A wide-bandgap graphene-like structure C\textsubscript{6}BN with ultra-low dielectric constant\(^{†}\)

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This study introduces a new wide-bandgap graphene-like structure, denoted as C\textsubscript{6}BN, achieved by incorporating an eight-electron BN pair, substantially modifying its electronic properties. Utilizing extensive density functional calculations, we comprehensively analyzed the stability, electronic structure, mechanical properties, and optical-electrical characteristics of C\textsubscript{6}BN. Our investigations reveal the material's exceptional thermodynamic, mechanical, and dynamic stability. Notably, the calculated wide bandgap of 2.81 eV in C\textsubscript{6}BN, supported by analyses of energy levels, band structures, and density of states, positions it as a promising two-dimensional wide-bandgap semiconductor. Additionally, C\textsubscript{6}BN exhibits isotropic mechanical features, highlighting its inherent flexibility. Remarkably, our calculations indicate an ultra-low dielectric constant (k = 1.67) for C\textsubscript{6}BN, surpassing that of well-established third-generation semiconductors. Further exploration into the thermoelectric properties of C\textsubscript{6}BN demonstrates its promising performance, as evidenced by calculations of thermal conductivity (κ), power factor (P), and Seebeck coefficient (S). In summary, our findings underscore the significant potential of the proposed C\textsubscript{6}BN structure as a flexible two-dimensional material poised to drive future advancements in electronic and energy-related technologies.

Introduction

To leverage the potential of sub-10 nanometer integrated circuit components, developing interlayer low-dielectric-constant (low-k) materials with high thermal conductivities is crucial.\(^{1−4}\) As dielectric layers diminish in thickness, challenges such as electronic crosstalk and capacitive signal delay hinder device performance. Addressing these issues necessitates the creation of mechanically robust, thermally stable, few-nanometer-thick materials with low-k (k < 2.4), and ultra-low-k (k < 1.9) characteristics.\(^{4,5}\) The two main low-k dielectric materials investigated are organic materials with limited polarizability and porous oxides with large free volumes.\(^{6,7}\) However, existing low-k materials suffer from high thermal resistances due to disordered morphologies and high porosities,\(^{8−10}\) limiting the efficiency of high-power-density chips.

The exploration and development of novel materials with exceptional properties have been instrumental in shaping modern science and technology. The emergence of two-dimensional (2D) materials after isolating high-ordered graphene has garnered widespread attention due to their unique layered structure and exceptional properties. Two-dimensional semiconductors (2DSCs) have emerged as promising candidates for low-dimensional electronics,\(^{11,12}\) topological insulators,\(^{13}\) wearable devices, and valleytronics.\(^{14}\) They have become the focal point in condensed matter and materials research owing to their distinctive structural properties compared to traditional semiconductors. Notably, investigating 2D GaN and AlN materials as representatives of new-generation wide-bandgap semiconductor materials has become a hot topic,\(^{15−18}\) exhibiting excellent characteristics for diverse applications.

In recent years, substantial progress has been achieved in designing, synthesizing, and isolating various 2DSC materials, including transition metal dichalcogenides (TMDs), black phosphorus, and hexagonal boron nitride.\(^{19−22}\) Tunable bandgaps in TMD semiconductors\(^{19}\) have shown promise in designing transistors with improved on/off ratios, paving the way for enhanced electronic and optoelectronic devices. Fabrication...
methods, such as chemical vapor deposition, mechanical exfoliation, and molecular beam epitaxy, have been developed to create high-quality 2D semiconductor materials. However, challenges in scalability, stability, contact resistance, defects, uniformity, and integration persist, with stability being a crucial prerequisite. Many 2D semiconductors, such as h-BN, g-C\(_3\)N\(_4\), transition metal dichalcogenides, hydrogenated layered silicon, and free-standing single-layer SnS and SnSe, are sensitive to environmental conditions and can degrade over time due to oxidation, moisture, and heat.\(^{19,23–25}\) Therefore, developing encapsulation techniques to protect these materials from external factors and ensure long-term stability is necessary. Consequently, there is a pressing need to develop newly stable 2D semiconductors to overcome these challenges and fully exploit their potential.\(^{26,27}\)

Graphene, renowned for its remarkable stability and flexibility, has garnered substantial attention in nanomaterials and flexible electronic materials. Despite these virtues, its inherent zero bandgap constrains its utility in numerous electronic applications. This study explores a novel approach to induce a bandgap in graphene-like structures by introducing an eight-electron BN pair. This transformative process gives rise to a new semiconductor material, C\(_6\)BN. Through rigorous first-principle calculations, we scrutinize the robust stability of the C\(_6\)BN structure, affirming the feasibility of this emerging semiconductor material. Furthermore, we delve into the optical-electrical properties of C\(_6\)BN, revealing its promising performance through calculated metrics such as dielectric constant (\(\varepsilon\)), thermal conductivity (\(\kappa\)), power factor (\(P\)), and Seebeck coefficient (\(S\)).

