Baghdad Science Journal

Volume 23 | Issue 3 Article 17

3-23-2026

Influence of Beryllium Substitution on Vibrational and Electronic Properties of Carbon Nano-Cone: Density Functional Theory

Rajaa K. Mohammad
Department of Physics, College of Science, University of Kerbala, Karbala, Iraq, rajaa.k@uokerbala.edu.iq

Hussein M. L.
Department of Physics, College of Science, University of Kerbala, Karbala, Iraq,
hussein.mohammed@uokerbala.edu.iq

Ammar S. Hameed
Department of Physics, College of Science, University of Kerbala, Karbala, Iraq,
ammar.s@uokerbala.edu.iq

Luma M. Ahmed
Department of Chemistry, College of Science, University of Kerbala, Karbala, Iraq,
luma.ahmed@uokerbala.edu.iq

Shurooq Sabah Abed AL-Abbas
Department of Physics, College of Education for Pure Sciences, University of Babylon, Babylon, Iraq,
pure.shurooq.sabah@uobabylon.edu.iq

How to Cite this Article

Mohammad, Rajaa K.; L., Hussein M.; Hameed, Ammar S.; Ahmed, Luma M.; and AL-Abbas, Shurooq Sabah Abed (2026) "Influence of Beryllium Substitution on Vibrational and Electronic Properties of Carbon Nano-Cone: Density Functional Theory," *Baghdad Science Journal*: Vol. 23: Iss. 3, Article 17.
DOI: https://doi.org/10.21123/2411-7986.5245

BAGHDAD SCIENCE JOURNAL 2026;23(3):943–952

Scan the QR to view the full-text article on the journal website

RESEARCH ARTICLE

Influence of Beryllium Substitution on Vibrational and Electronic Properties of Carbon Nano-Cone: Density Functional Theory

Rajaa K. Mohammad [1], **Hussein M. L.** [1,*], **Ammar S. Hameed** [1], **Luma M. Ahmed** [2], **Shurooq Sabah Abed AL-Abbas** [3]

[1] Department of Physics, College of Science, University of Kerbala, Karbala, Iraq
[2] Department of Chemistry, College of Science, University of Kerbala, Karbala, Iraq
[3] Department of Physics, College of Education for Pure Sciences, University of Babylon, Babylon, Iraq

ABSTRACT

Density Functional Theory (DFT) was employed to investigate the effects of beryllium (Be) substitution on the vibrational and electronic properties of a single-wall carbon nano-cone. The study aims to clarify how Be incorporation modifies the structural stability and electronic characteristics of this nanostructure. Electronic parameters including ionization potential (I), electron affinity (Eea), Fermi energy (Ef), HOMO–LUMO energies, total energy (E), and band gap (Eg) were calculated. Infrared (IR) spectra, optimized geometries, electrostatic potential maps, and electron density distributions were also analyzed. The results indicate that Be substitution reduces the ionization potential while increasing the electron affinity. Incorporation of Be atoms raises the HOMO level, Fermi energy, electron affinity, and total energy, whereas it lowers the LUMO energy and narrows the band gap. Vibrational analysis shows weakened vibrational stability upon substitution. Furthermore, electrostatic potential and charge density distributions are strongly influenced by the type, number, and position of substituted atoms, as well as by local charge redistribution. Positional dependence of Be substitution leads to noticeable variations in both electronic and vibrational responses. These findings demonstrate that controlled Be substitution can effectively tune the electronic structure of carbon nano-cones, enhancing their suitability for potential applications in nanoelectronics, catalysis, sensing, and energy storage systems.

Keywords: Beryllium substitution, DFT calculation, Electronic properties, IR spectra, Nano-cone molecule

Introduction

Understanding how beryllium substitution affects the properties of carbon nano-cones can provide insights into novel materials with tailored properties. This can potentially lead to developing of advanced materials for various applications such as electronics, sensors, and catalysis.

Comparing the results of this study with existing research on similar substitutions or modifications of nano-cones allows for a broader understanding of the effects of different dopants or substitutions on, nanostructure properties. It helps researchers identify trends, similarities, and differences across various systems, which can guide future investigations and potential applications, research has demonstrated that carbon nanotubes (CNTs) offer better mechanical and electrical capabilities than any other available materials. Due to their unique electrical, mechanical, and other capabilities, CNTs have the potential to be used in atomic-force microscopy as nano-fillers for composite materials, nano-actuators, nanomotors, nano-bearings, nano-springs, field emitters and in nano-scale electronic devices.[1–3] Thus, research in

Received 27 October 2023; revised 6 January 2025; accepted 8 January 2025.
Available online 23 March 2026

* Corresponding author.
E-mail addresses: rajaa.k@uokerbala.edu.iq (R. K. Mohammad), hussein.mohammed@uokerbala.edu.iq (H. M.L.), ammar.s@uokerbala.edu.iq (A. S. Hameed), luma.ahmed@uokerbala.edu.iq (L. M. Ahmed), pure.shurooq.sabah@uobabylon.edu.iq (S. S. A. AL-Abbas).

https://doi.org/10.21123/2411-7986.5245

computational nano-mechanics and computational condensed-matter physics, particularly on the vibrational behavior of CNTs, has made CNTs the center of these fields.[4] Two approaches are often utilized due to the tremendous difficulty associated with conducting controlled tests at the nanoscale scale.

