum value of IP and EA is observed for (6, 6) CNT. The maximum value of EA for Si doping is 4.538 eV corresponding to (5, 5) CNT whereas for Ge doping maximum value of EA is 4.07 eV

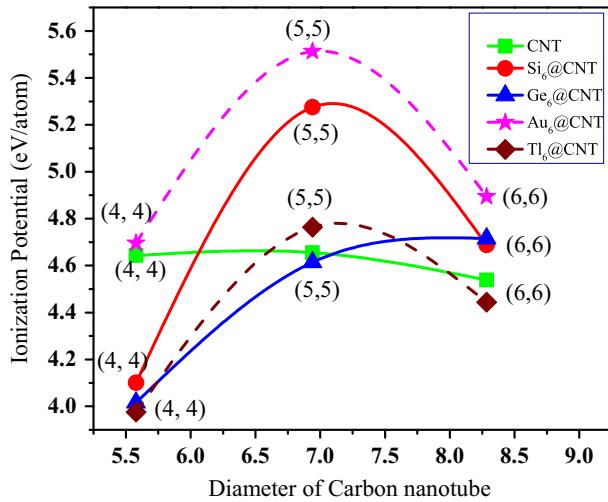


Fig. 8. The variation of ionization potential with diameter for Si, Ge, Au and Tl encapsulated armchair (n, n), $n=4-6$ CNTs.

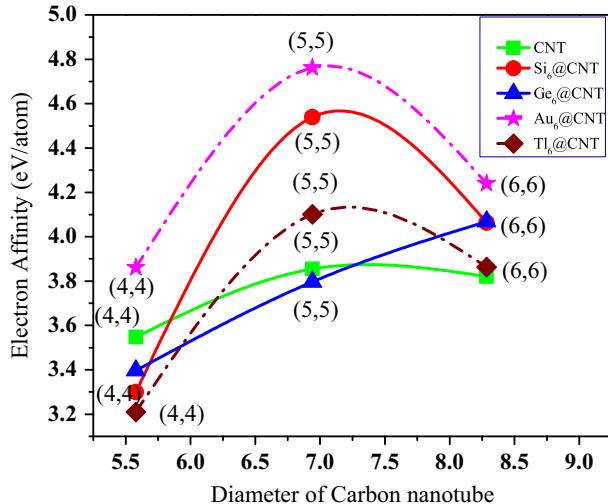


Fig. 9. The variation of electron affinity with diameter for Si, Ge, Au and Tl encapsulated armchair (n, n), $n=4-6$ CNTs.

corresponding to $\text{Ge}_6@\text{CNT}(6, 6)$. The maximum values of IP are 5.274 eV and 4.715 eV for $\text{Si}_6@\text{CNT}(5, 5)$ and $\text{Ge}_6@\text{CNT}(6, 6)$ respectively. On comparing IP and EA values we find that Si doped CNTs have higher values than Ge doped CNTs for (4, 4) and (5, 5) configurations which means that Ge doped CNTs are less reactive than Si doped CNTs. The value of IP for Si and Ge doped (6, 6) CNTs is same whereas value of EA for Ge doped (6, 6) CNT is slightly greater than that of corresponding Si doped CNT.

For metallic dopants, the maximum values of IP are 5.513 eV and 4.763 eV for Au and Tl doping in (5, 5) CNT respectively. As we move from (5, 5) to (6, 6) CNTs, the value of IP decreases. A similar trend is observed for EA values of Au and Tl encapsulated CNTs. Also IP of Au doped (4, 4) CNT is very close to that of pure (4, 4) CNT whereas EA of this CNT is greater as compared to corresponding pure CNT. Also IP and EA for Au doped CNTs are more as compare to Tl doped CNTs showing that Tl doped CNTs are less reactive than Au doped CNTs. The maximum and minimum values of Au encapsulated CNTs are 4.763 eV and 3.861 eV corresponding to (4, 4) and (5, 5) CNTs respectively. For Tl encapsulated CNTs the maximum and minimum values are 4.101 eV and 3.209 eV respectively for (4, 4) and (5, 5) CNTs. On comparing IP and EA values among various dopants then we find that IP and EA values are highest for Au doped CNTs followed by Si, Tl and Ge.