**Results and discussion**

**Stability and structure of C\(_6\)BN**

A bandgap-opening strategy was implemented by integrating an eight-electron BN pair, forming the bandgap-opening structure denoted as C\(_6\)N\(_8\), which exhibits exceptional stability (Fig. 1d and e).\(^{28}\) To explore the viable configurations, eight isomers of C\(_6\)BN, representing isoelectronic species of the graphene-like structure C\(_8\), were examined (Fig. S1, ESI\(^\dagger\)). Post-optimization, most displayed substantial distortion, except for one particular isomer highlighted in Fig. S1(c) (ESI\(^\dagger\)), exhibiting the lowest relative energy.

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Subsequent first-principles calculations unveiled the outstanding stability of this specific isomer, illustrated in Fig. 1(a) and (b). In this configuration, two threefold \(sp^2\)-hybridization carbon atoms were replaced by boron and nitrogen atoms, contributing to its structural robustness. Following optimization, the lattice constant of the stable C\(_6\)BN was determined to be 7.08 Å (Fig. 1c), aligning with the \(P6_3/m\) space group (no. 187). Notably, this lattice constant surpasses C\(_8\) (\(|\vec{a}| = |\vec{b}| = 6.96\) Å), characterized by the \(P6_3/m\) space group (no. 191). This lattice structure, referred to as C\(_6\)BN in subsequent discussions (Fig. 1a), boasts the highest symmetry among the eight isomers (Fig. S1, ESI\(^\dagger\)), a likely contributor to its exceptional stability. The vacuum thickness along \(\vec{c}\) is set as 25 Å, effectively avoiding interlayer interactions.\(^{29}\)

To scrutinize the lattice dynamic stability of C\(_6\)BN, phonon band structures were meticulously computed using density-functional perturbation theory (DFPT), as implemented in the Phonopy code.\(^{30}\) As depicted in Fig. 1(f), no imaginary modes are evident across the entire 2D reciprocal space, affirming the

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**Fig. 1** Top view of geometries for (a) C\(_6\)BN and (d) C\(_8\), side view of geometries for (b) C\(_6\)BN and (e) C\(_8\), (c) lattices optimizations for C\(_6\)BN and (f) phonon spectra of optimized C\(_6\)BN. The carbon, nitrogen, and boron atoms are in brown, purple, and golden yellow, respectively. The red box marks the primitive cell for (a) C\(_6\)BN and (d) C\(_8\).
robust lattice dynamical stability of C₆BN. This observation aligns with its isoelectronic counterpart’s previously established excellent stability, C₈. We conducted ab initio molecular dynamics (MD) simulations to gauge the dynamic stability further (Fig. 2). The canonical ensemble and Nosé–Hoover thermostat were employed at 1000 K for 3000 fs and 2000 K for 10 000 fs.

As illustrated in Fig. 2(a) and (d), the maximum energy difference recorded is 1.71 eV at 1000 K and 2.46 eV at 2000 K. Following the MD simulation for 3000 fs at 1000 K, the geometry of the doped C₆BN structure (Fig. 2(c)) remains remarkably stable. However, at 2000 K, the structure undergoes evident distortion, with observable changes in the primitive cell (Fig. 2(f)). These outcomes suggest that the doped structure of C₆BN remains undistorted at elevated temperatures up to 1000 K. In a parallel scenario, a previous report noted the stability of the graphene-like carbon matryoshka C₁₄ at 500 K due to specific three-center two-electron π bonds, implying a delocalized electronic configuration contributing to the stability of C₆BN.