When researching CNTs simulations of molecular dynamics are difficult to carry out and time-consuming when applied to large-scale systems. The second approach is called continuum mechanics and it involves modelling CNTs shells and beams.[5,6] In the field of nanotechnology, non-local theories have been used to examine the vibration and wave propagation of CNTs with the use of beam models.[7,8] The nonlinear vibration analysis of a single-walled carbon nanotube also interacts well with the medium that surrounds the nanotubes.[9] Buckling of CNTs was investigated by (Ru, He, and coworkers) using an elastic shell model.[10,11] They developed a continuous shell model to investigate various CNT instability patterns that occurred under various compressive stresses.[12,13] They utilized an elastic shell model integrated by the Van-der-Waals effect to investigate the buckling behavior of CNTs. In Muc Study Shell Structures,[14] the authors explained how the thin shell theory may be utilized to anticipate how CNTs behave. Changing the electronic band gap may be accomplished by various techniques, including filling, chemical doping, and the use of electric fields as an external stimulus.[15] The thermal characteristics of structural equivalents of carbon nanotubes BNNTs may be effectively altered and managed using adsorption. The electronic characteristics of the various diameters for zigzag ZSWBNNTs of varying diameters are modified when Fe atoms are incorporated into the material. According to (Alencar, Azevedo, and M. Machado), the Fe atoms that are contained within these tubes are more adversely affected than the tubes that are located on the outside. In addition, the electrical band gap decreases more when the Fe atom is located within the tube than outside the tube, The reason for choosing the iron atom is the iron-first-nitrogen-neighbor bond length works as a constraint in determining the most favorable position for the adsorbate, Also, the levels of the 3d and 4s orbitals of the iron atom present localized levels at the band gap of the nanotubes.[16] The incorporation of F, Cl, or Br into the molecule, determining the molecular structure of CNTs by using the Density Functional Theory DFT method is a highly fruitful endeavor. By using a DFT approach, which is computed in the quantum program, estimates are provided for the electrical construct, bandgap, IR spectrum, Raman spectrum, total energy, and depolarization spectrum.[17]

In this manuscript, molecular dynamics simulation together with density functional theory was used to investigate the Be substitution effect on the vibrational and electronic properties of the single wall carbon Nano-cone. The DFT method with this level has been chosen because of the accuracy associated. Where the DFT method focuses on the electron density function instead of wave function was used to study the interaction. Predicts a wide range of molecular properties are including molecular structure, atomization energies, vibrational frequencies, electrical and magnetic properties, and ionization energies, among others. They are applied to considerably bigger systems, with hundreds or even thousands of atoms.

Material and methods

Computational approach

The program Gaussian 09 was utilized to carry out the DFT procedures. B3LYP[18] is a hybrid function that combines the exchange and correlation function developed by Lee, Yang, and Parr,[18,19] where the Development of the Colic-Salvetti correlation-energy formula into a function of the electron density.[20] Geometrical optimization of (A) NANO-CON, (B) NANO-CON + Be(1), (C) NANO-CON + Be(2), and (D) NANO-CON + Be(3) simulations in the gas phase by using the B3LYP/3-21G level of theory was used to study the process involved in the substitution of atoms of Before atoms of (C) in different locations. The process of computing electronic characteristics including energy gaps (Eg), ionization potentials (Is), and electronic states by using the hybrid functional B3LYP basis set is highly successful. Computations of the exchange-correlation energy and the interaction effects between electrons produce the most precise results. Fig. 1 illustrates the geometrical optimization of (A) NANO-CON, (B) NANO-CON + Be(1), (C) NANO-CON + Be(2), and (D) NANO-CON + Be(3) in the gas-phase by utilizing DFT techniques at the B3LYP/3-21G level. EHOMO refers to the energy of the highest molecular orbital that is occupied, whilst ELUMO stands for the energy of the lowest molecular orbital used to calculate Eg as shown in the equations below.[21–23]

$$I = EHOMO \tag{1}$$

$$E = ELUMO \tag{2}$$

$$Eg = (ELUMO - EHOMO) \tag{3}$$

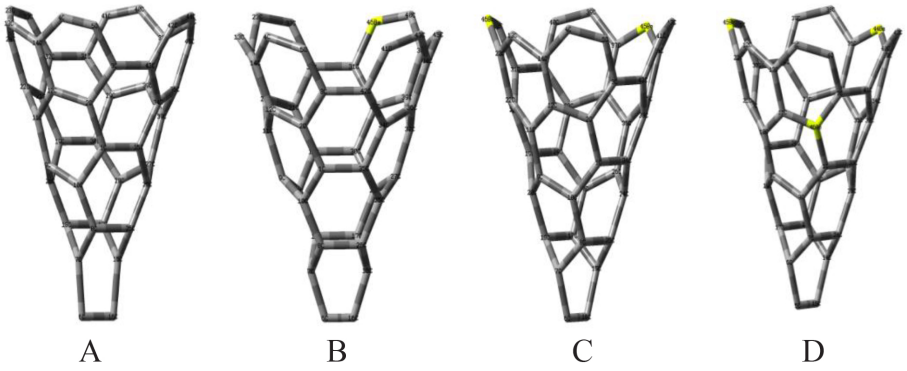


Fig. 1. Optimized structures of (A) NANO-CON, (B) NANO-CON+ Be (1), (C) NANO-CON+ Be (2), and (D) NANO-CON+ Be (3) molecules using DFT method with3-21G basis-set.

