TUNABLE ELECTRONIC AND MECHANICAL PROPERTIES OF BCN MONOLAYER UNDER STRAIN AND ELECTRIC FIELDS

Dinh The Hung
Phenikaa School of Engineering - Phenikaa University

ARTICLE INFO

Received: 01/5/2025
Revised: 22/5/2025
Published: 22/5/2025

KEYWORDS

BCN monolayer
Electronic properties
Structural stability
Biaxial strain
Direct semiconductor

ABSTRACT

This research uses first-principles calculations to investigate the structural stability, mechanical strength, and electronic properties of two-dimensional BCN monolayers. The study aims to understand how external perturbations like strain and electric fields influence the adaptability of BCN monolayers. The research employs Quantum Espresso software with advanced computational techniques such as the Perdew-Burke-Ernzerhof functional within the generalized gradient approximation and dynamic stability assessments through phonon dispersion. Key findings include the BCN monolayer's robust structural stability under dynamic, mechanical, and thermodynamic criteria and impressive mechanical strength, with maximum biaxial tensile stress reaching 25.73 N/m at 16% strain. Furthermore, the monolayer demonstrates a tunable direct band gap ranging from 0.90 eV to 1.747 eV under strain and a significant band gap reduction under electric fields, with a decrease of 79.55% at -1.0 V/Å. These insights underline the BCN monolayer's potential for applications in optoelectronic devices, flexible sensors, and field-controlled systems. The findings contribute valuable knowledge to material science, paving the way for future semiconductor technology and energy systems advancements.

ĐẶC TÍNH ĐIỆN TỬ VÀ CƠ HỌC CÓ THỂ ĐIỀU CHỈNH CỦA BCN ĐƠN LỚP DƯỚI TÁC ĐỘNG CỦA BIẾN DẠNG VÀ ĐIỆN TRƯỜNG

Đinh Thế Hưng
Trường Kỹ thuật Phenikaa - Đại học Phenikaa

THÔNG TIN BÀI BÁO

Ngày nhận bài: 01/5/2025
Ngày hoàn thiện: 22/5/2025
Ngày đăng: 22/5/2025

TỪ KHÓA

BCN đơn lớp
Tính chất điện tử
Độ ổn định
Biến dạng theo phương xy
Vật liệu bán dẫn trực tiếp

TÓM TẮT

Nghiên cứu này khám phá tính ổn định cấu trúc, độ bền cơ học và các đặc tính điện tử của BCN đơn lớp bằng các tính toán dựa trên nguyên lý đầu tiên. Mục tiêu là tìm hiểu cách các yếu tố bên ngoài như biến dạng và điện trường ảnh hưởng đến đặc tính điện tử và cơ học của BCN đơn lớp. Nghiên cứu sử dụng phần mềm Quantum Espresso cùng các kỹ thuật tính toán như hàm số Perdew-Burke-Ernzerhof trong khuôn khổ xấp xỉ gradient tổng quát và đánh giá độ ổn định động qua phổ dao động phonon. Các kết quả chính bao gồm tính ổn định cấu trúc của BCN đơn lớp theo các tiêu chí động, cơ học và nhiệt động; độ bền cơ học ấn tượng với ứng suất kéo căng hai chiều cực đại đạt 25,73 N/m tại biến dạng 16%. Hơn nữa, BCN đơn lớp cho thấy khả năng điều chỉnh độ rộng vùng cấm trực tiếp từ 0,90 eV đến 1,747 eV dưới tác động của biến dạng và sự giảm đáng kể của độ rộng vùng cấm dưới điện trường, giảm 79,55% ở - 1,0 V/Å. Những phát hiện này nhấn mạnh tiềm năng của BCN đơn lớp trong các ứng dụng thiết bị quang điện tử, cảm biến linh hoạt và hệ thống điều khiển bằng điện trường. Kết quả nghiên cứu cung cấp kiến thức giá trị cho khoa học vật liệu, mở đường cho các tiến bộ trong công nghệ bán dẫn và hệ thống năng lượng.

