สมบัติเชิงโครงสร้างและสมบัติเชิงอิเล็กโทรนิคของคาร์บอนนาโนแคปที่โดปด้วยโบรอนไนไตรด์โบรอนฟอสไฟด์อะลูมิเนียมไนไตรด์และอะลูมิเนียมฟอสไฟด์: การศึกษาเชิงทฤษฎี

Structural and electronic property of BN–, BP–, AlN–, and AlP–doped carbon nanocaps: A theoretical study

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บทคัดย่อ

ในงานวิจัยนี้ได้ใช้คาร์บอนนาโนแคป(CNC, $C_{60}H_{10}$)เป็นต้นแบบชนิดใหม่สำหรับการโดปด้วยสปีชีเชิงเคมี โดยได้ศึกษาการโดปอะตอมคู่ของโบรอนไนไตรด์ โบรอนฟอสไฟด์ อะลูมิเนียมไนไตรด์ และ อะลูมิเนียมฟอสไฟด์ลงบนคาร์บอนนาโนแคป ได้คำนวณหาสมบัติเชิงโครงสร้าง พลังงาน การเคลื่อนย้ายประจุ และสมบัติเชิงอิเล็กโทรนิคของคาร์บอนนาโนแคปและคาร์บอนนาโนแคปที่โดปด้วยอะตอมคู่ ด้วยทฤษฎีฟังก์ชันนัลความหนาแน่น ผลการคำนวณแสดงให้เห็นว่าการโดปด้วยอะตอมคู่นี้ให้โครงสร้างของสารประกอบเชิงซ้อนที่เสถียรและการโดปเกิดผ่านกระบวนการคายความร้อน โดยมีค่าพลังงานการยึดจับที่สูงที่สูงสุดเท่ากับ –280.80 kcal/molซึ่งเป็นการโดปด้วยโบรอนไนไตรด์นั่นคือโบรอนไนไตรด์สามารถเกิดอันตรกิริยาที่แข็งแรงที่สุดกับคาร์บอนนาโนแคป นอกจากนี้งานวิจัยนี้ยังได้ศึกษาและรายงานสมบัติเชิงโครงสร้าง การเคลื่อนย้ายประจุ และ สมบัติเชิงอิเล็กโทรนิค ของคาร์บอนนาโนแคปและคาร์บอนนาโนแคปที่โดปด้วยอะตอมคู่

คำสำคัญ: คาร์บอนนาโนแคป ดีเอฟที โบรอนไนไตรด์ โบรอนฟอสไฟด์ อะลูมิเนียมฟอสไฟด์ อะลูมิเนียมไนไตรด์

Abstract

In this research, the single–walled carbon nano cap (CNC, $C_{60}H_{10}$) was used as a new prototype for doping of chemical species. The atomic pairing BN, BP, AlN, and AlP doping on CNC were investigated. The structure, energy, charge transfer, and electronic properties of CNC and its co–doping structures were computed using density functional theory. The results indicated that the atomic co-doping generated the stable complexes and occurred viaexothermic process.The BN doping with the highest binding energy of -280.80 kcal/mol showed the strongest interaction with CNC. Furthermore, the structural, charge transfer,and electronic properties of CNC and its co–doping structures were reported.

Keywords: Carbon nanocap,DFT,BN, BP, AlN, AlP, CNC

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Introduction

Single–walled carbon nanotube (SWCNT) is a new kind of carbon–based nanostructure family, which was discovered since in 1991.[1] SWCNT shows outstanding structural and electronic properties depending on its chirality.[2] Therefore, SWCNT plays a good candidate for the promising materials in the future. So, many works have been investigated significantly to improve its structural and electronic properties. Due to excellence properties, its applications in materials science and nanotechnology field were widely studied.[3]

Recently, Yu and co-workers reported[4] that structural control and especially chirality control of SWCNTs were studied herein a rational approach to engineering fullerene caps for growing SWCNTs with controlled structures via chemical vapor deposition (CVD). Opening of fullerendione via thermal oxidation yields hemispherical caps which can initiate SWNT growth at their open ends. The size and structure of these caps can be engineered by tuning the temperature of thermal oxidation. Interestingly, SWNTs made using fullerene caps show step like diameter distributions relative to SWNTs catalyzed by Fe nanoparticles. This cap engineering using opened C_{60} provides a potential approach to grow SWCNTs with controlled structures.[4]