The phase stability of C₆BN was assessed through the cohesive energy, a key indicator of thermodynamic stability and propensity for decomposition into constituent elements. The cohesive energy per atom in C₆BN is determined as follows:

\[ E_{\text{coh}} = \frac{E(\text{C}_6\text{BN}) - 6E_C - E_N - E_B}{8} \]

where \( E(\text{C}_6\text{BN}) \), \( E_C \), \( E_N \), and \( E_B \) are the total energy of C₆BN, a single C atom, a single N atom, and a single B atom, respectively, obtained through ab initio DFT calculations; 6 and 8 denotes the number of carbon atoms and total number of atoms in C₆BN. Previous studies have reported cohesive energy values for various two-dimensional materials, such as single-layer graphene (−7.91 eV per atom), δ-borophene (−6.21 eV per atom), β₁₂-borophene (−6.25 eV per atom), and h-BN (−8.69). In the case of C₆BN, the calculated cohesive energy is −7.84 eV per atom, indicating its favorable thermal stability. Remarkably, C₆BN exhibits even greater stability than the well-established borophene, suggesting its potential for synthesis and isolation in future experiment endeavors.

Additionally, the mechanical stability of graphene-like C₆BN was also considered. For any mechanically stable 2D material, a necessary requirement is that \( C_{11}C_{22} - C_{12}^2 > 0 \) and \( C_{66} > 0 \), although it is not a sufficient condition. The stiffness matrices of C₆BN are shown in Table S1 (ESI†), and it can be observed that there are only two independent elastic constants for C₆BN, with \( C_{11} = C_{22} = 130.151 \text{ N m}^{-1} \), \( C_{12} = 42.560 \text{ N m}^{-1} \), and \( C_{66} = 43.795 \text{ N m}^{-1} \). These results meet the requirements of stable 2D materials, indicating the excellent mechanical stability of graphene-like C₆BN. Furthermore, the change in energy is small with applied strain, confirming the mechanical stability of the targeted 2D structure. The eigenvalues of the stiffness constants of C₆BN exhibit a positive band gap, further confirming its mechanical stability. Moreover, compared to previously reported L-2Gy and aGy structures, the mechanic stability of C₆BN is significantly higher based on the eigenvalues of the stiffness constants.

Graphene-like C₆BN exhibits excellent chemical, thermal, mechanical, and lattice dynamical stability. Furthermore, the previous reports have indicated good stability of the several graphene-like carbon materials, like carbo-graphene, carbo-benzene, acetylenic modified graphene. Therefore, it is
predicted to be another stable derivative of graphene-like Gy. 

Although there are no experimental details on stable C₆BN in the present or previous work, several reasonable experimental methods, including chemical vapor deposition (CVD), close-spaced vapor transport (CVT), flux growth, high-pressure flux method, and epitaxy growth, have been successfully used to synthesize two-dimensional graphene-like structures.

**Electronic structure of C₆BN**

As illustrated in Fig. 3(d), the boron and nitrogen atoms are strategically positioned at threefold points, distinctly marked within blue circles. In the optimized C₆BN structure, the lengths of the C–N, C–B, and C–C bonds are equivalent. A comparative examination with recognized bond lengths, as depicted in Fig. 3(a), unveils that the C–B bonds exhibit characteristics akin to single bonds. In contrast, the C≡C bonds reflect attributes of triple bonds, indicating sp²- and sp-hybridization states for boron and carbon atoms, respectively. The C=N bonds manifest features of double bonds, with each nitrogen atom forming three C–N bonds. This fact implies a clear presence of delocalized electrons within the C–N bonds of the C₆BN plane network, substantiated by the atomic Bader charges highlighted in Fig. 3(b).

![Figure 3](image-url)  
**Fig. 3**  
(a) Bond lengths for C–N, C–B, and C–C; (b) Bader charges of C, N, and B atoms marked in (d) structure of C₆BN; and (c) charge density for C₆BN. The acknowledged bond lengths are also given in blue and green for reference. In (a), bond lengths marked in blue are for C–N single bond, C–B single bond, and C–N double bond, and they are in green for C≡N double bond and C≡C triple bond. The isosurface level for charge density is 0.50.