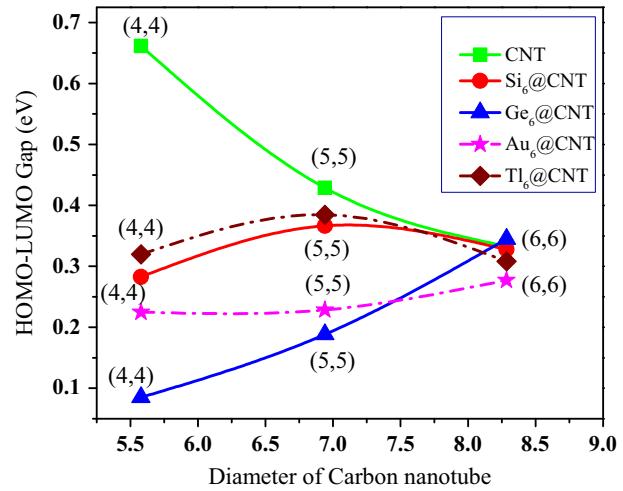


Fig. 10. The variation of HOMO-LUMO gap with diameter for Si, Ge, Au and Tl encapsulated armchair (n, n), $n=4-6$ CNTs.

The concepts of the highest occupied molecular orbital (HOMO), and lowest unoccupied molecular orbital (LUMO) are of fundamental crucial importance in understanding the charge transfer, stability and reactivity of many organic molecules. The calculated HOMO-LUMO gap of pure and doped armchair nanotubes is shown in Fig. 10. On doping of Si and Ge, HOMO-LUMO gap decreases for (4, 4) CNTs as compared to pure CNTs and hence exhibits metallic behavior. HOMO-LUMO gap of doped CNTs increases as we move from (4, 4) to (5, 5) CNTs. For Ge doped (6, 6) CNT, HOMO-LUMO gap increases as compared to (5, 5) CNTs while the HOMO-LUMO gap for Si doped (6, 6) CNTs decreases as compared to Si doped (5, 5) CNTs. Maximum HOMO-LUMO gap for $\text{Si}_6@\text{CNT}$ s is observed for (5, 5) CNT whereas for $\text{Ge}_6@\text{CNT}$ s maximum HOMO-LUMO gap is observed for (6, 6) CNT that mean the behavior of CNT is semiconducting for these configurations. For Au encapsulated CNTs, the gap increases as we move from (4, 4) to (5, 5) CNTs but with further increase in diameter, it decreases. Maximum HOMO-LUMO gap for $\text{Au}_6@\text{CNT}$ s is observed for (5, 5) CNT whereas for $\text{Tl}_6@\text{CNT}$ s HOMO-LUMO gap is maximum for (6, 6) CNT. Also it is clear from Fig. 10 that values of the HOMO-LUMO gap are approximately equal for pure and doped (6, 6) CNTs. In general, from Fig. 10, it can be inferred that doping makes armchair CNTs metallic and therefore makes them more suitable for applications involving conduction.

3.2. Zigzag SWCNTs

We have performed similar calculations for zigzag SWCNTs. We have placed six atoms chain of dopant atoms inside zigzag CNTs. We have considered (4, 0), (5, 0) and (6, 0) zigzag SWCNTs. The B.E./atom values are –7.219 eV, –7.356 eV, and –7.5405 eV for (4, 0), (5, 0) and (6, 0) pure zigzag CNTs respectively. Fig. 11 illustrates the optimized structure after doping the chain consisting of six atoms of Si and Ge in zigzag CNTs. We found that zigzag tubes bind Si and Ge atoms with less energy compared to armchair tubes of similar diameter. The B.E./atom for Si doped (4, 0) and Ge doped (4, 0), (5, 0) tube is positive which implies instability of the endohedral tube. However Ge doped (6, 0) tube gave negative binding energy. The B.E./atom for Au and Tl doped zigzag CNTs is positive for all the diameters. The various calculated parameters for doped stable CNTs are shown in Table 1. It is clear from Table 1 that IP and EA of doped CNTs are less than that of pure CNTs. IP and EA values of (5, 0) and (6, 0) CNTs decrease on doping. IP and EA values remain almost same for Si and Ge doping. Therefore we can say that both parameters remain almost independent of CNT

