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STABILITY AND CHARGE DISTRIBUTION IN CARBON NANOCONES: A COMPARATIVE STUDY USING GFN2-xTB AND g-xTB METHODS

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Abstract: Due to their unique geometry and favorable mechanical and electrical properties, carbon nanocones (CNCs) are increasingly studied for applications in electronics, optics, energy storage, and biomedicine. In this computational study, we investigate the structural and electronic stability of several CNC systems with different disclination angles, using two modern semi-empirical methods: GFN2-xTB and g-xTB. Geometry optimizations and property calculations were performed for each system, with particular focus on the HOMO-LUMO gap as a measure of molecular stability. In addition, dipole moments were computed to gain insight into charge separation and polarity across the nanocone series. All calculations were carried out using the Atomistica.online (https://atomistica.online/) 2025 platform. The results show that the NC60 nanocone, corresponding to a 60° disclination angle, exhibits the highest stability among the systems studied. This work provides valuable comparative data and further insight into the structure-property relationships of carbon nanocones, contributing to their potential application in nanotechnology and materials science.

Keywords: GFN2, g-xTB, nanomaterials

1. Introduction

Carbon nanocones (CNC) are hollow cone-shaped structures made of graphitic carbon [1]. Eight classes of different CNC structures were identified along with their subclasses [2]. These structures were first noticed in 1994 [3], but only in the following years was their significance and potential discovered. It is possible to mathematically model CNC as three-dimensional planar infinite graphs with the formation of a network of carbon atoms [4]. Unlike other carbon nanomaterials, CNC has an open structure, high mechanical strength and conductivity, as well as a larger surface area and porosity, which makes it useful for a wide range of potential applications [5].

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Because of its excellent mechanical and electrical properties, CNC has become an attractive nanomaterial that still attracts the attention of many scientists. It is increasingly used in gas storage devices, biofuel cells, supercapacitors and sensors such as biochemical and electrochemical [6–9]. It is useful in the fields of optics and electronics. CNC can also be used as an anode material for various ion batteries [10, 11]. Due to its curvature, it stands out as very successful in storing hydrogen [12–14]. This nanomaterial is characterized by biocompatibility, which makes it suitable for use in the medical field. [15, 16]. They have been investigated as possible carriers of platforms for the delivery of drugs, vaccines and gene therapy [17–19].

In this work, we investigated several nanocone structures that differ in their disclination angle, a geometric parameter that defines the opening angle of the cone. The number in each nanocone label (e.g., NC60, NC120) corresponds to the disclination angle in degrees. These nanocones were optimized using two modern semi-empirical quantum chemical methods: GFN2 and g-xTB. In addition to evaluating stability through the HOMO–LUMO gap, we also examined charge separation in these systems by calculating their dipole moments.

2. Computational details

The initial nanocone structures were generated using Nanotube Modeler (Generation of Nano-Geometries, JCrystalSoft, 2005–2018) [20,21], a software tool that allows the construction of carbon nanostructures based on user-defined parameters. Each nanocone was built with a specific disclination angle, which determines the cone's opening angle and corresponds to the value in the structure's label (e.g., NC60, NC120).

Geometry optimizations and property calculations were performed using two modern semi-empirical quantum chemical methods: GFN2-xTB [22] and g-xTB [23], developed by Prof. Grimme and coworkers. Both methods are part of the extended tight-binding framework developed to provide reliable results with reduced computational cost [24–26].

All calculations were conducted using the Atomistica.online 2025 platform [27,28], which integrates xtb and g-xtb codes into a browser-based environment for accessible atomistic modeling. The platform enabled efficient geometry optimization and analysis of electronic properties, including HOMO–LUMO gaps and dipole moments, for all nanocone systems investigated in this study.

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3. Results and discussion

3.1. Stability of nanocones

Optimization calculations were performed using two semi-empirical methods: GFN2 and g-xTB. Both methods yielded very similar geometries, which is expected due to the high symmetry and rigidity of the nanocone structures. These similarities suggest that either method can be reliably used for structural optimization of such systems. In addition, the optimized structures obtained here can serve as a suitable starting point for further refinement using more advanced quantum chemical methods. Optimized geometries of studied CNCs are presented in Figure 1.