Generally, modification of the cap or surface of SWCNT has been significantly changed the structural and electronic properties. The chemical doping includes the attendance of chemical groups such as N, B, Al, S, P, and Si as well as the systems of SWCNTs doping with transition metals (TM) such as Fe, Co, Ni, Cu, Pd, Os, Pt can be improved significantly its structural properties. Moreover, improvements of electronic property and chemical reactivity by doping were studied and reported.[5–8] Especially, substitutional doping in SWCNT indicated that carbon atoms in the hexagonal structure were replaced by heteroatoms, thus effect the sp^2 hybridization of the carbon atoms, and the electronic properties of SWCNT could be modified. Furthermore, the theoretical studies on reactivity and stability of capped and open–ended SWCNTs were reported. Saha and co-workers[9] using density functional theory (DFT) calculations predicted the reactivity pattern governing the nucleophilic, electrophilic, and radical attacks on the external surface of open and capped (5,5) armchair single–walled carbon nanotubes. The results revealed that the carbon atoms in edge or cap regions showed different reactivity pattern than those at the middle portion of the nanotubes. Comparison of chemical adsorption on SWCNT, graphene and C_{60} was reported.[10–12] Interaction of carbon nanostructure strongly depends on the curvature due to the bending of C–C bonds in their systems, which in directly implies the disturbance in the orientation of the π–orbitals due to the varying angular separation.[12]

In the present work, the single–walled carbon nano cap(CNC, $C_{60}H_{10}$) was used as a new prototype for chemical doping studies. The BN-, BP-, AlN-, and AlP-doped CNCs have been investigated. Therefore, the geometrical, charge transfer, and electronic properties of CNC and its co–doping structures have been theoretically investigated using the DFT method.

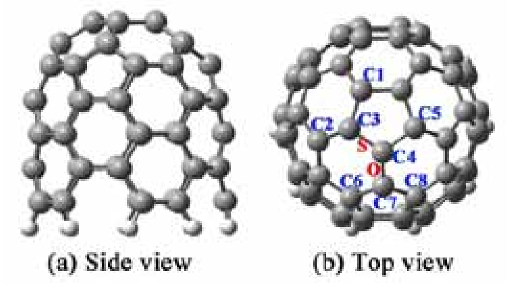

Figure 1. Modeled structures of a pristine CNC (a) side view and (b) top view with doping configuration sites labeled as red letters (slanted bond (s), orthogonal bond (o)) for various BN–, BP–, AlN–, and AlP–doped structures.

Computational details

Calculations of the present work were carried out using the Gaussian 09 computational package.[13]The geometrical structures of all systems have been fully optimized under gas phase by using the DFT method. The exchange and correlation functionals of the B3LYP, Becke's three parameter exchange functional with the Lee–Yang–Parr correlation functional was carried out to optimize the structure.[14,15]The LanL2DZ basis set was used.[16] The most stable structure from the optimized geometries of the system was taken for the last single point energy calculations.

For modeled structures of studied work, capped single–walled carbon nanotube, compose of 60 C atoms with 10 hydrogen atoms to saturate dangling bonds ($C_{60}H_{10}$), was used to model the single–walled carbon nano cap (CNC) as displayed in Figure 1. As in Figure 1b, the doping site configurations are labeled as red letters (slanted bond (s), orthogonal bond (o)) for various BN–, BP–, AlN–, and AlP–doped structures. The two different sites of the co–doping onto C–C bond of the CNC are (1) the bridge site of anorthogonal C4–C7 bond(as o in Figure 1b) and (2) the bridge site of a slantedC3–C4 bond (as s in Figure 1b).By taking the possibilities of the doped atoms and the sites of o and s, there are sixteen different configurations of BN-, BP-,AlN-, and AlP-doped CNCs. These included BN–doped CNC(o), BN–doped CNC(s), BP–doped CNC(o), BP–doped CNC(s), AlN–doped CNC(o), AlN–doped CNC(s), AlP–doped CNC(o), AlP–doped CNC(s), NB–doped CNC(o), NB–doped CNC(s), PB–doped CNC(o), PB–doped CNC(s), NAl–doped CNC(o), NAl–doped CNC(s), PAl–doped CNC(o), and PAl–doped CNC(s).

