Penta fever going on: conductive Penta-BCN₄ with negative differential resistance (NDR)

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ABSTRACT: Pentagonal 2D structures, surpassing conventional hexagonal sheets, are gaining increasing attention due to their exceptional properties and diverse applications. In this study, we investigate penta-BCN₄, a ternary monolayer 2D penta structure with intrinsically exceptional properties. Using Density Functional Theory calculations, we found that penta-BCN₄ is a conductive material with mechanical, thermal, and dynamic stability. Penta-BCN₄ exhibits a high Young's modulus and a small Poisson ratio, which are isotropic in different directions. In contrast, penta-BCN, which has been previously studied, is mechanically anisotropic. We also discovered that one of the most intriguing properties of penta-BCN₄'s band structure is the phenomenon of negative differential resistance (NDR). To assess NDR more precisely, we computed the transport in the direction of the N-N bond in addition to the throughput in the direction of the lattice vector (a). The intrinsic NDR of the penta-BCN₄ monolayer, combined with its vanishing band gap, makes this material appealing for technological applications, as B, C, and N are abundant resources, light in mass, and environmentally safe. This research expands the possibilities of monolayer 2D penta structures into new avenues.

TOC GRAPHICS



KEYWORDS. Two dimensional materials, Penat structure, Penta-Graphene, Negative differential resistance, NDR,

In the realm of materials science and nanotechnology, two-dimensional (2D) materials have emerged as a transformative class of substances with profound implications for a broad spectrum of applications. In the 1930s, research into monolayer structures was initiated, propelled by Langmuir's seminal investigations on the deposition of alkali metal atoms onto metal films. His pioneering work established the cornerstone of surface science ¹. Extensive research has been carried out on elemental monolayers and 2D materials ever since. The investigation into the extraordinary electrical and thermal behavior of graphene² has reignited interest in layered 2D materials such as MXenes, chalcogenides, and transition metal oxides ³. The revelation of concealed phenomena and physics, such as non-trivial topology, has sparked this interest, ⁴ valleytronics, ⁵ high temperature ballistic conduction ⁶ and further optoelectronic ⁷ properties primarily arising from their 2D nature have recently been addressed in several reviews ⁸. Research into these newly proposed 2D materials has also revealed abundant data on material structureproperty relationships, thus providing novel insights into topics of technological significance, thereby establishing the foundation for their utilization across various domains, including metalion batteries ⁹, thermoelectricity ¹⁰, spintronic ¹¹, water splitting ¹², heterojunctions¹³, and gas sensors ¹⁴. Consequently, materials with atomic-scale thickness are increasingly sought after for a variety of potentially important applications in next-generation technology, including spintronics, advanced nanoelectronics, nanosensing, and more.

Mathematicians are familiar with the pentagon because of its association with the golden ratio (0.618) and its representation as the fifth Platonic solid, a dodecahedron comprising 12 pentagonal faces. Chemists have identified a number of pentagonal molecules, such as the five-membered sulfur-pnictogen ring SN_2P_2 , cyclopentane, pyrrole, thiophene, tetrathiafulvalene terthienyl ¹⁵, the aromatic pentagonal anion P_2N_3 ¹⁶, and fullerene C_{20} ¹⁷. In physics, the Euclidean plane does not

allow for the tessellation of regular pentagons due to the lack of five-fold rotational symmetry present in triangles, squares, and hexagons. As a result, using regular pentagons in 2D space does not allow for the creation of a perfect mosaic.