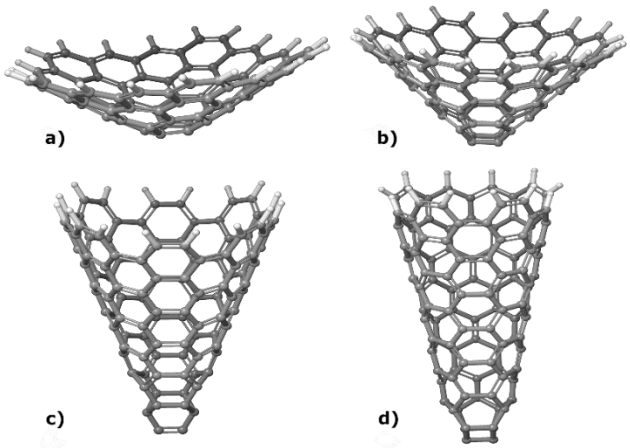

Figure 1. Geometrically optimized structures of the nanocones obtained by the g-xTB method: (a) NC60, (b) NC120, (c)NC240, (d) NC300

To assess the stability, we calculated the energy gap (Eg), defined as the difference between the energies of the lowest unoccupied molecular orbital (LUMO) and the highest occupied molecular orbital (HOMO):

$$E_g = E_{LUMO} - E_{HOMO} \quad (1)$$

The HOMO–LUMO gap (Eg) values for each nanocone system, calculated using both the GFN2 and g-xTB methods, are presented in Table 1.

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Table 1. The value of the HOMO-LUMO gap of systems optimized by the GFN2 method

Nanocone system	E_g [eV] GFN2	Eg [eV] g-xTB
NC60	1.43	5.18
NC120	0.15	3.47
NC240	0.37	3.67
NC300	0.19	3.75

Eg values for each nanocone system, calculated using both the GFN2 and g-xTB methods, are presented in Table 1. While both methods identify NC60 as the most stable system, they differ in the absolute Eg values. The g-xTB method consistently predicts significantly larger energy gaps than GFN2. For example, the Eg for NC60 is 1.43 eV with GFN2 and 5.18 eV with g-xTB. For NC120 and NC240, both methods follow the expected trend of decreasing stability with increasing size, as reflected by smaller Eg values. However, a slight discrepancy appears with NC300. The GFN2 method suggests a further decrease in the HOMO–LUMO gap for NC300 (0.19 eV), indicating continued destabilization. In contrast, g-xTB predicts a slightly larger gap for NC300 (3.75 eV) than for NC240 (3.67 eV), suggesting a slight reversal or plateau in the stability trend.

This difference may be a consequence of how each method treats the frontier orbitals in extended systems or from differences in basis set approximations and treatment of electronic delocalization. Despite this inconsistency for NC300, both methods agree on the general trend and relative ranking of smaller nanocones, particularly highlighting NC60 as the most electronically stable structure.

3.2. Charge separation

Dipole moment is a fundamental molecular property that gives insights into the separation of positive and negative charges within a molecule. It arises from an uneven distribution of electron density and is a direct measure of molecular polarity. Nanostructures like carbon nanocones often possess intrinsic asymmetry due to their conical geometry, because of which dipole moments can provide valuable insight into electronic distribution and surface reactivity. Even in systems composed of a single element such as carbon, the geometry alone can induce local polarizations, especially when the structure lacks mirror or inversion symmetry.

Understanding the dipole moment of nanocones is important because it affects how these structures behave in different environments. Charge separation plays a key role in how nanocones interact with electric fields, solvents, or polar molecules. This kind of information is especially useful when designing devices like sensors, capacitors, or electrochemical

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systems that rely on those interactions. Also, dipole moments can affect the orientation and self-assembly of nanostructures in complex environments. Finally, dipole moment values serve as an additional indicator of structural asymmetry and can complement other electronic parameters such as the HOMO-LUMO gap. By analyzing dipole moments of nanocones of different sizes, it is possible to obtain a better understanding of how structural growth impacts charge distribution and polarity. Dipole moments have also been calculated using the GFN2 method, and the results are presented in Table 2.

Table 2. Dipole moments of nanocone systems calculated with the GFN2 method

Nanocone system	Dipole moment GFN2	Dipole moment g-xTB
NC60	4.08	7.08
NC120	5.11	9.06
NC240	6.65	9.54
NC300	12.46	24.60

As shown in Table 2, the dipole moment increases with the size of the nanocone. This trend is expected due to the growing asymmetry and elongation of the structures as more atoms are added. The NC60 system, which is the smallest, has the lowest dipole moment, while NC300 exhibits the highest value, more than three times larger. This increase suggests a progressive polarization of the charge distribution as the nanocone becomes larger.