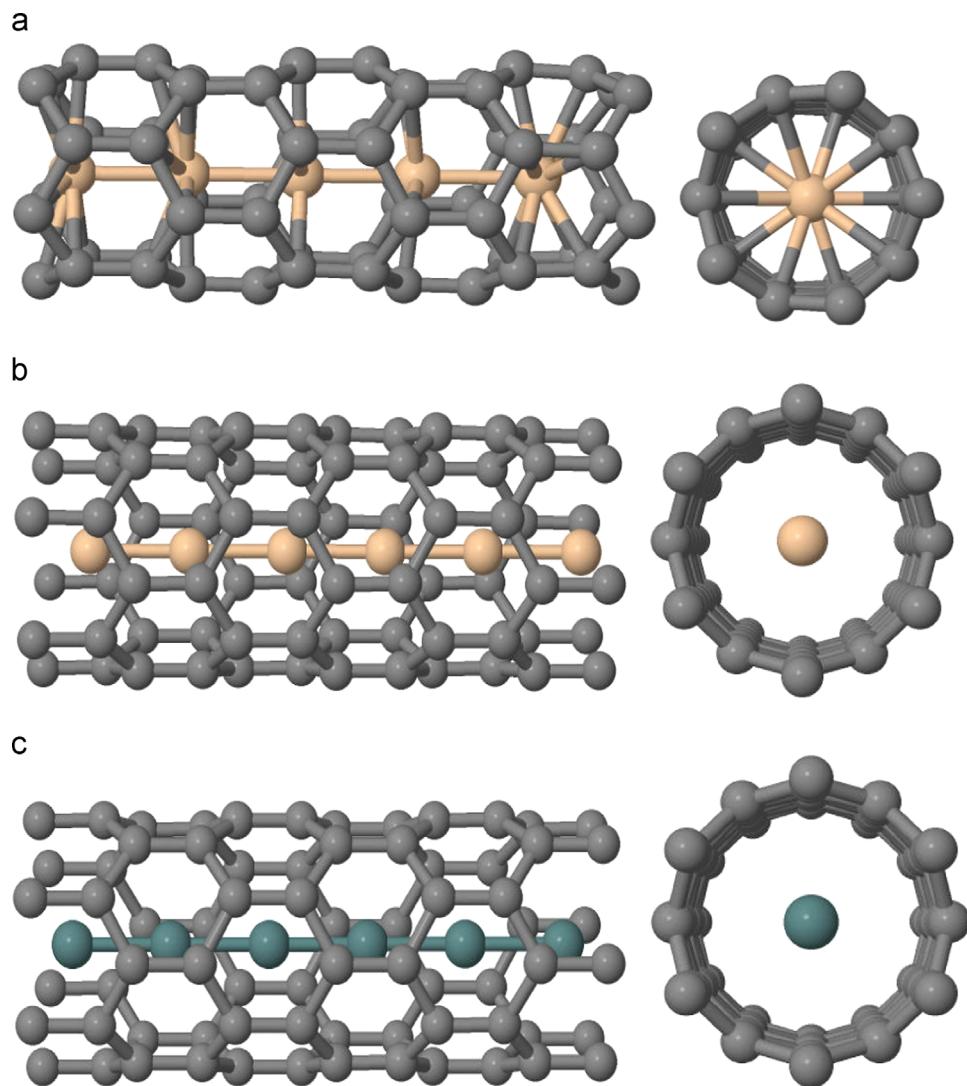


Fig. 11. The optimized structures of $\text{Si}_6@\text{CNTs}$ (a) (5, 0), (b) (6, 0), and (c) $\text{Ge}_6@\text{CNT}$ (6, 0).

Table 1

The variation of B.E./atom, IP, EA and HOMO–LUMO gap (in eV) for Si and Ge doped zigzag ($n, 0$); $n=5, 6$ CNTs.