DOI: https://doi.org/10.34238/tnu-jst.12710

Email: hung.dinhthe@phenikaa-uni.edu.vn

1. Introduction

Two-dimensional (2D) materials [1] - [3] have emerged as a pivotal class in materials science and nanotechnology due to their unique properties, including atomic-scale thickness, high surface-area-to-volume ratios, and highly tunable electronic and mechanical characteristics. These features have enabled a broad range of applications, spanning optoelectronic devices, flexible sensors, energy storage systems, and energy conversion technologies. Among the widely studied 2D materials, graphene [4], hexagonal boron nitride (hBN) [5], BC nanosheet [6], black phosphorus [7], and transition metal dichalcogenides (TMDs) [8] - [12] have demonstrated remarkable advancements. Recently, boron-carbon-nitride (BCN) monolayers [13] - [17] have attracted attention due to their excellent structural stability, mechanical robustness, and versatile electronic properties.

While previous research has explored BCN materials, critical knowledge gaps remain regarding their response to external perturbations, particularly mechanical strain and electric fields, which are essential for fine-tuning their properties in next-generation electronic devices. Some studies have investigated individual aspects of BCN monolayers but lacked a comprehensive approach to understanding their behavior under these external factors. Linh et al. [13] focused on the influence of doping on BCN monolayers under axial strain but did not systematically explore strain engineering as a means to modulate electronic properties. Ma et al. [14] studied atomic arrangements in BCN structures, identifying indirect semiconducting configurations without evaluating their adaptability for direct semiconductor applications. Yihua Lu et al. [15] examined BCN multilayers but primarily analyzed stacking-dependent electronic behaviors rather than monolayer responses to external stimuli. Similarly, Yadav et al. [16] investigated BCN's molecular adsorption characteristics but did not assess its intrinsic electronic tunability under applied fields. Wang et al. [17] explored substitutional doping techniques to manipulate BCN band gaps but overlooked strain engineering and field modulation as viable approaches to achieving desired electronic performance. Collectively, these studies provide foundational insights but fail to establish a systematic framework for BCN monolayer tuning under strain and electric fields, which is crucial for its integration into high-performance optoelectronic and flexible electronic systems.

To bridge this gap, the current study systematically evaluates BCN monolayers' structural stability, mechanical properties, and electronic characteristics under biaxial strain and external electric fields using first-principles calculations. Specifically, the research examines how strain influences mechanical behavior and band gap evolution while investigating the impact of electric fields on electronic properties. By identifying BCN monolayers' tunability, this study provides deeper insights into their adaptability, establishing a strong foundation for their integration into flexible electronics, optoelectronic devices, and field-controlled systems. The findings contribute to advancing the theoretical and practical understanding of BCN materials, reinforcing their potential for next-generation semiconductor technologies and innovative functional devices.

2. Simulation

This study leverages Density Functional Theory [18], [19], implemented via the Quantum Espresso (QE) software package [20], to perform all calculations. Vanderbilt pseudopotentials [21] are utilized to model electron interactions, while the exchange-correlation energies are computed using the Perdew-Burke-Ernzerhof (PBE) functional within the generalized gradient approximation (GGA) framework [22]. The plane wave basis set is examined with a cutoff energy of 70 Ry and a charge density threshold of 840 Ry. Sampling in the Brillouin zone is achieved through a $17 \times 17 \times 1$ k-point grid generated following the Monkhorst-Pack scheme [23].

The atomic structure models for the BCN monolayer are shown in Figure 1. Periodic boundary conditions are applied in all three spatial dimensions (x, y, and z). To eliminate inter-layer interactions along the z-axis, a vacuum region with a thickness of 30 Å is incorporated.

Structural optimization is performed using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) minimization algorithm under stringent conditions: stresses are constrained to below 5×10^{-3} GPa, and forces are minimized to less than 10^{-7} Ry/au at a temperature of 0 K. Elastic constants are derived through the Thermo-Pw module [24].

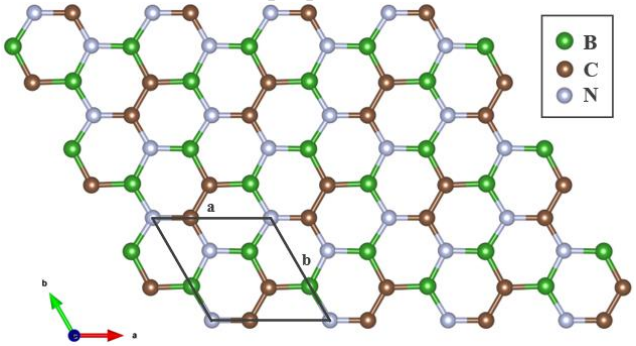

Figure 1. *The optimal structure of the BCN monolayer*

The mechanical response of the crystalline structure under strain in the x, y, and biaxial directions is quantified using the equation (1):

$$\varepsilon = (a - a_0)/a_0 * 100\% \quad (1)$$

where a and a_0 denote the lattice vectors before and after strain application, respectively. Strain levels ranging from 0% to 30%, in increments of 2%, are applied to the material. Following each deformation step, structural optimization is conducted to ensure stabilization, with residual stress components maintained below 5×10^{-2} GPa.