The binding energies (E_b) of CNC co–doping with pairedBN, BP, AlN, and AlP at the different sites were evaluated by using the following equations (eqs.):

$$E_b = E_{\text{BN-doped CNC}} - E_{\text{CNC -VAC}} - E_{\text{BN}} \quad (1)$$

$$E_b = E_{\text{BP-doped CNC}} - E_{\text{CNC -VAC}} - E_{\text{BP}} \quad (2)$$

$$E_b = E_{\text{AlN-doped CNC}} - E_{\text{CNC -VAC}} - E_{\text{AlN}} \quad (3)$$

$$E_b = E_{\text{AlP-doped CNC}} - E_{\text{CNC -VAC}} - E_{\text{AlP}} \quad (4)$$

Where $E_{\text{BN-doped CNC}}$, $E_{\text{BP-doped CNC}}$, $E_{\text{AlN-doped CNC}}$, and $E_{\text{AlP-doped CNC}}$ are the total energies for BN, BP, AlN, and AlP co–doping on to reactivity surface of a CNC with the different configurations, respectively. $E_{\text{CNC-VAC}}$ is the total energy of CNC with pairing C atom vacancy ($C_{58}H_{10}$) whereas E_{BN}, E_{BP}, E_{AlN}, and E_{AlP} are the total energies of isolated paired BN, BP, AlN, and AlP, respectively. A negative binding energy indicates that the system is an exothermic interaction.

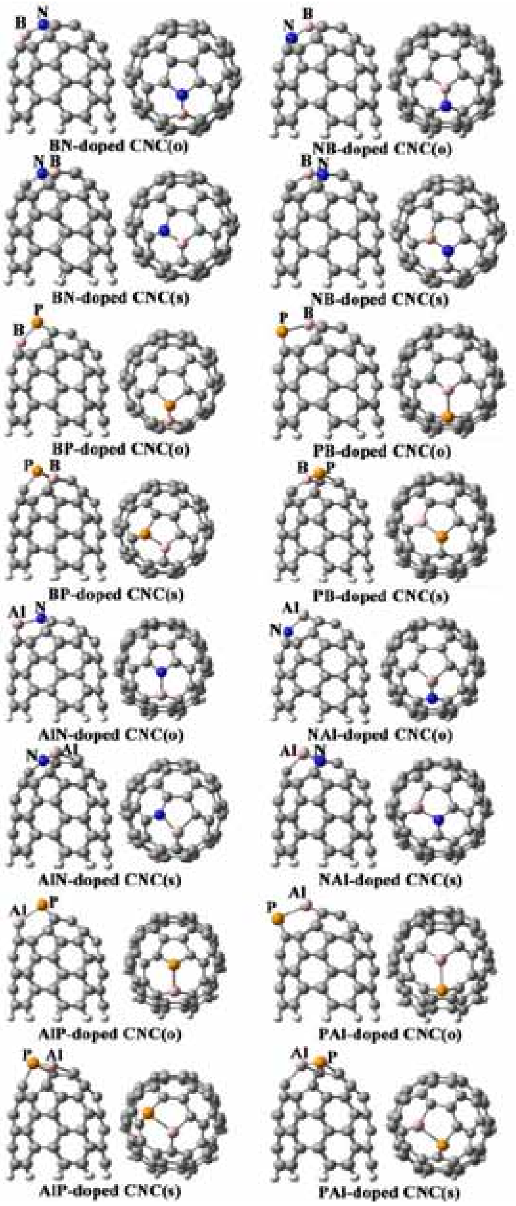

Figure 2. The Optimized structures of BN–, BP–, AlN–, and AlP–doped on to CNC at the various different sites as computed at the B3LYP/LanL2DZ level.