Parameters	Pure CNT (5,0)	Pure CNT (6,0)	$\text{Si}_6@\text{CNT}/$ (5,0)	$\text{Si}_6@\text{CNT}/$ (6,0)	$\text{Ge}_6@\text{CNT}/$ (6,0)
B.E./atom (eV)	−7.356	−7.5405	−1.623	−1.698	−0.545
I.P. (eV)	5.173	5.151	4.637	4.609	4.590
E.A. (eV)	4.053	4.092	3.389	3.553	3.552
HOMO–LUMO gap (eV)	1.099	0.683	0.986	1.458	0.953

diameter and dopant type. HOMO–LUMO gap of (5, 0) zigzag CNTs decreases on Si doping whereas it increases for Si and Ge doped (6, 0) CNTs. Also HOMO–LUMO gap of zigzag CNT has been found to be higher than doped or undoped armchair CNTs. This leads to the conclusion that zigzag CNTs are semiconducting.

4. Conclusion

The electronic properties of endohedrally doped armchair (n, n) and zigzag ($n, 0$); $n=4–6$, single wall carbon nanotubes (SWCNTs) with Si, Ge, Au and Ti atoms have been studied using the *ab-initio* method. We have considered doping of a linear chain of six atoms

inside SWCNTs of different diameters but of same length. The six atoms chain was chosen keeping in view maximum value of B.E./atom for doped CNTs. We have calculated the binding energy per atom, ionization potential, electron affinity and HOMO–LUMO gap of doped armchair and zigzag SWCNTs. For armchair undoped CNTs, the B.E./atom increases with the increase in diameter of the tubes. For Si, Ge and Ti doped CNTs, B.E./atom is maximum for (6, 6) CNT whereas for Au doped CNTs, it is maximum for (5, 5) CNTs. For pure CNTs, IP decreases slightly with increasing diameter whereas EA increases with diameter. For doped armchair CNTs, maximum IP and EA are observed for doped (5, 5) tube. In case of zigzag tubes only Si doped (5, 0), (6, 0) and Ge doped (6, 0) CNTs are stable. The calculated B.E./atom for rest of the complexes is positive indicating instability of these complexes. IP and EA of the doped zigzag CNTs are less than as compared to pure. Also IP and EA for doped zigzag CNTs remains almost independent of tube diameter and dopant type. The study of HOMO–LUMO gap shows that on doping metallic character of the armchair tubes increases whereas for zigzag CNTs semiconducting character increases.

Acknowledgments

Authors are thankful to the SIESTA group for providing the computational code and greatly acknowledge the HPCC facility provided by Department of Physics, Panjab University, Chandigarh.