Furthermore, to explore the influence of electric fields on the energy band structure of the BCN monolayer, band structure calculations are performed under electric fields varying between -1.0 V/Å and +1.0 V/Å with a step of 0.2 V/Å.

3. Results and discussion

3.1. Structural stability

This study explores four distinct two-dimensional BCN material monolayers, as illustrated in Figure 1. The values obtained for lattice constants strongly agree with previously reported data [25] with a deviation of no more than 1%. Specifically, the lattice constants are determined to be $a = b = 4.35$ Å. The mechanical properties of the BCN structure include C_{11} = 194.17 GPa, C_{12} = 42.81 GPa, C_{66} = 74.66 GPa.

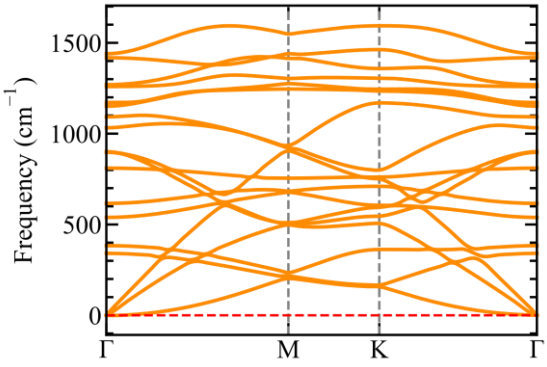

Figure 2. *Phonon dispersion curves of BCN monolayer materials in the Brillouin region*

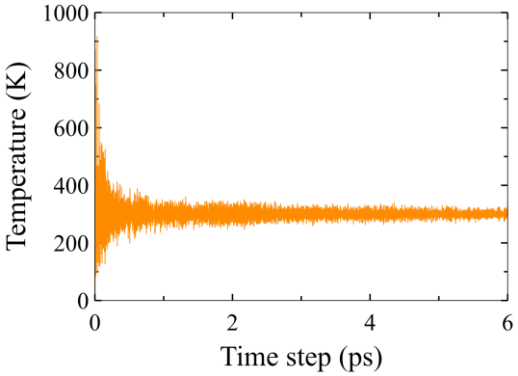

Figure 3. *Dynamic equilibrium graph of BCN monolayer using AIMD algorithm*

Three distinct stability criteria- dynamic, mechanical, and thermodynamic - are employed to evaluate the BCN monolayer structure's stability thoroughly.

Firstly, dynamic stability, Phonon lattice oscillations serve as the basis for assessing dynamic stability. As depicted in Figure 2, the BCN monolayer exhibits eighteen vibrational branches, including three low-frequency acoustic branches and fifteen high-frequency optical branches, corresponding to six atoms in a unit cell. The absence of negative frequency oscillations throughout the Brillouin zone attests to the high dynamic stability of the structure, with a maximum vibration frequency of 1594 cm^{-1}.

Secondly, mechanical stability is evaluated through elastic constants using the Born criterion, which stipulates that the $C_{11} > |C_{12}| > 0$ and $C_{66} > 0$ [26]. The computed results confirm that the BCN monolayer satisfies these criteria, affirming its mechanical robustness.

Finally, thermodynamic stability is determined through ab initio molecular dynamics (AIMD) simulations conducted at 300 K. Figure 3 illustrates the structural integrity of the BCN monolayer under thermal conditions, demonstrating no signs of structural deterioration. These findings confirm the material's stability against thermal fluctuations.

Through comprehensive analyses encompassing dynamic, mechanical, and thermodynamic criteria, the BCN monolayer is shown to exhibit exceptional stability, qualifying it for further scientific inquiry.

3.2. Mechanical properties

Figure 4 illustrates the stress-strain behavior of the BCN monolayer. As a two-dimensional material, stress is calculated as the product of unit cell stress (N/m) and unit cell thickness (30 Å). The stress-strain relationship reveals consistent trends under biaxial strain (ε_{bia}). For tensile strains up to ε_{bia} = 16%, the material exhibits a progressive increase in stress, peaking at a maximum stress of 25.73 N/m at ε_{bia}= 16%.