Considering the electronic properties, the single point energy calculations to study the properties of the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO), and the energy gaps (E_{gap}) referring to the energy difference between HOMO and LUMO orbitals ($E_{LUMO} - E_{HOMO}$) were taken at the same level. Natural bond orbital (NBO) analysis of all systems was carried out to estimate the partial charge transfer (Q_T).[17]The total density of states (DOSs) of all systems were also studied and reported.[18]

Results and discussion

Structural properties and binding energies

The B3LYP/LanL2DZ–optimized structures of BN–doped CNC, BP–doped CNC, AlN–doped CNC and AlP–doped CNC are displayed in Figure 2 and accompanying with the selected geometrical data are listed in Table 1.

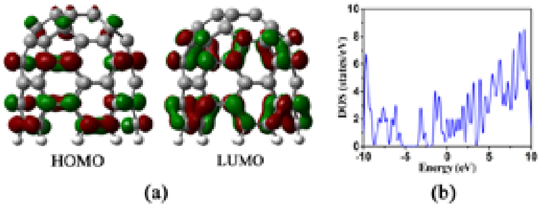

Figure 3. (a)The frontier molecular orbitals, HOMO and LUMO and (b) DOS of pristine CNC.

The calculation results indicated that when two carbon atoms (C3–C4 andC4–C7 in Figure 1b) of CNC substituted by one of pairing BN, BP, AlN and AlP atoms, the geometric structures of the CNC presented interesting changes caused from the co–doping effect comparing to pristine CNC. The corresponding bond lengths of C1–C3 (1.463 Å), C2–C3 (1.408 Å), C3–C4 (1.463 Å), C4–C5 (1.463 Å), C4–C7 (1.408 Å), C6–C7 (1.457 Å), C7–C8 (1.457 Å) of pristine CNC were observed. After co–doping, the Al–C (for AlN–CNC), Al–C (for AlP–CNC), P–C (for BP–CNC), and P–C (for AlP–CNC)bond lengths were elongated in comparison with the corresponding conventional C-C bond(see in Table 1) of the pristine CNC. This indicates that the co–doping makes the significantly changes of CNC configurations.

Table 1. Geometrical data of BN–, BP–, AlN–, and AlP–doped CNCs at the different sites as computed at the B3LYP/LanL2DZ level.

Systems[a]	Bond lengths[b]						
CNC	1.463	1.408	1.463	1.463	1.408	1.457	1.457
	(C1–C3)	(C2–C3)	(C3–C4)	(C4–C5)	(C4–C7)	(C6–C7)	(C7–C8)
BN–doped CNC(o)	–	–	1.442	1.442	1.446	1.539	1.539
			(C3–N)	(N–C5)	(B–N)	(C6–B)	(B–C8)
BN–doped CNC(s)	1.445	1.388	1.503	1.538	1.492	–	–
	(C1–N)	(C2–N)	(B–N)	(B–C5)	(B–C7)		
BP–doped CNC(o)	–	–	1.877	1.877	1.909	1.538	1.539
			(C3–P)	(P–C5)	(B–P)	(C6–B)	(B–C8)
BP–doped CNC(s)	1.877	1.828	1.944	1.550	1.504	–	–
	(C1–P)	(C2–P)	(B–P)	(B–C5)	(B–C7)		
AlN–doped CNC(o)	–	–	1.434	1.434	1.831	1.910	1.910
			(C3–N)	(N–C5)	(Al–N)	(C6–Al)	(Al–C8)
AlN–doped CNC(s)	1.441	1.389	1.892	1.910	1.867	–	–
	(C1–N)	(C2–N)	(Al–N)	(Al–C5)	(Al–C7)		
AlP–doped CNC(o)	–	–	1.929	1.929	2.311	1.912	1.912
			(C3–P)	(P–C5)	(Al–P)	(C6–Al)	(Al–C8)
AlP–doped CNC(s)	1.946	1.889	2.333	1.925	1.888	–	–
	(C1–P)	(C2–P)	(Al–P)	(Al–C5)	(Al–C7)		
NB–doped CNC(o)	–	–	1.541	1.541	1.451	1.432	1.432
			(C3–B)	(B–C5)	(N–B)	(C6–N)	(N–C8)
NB–doped CNC(s)	1.538	1.492	1.503	1.445	1.388	–	–
	(C1–B)	(C2–B)	(N–B)	(N–C5)	(N–C7)		
PB–doped CNC(o)	–	–	1.540	1.540	1.917	1.869	1.869
			(C3–B)	(B–C5)	(P–B)	(C6–P)	(P–C8)
PB–doped CNC(s)	1.550	1.505	1.944	1.877	1.828	–	–
	(C1–B)	(C2–B)	(P–B)	(P–C5)	(P–C7)		
NAl–doped CNC(o)	–	–	1.906	1.906	1.835	1.427	1.427
			(C3–Al)	(Al–C5)	(N–Al)	(C6–N)	(N–C8)
NAl–doped CNC(s)	1.910	1.867	1.892	1.441	1.389	–	–
	(C1–Al)	(C2–Al)	(N–Al)	(N–C5)	(N–C7)		
PAl–doped CNC(o)	–	–	1.912	1.912	2.316	1.919	1.919
			(C3–Al)	(Al–C5)	(P–Al)	(C6–P)	(P–C8)
PAl–doped CNC(s)	1.925	1.888	2.333	1.946	1.889	–	–
	(C1–Al)	(C2–Al)	(P–Al)	(P–C5)	(P–C7)		

