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ORIGINAL PAPER

Electric field effect on the *zigzag* (6,0) single-wall BC_2N nanotube for use in nano-electronic circuits

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Abstract We have analyzed the effect of external electric field on the *zigzag* (6,0) single-wall BC_2N nanotube using density functional theory calculations. Analysis of the structural parameters indicates that the nanotube is resistant against the external electric field strengths. Analysis of the electronic structure of the nanotube indicates that the applied parallel electric field strengths have a much stronger interaction with the nanotube with respect to the transverse electric field strengths and the nanotube is easier to modulate by the applied parallel electric field. Our results show that the properties of the nanotube can be controlled by the proper external electric field for use in nano-electronic circuits.

Keywords Dipole moment · Field effect · Nano-electronic device · Single-wall BC_2N nanotube

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Introduction

Since the synthesis of carbon nanotubes (CNTs) by Ijima in 1991 [1], single-walled carbon nanotubes (SWCNTs) have attracted great interest owing to their physical and chemical properties [1–3] and applications as novel materials [4, 5]. Recently, compounds containing boron, carbon, and nitrogen atoms have been an interesting subject of many theoretical and experimental works. $B_xC_yN_z$ nanotubes successfully have been synthesized by different methods [6–8]. Stability and electronic properties of these compounds are between the homogeneity of carbon nanotubes (CNTs) and the heterogeneity of boron nitride nanotubes (BNNTs), depending on their stoichiometry.

The electronic properties of the CNTs (metallic or semiconducting) depend on their tubular diameter and chirality, whereas BNNTs are always semiconductors. Therefore, the electronic properties of $B_xC_yN_z$ nanotubes can be controlled by suitable variations in their stoichiometry for fabrication of an electronic device material. Among such nanotubes, the single-wall BC_2N nanotube stoichiometry is the most stable stoichiometry [9]. The electronic structure properties of BC2NNTs have been theoretically studied by different groups [9–11]. Recently, theoretical calculations on the pristine $B_xC_yN_z$ compound nanotubes have shown that these nanostructures are very promising for energy-storage applications [12] and also for nanotube-based molecular sensors [13]. However, to our knowledge, no experiments and theoretical investigation have been reported on BC2N nanotube surfaces under both parallel and perpendicular static external electric fields, so further study of the electronic properties of BC2N nanotubes under external electric fields remains interesting.

Tuning the electronic structures of the BC2N nanotubes for specific application is important in building specific electronic and mechanical devices. Improving the sensing performance of the pristine nanotubes and nano sheets by

manipulating their structure is too expensive; and thus, finding highly sensitive pristine nanotubes is of scientific interest. Electric field effect is one of the best techniques used aimed at improvement of the electronic structure properties of nanotubes and adsorption of gaseous molecules on the tubes surface. In recent years, several studies have been done in the computational calculation of the field effects on the electronic and structural properties of nanotubes [14–16]. In a previous case [17] we have investigated zigzag single-walled aluminum nitride nanotube under the parallel and transverse electric field strengths. Our results showed that the nanotube is a stable molecule over the entire range of the applied electrical field strength.

The objective of the present work is to study the results of density functional calculations on the geometric and electronic properties of the (6,0) *zigzag* BC2N nanotube. We investigated the charge density distributions, electric dipole moments, molecular orbital energy analysis, energies, molecular volume, density of states, electronic spatial extent (*ESE*), and energy gap ($E_{HOMO} - E_{LUMO}$), of the nanotube under the influence of both parallel and perpendicular static external electric fields. The important results can be used in production of solid-state devices, mechanism of action of external electric fields in nanotubes, and design further molecules with better reactivity.

Computational methods

In the present work, we have studied influence of the static external electric field on structural and electronic properties of the (6,0) *zigzag* BC2N nanotube. The static external electric field is separately applied at the positive X- and positive Y-directions, which is parallel and perpendicular to X and Y plane (Fig. 1). Due to the absence of periodic boundary conditions in molecular calculations, it was necessary to saturate the B and N dangling bonds with H atoms. The hydrogenated model of the pristine (6,0) *zigzag* BC2N nanotube consist of 84 atoms with formula $B_{18}C_{36}N_{18}H_{12}$. In the first step, the atomic geometrical parameters of the structure was allowed to relax in the optimization at the DFT level of B3LYP exchange functional and 6–31 G* standard basis set. Then, the influence of the external electric field at various applied parallel and transverse electric field strengths on the nanotube was investigated. The numerical values of the external static electric field strengths in X and Y directions on the *zigzag* (6,0) BC2N nanotube model are 35×10^{-4}, 70×10^{-4}, 100×10^{-4}, and 140×10^{-4} a.u. (1 a.u.= 5.14224×10^{11} V/m) [18].

The structural and electronic properties was based on the B–C, C–C, C–N, and B–N bond lengths, bond angles, length of tube, tip diameters, molecular volume, dipole moments (μ), energy gaps (*Eg*), energies (E_T), atomic charges, molecular orbital energies, electronic spatial extent (*ESE*), and density of states for the nanotube in the above electric fields with X and Y orientations. All the calculations were carried out using a locally modified version of the GAMESS electronic structure program [19].

Results and discussion

Field effect on the structural parameters of the (6,0) zigzag BC2N nanotube

The structural properties consisting of the bond lengths, bond angles, tip diameters, length of tube, and molecular volume for the optimized structure of *zigzag* (6,0) BC2N nanotube at various applied parallel and transverse electric field strengths with significant changes in the parameters are summarized in Tables 1 and 2. The bond lengths obtained at different applied parallel and transverse electric field strengths with respect to the corresponding values at zero fields (E_X=E_Y=0) indicate that the changes of all B–C, C–C, C–N, and N–B bond lengths of the *zigzag* (6,0) BC2N nanotube model over the entire range of the applied parallel and transverse electric field strengths are <0.04 Å. The most significant changes in the bond lengths for the applied parallel electric field are observed for the N–B bond lengths that increase gradually from 1.445 Å at the zero field strength (E_X=0) to 1.479 Å at the field strength of 140×10^{-4} a.u. (E_X=140). In transverse applied electric field case, the most significant change is observed for the C–N bond lengths that increase gradually from 1.419 Å at the zero field