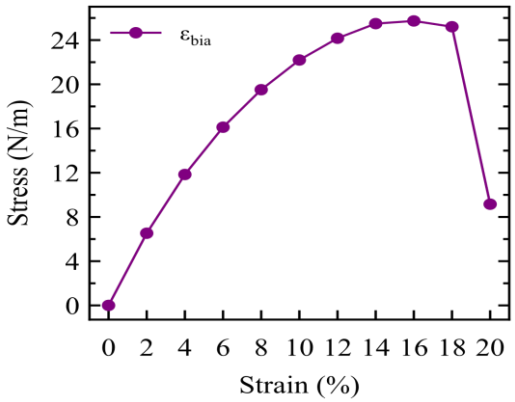

Figure 4. *The relationship between mechanical strain and stress of the BCN monolayer*

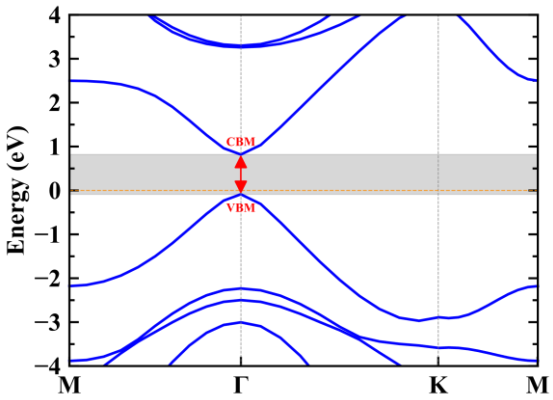

Figure 5. *Energy band structures of the BCN monolayer using the PBE functional*

To further characterize the strength and stability of the BCN material family, cohesive energy calculations were performed using the following formula (2):

$$E_{coh} = \frac{n_B E_B + n_C E_C + n_N E_N - E_{tot}}{n_B + n_C + n_N} \quad (2)$$

where, E_B, E_C, E_N, and E_{tot} represent the energies of the B, C, and N atoms and the total energy of the BCN structure, respectively. The variables of n_B, n_C, and n_N denote the atomic quantities of B, C, and N. The calculated cohesive energy (E_{coh}) in the natural state was 8.27 eV/atom, indicating robust binding within the BCN monolayer structures.

3.3. Electronic properties

To examine the electronic properties of the BCN monolayer, band gap energies were calculated using the PBE functional, as depicted in Figure 5. The results reveal the structure's

direct semiconductor characteristics, with a band gap energy of E_g = 0.90 eV, measured from the Valence Band Maximum (VBM) to the Conduction Band Minimum (CBM). These findings align with previous studies [25] confirming their reliability.

3.3.1. Effect of strain on electronic properties of BCN monolayer

The impact of biaxial strain on the band gap energy is illustrated in Figure 6, which contains eight subplots arranged sequentially. The band gap energy progressively increases from 0.916 eV at 2% strain to 1.747 eV at 16% strain, demonstrating a clear upward trend with rising strain levels. This adaptability highlights the exceptional ability of the BCN monolayer to modify its electronic properties through mechanical strain.

Remarkably, under natural conditions and applied strain, the BCN structure retains its direct semiconductor nature at the Gamma point, showcasing its structural and electronic stability. The gradual transformation of the band structure presents significant opportunities for designing advanced materials with enhanced functionalities. BCN material's tunable band gap via strain application holds immense promise for various applications, including optoelectronic devices, flexible sensors, and integrated electronic components.