These results indicate that larger nanocones may have a stronger interaction with external electric fields or polar environments, which could be important for applications in sensing, alignment in external fields, or self-assembly. Additionally, the presence of nonzero dipole moments in all systems, despite being composed only of carbon atoms, confirms that geometry alone can induce significant charge separation in conical nanostructures.

4. Conclusions

Based on the research conducted, it can be concluded that the electronic stability of carbon nanocones depends on their size, ie geometry. The values of the HOMO–LUMO gap (Eg) calculated using the GFN2 and g-xTB methods unambiguously indicate that the NC60 system is the most stable. The values of the dipole moment serve as a complement to the electronic parameters and increase with the size of the nanocone. The NC300 system has the highest dipole moment value, which is expected. Overall, the obtained results contribute to a better understanding of the structural and electronic stability of carbon nanocones, which contributes to further research and potential applications of the observed systems.

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References

[1] D.J. Klein, Topo-combinatoric categorization of quasi-local graphitic defects, Phys. Chem. Chem. Phys. 4 (2002) 2099–2110. https://doi.org/10.1039/b110618j.
[2] D.J. Klein, A.T. Balaban, The Eight Classes of Positive-Curvature Graphitic Nanocones, J. Chem. Inf. Model. 46 (2006) 307–320. https://doi.org/10.1021/ci0503356.
[3] H. Terrones, Curved graphite and its mathematical transformations, J Math Chem 15 (1994) 143–156. https://doi.org/10.1007/BF01277556.
[4] M. Asim, Z.S. Mufti, M.F. Hanif, A. Tabraiz, A topological and statistical perspective on carbon nanocones using Kulli-Basava indices, Chem. Pap. 79 (2025) 2955–2974. https://doi.org/10.1007/s11696-025-03980-2.
[5] A. Kumar, M.I. Sayyed, M.M. Sabugaa, M. Al-Bahrani, S. Sharma, M.J. Saadh, A DFT study on effective detection of ClCN gas by functionalized, decorated, and doped nanocone strategies, RSC Adv. 13 (2023) 12554–12571. https://doi.org/10.1039/D3RA01231J.
[6] K. Ajima, T. Murakami, Y. Mizoguchi, K. Tsuchida, T. Ichihashi, S. Iijima, M. Yudasaka, Enhancement of *In Vivo* Anticancer Effects of Cisplatin by Incorporation Inside Single-Wall Carbon Nanohorns, ACS Nano 2 (2008) 2057–2064. https://doi.org/10.1021/nn800395t.
[7] O.O. Adisa, B.J. Cox, J.M. Hill, Open Carbon Nanocones as Candidates for Gas Storage, J. Phys. Chem. C 115 (2011) 24528–24533. https://doi.org/10.1021/jp2069094.
[8] N. Karousis, I. Suarez-Martinez, C.P. Ewels, N. Tagmatarchis, Structure, Properties, Functionalization, and Applications of Carbon Nanohorns, Chem. Rev. 116 (2016) 4850–4883. https://doi.org/10.1021/acs.chemrev.5b00611.
[9] Masako Yudasaka, Sumio Iijim, Vincent H. Crespi, Single-Wall Carbon Nanohorns and Nanocones, (n.d.).
[10] Q.-Q. Ren, Z.-B. Wang, K. Ke, S.-W. Zhang, B.-S. Yin, NiCo2O4 nanosheets and nanocones as additive-free anodes for high-performance Li-ion batteries, Ceramics International 43 (2017) 13710–13716. https://doi.org/10.1016/j.ceramint.2017.07.083.
[11] Z. Duan, Q. Yin, C. Li, L. Dong, X. Bai, Y. Zhang, M. Yang, D. Jia, R. Li, Z. Liu, Milling force and surface morphology of 45 steel under different Al2O3 nanofluid concentrations, Int J Adv Manuf Technol 107 (2020) 1277–1296. https://doi.org/10.1007/s00170-020-04969-9.
[12] A.A. EL-Barbary, Hydrogen storage on cross stacking nanocones, International Journal of Hydrogen Energy 44 (2019) 20099–20109. https://doi.org/10.1016/j.ijhydene.2019.05.043.
[13] A.S. Shalabi, K.A. Soliman, H.O. Taha, A comparative theoretical study of metal functionalized carbon nanocones and carbon nanocone sheets as potential hydrogen storage materials, Phys. Chem. Chem. Phys. 16 (2014) 19333–19339. https://doi.org/10.1039/C4CP02726D.
[14] M.-L. Liao, A study on hydrogen adsorption behaviors of open-tip carbon nanocones, J Nanopart Res 14 (2012) 837. https://doi.org/10.1007/s11051-012-0837-1.
[15] N. Wohner, P. Lam, K. Sattler, Energetic stability of graphene nanoflakes and nanocones, Carbon 67 (2014) 721–735. https://doi.org/10.1016/j.carbon.2013.10.064.
[16] J.H. Lee, B.S. Lee, Modal analysis of carbon nanotubes and nanocones using FEM, Computational Materials Science 51 (2012) 30–42. https://doi.org/10.1016/j.commatsci.2011.06.041.