Two planar pentagonal configurations were among the fictitious forms of carbon that Balaban theoretically explored, as research interest in elemental materials has recently resurged among stacked 2D materials ¹⁸. Based on extensive theoretical calculations, a 2D monolayer carbon structure referred to as penta-graphene (PG)¹⁹ was hypothesized, which mimics the type-4 pentagonal tiling's mathematical structure and it may peeled off from T12-carbon²⁰. The addition of hydrogen molecules to a thin film of T12-carbon with 4-layer in 001 direction, as revealed by ab initio molecular dynamics (AIMD) calculations, leads to the breaking of C-C bonds. As a result, this leads to the separation of a PG sheet from the T12-carbon which is partially hydrogenated ¹⁹. Dehydrogenation can then be used to create pure PG sheet ²¹. Due to its remarkable properties and special atomic layout, PG has attracted significant attention and served as a new pattern for exploring monolayer 2D penta structures, leading to the prediction of various types of single atom pentagonal sheets (penta-germanene ²², penta-tellurene ²³, and penta-silicene ^{24, 25}) to pentagonal sheets with binary atomic types (penta-CNP ²⁶, penta-B₂C ²⁷, penta-BN₂ ¹⁴, penta-CN₂ ²⁸, penta-PdSe2 ²⁹, etc.), ternary atomic types (penta-BCN ³⁰, penta-PdSSe ³¹, , penta-Zn₂C₂P₂ ³², etc.), and their fluorinated/hydrogenated derivatives ³³. Primarily, theoretical investigations based on density functional theory (DFT) and classical molecular dynamics (MD) were conducted to predict novel configurations of penta materials and analyze their properties. Utilizing theoretical approaches such as cohesive energy analysis, phonon dispersion calculations, and AIMD investigations, a wide range of penta structures with various elemental compositions were predicted. To the best of our knowledge, more than 126 binary and ternary monilayer based on pentagons have been

predicted. Many of them can be created by completely or partially swapping out the carbon atom in the PG's atomic configuration ^{29, 34}. Penta- PdS₂ ³⁵, penta-PdSe₂ ^{29, 34}, penta-NiN₂ ³⁶, and pentasilicene nanoribbons ³⁷ have been successfully synthesized. Interesting physical and chemical characteristics of these pentagon-based 2D materials, consisting of a negative Poisson's ratio ^{14, 19,} ^{26, 38}, second harmonic generation ³⁹, spontaneous polarization and intrinsic piezoelectricity ^{26, 30,} ⁴⁰, ferroelectricity ²⁵, and ferromagnetism ⁴¹.

Carbide penta structures demonstrate the highest stability among all predicted penta materials to date. A special role in the stability of carbides is also played by C_2 dimers, which, unlike individual carbon atoms, are a crucial building block in the growth of many carbon structures ⁴². Penta-CN₂ sheet ²⁸ has significant energy density (4.41 kJ/g), and exhibits robust mechanical properties, including a Young's modulus of 319 N/m, surpassing that of h-BN. Furthermore, the band structure of penta-CN₂ reveals a symmetry-protected double degeneracy. Because of its distinctive ⁴³ shape, the penta-CN₂ sheet likewise exposed for having high lattice thermal conductivity (660.71 W m⁻ ¹K⁻¹), proving wrong the theory that lone-pair electrons have poor thermal conductivity in the lattice. Penta-BN2¹⁴ penta-CB2²⁷ were systematically studied in parallel with the study of a penta-CN₂ sheet. whereas the penta-BN₂ doesn't have a bandgap, making it conductive, and it also exhibits strong elastic properties with a Young's Modulus of 271 N/m, and the penta-CB₂ is an indirect semiconductor with a bandgap of 2.47 eV, and it's also a promising candidate for use as an anode for Li/Na batteries due to its high theoretical capacity of 1594 mA.h.g⁻¹ for Li and 2391 mA.h.g⁻¹ for Na⁴⁴. Due to their intriguing properties, penta-sheets hold promise for a variety of applications. In electronic devices, an ohmic contact can be established between penta-graphene and nitrogen-doped graphene under a negative electric field ¹³. A Schottky contact is formed between bilayer penta-graphene and penta-BN₂ by adjusting the vertical distance between the two

layers, causing a transition from n-type to p-type behavior ⁴⁵. This property makes penta materials promising candidates for use as anode materials in Li/Na-ion batteries ⁴⁶.

In the present contribution, with the help of first principle DFT calculations, we created a 2D penta-BCN₄ structure, which was inspired by pentagonal-based framework structures and their appealing properties for nano-electronics. By comparing total energy calculations, phonon lattice dynamics calculations, AIMD calculations, and elastic constant calculations, respectively, the dynamic, thermal, mechanical, and transport properties of penta-BCN₄ have been examined. After confirming their outstanding stabilities, we thoroughly investigated each of their structural, mechanical, electronic, and optical characteristics before revealing their potential uses in nanoelectronics. The intrinsic NDR and lack of band gap characteristics in the penta-BCN₄ monolayer made it attractive for technological applications because B, C, and N are abundant in resources, light in mass, and environmentally safe.