[a]All systems weredisplayed in Figure 2.[b] In Å.

The values of binding energies computed by using eqs. 1–4 of BN–doped CNC, BP–doped CNC, AlN–doped CNC and AlP–doped CNC are listed in Table 2. The results showed that the highest and the lowest E_b values were –280.80 kcal/mol (NB–doped CNC(o)) and –129.35 kcal/mol (AlP–doped CNC(s),(PAl–doped CNC(s)), respectively. This indicated that NB–doped CNC(o) displays the strongest interaction with CNC whereas AlP–doped CNC(o) and AlP–doped CNCs(s) display the weakest interaction with CNC. In addition, E_b values of other co–doping CNC were in the range of–152.97 to –275.31 kcal/mol.

In addition, Q_T is defined as a change of dopant charges during structural doping. As also listing in Table 2, the Q_T of all systems, BN–doped CNC, BP–doped CNC, AlN–doped CNC and AlP–doped CNC, were found in the range of 0.197 to 1.814 e. A positive charge of all Q_T

indicates that the total charges from the dopant transferred to carbon nano cap.

Table 2. Binding energy (E_b), partial charge transfer (Q_T), frontier molecular orbital energies (E_{HOMO} and E_{LUMO}), energy gaps (E_{gap}), and chemical indices of BN–, BP–, AlN–, and AlP–doped on to CNC at the difference sites as computed at the B3LYP/LanL2DZ level.

systems	E_b[a]	Q_T[b]	E_{HOMO}[c]	E_{LUMO}[c]	E_{gap}[c, d]	□[c, e]	□[c, f]	□[c, g]
CNC	–	–	–5.660	–3.184	2.476	1.238	–4.422	4.422
BN–doped CNC(o)	–275.31	0.197	–5.524	–3.129	2.395	1.197	–4.327	4.327
BN–doped CNC(s)	–248.09	0.192	–5.633	–3.402	2.231	1.116	–4.517	4.517
BP–doped CNC(o)	–228.96	1.146	–5.524	–3.429	2.095	1.048	–4.476	4.476
BP–doped CNC(s)	–202.26	1.156	–5.660	–3.919	1.742	0.871	–4.789	4.789
AlN–doped CNC(o)	–214.52	0.880	–5.306	–3.374	1.932	0.966	–4.340	4.340
AlN–doped CNC(s)	–188.39	0.902	–5.361	–3.238	2.123	1.061	–4.299	4.299
AlP–doped CNC(o)	–152.97	1.802	–5.306	–3.320	1.986	0.993	–4.313	4.313
AlP–doped CNC(s)	–129.35	1.814	–5.524	–3.782	1.742	0.871	–4.653	4.653
NB–doped CNC(o)	–280.80	0.202	–5.551	–3.238	2.313	1.157	–4.395	4.395
NB–doped CNC(s)	–248.04	0.192	–5.633	–3.402	2.231	1.116	–4.517	4.517
PB–doped CNC(o)	–230.96	1.143	–5.524	–3.238	2.286	1.143	–4.381	4.381
PB–doped CNC(s)	–202.26	1.156	–5.660	–3.919	1.742	0.871	–4.789	4.789
NAl–doped CNC(o)	–221.35	0.908	–5.306	–3.265	2.041	1.020	–4.286	4.286
NAl–doped CNC(s)	–188.39	0.902	–5.361	–3.238	2.123	1.061	–4.299	4.299
PAl–doped CNC(o)	–156.47	0.359	–5.334	–3.238	2.095	1.048	–4.286	4.286
PAl–doped CNC(s)	–129.35	1.814	–5.524	–3.782	1.742	0.871	–4.653	4.653