[17] C.Y. Hsu, M.J. Saadh, A.F. Mutee, H. Mumtaz, G.U. Tillaeva, M. Mirzaei, M. Da'i, F. Mascarenhas-Melo, M.M. Salem-Bekhit, Assessing the metronidazole adsorption by an iron-enhanced nanocone along with DFT calculations regarding the conjugated system formations for developing the drug delivery platforms, Inorganic Chemistry Communications 165 (2024) 112496. https://doi.org/10.1016/j.inoche.2024.112496.
[18] R. Bhuvaneswari, V. Nagarajan, R. Chandiramouli, First-principles insights on the electronic and field emission properties of Ga and Al doped germanium nanocones, Journal of Electron Spectroscopy and Related Phenomena 227 (2018) 15–22. https://doi.org/10.1016/j.elspec.2018.06.002.
[19] M. Arockiaraj, J. Clement, K. Balasubramanian, Topological Properties of Carbon Nanocones, Polycyclic Aromatic Compounds 40 (2020) 1332–1346. https://doi.org/10.1080/10406638.2018.1544156.
[20] S. Melchor, J.A. Dobado, CoNTub: An Algorithm for Connecting Two Arbitrary Carbon Nanotubes, J. Chem. Inf. Comput. Sci. 44 (2004) 1639–1646. https://doi.org/10.1021/ci049857w.
[21] Nanotube Modeler (Nanocones, Bucky-Ball, Fullerenes, Simulation Software), (n.d.). http://www.jcrystal.com/products/wincnt/index.htm (accessed August 1, 2025).
[22] C. Bannwarth, S. Ehlert, S. Grimme, GFN2-xTB—An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions, J. Chem. Theory Comput. 15 (2019) 1652–1671. https://doi.org/10.1021/acs.jctc.8b01176.
[23] T. Froitzheim, M. Müller, A. Hansen, S. Grimme, g-xTB: A General-Purpose Extended Tight-Binding Electronic Structure Method For the Elements H to Lr (Z=1–103), (2025). https://doi.org/10.26434/chemrxiv-2025-bjxvt.
[24] C. Bannwarth, E. Caldeweyher, S. Ehlert, A. Hansen, P. Pracht, J. Seibert, S. Spicher, S. Grimme, Extended tight-binding quantum chemistry methods, WIREs Computational Molecular Science 11 (2021) e1493. https://doi.org/10.1002/wcms.1493.
[25] S. Ehlert, M. Stahn, S. Spicher, S. Grimme, Robust and Efficient Implicit Solvation Model for Fast Semiempirical Methods, J. Chem. Theory Comput. 17 (2021) 4250–4261. https://doi.org/10.1021/acs.jctc.1c00471.
[26] S. Grimme, C. Bannwarth, P. Shushkov, A Robust and Accurate Tight-Binding Quantum Chemical Method for Structures, Vibrational Frequencies, and Noncovalent Interactions of Large Molecular Systems Parametrized for All spd-Block Elements (Z = 1–86), J. Chem. Theory Comput. 13 (2017) 1989–2009. https://doi.org/10.1021/acs.jctc.7b00118.
[27] S. Armaković, S.J. Armaković, Atomistica.online – web application for generating input files for ORCA molecular modelling package made with the Anvil platform, Molecular Simulation 49 (2023) 117–123. https://doi.org/10.1080/08927022.2022.2126865.
[28] S. Armaković, S.J. Armaković, Online and desktop graphical user interfaces for xtb programme from atomistica.online platform, Molecular Simulation 50 (2024) 560–570. https://doi.org/10.1080/08927022.2024.2329736.

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