The ternary penta-structure of boron, carbon, and nitrogen atoms obtained in this work is shown in Figure 1. This structure has one boron atom, one carbon atom, and four nitrogen atoms. Pentagonal structures are made up of three layers of atoms, with boron and carbon atoms sandwiched between two layers of nitrogen atoms in Penta-BCN₄.



Figure 1. Unit cell of Penta-BCN₄ structure from top and side view.

Penta-BCN₄'s lattice vector lengths a=b=3.46 Å were derived after structural optimization. The vacuum separation is c=20 Å in order to prevent the layers from interacting with each other. B-N, N-N, and C-N bonds have lengths of 1.53, 1.39, and 1.48 Å, respectively. The length of the N-N bond in the Penta-BCN₄ structure is larger than that of the N₂ molecule (1.09 Å). ⁴⁷. All parameters are compiled in Table 1, which also contains information on other materials. Noticeably, the data given in Table 1 reveals that the lattice parameter of BCN₄ (3.46 Å) is 5.2% smaller than that of penta-graphene, approximately 4.3% larger than CN₂, and about 6% smaller than the BCN structure.. Considering the h parameter BCN₄ is about 15% and 5% greater than graphene and BCN respectively, but about 8% smaller than CN₂. By noticing the bonds, the N-N bonds of BCN₄ are about 3.5% smaller than CN₂, for C-N bonds BCN₄ is about 2% smaller than BCN and 1.5% greater than CN₂. Considering the B-N bonds the BCN₄ is about 8% greater than BCN.

Structures	a (Å)	b (Å)	h (Å)	<i>l</i> ₁ (Å)	l2 (Å)	<i>l</i> 3 (Å)	θ_1 (deg)	θ_2 (deg)	θ_3 (deg)
Penta-Graphene ¹⁹	3.64		1.20	C1-C2	C2-C2		134.2		
				1.55	1.34				
Penta-BCN	3.46		1.41	B-N	N-N	C-N	108 34	108.07 112.86	112.86
renta-DCIN4	5.40		1.41	1.53	1.39	1.48	108.54		112.00
Penta-CN ₂ ⁴³	3 31		1.52	C-N	N-N		105 3	107 74	
	5.51		1.02	1.46	1.44		100.0	107.71	
Penta-BCN ³⁰	3.67	3 63	1 34	C-B	B-N	C-N			
Tonu Derv	5.07	5.05	1.54	1.62	1.41	1.51			

Table 1. structural information for different materials including bond length (l_1, l_1, l_1) in angstrom unit, lattice vectors (a, b, c) in angstrom and angle between atoms $(\theta_1, \theta_2, \theta_3)$ in degree unit.

After optimizing the structure of Penta-BCN₄ in order to check the stability of this material, its cohesive energy has been calculated using the following equation 48 :

$$E_{coh} = (E - n_B E_B - n_C E_C - n_N E_N) / N$$
(1)

E represents the overall energy of the Penta-BCN₄ system after optimization, whereas E_B , E_C , and E_N represent the energy of the isolated atoms of B, C, and N, respectively. In addition, n_B , n_C , and n_N represent the number of B, C, and N atoms in the Penta-BCN₄ structure, respectively. The results, which are displayed in Table 2, indicate that the Penta-BCN₄ structure has a binding energy of 7.04 eV/atom, indicating high stability. This energy is close to graphene's (7.85 eV/atom) and h-BN's (7.07 eV/atom) adhesion energies, and it exceeds Silicene's (5.16 eV/atom) and MoS₂'s (5.02 eV/atom) adhesion energies.

Table 2. Data from the literature was gathered in order to compare the computed cohesive energy of penta-BCN₄ with other known pentagonal structures. Available experimental data has also been included in the table. Cohesive energies are measured in electron volts per atom.

energies						
G	Cohesive energy (eV/atom)					
Structures						
	experimental	theory				
Penta-BCN ₄	_	7.04				
Penta-Graphene	-	7.08 49				
1						
Penta-Silicene	_	3.92 49				
Penta-PtAs ₂	_	4.30 49				
Penta-NiP ₂	_	3.94 49				
Graphene	_	7.85 49				
1						
h-BN	_	7.07				
Silicene	5.16 50					
MoS ₂		5.02				
Germanene	4.15 51					
	_					

The dynamic stability of the Penta-BCN₄ structure was assessed after the geometry of the structure was optimized and the phonon bandstructure and phonon density of states (DOS) were obtained. Figure 2 shows that no 'negative' frequencies are found in the Brillouin zone, signifying that the structure of Penta-BCN₄ is dynamically stable.