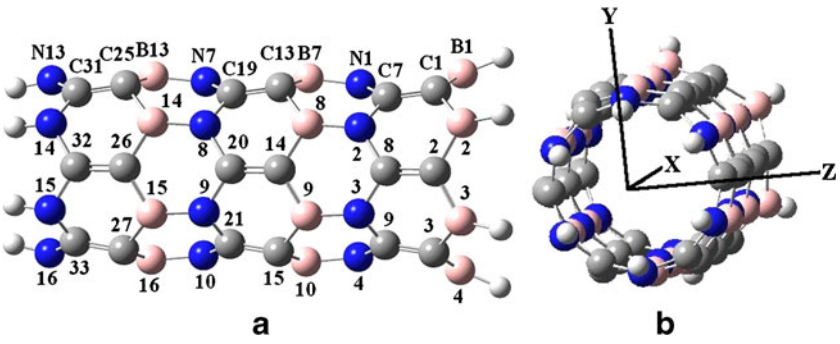

Fig. 1 (**a**) Two-dimensional (2D) and (**b**) Three-dimensional (3D) views of the *zigzag* (6,0) BC2N nanotube

Table 1 Optimized bond lengths (Å), bond angles (°), diameters (Å), length of tube (Å), and molecular volume ($cm^3\ mol^{-1}$) of the *zigzag* (6,0) BC2N nanotube at different applied parallel and transverse electric field strengths

Bond length	*Zigzag* (6,0) BC2N nanotube									
	X					Y				
	0	35	70	100	140	0	35	70	100	140
B1-C1	1.554	1.551	1.548	1.545	1.542	1.554	1.553	1.552	1.551	1.551
B2-C1	1.555	1.551	1.548	1.545	1.542	1.555	1.556	1.558	1.560	1.563
B2-C2	1.555	1.552	1.548	1.546	1.543	1.555	1.552	1.548	1.545	1.540
B3-C2	1.555	1.552	1.548	1.546	1.543	1.555	1.558	1.561	1.564	1.566
B3-C3	1.555	1.551	1.548	1.545	1.542	1.555	1.553	1.552	1.551	1.550
B4-C3	1.554	1.551	1.548	1.545	1.542	1.554	1.556	1.558	1.561	1.566
C7-C1	1.365	1.369	1.374	1.378	1.383	1.365	1.366	1.367	1.367	1.367
C8-C2	1.365	1.368	1.373	1.377	1.383	1.365	1.365	1.365	1.367	1.370
C9-C3	1.365	1.369	1.374	1.378	1.383	1.365	1.364	1.363	1.362	1.359
C7-N1	1.428	1.425	1.423	1.421	1.418	1.428	1.429	1.431	1.433	1.438
C7-N2	1.429	1.426	1.423	1.421	1.418	1.429	1.426	1.424	1.421	1.417
C8-N2	1.429	1.426	1.423	1.421	1.418	1.429	1.432	1.435	1.437	1.438
C8-N3	1.429	1.426	1.423	1.421	1.418	1.429	1.425	1.422	1.419	1.413
C9-N3	1.429	1.426	1.423	1.421	1.418	1.429	1.431	1.433	1.435	1.436
C9-N4	1.428	1.425	1.423	1.421	1.418	1.428	1.428	1.427	1.428	1.431
N1-B7	1.443	1.451	1.459	1.467	1.477	1.443	1.443	1.443	1.443	1.439
N2-B8	1.442	1.450	1.459	1.466	1.477	1.442	1.443	1.444	1.445	1.447
N3-B9	1.442	1.450	1.459	1.466	1.477	1.442	1.442	1.442	1.443	1.445
N4-B10	1.443	1.451	1.459	1.467	1.477	1.443	1.442	1.441	1.439	1.433
B7-C13	1.538	1.533	1.529	1.525	1.521	1.538	1.537	1.538	1.538	1.541
B8-C13	1.538	1.534	1.529	1.525	1.521	1.538	1.540	1.542	1.543	1.546
B8-C14	1.538	1.534	1.530	1.526	1.521	1.538	1.536	1.533	1.530	1.524
B9-C14	1.538	1.534	1.530	1.526	1.521	1.538	1.540	1.542	1.543	1.541
B9-C15	1.538	1.534	1.529	1.525	1.521	1.538	1.536	1.535	1.534	1.533
B10-C15	1.538	1.533	1.529	1.525	1.521	1.538	1.538	1.540	1.541	1.546
C13-C19	1.360	1.364	1.368	1.372	1.378	1.360	1.361	1.362	1.362	1.362
C14-C20	1.360	1.364	1.368	1.372	1.378	1.360	1.360	1.360	1.361	1.365
C15-C21	1.360	1.364	1.368	1.372	1.378	1.360	1.359	1.358	1.357	1.354
C19-N7	1.435	1.432	1.428	1.426	1.423	1.435	1.437	1.439	1.442	1.447
C19-N8	1.435	1.432	1.429	1.426	1.423	1.435	1.433	1.430	1.428	1.426
C20-N8	1.435	1.432	1.429	1.426	1.423	1.435	1.439	1.442	1.445	1.448
C20-N9	1.435	1.432	1.429	1.426	1.423	1.435	1.431	1.427	1.423	1.414
C21-N9	1.435	1.432	1.429	1.426	1.423	1.435	1.437	1.440	1.441	1.438
C21-N10	1.435	1.432	1.428	1.426	1.423	1.435	1.433	1.432	1.432	1.441
N7-B13	1.445	1.452	1.461	1.468	1.479	1.445	1.445	1.445	1.444	1.440
N8-B14	1.445	1.452	1.461	1.468	1.479	1.445	1.445	1.446	1.447	1.448
N9-B15	1.445	1.452	1.461	1.468	1.479	1.445	1.445	1.445	1.445	1.454
N10-B16	1.445	1.452	1.461	1.468	1.479	1.445	1.444	1.443	1.442	1.429
B13-C25	1.538	1.533	1.529	1.525	1.521	1.538	1.538	1.539	1.541	1.547
B14-C25	1.538	1.533	1.529	1.525	1.521	1.538	1.540	1.542	1.544	1.549
B14-C26	1.538	1.534	1.529	1.526	1.521	1.538	1.536	1.533	1.530	1.527
B15-C26	1.538	1.534	1.529	1.526	1.521	1.538	1.540	1.541	1.542	1.533
B15-C27	1.538	1.533	1.529	1.525	1.521	1.538	1.536	1.534	1.532	1.527
B16-C27	1.538	1.533	1.529	1.525	1.521	1.538	1.538	1.538	1.540	1.561
C25-C31	1.362	1.365	1.369	1.372	1.377	1.362	1.362	1.363	1.363	1.363