[a] Inkcal/mol

[b] Defined as a change of dopant charges during structural doping, in e.

[c] In eV.

[d] $E_{gap} = E_{LUMO} – E_{HOMO}$.

[e] Chemical hardness. □ = $E_{gap}/2$.

[f] Chemical potential. □ = $(E_{LUMO} + E_{HOMO})/2$.

[g] The Mulliken electronegativity, □ = $–(E_{LUMO} + E_{HOMO})/2$.

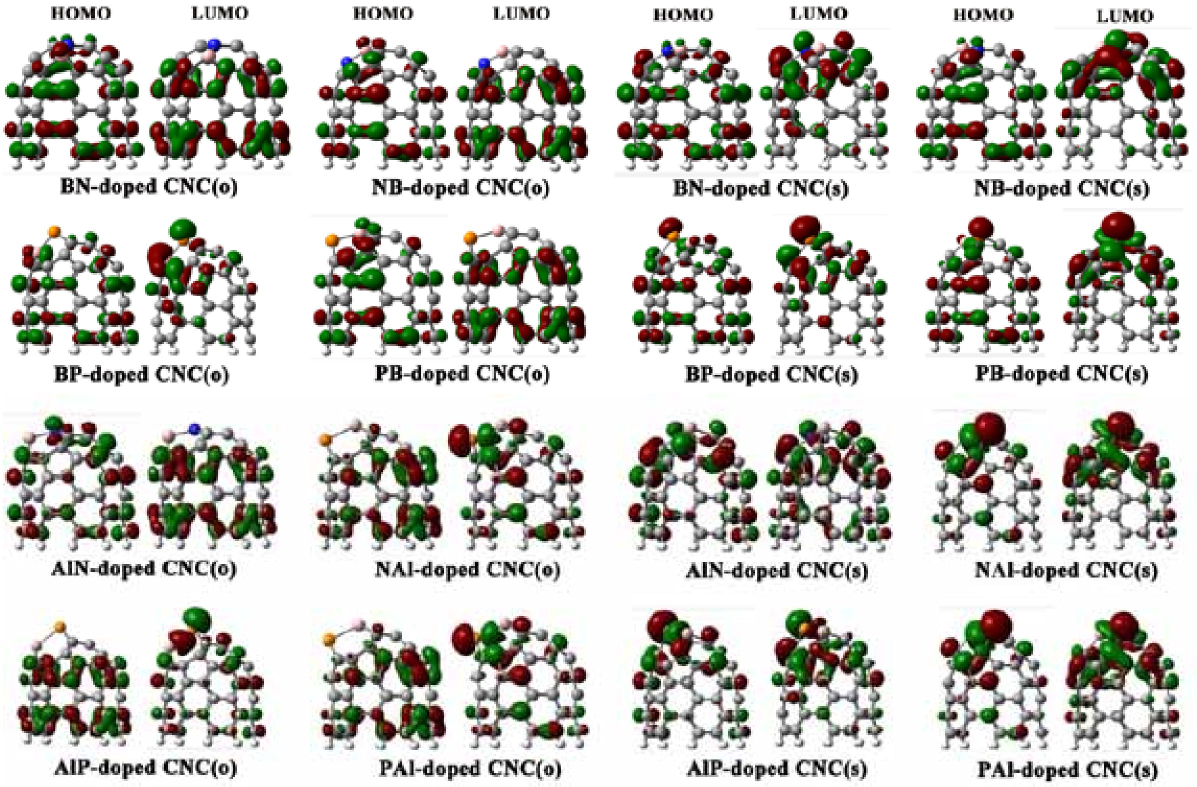

Figure 4. The frontier molecular orbitals, HOMO and LUMO, of BN–, BP–, AlN–, and AlP–dopedCNCsat the difference sites as computed at the B3LYP/LanL2DZ level.