Figure 2. Phonon bandstructure (a) and density of states (b) of Penta-BCN₄ structure.

For the evaluation of the thermodynamic stability, AIMD simulations on the $3 \times 3 \times 1$ supercell were done for a length of 6 ps with a time step of 1 fs. Figure 3 exhibits that at 300 K temperature, the structure doesn't show large potential energy fluctuations, and after 6 ps, the structure has not experienced any significant changes. AIMD computations have been continued at temperatures greater than 300 K, including 600, 1000, 1100, and 1200 K. Penta-BCN₄ is still stable at 1100 K, and at 1200 K, consequently, N₂ molecules are formed and extracted from the structure and afterwards separated from the Penta-BCN₄ surface. The temperature stability of various pentagonal configurations is given as well in Table 3.



Figure 3. Fluctuation of potential energy of penta-BCN₄ (3×3×1 supercell) during a NVT AIMD simulation at 300, 600, 1000, 1100, 1200 K.

Table 3. Gathered data from literature in order to have a compar	rison with the calculated stability temperature of
penta-BCN ₄ with other reported pe	entagon structures.

Structures	Temperature (K)
Penta-BCN ₄	1100
Penta-BCN ³⁰	1200
Penta-Graphene ¹⁹	1000
Penta-B ₂ C ²⁷	1000
Penta-BN ¹⁴	450
Penta-BN ₂ ¹⁴	1000
Penta-Ge ⁵²	300
Penta-PdN ₂ ⁵³	700
Penta-PtN ₂ ⁵³	2000
Penta-ZnS ₂ ³⁹	1200

After determining that the Penta-BCN₄ structure is stable in terms of dynamically and thermally considerations, we focus on the mechanical stability. The elastic coefficients are calculated by subjecting the Penta-BCN₄ structure to uniaxial and biaxial deformations. Figure 4 depicts the energy-strain curve produced by uniaxial and biaxial deformations. The elastic coefficients were calculated using the following relations: ⁵⁴:

$$C_{11} = \frac{1}{A_0} \left(\frac{\partial^2 E}{\partial \varepsilon^2} \right) \bigg|_{\varepsilon=0}$$
(2)

$$2(C_{11} + C_{12}) = \frac{1}{A_0} \left(\frac{\partial^2 E}{\partial \varepsilon^2} \right) \Big|_{\varepsilon=0}$$
(3)

$$C_{66} = \frac{C_{11} - C_{12}}{2} \tag{4}$$

E, ε and A₀ represent the total energy of the system, the strain, and the cross-sectional area of the unit cell in the equilibrium state, respectively, in these equations. C₁₁=C₂₂ and C₁₂=C₂₁, according to the tetragonal symmetry of the Penta-BCN₄ structure. The Born-Huang criteria must be satisfied for a structure to be considered mechanically stable ⁵⁵:

$$C_{11}C_{12} - C_{12}^{2} > 0, \ C_{66} > 0$$
 (5)

The estimated elastic coefficients for the Penta-BCN₄ structure are shown in Table 4, indicating that the structure is mechanically stable. Important mechanical characteristics may be computed by taking elastic coefficients into account, as shown in Table 4. The elastic coefficients are used to compute Young's modulus (Y) and Poisson's ratio (v) using the following relations:

$$Y = \frac{C_{11}^2 - C_{12}^2}{C_{11}} \tag{6}$$

$$\nu = \frac{C_{12}}{C_{11}} \tag{7}$$

By utilizing Young's modulus and Poisson's ratio, the bulk modulus is calculated and the shear modulus has a direct relationship with C_{66} :

$$B = \frac{Y}{2(1-\nu)} \tag{8}$$

$$G = C_{66} \tag{9}$$

In Table 4, the mechanical parameters of Young's modulus, bulk, shear and Poisson's ratio are reported.



Figure 4. Energy-strain diagram of Penta-BCN₄ structure under biaxial and uniaxial strains deformations. At large positive strains, C-N and B-N bonds break, causing the energy-strain diagram to deviate from the expected quadratic behavior. This deviation ultimately resulted in the complete breakdown of the curve, leading to fracture..

Table 4. Elastic coefficients (C₁₁, C₁₂, C₂₂, C₆₆,), Young's modulus (Y), bulk (B), shear and Poisson's coefficient (G, v) of Penta-BCN₄ and other pentagonal systems.