Table 1 (continued)

Bond length	*Zigzag* (6,0) BC2N nanotube									
	X					Y				
	0	35	70	100	140	0	35	70	100	140
C26-C32	1.362	1.365	1.369	1.372	1.377	1.362	1.362	1.362	1.363	1.370
C27-C33	1.362	1.365	1.369	1.372	1.377	1.362	1.361	1.361	1.360	1.359
C31-N13	1.419	1.415	1.412	1.410	1.408	1.419	1.422	1.426	1.431	1.439
C31-N14	1.419	1.415	1.412	1.410	1.408	1.419	1.417	1.415	1.413	1.411
C32-N14	1.419	1.415	1.412	1.410	1.408	1.419	1.424	1.428	1.431	1.435
C32-N15	1.419	1.415	1.412	1.410	1.408	1.419	1.414	1.409	1.404	1.383
C33-N15	1.419	1.415	1.412	1.410	1.408	1.419	1.421	1.423	1.425	1.401
C33-N16	1.419	1.415	1.412	1.410	1.408	1.419	1.416	1.413	1.411	1.456
Average B-C	1.544	1.539	1.535	1.532	1.528	1.544	1.544	1.544	1.544	1.545
Average C-C	1.362	1.366	1.370	1.374	1.379	1.362	1.362	1.362	1.362	1.363
Average C-N	1.428	1.424	1.421	1.419	1.416	1.428	1.428	1.428	1.428	1.428
Average N-B	1.444	1.451	1.460	1.467	1.478	1.444	1.444	1.444	1.444	1.442
Bond angles										
N2-C8-N3	112.89	112.96	113.03	113.07	113.12	112.89	112.90	112.93	112.99	113.14
B8-C14-B9	110.69	110.62	110.55	110.48	110.39	110.69	110.72	110.82	110.98	111.44
C13-B8-C14	116.78	117.05	117.28	117.44	117.64	116.78	116.90	117.05	117.21	117.42
C19-N8-C20	112.84	112.84	112.83	112.80	112.76	112.84	112.84	112.90	113.02	113.14
B8-C14-C20	116.19	116.07	115.97	115.91	115.85	116.19	116.23	116.29	116.36	116.60
C15-C21-N9	122.30	122.27	122.24	122.22	122.20	122.30	122.28	122.30	122.32	122.80
B2-C2-B3	120.99	120.36	119.87	119.51	119.13	120.99	121.03	121.16	121.35	121.72
N14-C32-N15	114.36	114.47	114.58	114.65	114.74	114.36	114.36	114.36	114.38	114.38
Diameters										
(B-tip)	5.42	5.40	5.37	5.35	5.33	5.42	5.42	5.43	5.47	5.56
(N-tip)	4.77	4.76	4.75	4.75	4.74	4.77	4.77	4.80	4.83	4.86
Length of tube (*l*)	11.31	11.32	11.33	11.35	11.37	11.31	11.31	11.31	11.32	11.33
Molecular volume (*V*)	481.81	513.35	500.38	528.09	466.08	481.81	526.47	495.87	495.97	517.84

strength (E_Y=0) to 1.456 Å at the field strength of 140×10^{-4} a.u. (E_Y=140).

The variations in bond angles for applied parallel and transverse electric field strengths in Table 2 indicate that the maximum deviation of optimized bond angles with respect to the zero electric field (E_X=E_Y=0) at various parallel and transverse electric field strengths is less than 2°. The most significant change in the bond angles is observed for the B2-C2-B3 angle that decreases gradually from 120.99° at the zero field strength (E_X and E_Y=0) to 119.13 (E_X=140) and 121.72° (E_Y=140). The results in Tables 1 and 2 show that the values of bond lengths and bond angles for the applied parallel and transverse electric field strengths in the *zigzag* (6,0) BC2N nanotube model change only slightly. Therefore, the nanotube is resistant against the applied parallel and transverse electric field strengths.

Length of the BC2N nanotube is an important parameter characterizing its structural response to the applied parallel and transverse electric field in the nano-electronic circuit. The distance between the B2 and N14 atoms of the BC2N nanotube model considered as the length (*l*) of the tube (see Fig. 1a). The calculated lengths and tip diameters of the nanotube at various parallel and transverse electric field strengths with respect to the corresponding values at zero field (E_X=E_Y=0) with significant changes in the parameters are presented in Tables 1 and 2. The results indicate that length of the nanotube does not change significantly with an increase in the electric field strengths (<1 %). The length resistance of the nanotube against external electric field can be considered as an advantage of the nanotube in molecular scale device. The most significant changes for the B-tip and N-tip diameters of the nanotube are observed for the applied transverse electric field that increases gradually from 5.42 and 4.77 Å at the zero field strength (E_Y=0) to 5.56 and 5.24 Å at the field strength of 140×10^{-4} a.u (E_Y=140). Also, the results indicate that

Table 2 Differential values of optimized bond lengths (Å), bond angles (°), diameters (Å), length of tube (Å), and molecular volume ($cm^3\ mol^{-1}$) of the *zigzag* (6,0) BC2N nanotube at different applied parallel and transverse electric field strengths