Eq. (4) could be used to compute the Fermi energy as follows23:

$$E_f = -(I + E)/2 \quad (4)$$

Results and discussion

NANO-CON (A), NANO-CON+, NANO-CON+ Be (2) (C), and NANO-CON+ (D) were the optimized structures. Be (3) (C) and Be (3)(D) molecules were computed in the gas phase by using DFT methods with a 3-21G basis set, as shown in Fig. 1

Electronic properties

Electronic properties, such as HOMO and LUMO energies, and electronic characteristics I, E, Eg, and Ef in electron Volt units were computed using the DFT method with a 3-21G basis set for NANO-CON (A), NANO-CON+ Be (1) (B), NANO-CON+ Be (2) (C) and NANO-CON+ Be (3) (D) molecules. The ionization potential was calculated by deducting one electron from NANO-CON+ Be (1). Table 1. Displays these quantities, which provide insights into the chemical reactivity of substitute NANO-CON. The electron distribution of Be at $1S^2$ $2S^2$ is assumed to be inactivation in chemical bonding for(C) atoms. As a result, electron substitution reduces the values of I whilst increasing the values of total energy E. According to Table 1. Be impurity increases HOMO, E, and total energy while NANO-CON decreases LUMO, I, and Eg. The I for NANO-CON+ Be (1) and NANO-CON+ Be (3) is lower than that for pristine tubes, indicating that the NANO-CONs require less energy to become cations than pristine tubes and confirming their electron-donating properties. NANO-CON+ Be (1) and NANO-CON+ Be (3) may be useful for high-energy particle detectors or catalysis due to their small I. The existence of an Eg shed light on how the molecule functioned. The NANO-CON+ Be(1) molecule also has a small Eg of 1.209257 eV. A relatively narrow Eg is indicative of the molecule's level of activity. Meanwhile NANO-CON+ Be (2) has a high Eg of 1.919736 eV.

Table 1. The predicted HOMO and LUMO energies and the electronic characteristics (I, E, Eg, Ef, and ET) in eV for NANO-CON (A), NANO-CON+ Be (1) (B), NANO-CON+ Be (2) (C) and NANO CON+ Be (3) molecules.

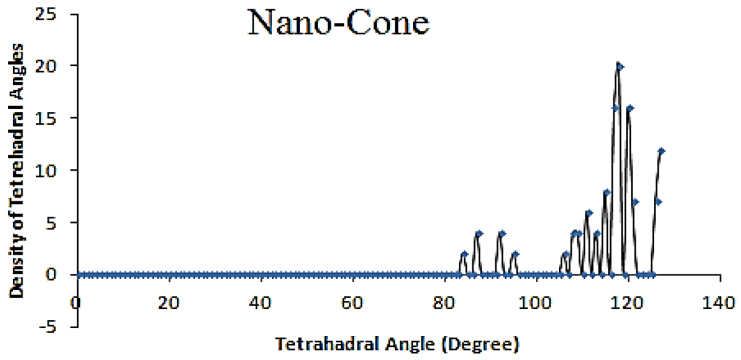
Molecules	HOMO	LOUMO	Eg
NANO-CON	−6.82561	−5.03295	1.792661
NANO-CON+ Be(1)	−5.61309	−4.40383	1.209257
NANO-CON+ Be(2)	−5.83132	−3.91158	1.919736
NANO-CON+ Be(3)	−5.75594	−4.10968	1.646266

Density of tetrahedral angles

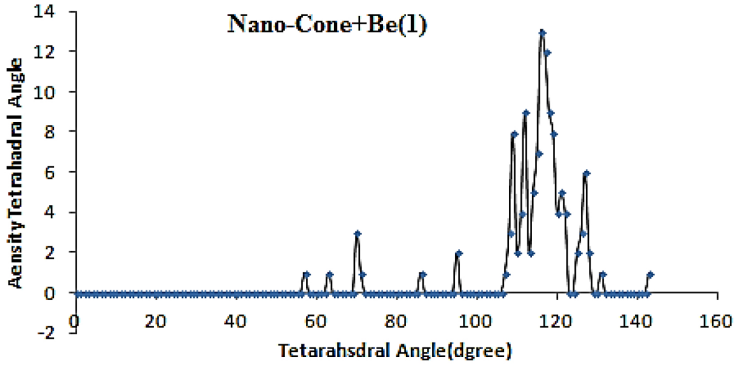
Densities and their values of tetrahedral angles for the molecules are presented in Fig. 2. [NANO-CON (A), NANO-CON+ Be (1) (B), NANO-CON+ Be (2) (C) and NANO-CON+ Be (3) (D)]. The tetrahedral angles of NANO-CON are located at an angle of 87.80–127.97 AO, whereas those of NANO-CON+ Be (1) (B), NANO-CON+ Be (2) (C) and NANO-CON+ Be (3) (D) molecules are located at angles of 57.06–143.96, 58.33–155.69 and 49.79–154.52 AO. The introduction of Be atoms into this molecule in place of C atoms causes a reduction in the tetrahedral angles.