Structures	C11	C12	C22	C66	Y	В	G	v
Penta-BCN ₄	257.32	2.62		127.35	257.30	129.97	127.35	0.01
Penta-BCN ³⁰	223.56	4.90	189.16	104.88	223.45 ª	-	-	0.022 ª
T child-Derv					189.03 ^b			0.026 ^b
Penta-Graphene ¹⁹	265	-18	-	-	263.8	-	-	-0.068
Penta-BN ¹⁴	133.67	5.48	133.67	65.60	-	-	-	0.04
Penta-BN ₂ ¹⁴	224.18	-7.03	224.18	120.48	224	-	-	-0.03
Penta-CN ₂ ²⁸	319	22			318.5	-	-	0.068
Penta-P ₂ C ⁵⁶	84.11	44.72	84.11	79.18	60.33	-	-	0.53
Graphene 57	352.0	62.6	-	-	340.8	-	-	0.178
Graphane 57	248.2	19.4	-	-	246.7	-	-	0.078

^{a,b} The Penta-BCN is mechanically anisotropic, and a is related to the *a* direction and b is related to the *b* direction.

To assess the anisotropy of Young's modulus and Poisson's ratio within the Penta-BCN₄ plane in various directions, calculations were performed using the following relationships⁵⁸:

$$Y(\theta) = \frac{\Delta}{C_{11}s^4 + C_{22}c^4 + (\frac{\Delta}{C_{66}} - 2C_{12})c^2s^2}$$
(10)

$$\nu(\theta) = \frac{\left(C_{11} + C_{22} - \frac{\Delta}{C_{44}}\right)c^2 s^2 - C_{12}(c^4 + s^4)}{C_{11}s^4 + C_{22}c^4 + (\frac{\Delta}{C_{66}} - 2C_{12})c^2 s^2}$$
(11)

Figure 5 demonstrates the isotropic mechanical characteristics of Penta-BCN₄, attributed to its high structural symmetry in various orientations. In contrast Penta-BCN, which has previously been studied, is mechanically anisotropic ³⁰.



Figure 5. Diagram of Young's modulus and Poisson's ratio of Penta-BCN₄ structure in different crystal directions. As it is illustrated the mechanical parameters of Penta-BCN₄ are isotropic in different directions.

The strain-stress diagram was analyzed using the data depicted in Figure 6. The elastic to plastic transition zone in Penta-BCN₄ is 10.5% for biaxial strains and 11% for uniaxial strains, according to Table 5. If the external force is removed in the elastic zone, the material can return to its original condition; however, after the material reaches the plastic region, even if the external force is removed, the material will not return to its original shape. In reality, in the plastic zone, where it causes certain bonds to break and other ones to form, the atoms of the material take on new forms and lose their original characteristics. Figure 7 exhibits the deformation and fraction of structure atomic bonds, as it can be observed at 12% uniaxial strains the C-N bond is broken and at 14% strains B-N bonds are broken while for biaxial strains the C-N bond becomes broken at 11%, after 17.5% strains just one B-N bond breaks and continuously at 18% strain the other B-N bond becomes broken.



Figure 6. Diagram of stress-strain/ energy-strain and elastic-plastic transition zone for Penta-BCN₄. (a) shows the results for uniaxial and (b) shows the results for biaxial strain.

Structures	bia	xial	uniaxial		
	εc1 (%)	EC2 (%)	ε _{C1} (%)	εc2 (%)	
Penta-BCN ₄	10	17.5	10.5	11	
Penta-BCN 59	24.3	18.4	-	-	
Penta-Graphene ⁶⁰	23	-	19.5		
Penta-BN ¹⁴	12	-	-	-	
Penta-BN ₂ ¹⁴	12	-	-	-	
Penta-CN ₂ ⁶¹	-	-	12.5	-	
Graphene 57	23	-	23 ^z , 19 ^a	-	
Graphane ⁶²	24	34	-	-	

Table 5. Elastic-plastic transition zone in Penta-BCN4 for uniaxial and biaxial stress/strain. ε_{C1} is the maximum ofstress-strain and ε_{C2} is the maximum of energy-strain in harmonic region.

^{z,a} Responses for armchair (a), and zigzag (z) strains of graphene.