ΔBond length	*Zigzag* (6,0) BC2N nanotube									
	X					Y				
	0	35	70	100	140	0	35	70	100	140
B1-C1	0.000	−0.003	−0.006	−0.009	−0.012	0.000	−0.001	−0.002	−0.003	−0.003
B2-C1	0.000	−0.004	−0.007	−0.010	−0.013	0.000	0.001	0.003	0.005	0.008
B2-C2	0.000	−0.003	−0.007	−0.009	−0.012	0.000	−0.003	−0.007	−0.010	−0.015
B3-C2	0.000	−0.003	−0.007	−0.009	−0.012	0.000	0.003	0.006	0.009	0.011
B3-C3	0.000	−0.004	−0.007	−0.010	−0.013	0.000	−0.002	−0.003	−0.004	−0.005
B4-C3	0.000	−0.003	−0.006	−0.009	−0.012	0.000	0.002	0.004	0.007	0.012
C7-C1	0.000	0.004	0.009	0.013	0.018	0.000	0.001	0.002	0.002	0.002
C8-C2	0.000	0.003	0.008	0.012	0.018	0.000	0.000	0.000	0.002	0.005
C9-C3	0.000	0.004	0.009	0.013	0.018	0.000	−0.001	−0.002	−0.003	−0.006
C7-N1	0.000	−0.003	−0.005	−0.007	−0.010	0.000	0.001	0.003	0.005	0.010
C7-N2	0.000	−0.003	−0.006	−0.008	−0.011	0.000	−0.003	−0.005	−0.008	−0.012
C8-N2	0.000	−0.003	−0.006	−0.008	−0.011	0.000	0.003	0.006	0.008	0.009
C8-N3	0.000	−0.003	−0.006	−0.008	−0.011	0.000	−0.004	−0.007	−0.010	−0.016
C9-N3	0.000	−0.003	−0.006	−0.008	−0.011	0.000	0.002	0.004	0.006	0.007
C9-N4	0.000	−0.003	−0.005	−0.007	−0.010	0.000	0.000	−0.001	0.000	0.003
N1-B7	0.000	0.008	0.016	0.024	0.034	0.000	0.000	0.000	0.000	−0.004
N2-B8	0.000	0.008	0.017	0.024	0.035	0.000	0.001	0.002	0.003	0.005
N3-B9	0.000	0.008	0.017	0.024	0.035	0.000	0.000	0.000	0.001	0.003
N4-B10	0.000	0.008	0.016	0.024	0.034	0.000	−0.001	−0.002	−0.004	−0.010
B7-C13	0.000	−0.005	−0.009	−0.013	−0.017	0.000	−0.001	0.000	0.000	0.003
B8-C13	0.000	−0.004	−0.009	−0.013	−0.017	0.000	0.002	0.004	0.005	0.008
B8-C14	0.000	−0.004	−0.008	−0.012	−0.017	0.000	−0.002	−0.005	−0.008	−0.014
B9-C14	0.000	−0.004	−0.008	−0.012	−0.017	0.000	0.002	0.004	0.005	0.003
B9-C15	0.000	−0.004	−0.009	−0.013	−0.017	0.000	−0.002	−0.003	−0.004	−0.005
B10-C15	0.000	−0.005	−0.009	−0.013	−0.017	0.000	0.000	0.002	0.003	0.008
C13-C19	0.000	0.004	0.008	0.012	0.018	0.000	0.001	0.002	0.002	0.002
C14-C20	0.000	0.004	0.008	0.012	0.018	0.000	0.000	0.000	0.001	0.005
C15-C21	0.000	0.004	0.008	0.012	0.018	0.000	−0.001	−0.002	−0.003	−0.006
C19-N7	0.000	−0.003	−0.007	−0.009	−0.012	0.000	0.002	0.004	0.007	0.012
C19-N8	0.000	−0.003	−0.006	−0.009	−0.012	0.000	−0.002	−0.005	−0.007	−0.009
C20-N8	0.000	−0.003	−0.006	−0.009	−0.012	0.000	0.004	0.007	0.010	0.013
C20-N9	0.000	−0.003	−0.006	−0.009	−0.012	0.000	−0.004	−0.008	−0.012	−0.021
C21-N9	0.000	−0.003	−0.006	−0.009	−0.012	0.000	0.002	0.005	0.006	0.003
C21-N10	0.000	−0.003	−0.007	−0.009	−0.012	0.000	−0.002	−0.003	−0.003	0.006
N7-B13	0.000	0.007	0.016	0.023	0.034	0.000	0.000	0.000	−0.001	−0.005
N8-B14	0.000	0.007	0.016	0.023	0.034	0.000	0.000	0.001	0.002	0.003
N9-B15	0.000	0.007	0.016	0.023	0.034	0.000	0.000	0.000	0.000	0.009
N10-B16	0.000	0.007	0.016	0.023	0.034	0.000	−0.001	−0.002	−0.003	−0.016
B13-C25	0.000	−0.005	−0.009	−0.013	−0.017	0.000	0.000	0.001	0.003	0.009
B14-C25	0.000	−0.005	−0.009	−0.013	−0.017	0.000	0.002	0.004	0.006	0.011
B14-C26	0.000	−0.004	−0.009	−0.012	−0.017	0.000	−0.002	−0.005	−0.008	−0.011
B15-C26	0.000	−0.004	−0.009	−0.012	−0.017	0.000	0.002	0.003	0.004	−0.005
B15-C27	0.000	−0.005	−0.009	−0.013	−0.017	0.000	−0.002	−0.004	−0.006	−0.011
B16-C27	0.000	−0.005	−0.009	−0.013	−0.017	0.000	0.000	0.000	0.002	0.023
C25-C31	0.000	0.003	0.007	0.010	0.015	0.000	0.000	0.001	0.001	0.001

Table 2 (continued)