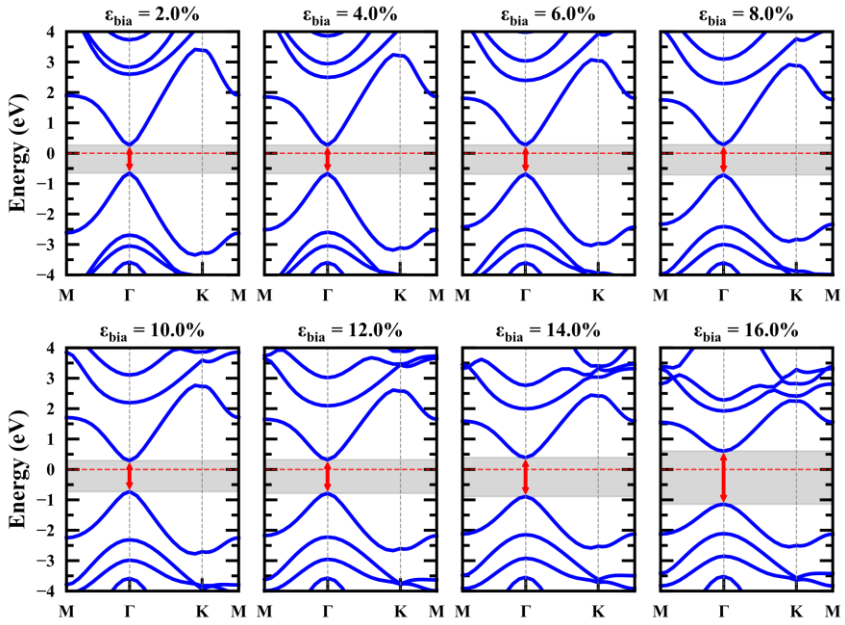

Figure 6. *Energy band structures under biaxial strains for the BCN monolayer*

Moreover, Figure 7 highlights the correlation between biaxial strain and the band gap energy. The data indicates a substantial increase in band gap energy from 0.905 eV at 0% strain to 1.747 eV at 16% strain, representing a near-exponential rise. This trend suggests potential applications in optoelectronics, such as developing sensitive sensors and solar energy components. These findings advance the study of materials science and pave the way for innovative solutions in the mechanical tuning of electronic properties.

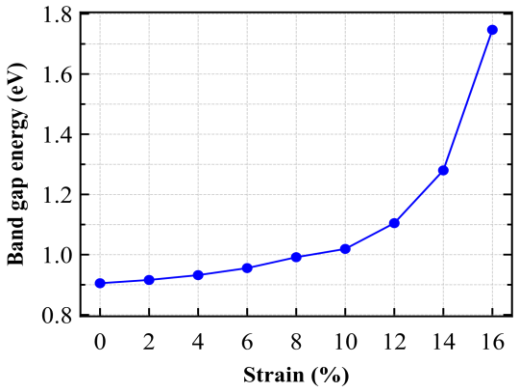

Figure 7. *Effect of biaxial strain on band gap energies of the BCN monolayer*

3.3.2. Effect of electric field on electronic properties of BCN monolayer

The influence of an external electric field on the band gap energy was investigated, with results depicted in Figure 8. As the electric field strength varies from -1.0 V/Å to +1.0 V/Å, the BCN monolayer maintains its direct band gap nature at the Gamma point, a critical attribute for optical and electronic applications. The most significant band gap reduction occurs under an electric field of -1.0 V/Å, with a decrease of approximately 79.55% compared to its value at 0.0 V/Å. For other field strengths, reductions remain below 8.51%.

Additionally, the symmetrical change in the band gap as the electric field transitions from negative to positive reflects the intrinsic atomic symmetry of the BCN monolayer. This remarkable ability to modulate electronic properties under varying field strengths underscores its suitability for applications in flexible electronics, sensors, and electric field-controlled systems.