Figure 7. Deformation and fraction of the elastic to plastic transition zone in Penta-BCN₄.

Although Penta-BCN₄ can tolerate up to 10.5% biaxial strain, phonon simulations suggest that this material is only dynamically stable in the -4% to +5% biaxial strain range. Negative modes arise in the phonon structure of Penta-BCN₄ beyond -4% and +5% strains, as shown in Figure 8, indicating the dynamic instability of this structure. Thus, Penta-BCN₄ has somewhat superior dynamic stability under biaxial strains (-4%,+5%) than Penta-BCN (-4%,+4%) ⁵⁹.



Figure 8. Phonon dispersion of Penta-BCN₄ under biaxial strains ranging from -4 to +6%. Negative modes occur in the phonon structure of Penta-BCN₄ beyond +5% strains, indicating the dynamic instability of this structure.

Figure 9 shows the band structure diagram and DOS of the Penta-BCN₄ structure for evaluating its electronic characteristics. According to the calculations, Penta-BCN₄ is conductive and has no band gap.

Figure 9c depicts the partial (P)DOS in order to analyze the influence of atomic orbitals on the electronic characteristics of the Penta-BCN₄ structure. According to the PDOS diagram, the p_z orbital of nitrogen has the largest contribution at the Fermi level and contributes the most to the conductivity of Penta-BCN₄.



Figure 9. Electronic properties of Penta-BCN₄ (a) band structure, (b) DOS, and (c) partial DOS (with respect to Fermi level). According to the PDOS, the p_z orbital of nitrogen atoms has the largest contribution at the Fermi level and contributes the most to the conductivity of Penta-BCN₄.

For charge distribution assessment in Penta-BCN₄, Bader charge analysis has been performed. Calculations show that each nitrogen atom has absorbed 0.8 e charge from carbon and boron atoms around it, and carbon and boron atoms have lost 1 and 2.2 electrons, respectively. Noteworthy, the reason for this charge transfer is the greater electronegativity of the nitrogen atom $(3.04)^{63}$ compared to the carbon $(2.55)^{63}$ and boron $(2.04)^{63}$. Thus, the accumulation of charge on nitrogen atoms is increased.

The Electron Localization Function (ELF), based on Pauli repulsion, shows the degree of electron localization in solids and can provide a direct image of lone-pair electrons. In Figure 10b-f, the red area next to the nitrogen atoms is the location of the s² orbital electron pairs of the nitrogen atom.

In the ELF diagram of Figure 10, a strong reduction of the electron cloud around the boron and carbon atoms can be seen, which has led to the condensation of the electron cloud around the nitrogen atoms.



Figure 10. Electron localization function diagram of each bonding in Penta-BCN₄ structure. The electron density shown from top(a) and side view (c). The electron density shown for N-N bonds from top (b) and side (d) view. The electron localization depicted for N-B-N, and N-C-N bonds shown in (e) and (f) respectively.

Inspecting Figure 11 it can be concluded that the lone pair of s orbital electrons of the nitrogen atom formed an isolated band in the valence band at the energy of -14.1 eV, which are far from the Fermi energy level. But these electron pairs lead to a 5 eV upshift of the Fermi level compared to Penta-Graphene ^{19, 43}. As a result, the p_z orbital of the nitrogen atom is completely placed at the Fermi level, leading to the conduction of Penta-BCN₄.



Figure 11. Density of local states of nitrogen atom in penta-BCN₄ structure illustrated for s, p_x, p_y, and p_z orbitals. The pair of s orbital electrons of the nitrogen atom formed an isolated band in the valence band at the energy of -14.1 eV, which are far from the Fermi energy level. But these electron pairs lead to a 5 eV upshift of the Fermi level.

Figure 12 illustrates the band structure diagram of Penta-BCN₄ under uniaxial and biaxial strains. Under uniaxial and biaxial strains, the structure of Penta-BCN₄ remains conductive, and no band gap occurs in its band structure. As a result, Penta-BCN₄ exhibits remarkable resilience to external loads, particularly when subjected to substantial mechanical strains..