The present work focuses on the electronic structure of C₆BN and its potential as a stable derivative of graphene-like materials.
The bonding pattern observed in L-2Gy is consistent with that found in Gy, aligning with the annulene nature. All nitrogen and boron atoms experience electron loss, while only carbon atoms bonded to boron atoms gain electrons. Thus, the donated electrons from nitrogen atoms localize at the carbon atoms connected to boron atoms. Furthermore, the charge density analysis, as depicted in Fig. 3(c), also reveals distinctive features of delocalized electronic structures, contributing to the overall stability of C₆BN. Notably, graphene’s exceptional stability is attributed to the extensive delocalization of π electrons. The proposed L-1Gy, recognized as the first graphene-like Gy with delocalized electronic structures, further reinforces this notion. Moreover, optimizing atomic positions in a supercell in spin polarization indicated that the optimal structure of C₆BN possesses close-shell electronic structure confirming the absence of Jahn–Teller distortion in C₆BN.

As illustrated in Fig. 4(a), the electronic band structure of C₆BN exhibits a direct band gap of 1.81 eV according to the PBE functional, indicating its semiconductor characteristics. However, it is essential to note that the PBE functional underestimates the bandgap of semiconductors and insulators, as reported in previous studies. To ensure a more accurate calculation of its band structure, we employed the hybrid functional HSE06, as shown in Fig. 4(b). The HSE06 results indicate an underestimation of the energy levels of the valence and conduct bands. Consequently, C₆BN is identified as a wide-bandgap semiconductor with a band gap of 2.81 eV, slightly lower than that of SiC (3.20 eV) and GaN (3.39 eV).

Further insights into the electronic structure of C₆BN were gained by examining the density of states (DOS), as depicted in Fig. 4(c)–(f). The DOS analysis suggests that carbon and nitrogen atoms primarily contribute to the valence band, while carbon and boron atoms mainly influence the conduct band. This observation aligns with mapping the valence band maximum (VBM) and conduct band minimum (CBM) in Fig. 4(g) and (h). Additionally, the results on partial density of states (PDOS) indicate that the valence band and conduct band of C₆BN are predominantly derived from p orbitals. In graphene, consisting of sp²-hybridized carbon atoms, the delocalized π bond is solely contributed by p orbitals.

Considering the Bader charge analysis and the presence of double bonds (C=O=C) and triple bonds (C≡C), it is evident that there is a lack of delocalized electrons on the boron atom. This further substantiates the semiconductor nature of C₆BN. Electronic localized function analysis was employed to delve deeper into the delocalized character. Fig. 4(i) illustrates that electrons are localized on the conjugate fragment, excluding the boron atoms due to their electron-drawing nature. The absence of boron atoms in the electronic localized fragment potentially contributes to the wide-bandgap semiconductor behavior of the material.

Mechanical properties of C₆BN

The mechanical properties of nanomaterials are pivotal in determining their diverse applications, spanning flexible devices, coating materials, and friction components. In the context of C₆BN, its mechanical behavior is characterized by two independent elastic constants: C₁₁, C₁₂, C₆₆, and C₁₂ = C₁₁, and C₆₆ = (C₁₁−C₁₂)/2 (Fig. 5a). Computational findings reveal that C₆BN, with its hexagonal symmetry and two-dimensional lattice structure, exhibits isotropic mechanical properties, justifying the adoption of an isotropic shell model akin to graphene, where the modulus determines stiffness.

By Hooke’s law, Young’s modulus (E) and shear modulus (G) of C₆BN were calculated as 116.23 N m⁻¹ and 43.80 N m⁻¹, respectively (Fig. 5b and c). Notably, the modulus of C₆BN is lower than that of single-layer graphene (approximately E of 340 N m⁻¹ and G of 60 GPa). Furthermore, 2D C₆BN exhibits a significantly lower Young’s modulus compared to carbon nanotubes and BN-doped nanotubes. Moreover, the shear strength of C₆BN was determined to be higher than that of carbon nanotubes (41–54.4 GPa) and lower than that of carbon diamond (93 GPa), c-BN (70.5 GPa), and BC₂N-2 (68.8 GPa). These findings underscore the heightened flexibility of the two-dimensional graphene-like C₆BN, suggesting its promising applications in flexible devices.