ΔBond length	*Zigzag* (6,0) BC2N nanotube									
	X					Y				
	0	35	70	100	140	0	35	70	100	140
C26-C32	0.000	0.003	0.007	0.010	0.015	0.000	0.000	0.000	0.001	0.008
C27-C33	0.000	0.003	0.007	0.010	0.015	0.000	−0.001	−0.001	−0.002	−0.003
C31-N13	0.000	−0.004	−0.007	−0.009	−0.011	0.000	0.003	0.007	0.012	0.020
C31-N14	0.000	−0.004	−0.007	−0.009	−0.011	0.000	−0.002	−0.004	−0.006	−0.008
C32-N14	0.000	−0.004	−0.007	−0.009	−0.011	0.000	0.005	0.009	0.012	0.016
C32-N15	0.000	−0.004	−0.007	−0.009	−0.011	0.000	−0.005	−0.010	−0.015	−0.036
C33-N15	0.000	−0.004	−0.007	−0.009	−0.011	0.000	0.002	0.004	0.006	−0.018
C33-N16	0.000	−0.004	−0.007	−0.009	−0.011	0.000	−0.003	−0.006	−0.008	0.037
Average B-C	0.000	−0.005	−0.009	−0.012	−0.016	0.000	0.000	0.000	0.000	0.001
Average C-C	0.000	0.004	0.008	0.012	0.017	0.000	0.000	0.000	0.000	0.001
Average C-N	0.000	−0.004	−0.007	−0.009	−0.012	0.000	0.000	0.000	0.000	0.000
Average N-B	0.000	0.007	0.016	0.023	0.034	0.000	0.000	0.000	0.000	−0.002
ΔBond angles										
N2-C8-N3	0.00	0.07	0.14	0.18	0.23	0.00	0.01	0.04	0.10	0.25
B8-C14-B9	0.00	−0.07	−0.14	−0.21	−0.30	0.00	0.03	0.13	0.29	0.75
C13-B8-C14	0.00	0.27	0.50	0.66	0.86	0.00	0.12	0.27	0.43	0.64
C19-N8-C20	0.00	0.00	−0.01	−0.04	−0.08	0.00	0.00	0.06	0.18	0.30
B8-C14-C20	0.00	−0.12	−0.22	−0.28	−0.34	0.00	0.04	0.10	0.17	0.41
C15-C21-N9	0.00	−0.03	−0.06	−0.08	−0.10	0.00	−0.02	0.00	0.02	0.50
B2-C2-B3	0.00	−0.63	−1.12	−1.48	−1.86	0.00	0.04	0.17	0.36	0.73
N14-C32-N15	0.00	0.11	0.22	0.29	0.38	0.00	0.00	0.00	0.02	0.02
ΔDiameters										
(B-tip)	0.00	−0.02	−0.05	−0.07	−0.09	0.00	0.00	0.01	0.05	0.14
(N-tip)	0.00	−0.01	−0.02	−0.02	−0.03	0.00	0.00	0.03	0.06	0.09
Length of tube (Δ*l*)	0.00	0.01	0.02	0.04	0.06	0.00	0.00	0.00	0.01	0.02
Molecular volume (Δ*V*)	0.00	31.54	18.57	46.28	−15.73	0.00	44.66	14.06	14.16	36.03

resistance of the N-tip of the nanotube against the applied external electric field is more than the resistance of the B-tip of the nanotube against the external electric field (see Table 2).

Molecular volume (cm^3 mol^{-1}) is one of the important parameters that reflects the molecular geometric response to the applied parallel and transverse electric field strengths. This parameter is defined as the volume inside a contour of 0.001 electron/$bohr^3$ density. The calculated molecular volume of the *zigzag* (6,0) BC2N nanotube at various parallel and transverse electric field strengths with respect to the corresponding values at zero fields (E_X=E_Y=0) with significant changes in the parameter are presented in Tables 1 and 2. The results presented in the tables indicate that variations of the molecular volume for the applied parallel and transverse electric field strengths do not have any well-defined trend from zero to 140×10^{-4} a.u..

Field effect on electronic properties of the (6,0) zigzag BC2N nanotube densities of states (DOS)

We studied the influence of external electric field on the electronic properties of the nanotube. The total densities of states (DOS) of the nanotube at various applied parallel and transverse electric field strengths are shown in Figs. 2 and 3. As is shown in Figs. 2 and 3, the energy gap obtained from these calculations at different applied transverse electric field strengths with respect to the corresponding values at zero fields (E_Y=0) are decreased. The energy gap value for the applied parallel electric field is gradually increased from 2.00 eV at the zero field strength (E_X=0) to 2.25 eV at the field strength of 70×10^{-4} a.u. (E_X=70) and then by increasing the applied parallel electric field, the parameter is gradually decreased to 1.67 eV at the field strength of 140×10^{-4} a.u. (E_X=140). The energy gap value for the applied