References

- [1] S. Iijima, Nature 354 (1991) 56.
- [2] T.W. Odom, J.L. Huang, P. Kim, C.M. Lieber, Nature 391 (1998) 62.
- [3] D.H. Robertson, D.W. Brenner, J.W. Mintmire, Phys. Rev. B 45 (1992) 12592.
- [4] M.F. Yu, B.S. Files, S. Arepalli, R.S. Ruoff, Phys. Rev. Lett. 84 (2002) 5552.
- [5] S. Reich, C. Thomsen, P. Ordejon, Phys. Rev. B 65 (2002) 155411.
- [6] Y.K. Kwon, S. Saito, D. Tomanek, Phys. Rev. B 58 (1998) R13314.
- [7] R. Saito, M. Fujita, G. Dresselhaus, M.S. Dresselhaus, Appl. Phys. Lett. 60 (1992) 2204.
- [8] I. Zanella, S.B. Fagan, R. Mota, A. Fazzio, Chem. Phys. Lett. 439 (2007) 348.
- [9] S.B. Fagan, R. Mota, R.J. Baierle, A.J.R. da Silva, A. Fazzio, Mater. Charact. 50 (2003) 183.
- [10] R.J. Baierle, S.B. Fagan, R. Mota, A.J.R. da Silva, A. Fazzio, Phys. Rev. B 64 (2001) 085413.
- [11] A. Galano, M.F. Marquez, Chem. Phys. 345 (2008) 87.
- [12] B.B. Shirvani, M.B. Shirvani, J. Beheshtian, N.L. Hadipour, J. Iran. Chem. Soc. 8 (2011) S110.
- [13] H.J. Shin, S.M. Kim, S.M. Yoon, A. Benayad, K.K. Kim, S.J. Kim, H.K. Park, J. Y. Choi, Y.H. Lee, J. Am. Chem. Soc. 130 (2008) 2062.
- [14] R. Voggu, C.S. Rout, A.D. Franklin, T.S. Fisher, C.N.R. Rao, J. Phys. Chem. C 112 (2008) 13053.
- [15] M.S. Strano, C.A. Dyke, M.L. Usrey, P.W. Barone, M.J. Allen, H. Shan, C. Kittrell, R. Hauge, J.M. Tour, R.E. Smalley, Science 301 (2003) 1519.
- [16] L. Lai, J. Lu, W. Song, M. Ni, L. Wang, G. Luo, J. Zhou, W.N. Mei, Z. Gao, D. Yu, J. Phys. Chem. C 112 (2008) 16417.
- [17] T. Kimura, T. Sugai, H. Shinohara, Chem. Phys. Lett. 256 (1996) 269.
- [18] C. Ray, M. Pellarin, J.L. Lerme, J.L. Vialle, M. Broyer, X. Blase, P. Melinon, P. Keghelian, A. Perez, Phys. Rev. Lett. 80 (1998) 5365.
- [19] M. Pellarin, C. Ray, J. Lerme, J.L. Vialle, M. Broyer, X. Blase, P. Keghelian, P. Melinon, A. Perez, J. Chem. Phys. 110 (1999) 6927.
- [20] M. Pellarin, C. Ray, J. Lerme, J.L. Vialle, M. Broyer, X. Blase, P. Keghelian, P. Melinon, A. Perez, Eur. Phys. J. 9 (1999) 49.
- [21] J.L. Fye, M.F. Jarrold, J. Phys. Chem. A 101 (1997) 1836.
- [22] T. Kimura, T. Sugai, H. Shinohara, Chem. Phys. Lett. 256 (1996) 269.
- [23] T. Takenobu, T. Kambara, N. Akima, T. Takahashi, M. Shiraishi, K. Tsukagoshi, H. Kataura, Y. Aoyagi, Y. Iwasa, Adv. Mater. 17 (2005) 2430.
- [24] J. Chen, M.A. Hamon, H. Hu, Y. Chen, A.M. Rao, P.C. Eklund, R.C. Haddon, Science 282 (1998) 95.
- [25] S. Janietz, D.D.C. Bradley, M. Grell, G. Giebel, M. Inbasekaran, E.P. Woo, Appl. Phys. Lett. 73 (1998) 2453.
- [26] Z. Li, Z.X. Chen, G.J. Kang, X. He, Catal. Today 165 (2011) 25.
- [27] J.M. Soler, E. Artacho, J.D. Gale, A. Garcia, J. Junquera, P. Ordejon, D. Sanchez-Portal, J. Phys.: Condens. Matter. 14 (2002) 2745.
- [28] N. Troullier, J.L. Martins, Phys. Rev. B, 43 (1991) 1993.
- [29] J.P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 77 (1996) 3865.
- [30] P. Jensen, J. Gale, X. Blase, Phys. Rev. B 66 (2002) 193403.
- [31] M. Matsubara, C. Massobri, Jean-Claude Parlebas, Comp. Mater. Sci. 33 (2005) 237.
- [32] M. Anafcheh, R. Ghafouri, Superlattices Microstruct. 60 (2013) 1.
- [33] B.B. Shirvani, J. Beheshtian, M.D. Esrafil, N.L. Hadipour, Physica B 405 (2010) 1455.
- [34] N.A. Poklonski, E.F. Kislyakov, O.N. Bubel, S.V. Ratkevich, S.A. Vyrko, A. M. Popov, N.N. Hieu, N.A. Viet, Nanoscale Res. Lett. 6 (2011) 216.
- [35] N.M. Umran, R. Kumar, Physica B 437 (2014) 47.
- [36] H.H. Akkinen, M. Moseler, U. Landman, Phys. Rev. Lett. 89 (2002) 033401.