Density of dihedral angles

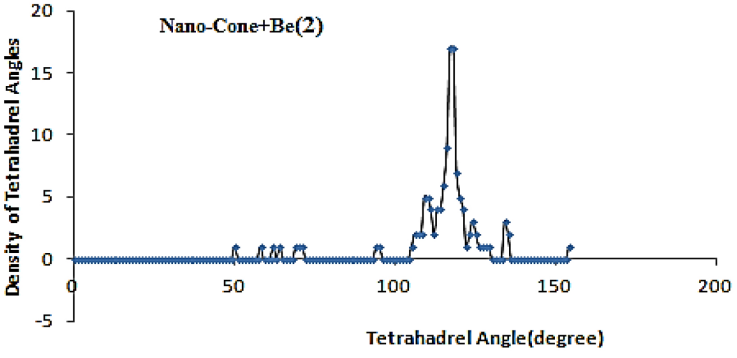
The density of the dihedral angle may be used as a measurement tool for determining the change in dihedral angle value. The calculations show that the reason because the dihedral angle falls within the range of a pure molecule or one in which deformation happened, the molecule is pure. The



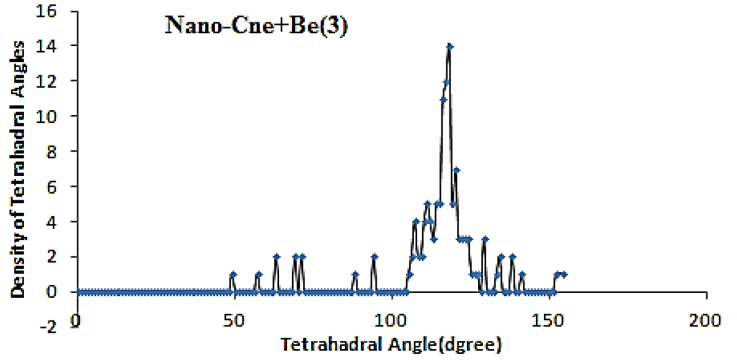
A



B

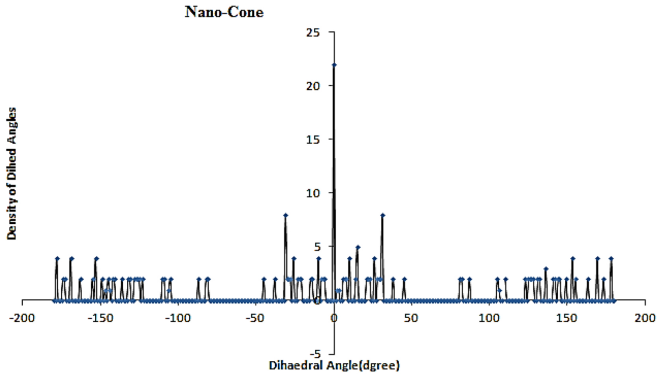


C

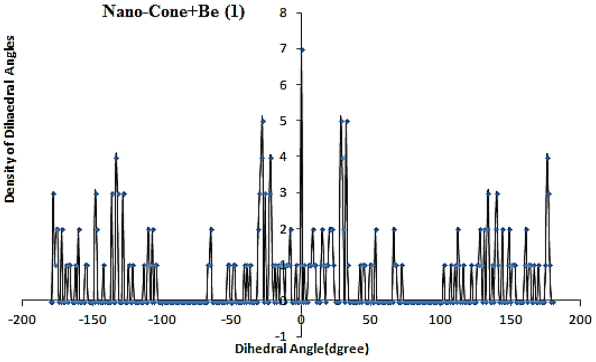


D

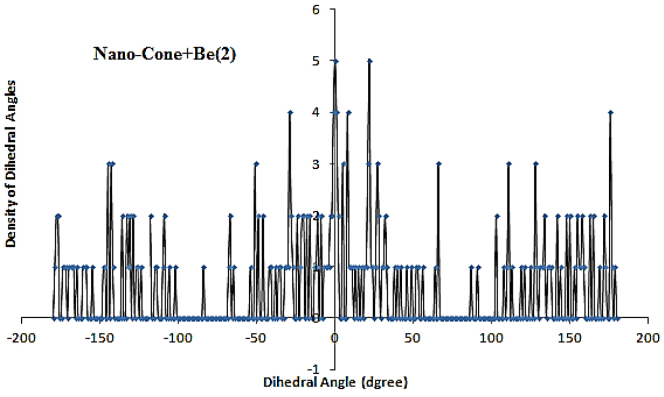
Fig. 2. Density of tetrahedral angles for NANO-CON, A. NANO-CON+ Be (1), B. NANO-CON+ Be (2), C. NANO-CON+ Be (3) (D)molecules.