Electronic properties

To investigate the electronic properties of BN–doped CNC, BP–doped CNC, AlN–doped CNC and AlP–doped CNC, thus the frontier molecular orbital energies, energy gaps(E_{gap}), and chemical indices of CNC and their chemical doped structures were investigated and listed in Table 2.The value of energy gap of pristine CNC was observed to be 2.476 eV suggesting a semi–conducting behavior.[19]Afterco–doping, the HOMO-LUMO energy gap of BN–doped CNC, BP–doped CNC, AlN–doped CNC and AlP–doped CNC were narrowed to approach a conductor. Outstanding E_{gap} of 1.742 eV (BP–doped CNC(s), PB–doped CNC(s), AlP–doped CNC(s), and PAl–doped CNC(s)), 1.932 eV (AlN–doped CNC(o)), 1.986 eV (AlP–doped CNC(o)) was occurred. Chemical reactivity indices of the all systems derived from Koopmans theorem[20] are also listed in Table 2. These three parameters are important tools to study the relative stability of the molecular systems. Based on the energy gap, the relative stability and chemical hardness are in decreasing from pristine CNC to the co–doping CNCs. The Mullikenelectronegativities of all systems were found in the range of 4.286 to 4.789 eV.

The plots offrontier molecular orbitals, HOMO and LUMO, and DOS of pristine CNC are displayed in Figure 3. Both HOMO and LUMO orbitals of pristine CNC were located vicinity around the tube of carbon nano cap. However, disappeared electron densities on the top of nano cap were obtained. The energy gap of 2.476 eV makes DOS platen and displayed a narrow–gap semiconductor. The plots of frontier molecular orbitals of all chemical–doped CNCs are displayed in Figure 4.Similar to the case of pristine, the HOMO of all BN–doped CNC, BP–doped CNC, AlN–doped CNC and AlP–doped CNC were located vicinity around the tube, except for in NAl–doped CNC(s), AlP–doped CNC(s),and PAl–doped CNC(s), they were mostly located on the top of dopants. In similar way, the frontier orbitals of LUMO are mostly located on the top of dopants. This suggested that the chemical dopants are more affected to streng then inter action with CNC to give the most stable complexes.