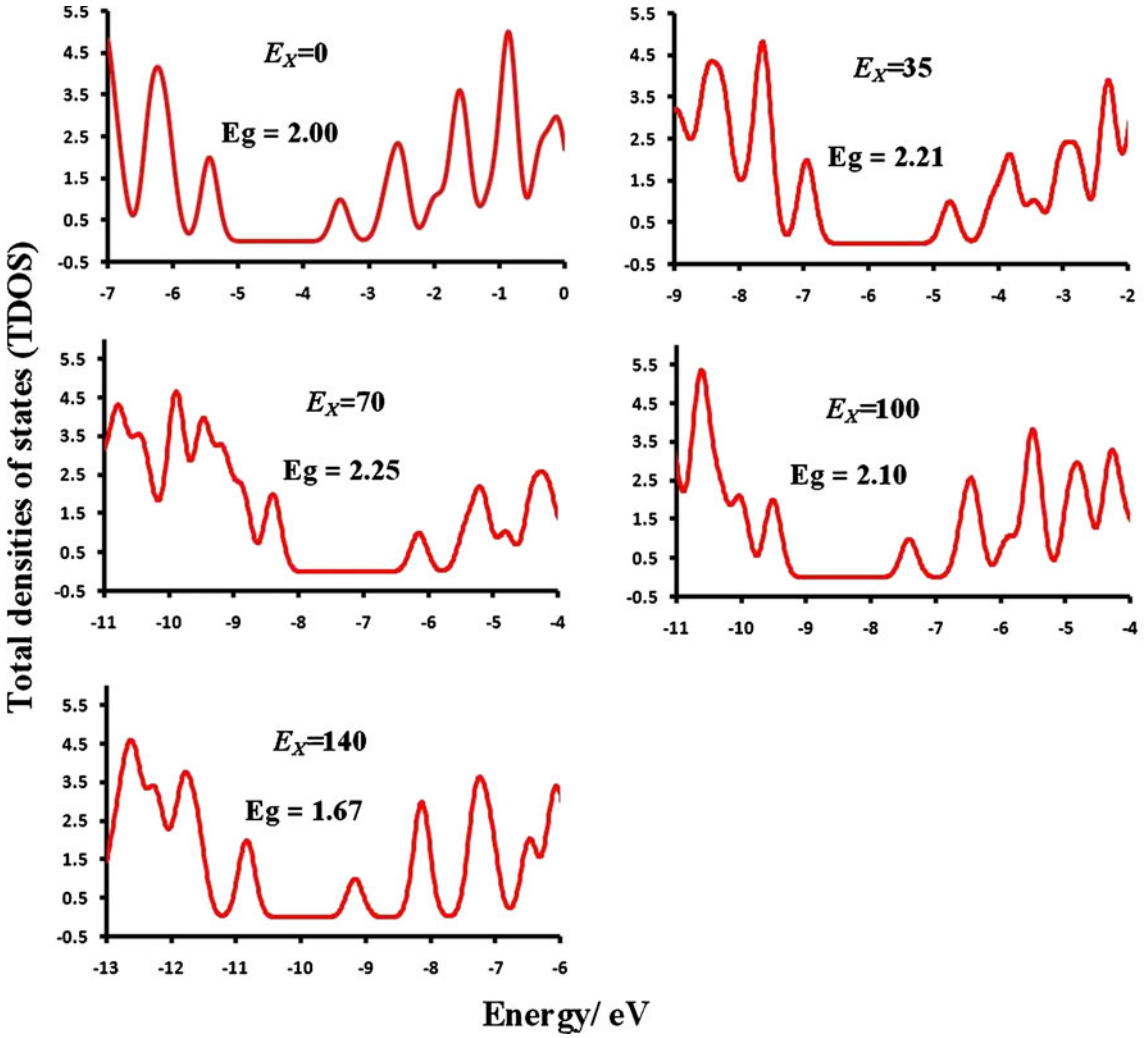

Fig. 2 Total densities of states (DOS) for the *zigzag* (6,0) BC2N nanotube at different applied parallel electric field strengths

transverse electric field is also gradually decreased from 2.00 eV at the zero field strength (E_Y=0) to 1.55 eV at the field strength of 140×10^{-4} a.u. (E_Y=140). The total densities of states (TDOS) of these tubes show the significant changes due to external electric field in the gaps regions of the TDOS plots. In comparison with the zero field strength, the energy gap of the nanotube in high external electric field is decreased while their electrical conductance is increased. Also, the total energy (E_T) value of the nanotube is increased with any increase in the applied external electric field strengths, especially for the applied parallel electric field. This results show that the applied parallel electric field has more influence on the stability of the nanotube than the applied transverse electric field (see Table 3).

Electronic spatial extent (ESE)

The electronic spatial extent (*ESE*) for every nanotube is defined as the surface area covering a volume around the nanotube and describes the gross receptivity of the nanotube from an external electric field. The *ESE* of the *zigzag* (6,0) BC2N nanotube at various parallel and transverse electric fields with significant changes in the parameter are summarized in Table 3. The results indicate that the *ESE* of the nanotube does not change significantly by increasing electric field strengths from $0-140\times10^{-4}$ a.u. (<0.2 %). This slight change of *ESE* against external electric field can be regarded as a positive index for the nanotube as a nano-device in nano-circuits.

Molecular orbital (MO)

To better understand the electric response and electrical transport in the *zigzag* (6,0) BC2N nanotube, we studied the electronic energies of the nanotube at different applied parallel and transverse electric field strengths. The reason is that the electric response and electrical transport

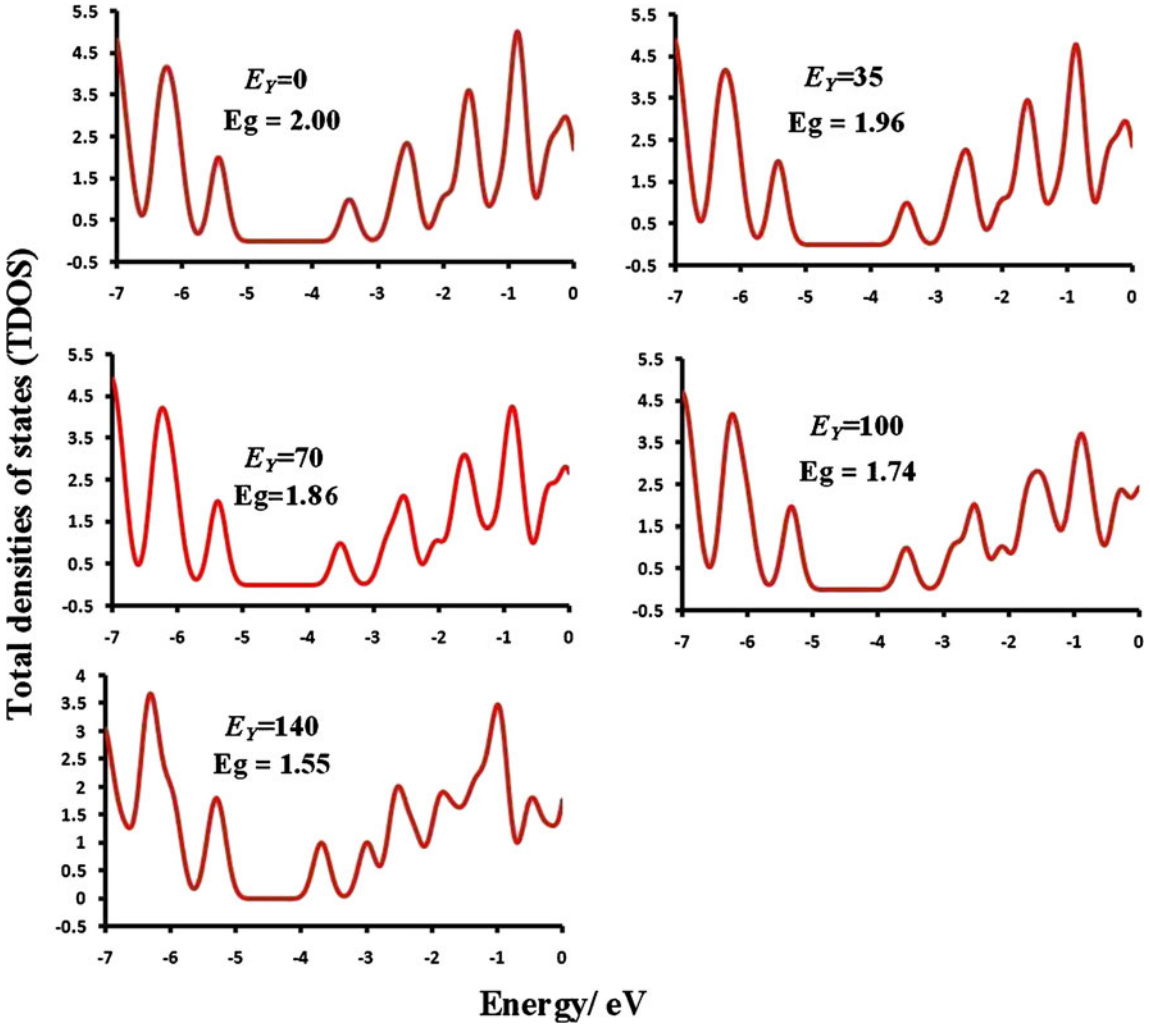

Fig. 3 Total densities of states (DOS) for the *zigzag* (6,0) BC2N nanotube at different applied transverse electric field strengths