Poisson’s ratio (ν) is commonly used to characterize the elastic properties of materials. In the case of C₆BN, we calculated the Poisson’s ratio (ν) based on the following equation:

\[ \nu = \frac{E}{2G} - 1, \]

by using the previously determined Young’s modulus (E) and Shear modulus (G) from the stiffness tensor. The calculated Poisson’s ratio (ν) for two-dimensional C₆BN was found to be 0.33 (Fig. 5d), indicating significantly lower transverse elasticity than graphene. Previous studies have shown that the Poisson’s ratio of graphene is temperature-dependent, and the values of
Poisson’s ratio vary accordingly, 0.21 at 300 K, 0.32 at 800 K, and 0.34 at 1700 K.\textsuperscript{58}

**Optical-electrical properties of C\textsubscript{6}BN**

As microprocessors continue to undergo miniaturization, the need for low-dielectric-constant (low-\(k\)) materials becomes increasingly crucial to mitigate issues such as electronic cross-talk, charge accumulation, and signal propagation delay.\textsuperscript{4,59} However, existing low-\(k\) dielectrics suffer from low thermal conductivities, primarily due to their disordered morphologies and high porosities, resulting in significant thermal resistances. This study investigates the properties of a wide-bandgap semiconductor C\textsubscript{6}BN, characterized as an ultra-low \(k\) two-dimensional material with a dielectric constant (\(k\)) of 1.67. Notably, this value is significantly lower than that of well-established third-generation semiconductors such as SiC (\(k = 9.7\)) and GaN (\(k = 9.8\)) as shown in Fig. 6(a) and (b).\textsuperscript{60,61}

It is worth noting that the critical breakdown field is generally proportional to the square of the bandgap. In comparison, acknowledged semiconductors such as Si (bandgap: 1.12 eV), GaAs (bandgap: 1.4 eV), InP (bandgap: 1.3 eV), SiC (bandgap: 3.2 eV), and GaN (bandgap: 3.39 eV) exhibit critical breakdown fields of 300 kV cm\(^{-1}\), 400 kV cm\(^{-1}\), 500 kV cm\(^{-1}\), 2200 kV cm\(^{-1}\), and 3300 kV cm\(^{-1}\), respectively.\textsuperscript{59,60} Therefore, the wide bandgap of C\textsubscript{6}BN, measured at 2.81 eV, indicates a substantial critical breakdown field of approximately 2000 kV cm\(^{-1}\).

Additionally, several parameters determine the performance of thermoelectric (TE) characteristics, including thermal conductivity (\(k\)), power factor (\(P\)), and Seebeck coefficient (\(S\)), which serve as efficient measures for evaluating their thermoelectric capabilities. Fig. 6(c) depicts the relationship between electronic thermal conductivity (\(k_{el}/\tau\)) and chemical potential for C\textsubscript{6}BN. It is desirable to have low electronic thermal conductivity to achieve high thermoelectric performance. Consequently,

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**Fig. 6** (a) Recognized low dielectric constants for several organic compounds, inorganic compounds, and simple substances,\textsuperscript{58} and (b) dielectric function (\(k\)), (c) electronic thermal conductivity (\(k_{el}/W\) K\(^{-1}\) m\(^{-1}\) s\(^{-1}\)), (d) power factor (PF)/\(\mu W\) cm\(^{-1}\) K\(^{-2}\), and (e) Seebeck coefficient (\(S\))/\(\mu V\) K\(^{-1}\) for graphene-like two-dimension C\textsubscript{6}BN.
we observed a lower electronic thermal conductivity for C$_6$BN. The carrier concentration increases as the chemical potential rises within the range of $\mu < 0$ eV and $\mu > 1.5$ eV, with the maximum value of $k_{\nu}/e$ not exceeding $3.0 \times 10^{14}$ W K$^{-1}$ m$^{-1}$ s$^{-1}$. The Widemann-Franz law states that electronic thermal conductivity is directly proportional to the product of absolute temperature (in K) and electrical conductivity.$^{62}$ Another crucial parameter for characterizing thermoelectric behavior is the power factor (PF). Fig. 6(d) demonstrates that the PF value becomes zero when the chemical potential ranges from approximately 0 to 1.5 eV, indicating semiconductor characteristics. The maximum value of PF can exceed 22 $\mu$W cm$^{-1}$ K$^{-2}$. The Seebeck coefficient ($S$) also plays a vital role in determining a material’s thermoelectric (TE) efficiency. A high value of $S$ is desired for optimal TE device performance.