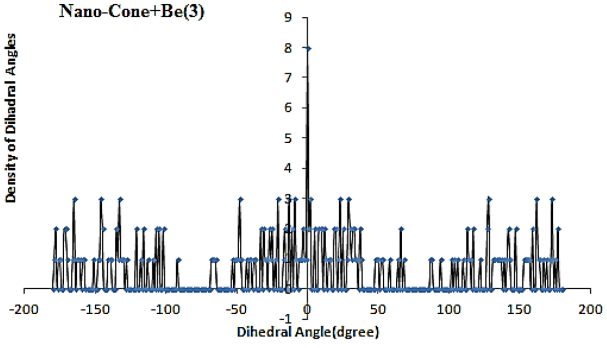
A



B

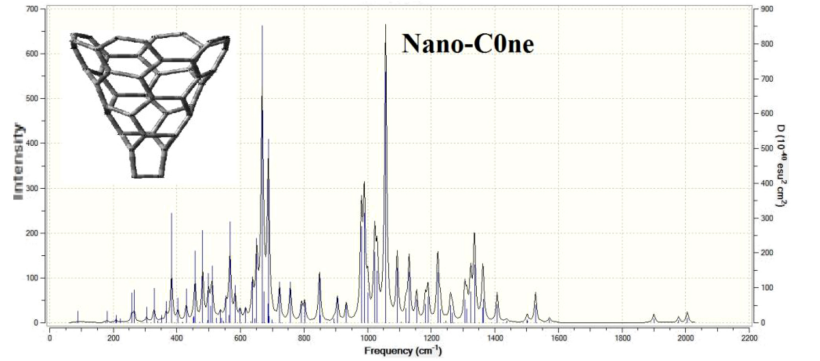


C

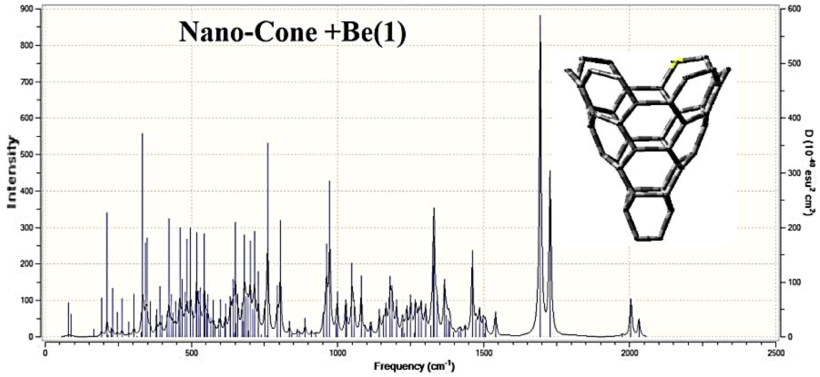


D

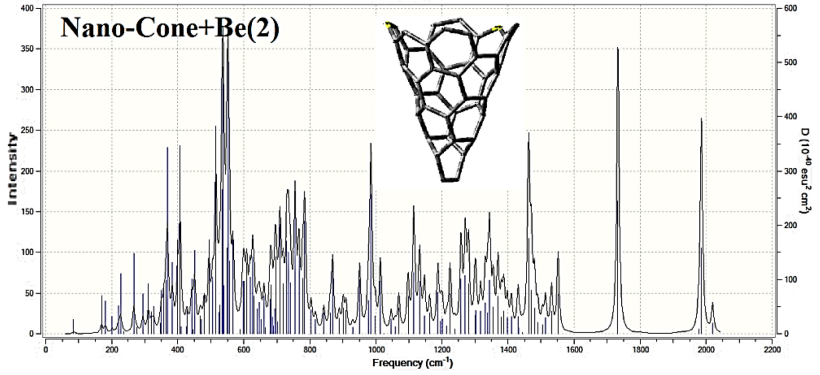
Fig. 3. Density of dihedral angles for NANO-CON, A. NANO-CON+ Be (1), B. NANO-CON+ Be (2), C. and NANO-CON+ Be (3), D. molecules by using DFT method and 3-21G basis set.



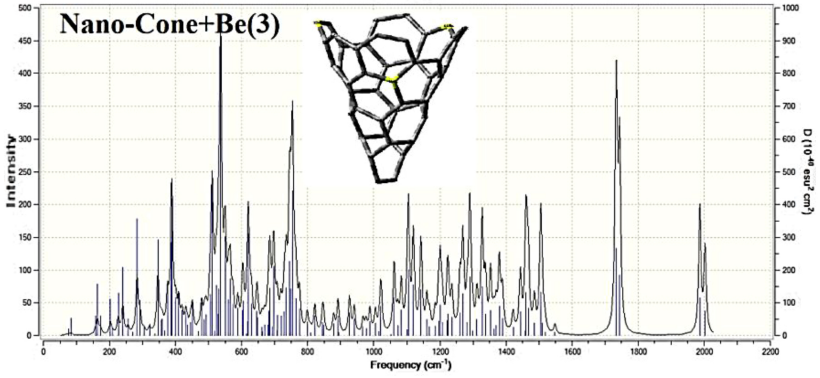
A



B



C



D

Fig. 4. IR spectra, displacement and dipole derivative vector for, A. NANO-CON, B. NANO-CON+ Be (1), C. NANO-CON+ Be(2) and, D. NANO-CON+ Be(3) molecules.

number of dihedral angles based on DFT method with the 3-21G basis set are178.79° and −178.44° for NANO-CON,178.67° and −177° for NANO-CON + Be(1), −179.92° and 179° for NANO-CON + Be(2) and −179.1° and 177.85° for NANO-CON + Be(3). Fig. 3 shows that the substitution is the responsible for the slight variation in density exhibited by the molecules.

IR spectra

The IR spectrum for the following types (C=C) and(C–C), stretching C–C rocking and C–C waging studied in the regions 1900.19, 2004.96, 1120.15 and 1407.23 cm^{-1} is weak for NANO-CON. Fig. 4 shows that the C–C,C=C and C–Be stretching for NANO-CON + Be(1) (B), NANO-CON + Be(2) (C) and NANO-CON + Be(3) (D) in the region 2019.31–2002.64cm^{-1}, C–C stretching, (C=C) stretching researched for the area1733.04–1363.45 cm^{-1} and C–Be stretching studied in the region 1504.55–1312.45 cm^{-1}. NANO-CON + Be (3) is out of plan is the modes of vibration for all ring modes in 926.68 cm^{-1}. Fig. 5 also shows the displacement and dipole derivative vector for (A) NANO-CON, (B) NANO-CON + Be(1), (C) NANO-CON + Be(2) and (D) NANO-CON + Be(3). The impurities lead to increasing vibration modes and displacement and a dipole derivative vector appears in NANO-CON. NANO-CON + Be (3) has C–C-crocking and C–Be–C– waging in regions 1222.23 and 1021.77 cm^{-1} is weak. The effect of Be atoms is that they lead to the vibration of harmonic waves that are weak.