depend on all the molecular orbital energy spacing's between the occupied and virtual molecular orbitals. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energies for the nanotube as functions of the different applied parallel, E_X, and perpendicular, E_Y, electric field strengths are plotted in Fig. 4. As shown in Fig. 4, for the parallel case, both the HOMO and LUMO are more stabilized in comparison with the zero field strength. The HOMO and LUMO values in the applied parallel electric field is strongly increased from −5.44 and −3.44 eV at the zero field strength (E_X=0) to −10.83 and −9.16 eV at the field strength of 140×10^{-4} a.u. (E_X=140). For the applied transverse electric field, by increasing the external electric field, the HOMO values become more unstable, whereas the LUMO values are slightly more stabilized. This results show that the applied parallel electric field has more influence on the molecular orbital of the nanotube than the applied transverse electric field.

Dipole moment (μ)

When a nanotube is placed in an external electric field, its atomic charge distribution are easily changed and the centers of the positive and negative charges of the nanotube change due to charge redistribution, consequently leads to the polarization of the nanotube and gives it an induced electric dipole moment. As is evident from Table 3, the values of the induced electric dipole moment (μ_{Tot}) vector obtained from these calculations increases linearly with an upward trend in the applied external electric field strengths. Therefore, the electric dipole moment of a nanotube is an important property that characterizes its electronic and geometrical structure. The size and components of the electric dipoles moment (in Debye) for the nanotube at various applied parallel and transverse electric field strengths are shown in Fig. 5. μ_{Tol} and $|\mu_X|$ for the applied parallel electric field are gradually increased from 27.48 and −27.48 Debye at the zero field strength (E_X=0) to 75.01

Table 3 Optimized properties of the *zigzag* (6,0) BC2N nanotube at different applied parallel and transverse electric field strengths

Property	*Zigzag* (6,0) BC2N nanotube										
	X					Y					
	0	35	70	100	140	35	70	100	140		
E_T *BC2NNT/keV*	−76.5264	−76.5276	−76.5293	−76.5311	−76.5340	−76.5264	−76.5267	−76.5271	−76.5281		
ΔE_T *BC2NNT/eV*	0.00	−1.20	−2.90	−4.70	−7.60	0.00	−0.30	−0.70	−1.70		
Eg/eV	2.00	2.21	2.25	2.10	1.67	1.96	1.86	1.74	1.55		
Δ *Eg/eV*	0.00	0.21	0.25	0.10	−0.33	−0.04	−0.14	−0.26	−0.45		
ESE/bohr^2=a_0^2	114274.0	114420.2	114582.8	114733.2	114950.2	114275.3	114280.55	114286.8	114024.0		
ΔESE/bohr^2=a_0^2	0.0	146.2	308.8	459.2	676.2	1.3	6.55	12.8	−250.0		
μ_{Tot}/*Debye*	27.48	39.56	51.48	61.60	75.01	27.89	29.09	30.71	32.60		
$\Delta\mu_{Tot}$/*Debye*	0.00	12.80	24.00	34.12	47.53	0.41	1.61	3.23	5.12		

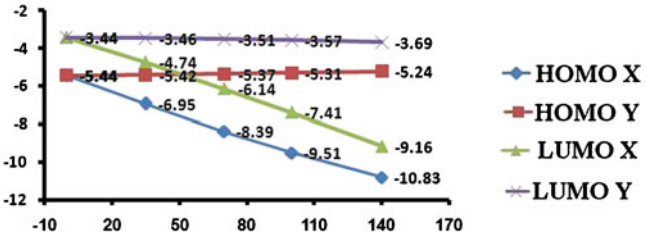

Fig. 4 HOMO and LUMO for the *zigzag* (6,0) BC2N nanotube at different applied parallel and transverse electric field strengths

and −75.01 Debye at the field strength of 140×10^{-4} a.u. (E_X=140). μ_{Tol} and $|\mu_Y|$for the applied transverse electric field are also gradually increased from 27.48 and 0.00 Debye at zero field strength (E_Y=0) to 32.60 and −19.94 Debye at the field strength of 140×10^{-4} a.u. (E_Y=140). These results show that when the nanotube is exposed to external electric field, it has a much stronger interaction with the electrodes of the nano-electronic circuit, especially for the applied parallel electric fields. Also, analysis of the dipole moments shows that the applied parallel electric field strength has a much stronger interaction with the nanotube with respect to the transverse electric field strengths and the nanotube is easier to modulate by the applied parallel electric field.

Charge density distribution

As is discussed in the previous section, because of applied external electric field strengths, the electronic charge distribution on atoms of the nanotube is changed. Consequently, all charge-related molecular properties became different. Therefore, the study of the electric field-dependent charge distribution that directly determined molecular behavior is important. In order to study the atomic charge distribution as a function of parallel and transverse electric field strengths (E_X and E_Y), the natural bond orbital charges (NBO) on the C, B, and N atoms have been calculated and plotted in Fig. 6. As shown in Fig. 6, the atomic charge variations obtained from these calculations increases with any upward trend in the applied external electric field strengths. Moreover, the separation of the center of the positive and the negative electric charges of the *zigzag* (6,0) BC2N nanotube increases with an increase in the applied external electric field strengths.