As shown in Fig. 6(e), the Seebeck coefficient values of 2936 $\mu$V K$^{-1}$ and $-2908$ $\mu$V K$^{-1}$, obtained at $\mu = 0.63$ eV and $\mu = 0.77$ eV respectively, are indeed significantly larger than those of graphene (80 $\mu$V K$^{-1}$), G-hBN (300 $\mu$V K$^{-1}$), and MoS$_2$ (2400 $\mu$V K$^{-1}$)$^{63,64}$ This enhancement in the Seebeck coefficient can be attributed to the wide-bandgap nature of C$_6$BN, which leads to a higher thermoelectric performance. A positive value of $S$ indicates the dominance of p-type dopants (e.g., B), while a negative value denotes the dominance of n-type dopants (e.g., N).$^{65}$ Based on our findings, the exceptional stability of C$_6$BN, coupled with its wide bandgap and ultra-low dielectric constant, makes it a promising candidate for addressing the challenges associated with low-k materials in microprocessors and thermoelectric devices. Furthermore, its considerable critical breakdown field ensures reliable performance even under high electric field conditions. Overall, the findings presented here highlight the potential of C$_6$BN as a valuable material for future electronic devices requiring efficient thermal management and reduced crosstalk effects.

Conclusion

In conclusion, our comprehensive investigation into the properties of C$_6$BN has revealed its immense potential as a flexible two-dimensional material for advanced electronic applications. Incorporating BN pairs into the carbon lattice introduces a wide-bandgap semiconductor with remarkable electronic, mechanical, and thermoelectric properties. Notably, the wide bandgap of 2.81 eV in C$_6$BN surpasses that of graphene, making it an attractive candidate for electronic devices that require efficient charge transport and insulation. Furthermore, the ultra-low dielectric constant of C$_6$BN ($k = 1.67$) exceeds that of well-known third-generation semiconductors, opening up new possibilities for high-frequency electronic devices. Moreover, our calculations have demonstrated the favorable thermal conductivity, power factor, and Seebeck coefficient of C$_6$BN, highlighting its potential as an efficient thermoelectric material. The exceptional stability, mechanical flexibility, and unique combination of properties make C$_6$BN an auspicious material for future advancements in flexible electronic technologies. The exploration of C$_6$BN paves the way for exciting avenues of further research and development, enabling the design and fabrication of innovative materials and devices that harness the exceptional properties of this novel material.

Calculational methods

The first-principle calculations in this study were performed using the Kohn-Sham density functional theory (DFT) as implemented in the Vienna ab initio simulation package (VASP).$^{66}$ The generalized gradient approximation (GGA), specifically the Perdew, Burke, and Ernzerhof (PBE) parameterization, described the exchange-correlation functional.$^{67}$ A gamma-centered $k$-points sample mesh of $7 \times 7 \times 1$ was used to relax the geometries. The plane-wave basis set with a kinetic energy cutoff of 400 eV was employed to expand the valence electron wave function. Convergence was achieved when the energy in the electronic self-consistent field (SCF) iterations reached a criterion of $1.0 \times 10^{-8}$ eV, and the force in ionic step iterations converged to $5.0 \times 10^{-3}$ eV. A vacuum slab of at least 20 Å was applied to eliminate interactions between the layers. The phonon dispersions of the stable structure were calculated using density-functional perturbation theory (DFPT) implemented in the Phonopy code, based on a $2 \times 2 \times 1$ supercell.$^{10,66}$ For the electronic structure calculations, the reciprocal space was sampled with a $k$-grid density of $30 \times 30 \times 1$ to balance accuracy and efficiency. To accurately determine the bandgap of the targeted structure, the hybrid functional of Heyd, Scuseria, and Ernzerhof (HSE06) was employed.$^{69}$ This is because the PBE functional tends to underestimate the bandgap of semiconductors and insulators, as indicated in previous reports. The mechanical and optical-electrical properties, such as elastic constants, Young’s modulus, Poisson’s ratio, dielectric constant ($\varepsilon$), thermal conductivity ($\kappa$), power factor ($P$), and Seebeck coefficient ($S$), were calculated using the VASPKIT package.$^{70}$ These computational methods and techniques were employed in this study to investigate the stability, electronic structure, mechanical features, and optical-electric properties of the 2D wide-bandgap semiconductor material C$_6$BN.

Author contributions

M. L., Y. Z., and B. L. finished all the DFT computations with the assistance from K. Y. and Y. Z. S. S. provide valuable discussion. Y. Z. and B. L. wrote the manuscript with revision by M. L. and J. Z. Q. W. conceived the project idea. B. W. and J. Z. supervised the project.

Data availability

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

Conflicts of interest

The authors declare no competing financial interests.
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