Electrostatic potential and electron density surfaces

Fig. 6 illustrates the electrostatic potential and electron density surfaces of the molecules NANO-CON, NANO-CON + Be (1), NANO-CON + Be (2), and NANO-CON + Be (3). These surfaces were estimated using the DFT technique with the 3-21G basis set. The kind, position, and amount of replacement atoms and the positive and negative charges were determined. All of these factors affect how electrostatic potential for the effect of the electronegativity of the atom used electron density is distributed across surfaces. The density distribution on the NANO-CON molecule is shown to be homogeneous in the picture. Meanwhile, the distribution of Be atoms in NANO-CON + Be (1), NANO-CON + Be (2), and NANO-CON + Be (3) molecules is shown to be heterogeneous because these atoms have the highest electron negativity, which allows them to attract charge to themselves. [24,25]

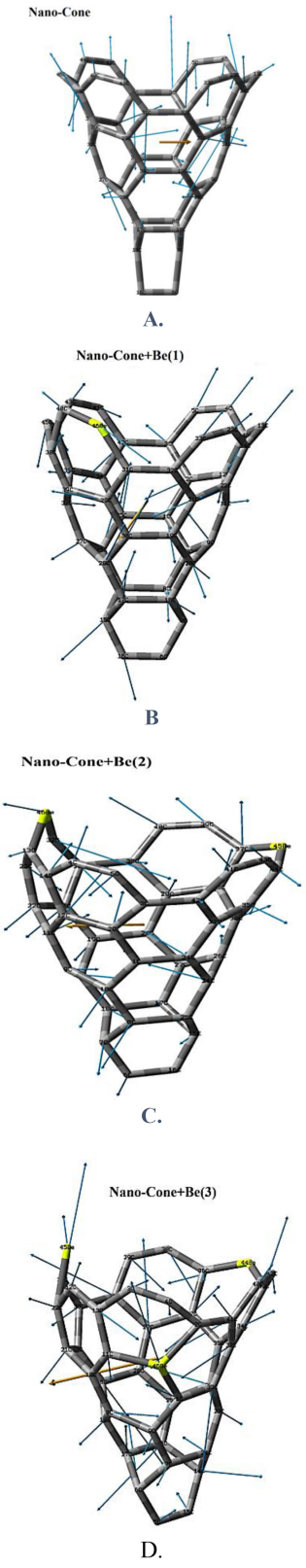


Fig. 5. Displacement and dipole derivative vector for, A. NANO-CON, B. NANO-CON+ Be(1), C. NANO-CON+ Be(2), and (D) NANO-CON+ Be(3) molecules by using DFT method with 3-21G basis set.

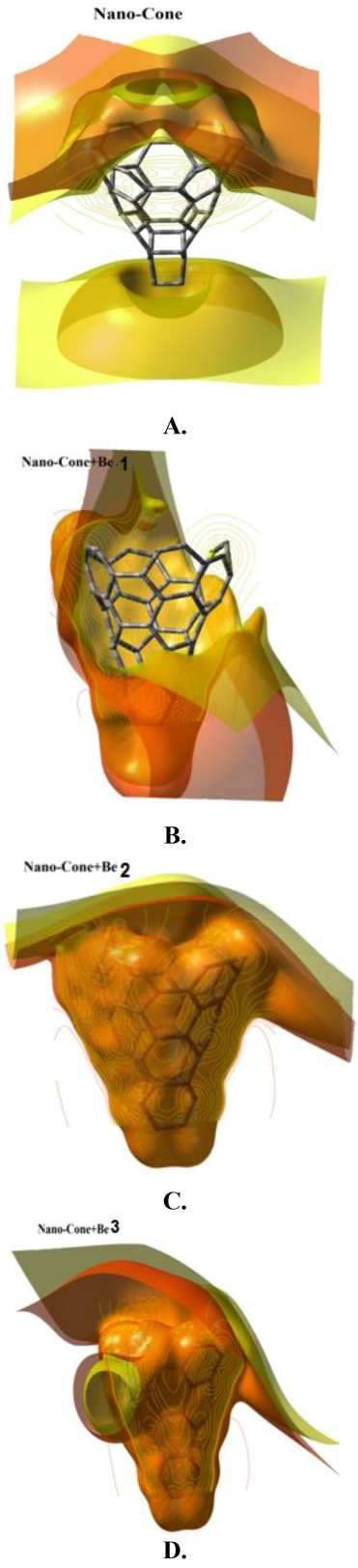


Fig. 6. Electrostatic potential and electron density surfaces for, A. NANO-CON, B. NANO-CON+ Be(1), C. NANO-CON+ Be(2), and,D. NANO-CON+ Be(3) molecules by using DFT method with 3-21G basis set.

Conclusion

The impact of Beryllium (Be) substitution on the single-wall carbon nano-cone's electrical and vibrational characteristics was examined using the DFT approach. The IR spectral characteristics of NANO-CONE molecules which look homogeneous through the charge distribution in Fig. 6, the optimization structure, and the electronic properties, which stand for ionization potential (I) and electron affinity (Eea), were evaluated. The computed values of electron substitution result in a decrease in I values and an increase in E values. Be atom insertion increases total energy, HOMO, E, and Ef. In contrast, nano-con reduces LUMO, I, and Eg. Be atoms also result in a faint vibrational harmony. The kind, location, and amount of replacement atoms as well as the positive and negative charges have an impact on the electron density surface distributions and electrostatic potential.

Acknowledgment

The authors wish to express their gratitude to the Department of Physics, and the Department of Chemistry College of Science, University of Kerbala, also the authors wish to express their gratitude to the Department of Physics College of Education for Pure Sciences, University of Babylon, for their support.