Conclusions

We studied the structure and electronic properties including bond lengths, bond angles, length of tube, tip diameters, molecular volume, dipole moments, energy gaps, energies, atomic charges, molecular orbital energies,

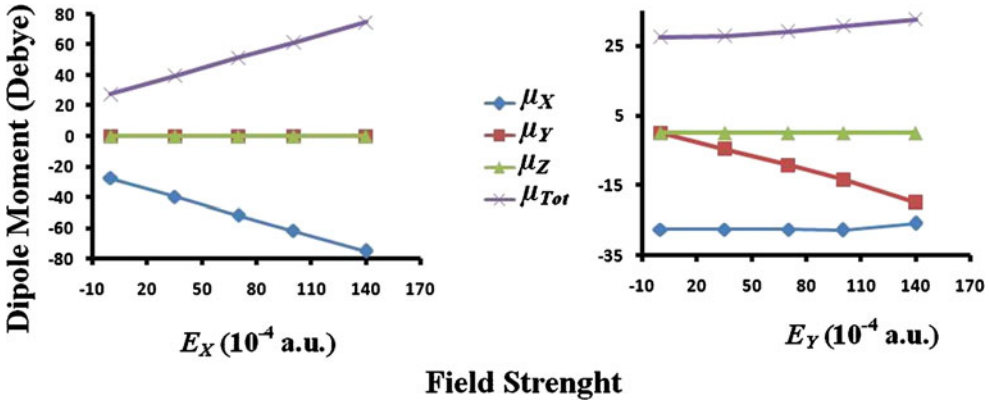

Fig. 5 Size of the electric dipole moment vector and its components (in Debye) for the *zigzag* (6,0) BC2N nanotube at different applied parallel and transverse electric field strengths

electronic spatial extent, and density of states for the *zigzag* (6,0) BC2N nanotube. This study was done at different applied parallel and transverse electric field strengths by means of density functional theory (DFT) calculations. We compared all the parameters in the applied external electric field strengths. Analysis of the structural parameters indicates that the nanotube is resistant against the applied parallel and transverse electric field strengths. Also, the length, tip diameters, electronic spatial extent, and molecular volume of the (6,0) *zigzag* BC2N nanotube do not significantly change with increasing electric field strength and indicated that the nanotube

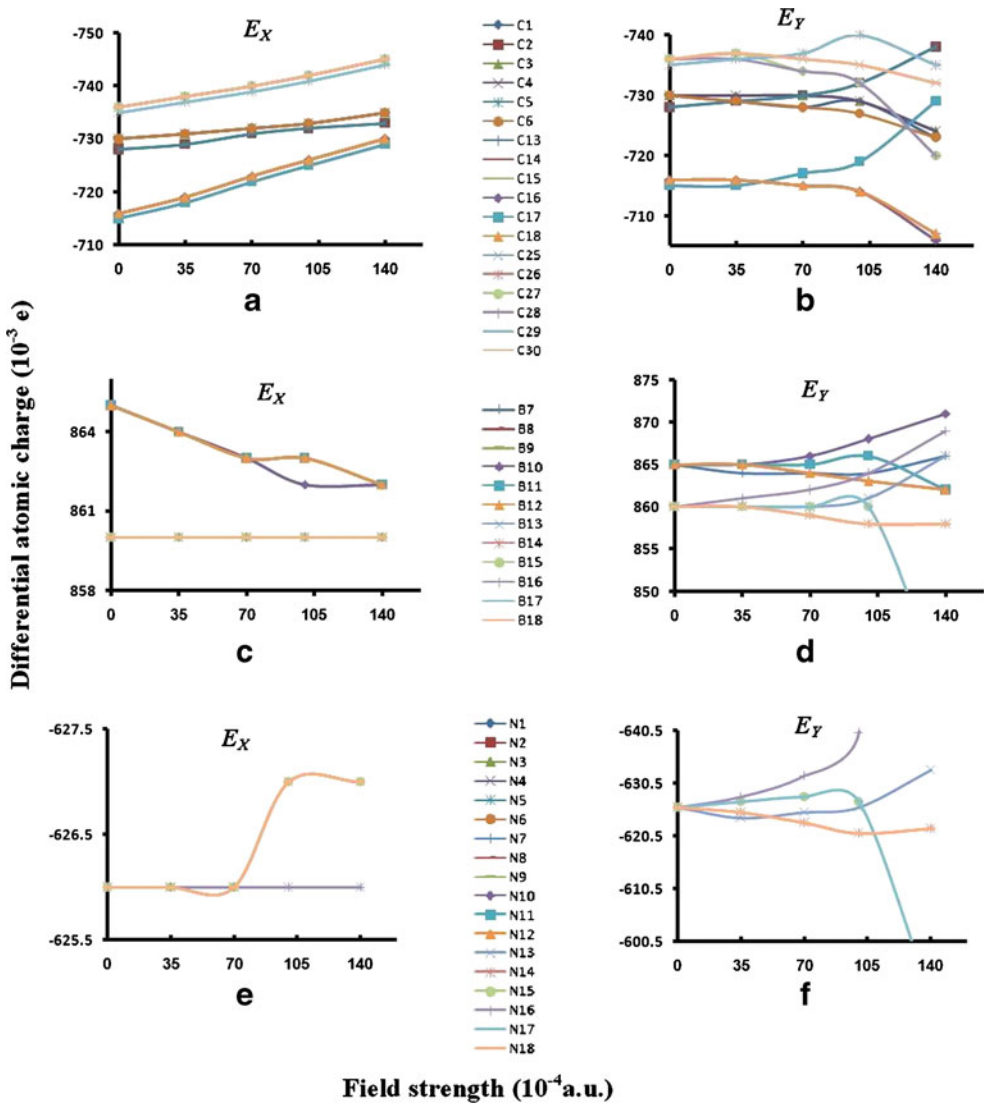

Fig. 6 Natural bond orbital charges (NBO) at different applied parallel and transverse electric field strengths on the C atoms (**a**, **b**), B atoms (**c**, **d**), and N atoms (**e**, **f**)

is a stable molecule over the entire range of the applied electrical field strength. Analysis of the densities of states, molecular orbital, dipole moment, and total energy of the (6,0) *zigzag* BC2N nanotube under external electrical field indicates that the applied parallel electric field strength has a much stronger interaction with the nanotube with respect to the transverse electric field strengths and the nanotube is easier to modulate by the applied parallel electric field. According to the structural resistance and electronic properties of the nanotube under influence of external electric field strengths, it can be said that electric field study of the nanotube is very important in relation to proposing or designing BC2N nanotubes as a molecular scale device for a nanoelectronic circuit and properties of the nanotube can be controlled by the proper external electric field.

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