(a)



Figure 12. Band structure of Penta-BCN₄ under (a) uniaxial and (b) biaxial strains. Considering the diagrams, the structure of Penta-BCN₄ remains conductive under uniaxial and biaxial strains, and no band gap appears in its band structure

The electron transport of the Penta-BCN₄ structure has been calculated using the non-equilibrium Green's function (NEGF) method. The transmission function is calculated using the following equation ⁶⁴:

$$T(E, V_b) = Tr(\Gamma_L G^D \Gamma_R G^A)$$
(12)

The current passing through the scattering region can then be calculated using the Landauer-Büttiker formula⁶⁴:

$$I = \frac{2e}{h} \int T(E, V_b) [f_L(E - \mu_L) - f_R(E - \mu_R)] dE$$
(13)

Here $\Gamma_{R(L)}$, $\mu_{R(L)}$, $G^{D(4)}$, are the right(left) broadening functions, the chemical potential of the right (left) electrode, and the delayed (advanced) Green function of the scattering area, respectively. The presence of a gap between the energy levels of -1.45 to -3.08 eV in the valence band is remarkable in the Penta-BCN₄ band structure. This splitting between bands offers a unique opportunity for novel electrical and optical behaviors. Here we investigate the negative differential resistance (NDR) phenomenon that is one of the most intriguing properties of Penta-BCN₄'s band structure. In order to investigate the transport properties of Penta-BCN₄, a transfer channel (ballistic region) with a length of more than 10 angstroms has been made which it is shown in Figure 13. This distance of 10 angstroms prevents the left and right electrodes from affecting each other. The left and right electrodes of this transfer channel are also made of Penta-BCN₄ material. In order to evaluate more precisely, in addition to calculating the throughput in the direction of the lattice vector (a), the transport in the direction of the N-N bond (Figure 13b) has also been calculated. The voltage range is from -3 volts to +3 volts.



Figure 13. Transfer channel of Penta-BCN₄ structure a) along vector a b) along N-N bonds and current-voltage diagram c) along vector a d) along N-N bonds

The results of transport calculations (Figure 13) show that the current passing through the Penta-BCN₄ transfer channel is of the order of microamperes. The maximum current passing through the Penta-BCN₄ transfer channel in the direction of lattice vector (a) is 5 μ A and in the direction of the N-N bond 35 μ A resulted. Thus, it is concluded that in terms of electron transport Penta-BCN₄ is anisotropic. Figure 13 exhibits the phenomena of NDR in the Penta-BCN₄ transfer channel using a currentvoltage diagram. Because Penta-BCN₄ is conductive, the current increases rapidly and reaches its maximum value once the voltage is increased. The passing current then hits zero at 1.45 V, indicating the negative differential resistance in the Penta-BCN₄ structure.

The electrons on the Fermi level are gradually transferred to the conduction band and generate the current at the beginning of the voltage increase from zero bias. As mentioned in the electronic properties section, most of these electrons belong to the nitrogen atom's p_z orbital. Subsequently, by increasing the voltage up to 1.45 V, as well as all the p_z orbital electrons, all the electrons on the Fermi level, in which they are distributed up to -1.45 eV below the Fermi level, are transferred to the conduction band and participate in the electric current. In this manner, the Penta-BCN₄ transfer channel is in the ON state from 0 to 1.45 volts. Following that, when the voltage increases, there will be no electron states in the valence band to supply current electrons, resulting in zero current and an OFF state until the voltage is increased to 3 V. As soon as the voltage approaches 3 V, the p_z orbital electrons at -3 eV located in the valence band will be able to gradually reach the conduction band.

The peak-to-valley ratios (PVRs) for the flow in the lattice vector (a) direction are 10^3 and, in the N-N direction 3.2×10^5 . An example of PVR of other materials is included in Table 6. The results of Table 6 show that the PVR of Penta-BCN₄ in the N-N direction is even greater than that of SiC $(3.6 \times 10^4)^{65}$. One of the applications of materials with a large PVR is the usage of tunnel diodes. The large PVR leads to the reduction of switching time in tunnel diodes.

Material	PVR
Penta-BCN ₄ (a direction)	10 ³
Penta-BCN ₄ (N-N direction)	3.2×10 ⁵
SiC ⁶⁵	3.6×10 ⁴
TMDC ⁶⁶	10 ³
GNR ⁶⁷	17.3
GaAs ⁶⁸	10
SiGe ⁶⁹	300
ZaGYNR ⁷⁰	4696

 Table 6. Calculated PVRs of different structures from literature in order to have a comparison with calculated data for penta-BCN4 structure.