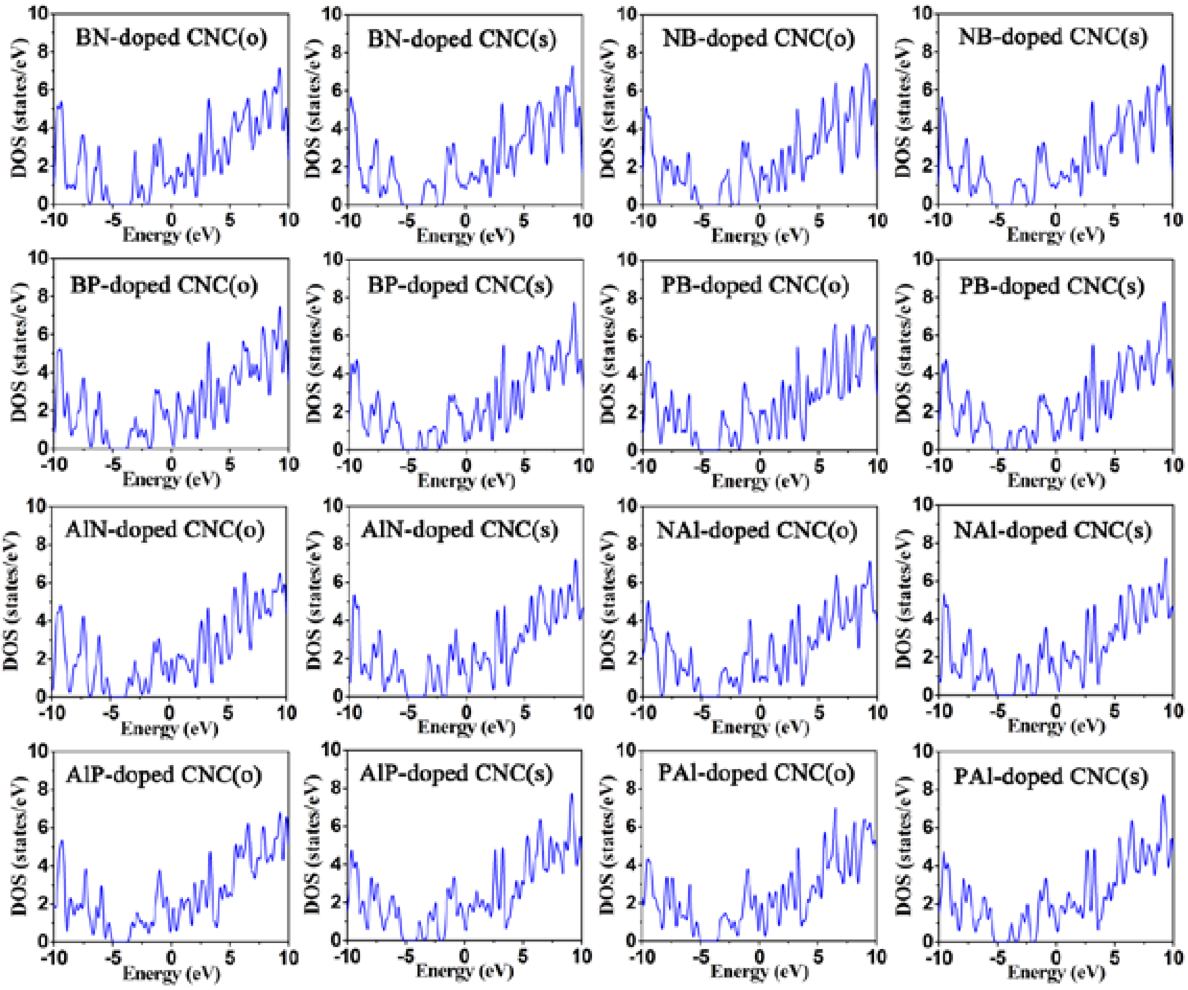

Figure 5. The density of states (DOS) of BN–, BP–, AlN–, and AlP–doped on to CNC at the various difference sites as computed at the B3LYP/LanL2DZ level.

Furthermore, theB3LYP/LanL2DZ–electronic DOSs determined for allco–doped CNCs are displayed in Figure5. The DOSs of the co–doped CNCs exhibited the different patterns and band gaps. Interestingly, from the DOS plots the results displayed that the DOSs of the co–doped CNCs showed a significant narrow change in their peaks, when comparing with pristine CNC. The se indicated that the co–doped CNCs corresponded nearly to approach a conductor after doping with chemical atoms.

Conclusion

Carbon nano cap was used as a new prototype for doping with paired BN, BP, AlN, and AlP atoms. The structures, energies, charge transfer, and electronic properties of CNC and its co–doping structures were theoretically investigated using the DFT methods. Calculated results showed that the value of energy gap of CNC was observed to be 2.476 eV, leading to semi–conducting behavior. After co–doping CNCs, binding energies of co-doping showed the exothermic processes with the highest and the lowest binding interactions of –280.80kcal/mol (NB–dopedCNC(o)) and–129.35kcal/mol (AlP–doped CNC(s) and PAl–doped CNC(s)), respectively, resulting that NB displayed the strongest interaction whit CNC whereas AlP displayed the weakest interaction with CNC. However, the charge transfers of all systems are found to be apositive charge indicating the total charges from the dopant transferred to nano cap. For electronic properties, the BN–doped CNC, BP–doped CNC, AlN–doped CNC and AlP–doped CNC resulted to the narrowed energy gap to nearly approach a conductor. Furthermore, frontier molecular orbitals and DOS properties ofBN–, BP–, AlN–, and AlP–doped CNC were investigated and reported.

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