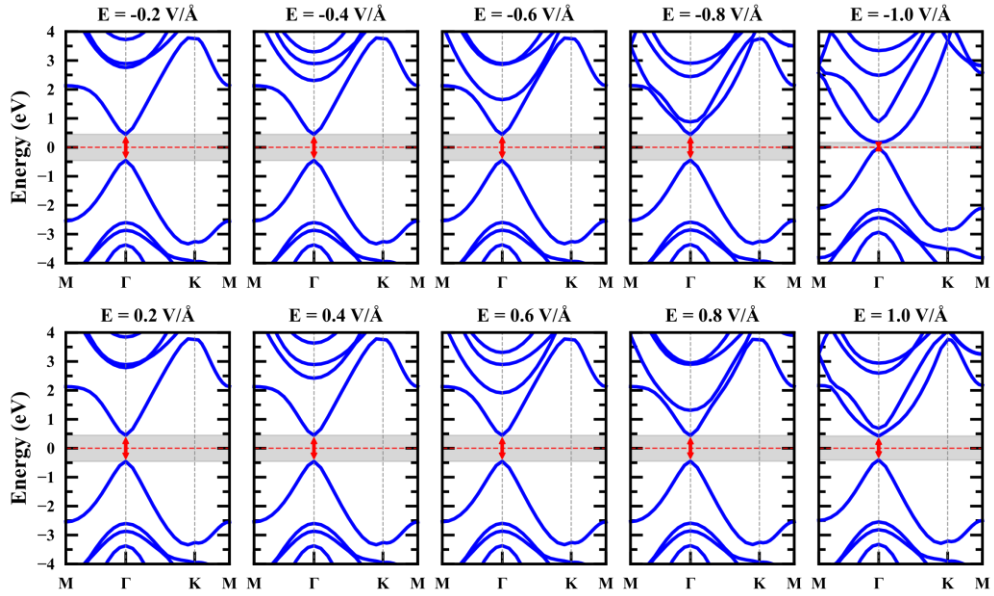

Figure 8. *Energy band structures at different electric field strengths for the BCN monolayer*

4. Conclusion

The BCN monolayer exhibits exceptional structural stability, confirmed through dynamic, mechanical, and thermodynamic analyses. Its robust framework ensures suitability for further exploration and applications.

In terms of mechanical properties, the material demonstrates impressive strength, reaching a peak stress of 25.73 N/m under 16% biaxial strain, surpassing comparable materials. This highlights its potential for flexible devices and mechanical sensors.

Regarding electronic properties, the BCN monolayer maintains a direct semiconductor nature at the Gamma point with an initial band gap of 0.90 eV. Notably, its band gap is highly tunable, ranging up to 1.747 eV under mechanical strain and decreasing by approximately 79.55% under an electric field of -1.0 V/Å.

With its adjustable electronic characteristics and structural stability, the BCN monolayer presents vast opportunities for optoelectronic devices, flexible sensors, and electric field-controlled applications, paving the way for innovations in advanced materials science.

REFERENCES

[1] M. Marian, D. Berman, D. Nečas, N. Emani, A. Ruggiero, and A. Rosenkranz, "Roadmap for 2D Materials in Biotribological/Biomedical Applications-A Review," *Adv. Colloid. Interf. Sci.*, vol. 307, Sep. 2022, doi: 10.1016/j.cis.2022.102747.