Authors' declaration

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are ours. Furthermore, any Figures and images, that are not ours, have been included with the necessary permission for republication, which is attached to the manuscript.
- No animal studies are present in the manuscript.
- No human studies are present in the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee at University of Kerbala.

Authors' contribution statement

R.K.M. and S.S.A.A. performed the DFT calculations and computational simulations. H.M.L. and A.S.H. prepared the first draft of the manuscript and contributed to the organization of the results and discussion sections. L.M.A. supervised the research work, contributed to the study design, and critically revised the manuscript for important intellectual content. All authors participated in data interpretation,

reviewed the manuscript, and approved the final version for publication.

Data availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

References

1. Wategaonkar SB, Parale VG, Pawar RP, Mali SS, Hong CK, Powar RR, *et al.* Structural, morphological, and optical studies of hydrothermally synthesized Nb-added TiO2 for DSSC application. Ceram Int. Elsevier. 2021;47(18):25580–25592. https://doi.org/10.1016/j.ceramint.2021.05.284.
2. Shirazi Z, Golikand AN, Keshavarz MH. A new nanocomposite based on poly (o-anthranilic acid), graphene oxide and functionalized carbon nanotube as an efficient corrosion inhibitor for stainless steel in severe environmental corrosion. Compos Commun. Elsevier. 2020;22:100467. https://doi.org/10.1016/j.coco.2020.100467.
3. Toh P-L, Naqvi SAAS, Wang S-M. Density functional theory investigation on the structural and electronic properties of pristine, vacancy, and group IV doped Zigzag Boron Nitride Nanotubes. Mal J Fund Appl Sci. Penerbit UTM Press. 2023;19(1):19–29. https://doi.org/10.11113/MJFAS.V19N1.2639.
4. Mahesh V. Active control of nonlinear coupled transient vibrations of multifunctional sandwich plates with agglomerated FG-CNTs core/magneto-electro-elastic facesheets. Thin-Walled Struct. 2022;179. https://doi.org/10.1016/j.tws.2022.109547.
5. Awrejcewicz J, Krysko A V, Zhigalov M V, Krysko VA, Awrejcewicz J, Krysko A V, *et al.* Vibrations of size-dependent beams under topologic optimization and temperature field. Mathematical Modelling and Numerical Analysis of Size-Dependent Structural Members in Temperature Fields. Adv Struct Mater. Springer. 2021;333–402. https://doi.org/10.1007/978-3-030-55993-9.
6. Thess A, Lee R, Nikolaev P, Dai H, Petit P, Robert J, *et al.* Crystalline ropes of metallic carbon nanotubes. Science. 1996;273(5274):483–487. https://doi.org/10.1126/science.273.5274.483.
7. Ke LL, Xiang Y, Yang J, Kitipornchai S. Nonlinear free vibration of embedded double-walled carbon nanotubes based on nonlocal Timoshenko beam theory. Comput Mater Sci. Elsevier. 2009;47(2):409–417. https://doi.org/10.1016/j.commatsci.2009.09.002.
8. Wang Q, Varadan VK. Vibration of carbon nanotubes studied using nonlocal continuum mechanics. Smart Mater Struct. IOP Publishing. 2006;15(2):659–666. https://doi.org/10.1088/0964-1726/15/2/050.
9. Mustapha KB, Zhong ZW. Free transverse vibration of an axially loaded non-prismatic single-walled carbon nanotube embedded in a two-parameter elastic medium. Comput Mater Sci. Elsevier. 2010;50(2):742–751. https://doi.org/10.1016/j.commatsci.2010.10.005.
10. National Research Council (US). Committee on CMMP 2010, Solid State Sciences Committee. Condensed-Matter and Materials Physics: The Science of the World Around Us. Washington (DC): National Academies Press. 2007.
11. He XQ, Kitipornchai S, Liew KM. Buckling analysis of multi-walled carbon nanotubes: a continuum model accounting for van der Waals interaction. J Mech Phys Solids. Elsevier. 2005;53(2):303–326. https://doi.org/10.1016/j.jmps.2004.08.003.
12. Olaniyan O, Maphasha RE, Madito MJ, Khaleed AA, Igumbor E, Manyala N. A systematic study of the stability, electronic and optical properties of beryllium and nitrogen co-doped graphene. Carbon. Elsevier. 2018;129:207–227. https://doi.org/10.1016/j.carbon.2017.12.014.
13. Liew KM, Alibeigloo A. Predicting bucking and vibration behaviors of functionally graded carbon nanotube reinforced composite cylindrical panels with three-dimensional flexibilities. Compos Struct. Elsevier. 2021;256:113039. https://doi.org/10.1016/j.compstruct.2020.113039.
14. Muc A. Modeling of carbon nanotubes with the use of thin shell theory. Shell Structures: Theory and Applications - Proceedings of the 9th SSTA Conference. 2010;87–90. https://doi.org/10.1016/10.1201/9780203859766.ch16.
15. Zhang HT, Zhang Z, Zhou H, Tanaka H, Fong DD, Ramanathan S. Beyond electrostatic modification: design and discovery of functional oxide phases via ionic-electronic doping. Adv Phys.: X. Taylor & Francis. 2019;4(1). https://doi.org/10.1080/23746149.2018.1523686.
16. Alencar A, Azevedo S, Machado M. First-principles studies of zigzag pristine boron nitride nanotubes doped with one iron atom. Appl Phys A: Mater Sci. Process. Springer Verlag. 2011;102(3):583–591. https://doi.org/10.1007/s00339-010-5963-y.
17. Moncada F, Reyes A. Multicomponent wavefunction-in-DFT embedding for positronium molecules. J Chem Phys. AIP Publishing. 2023;158(13):134101. https://doi.org/10.1063/5.0139813/2883242.
18. Stephens PJ, Devlin FJ, Chabalowski CF, Frisch MJ. Ab Initio calculation of vibrational absorption and circular dichroism spectra using density functional force fields. J Phys Chem. 1994;98(45):11623–11627. https://doi.org/10.1021/j100096a001.
19. Lee C, Yang W, Parr RG. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. Phys Rev B. 1988;37(2):785. https://doi.org/10.1103/physrevb.37.785.
20. Petersson GA, Al-Laham MA. A complete basis set model chemistry. II. Open-shell systems and the total energies of the first-row atoms. J Chem Phys. 1991;94(9):6081–6090. https://doi.org/10.1063/1.460447.
21. Mohammad RK, Al-Abbas SSA. The effects of cycloepentanes on electronic and spectra properties of nanotubes molecules. J Eng Sci Technol. 2022;17:59–66.
22. Hammer M, Bauer G, Stierle R, Gross J, Wilhelmsen Ø. Classical density functional theory for interfacial properties of hydrogen, helium, deuterium, neon, and their mixtures. J Chem Phys. 2023;158(10):104107. https://doi.org/10.1063/5.0137226/2881411.
23. Mohammad RK, Nowfal SH, Al-Seady MA, Abduljalil HM. Investigation ability of single walled carbon nanotubes to detection toxic gases utilizing DFT calculations. Egypt J Chem. 2022;65(6):89–98. https://doi.org/10.21608/EJCHEM.2021.87777.4232.
24. Wang D-W, Su D. Heterogeneous nanocarbon materials for oxygen reduction reaction. Energy Environ Sci. 2014;7(2):576–591. https://doi.org/10.1039/C3EE43463J.
25. Mahmood SS, Hussien FH, Atiyah AJ. Carbon Nanotubes: Synthesis via Flame Fragment Deposition (FFD) Method from Liquefied Petroleum Gas. Baghdad Sci J. 2023;20(2):Article 17. https://doi.org/10.21123/bsj.2022.6966.