In this study, we have predicted and introduced a novel ternary penta-structure composed of one boron atom, one carbon atom, and four nitrogen atoms.Pentagonal structures are made up of three layers of atoms, with boron and carbon atoms sandwiched between two layers of nitrogen atoms in Penta-BCN4. The results demonstrate that the Penta-BCN4 structure has a cohesive energy of 7.04 eV/atom, indicating that it is stable. At 1100 K, Penta-BCN4 remains stable, and at 1200 K, N₂ molecules are separated from the Penta-BCN4 surface. To consider mechanical stability of the structure, the results of calculated elastic coefficients for the Penta-BCN4 structure are reported, indicating that the Penta-BCN4 structure is mechanically stable. The PDOS diagram shows that the p_z orbital of nitrogen atoms has the highest contribution on the Fermi level and contributes significantly to the conductivity of Penta-BCN4. The nitrogen atom's pair of s orbital electrons formed an isolated band in the valence band at -14.1 eV, which is far from the Fermi energy level. To investigate the transport properties of Penta-BCN4, a transfer channel with a length of more than 10 angstroms was created. According to the results of transport calculations, the current passing through the Penta-BCN4 transfer channel is in the microampere range. The maximum

current passing through the Penta-BCN₄ transfer channel is 5 μ A in the direction of the lattice vector (a), and 35 μ A in the direction of the N-N bond. The passing current reaches zero at 1.45 V, indicating a negative differential resistance in the Penta-BCN₄ transport channel. The existence of a stateless space in the valence band of the Penta-BCN₄ band structure between -1.45 and 3.08 eV is the cause of this phenomenon. This gap provides the potential for the emergence of novel electronic and optical behaviors. This property of Penta-BCN₄ could be employed, for instance, in THz detection, oscillators, resonant tunneling diodes, multi-input and reconfigurable circuits, and fast-switching circuits. Further, Penta-BCN₄ could be utilized as a gate in the structure of interlayer tunneling field-effect transistors (ITFETs) for usage in Boolean and non-Boolean logic since it has NDR in forward and reverse bias. Also, since NDR occuring at low voltage will reduce power consumption in devices that use Penta-BCN₄ which makes it interesting for devices such as memory devices and RF oscillators. Finally, the results show that the PVR of Penta-BCN₄ in the N-N direction surpasses even that of SiC (3.6×10^4) . This noteworthy PVR value holds potential for various applications, including the use of tunnel diodes, where a large PVR contributes to reduced switching times and enhanced performance

COMPUTATIONAL METHODS

In this study, all investigated properties, including structural, electronic, and mechanical characteristics, were calculated using DFT as implemented in the VASP ⁷¹. The generalized gradient approximation, specifically the Perdew-Burke-Ernzerhof (PBE) approximation, has been chosen for the exchange-correlation functional ⁷². To facilitate a high accuracy of electronic property calculations, the projector augmented wave (PAW) pseudo-potentials are used, which are known to give a good agreement with all-electron calculations ⁷³. The first Brillouin zone is

sampled with $21 \times 21 \times 1$ points according to the Monkhorst-Pack mesh ⁷⁴, and 600 eV is chosen for cut off energy. The Gaussian smearing method was employed with the smearing parameter of 0.1 eV. The convergence limits for energy and forces are established to be 10^{-6} eV and 10^{-5} eV/Å, respectively. In addition, the PHONOPY package is used to calculate the phonon dispersion by means of the supercell method ⁷⁵. The atomic displacements are set to 0.01 Å. A $3 \times 3 \times 1$ supercell is used for the calculation. Correspondingly, the Brillouin zone of the above supercell was sampled by a $8 \times 8 \times 1$ mesh for the phonon momentum.

Ab-initio molecular dynamics simulations have been done using 3×3 supercells with 8×8×1 kpoints. AIMD simulations with NVT ensemble were carried out at 300, 600, 1000, 1100 and 1200 K respectively, for 0 to 6000 fs using a 1 fs time step. To calculate transport properties, the Siesta and TranSiesta packages were utilized. For electrode and scattering region calculations in TranSIESTA ⁷⁶ we used 1×1×100 k-points, respectively, and a cutoff value of 400 eV. For the transport calculations Troullier-Martins pseudopotentials were used ⁷⁷. In this work all calculations were implemented in non-polarized spin form because this structure has not shown any polar behavior.

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Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENT

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - SFB

1477 "Light-Matter Interactions at Interfaces", project number 441234705" (O.K.).

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