[2] P. Kumbhakar *et al.*, "Prospective applications of two-dimensional materials beyond laboratory frontiers: A review," *iScience*, vol. 26, no. 5, May 2023, Art. no. 106671, doi: 10.1016/j.isci.2023.106671.
[3] D. Akinwande *et al.*, "A Review on Mechanics and Mechanical Properties of 2D Materials-Graphene and Beyond," *Extreme Mech Lett.*, vol 13, May 2017, doi: 10.1016/j.eml.2017.01.008.
[4] C. Ye and Q. Peng, "Mechanical Stabilities and Properties of Graphene-like 2D III-Nitrides: A Review," *Crystals*, vol. 13, no. 1, 2023, doi: 10.3390/cryst13010012.
[5] S. Thomas, M. S. Manju, K. M. Ajith, S. U. Lee, and M. A. Zaeem, "Strain-induced work function in h-BN and BCN monolayers," *Physica E. Low Dimens. Syst. Nanostruct*, vol. 123, Sep. 2020, doi: 10.1016/j.physe.2020.114180.
[6] L. Zhu *et al.*, "Tunable electronic and optical properties of two-dimensional SnTe/InBr van der Waals heterostructures: A first-principles study," *Surfaces and Interfaces*, vol. 56, Jan. 2025, doi: 10.1016/j.surfin.2024.105715.
[7] Q. Wei and X. Peng, "Superior mechanical flexibility of phosphorene and few-layer black phosphorus," *Appl. Phys. Lett.*, vol. 104, no. 25, Jun. 2014, doi: 10.1063/1.4885215.
[8] S. Joseph *et al.*, "A review of the synthesis, properties, and applications of 2D transition metal dichalcogenides and their heterostructures," *Mater Chem. Phys.*, vol. 297, Mar. 2023, Art. no. 127332, doi: 10.1016/j.matchemphys.2023.127332.
[9] S. Ahmed and J. Yi, "Two-dimensional transition metal dichalcogenides and their charge carrier mobilities in field-effect transistors," *Nanomicro Lett.*, vol. 9, no. 4, pp. 1–23, Oct. 2017, doi: 10.1007/s40820-017-0152-6.
[10] L. Meng, Y. Ma, K. Si, S. Xu, J. Wang, and Y. Gong, "Recent advances of phase engineering in group VI transition metal dichalcogenides," *Tungsten*, vol. 1, pp. 46–58, 2019, doi: 10.1007/s42864-019-00012-x.
[11] X. Yin *et al.*, "Recent developments in 2D transition metal dichalcogenides: Phase transition and applications of the (quasi-)metallic phases," *Chemical Society Reviews*, vol. 18, 2021, doi: 10.1039/d1cs00236h.
[12] A. A. Tedstone, D. J. Lewis, and P. O'Brien, "Synthesis, Properties, and Applications of Transition Metal-Doped Layered Transition Metal Dichalcogenides," *Chem. Mater*, vol. 28, pp. 1965-1974, Apr. 2016, doi: 10.1021/acs.chemmater.6b00430.
[13] T. H. Dinh, H. L. Nguyen, and V. T. Do, "DFT Study on the Electronic and Mechanical Properties of BCN Monolayer," *Lecture Note in Networks and Systems*, vol. 943, pp. 472–477, 2024, doi: 10.1007/978-3-031-62238-0_49.
[14] Z. Ma, C. Tang, and C. Shi, "A New BCN Compound with Monoclinic Symmetry: First-Principle Calculations," *Materials*, vol. 15, no. 9, May 2022, doi: 10.3390/ma15093186.
[15] Y. Lu, Y. Yu, X. Zhu, and M. Wang, "Two predicted two-dimensional BCN structures: A first-principles study," *Physica. E. Low Dimens. Syst. Nanostruct.*, vol. 125, Jan. 2021, doi: 10.1016/j.physe.2020.114413.
[16] V. K. Yadav, S. H. Mir, and J. K. Singh, "Density Functional Theory Study of Aspirin Adsorption on BCN Sheets and their Hydrogen Evolution Reaction Activity: a Comparative Study with Graphene and Hexagonal Boron Nitride," *ChemPhysChem*, vol. 20, no. 5, pp. 687–694, Mar. 2019, doi: 10.1002/cphc.201801173.
[17] J. Wang and X. Luo, "Theoretical Investigation of the BCN Monolayer and Their Derivatives for Metal-free CO2 Photocatalysis, Capture, and Utilization," *ACS Omega*, vol. 9, 2024, doi: 10.1021/acsomega.3c07795.
[18] R. G. Parr and W. Yang, *Density Functional Theory of Atoms and Molecules*, Oxford: Oxford University Press, 1989.
[19] R. M. Dreizler and E. K. U. Gross, *Density Functional Theory*, Berlin: Springer, 1990.
[20] P. Giannozzi *et al.*, "QUANTUM ESPRESSO: A modular and open-source software project for quantum simulations of materials," *Journal of Physics Condensed Matter*, vol. 21, no. 39, 2009, doi: 10.1088/0953-8984/21/39/395502.
[21] D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism," *Phys. Rev. B*, vol. 41, Apr. 1990, doi: 10.1103/PhysRevB.41.7892.
[22] J. P. Perdew, K. Burke, and M. Ernzerhof, "Generalized Gradient Approximation Made Simple," *Phys. Rev. Lett.*, vol. 77, Oct. 1996, doi: 10.1103/PhysRevLett.77.3865.
[23] H. J. Monkhorst and J. D. Pack, "Special points for Brillonin-zone integrations," *Phys. Rev. B*, vol. 13, Jun. 1976, doi: 10.1103/PhysRevB.13.5188.
[24] A. D. Corso, "Clean Ir(111) and Pt(111) electronic surface states: A first-principle fully relativistic investigation," *Surf. Sci.*, vol. 637–638, pp. 106–115, Jul. 2015, doi: 10.1016/j.susc.2015.03.013.
[25] A. Bafekry *et al.*, "A novel two-dimensional boron-carbon-nitride (BCN) monolayer: A first-principles insight," *J. Appl. Phys.*, vol. 130, no. 11, Sep. 2021, doi: 10.1063/5.0062323.
[26] F. Mouhat and F. X. Coudert, "Necessary and sufficient elastic stability conditions in various crystal systems," *Phys. Rev. B Condens. Matter. Mater. Phys.*, vol. 90, no. 22, Dec. 2014, doi: 10.1103/PhysRevB.90.224104.