تأثير استبدال البريليوم على الخواص الاهتزازية والإلكترونية لمخروط الكربون النانوي: نظرية دالة الكثافة الوظيفي

رجاء خضر محمد [1]، حسين محمدعلي لطيف [1]، عمار صلاح حميد [1]، لمى مجيد احمد [2]، شروق صباح عبد العباس[3]

[1]الفيزياء، كلية العلوم ، جامعة كربلاء، كربلاء المقدسة ، العراق.
[2]الكيمياء، كلية العلوم ، جامعة كربلاء، كربلاء المقدسة ، العراق.
[3]الفيزياء، كلية التربية للعلوم الصرفة ، جامعة بابل ، الحلة، العراق.

الخلاصة

تم استخدام طريقة نظرية الكثافة الوظيفية (DFT) لدراسة تأثيرات الخواص الاهتزازية والإلكترونية لاستبدال البريليوم (Be) لمخروط الكربون النانوي أحادي الجدار. حيث يهدف الباحثون إلى فهم كيفية تأثير هذا التغيير على الخصائص الهيكلية والإلكترونية للبنى النانوية من خلال عمليات محاكاة DFT، حيث تتم دراسة الخصائص الإلكترونية والتي تمثل احتمال التأين (I) والألفة الإلكترونية (Eea)، والخصائص الطيفية للأشعة تحت الحمراء لـ NANO-CONE تم تقدير الجزيئات والهيكل الأمثل. القيم المحسوبة لاستبدال الإلكترون تقلل من قيم I، مع زيادة الالفة الالكترونية (Eea). يؤدي إدخال ذرات Be إلى زيادة أعلى مدار جزيئي مشغول (HOMO) , والألفة الإلكترونية (Eea)، وطاقة فيرمي (Ef)، والطاقة الكلية (E)، في حين أن NANO-CONE يقلل (LUMO)، وI، والطاقات. فجوة الطاقة (على سبيل المثال). كما أن ذرات البيريليوم (Be) تؤدي إلى ضعف تناغم الاهتزازات، ويتأثر الجهد الكهروستاتيكي وتوزيعات الكثافة الإلكترونية السطحية بنوع وموقع وعدد ذرات الاستبدال والشحنات السالبة والموجبة. ومن خلال دراسة هذه التأثيرات على الخواص الاهتزازية والإلكترونية لاستبدال البريليوم (Be) لمخروط الكربون النانوي أحادي الجدار، يمكن معرفة التطبيقات المحتملة لهذه الهياكل النانوية المعدلة في مجالات مختلفة مثل الإلكترونيات النانوية، والمحفز الكيميائي، وتقنيات الاستشعار,و تخزين الطاقة . بشكل عام، يوفر التحقيق في تأثير استبدال البريليوم على مخاريط الكربون النانوية رؤى قيمة في كل من العلوم الأساسية والتطبيقات التكنولوجية المحتملة، وتساعد مقارنة هذا العمل مع الدراسات الحالية حول البدائل أو التعديلات المماثلة في وضع النتائج في سياق المشهد الأوسع لأبحاث البنية النانوية.

الكلمات المفتاحية: استبدال البريليوم، حساب DFT، الخواص الإلكترونية، أطياف الأشعة تحت الحمراء، جزيء النانو المخروط.