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Penta-C$_{20}$: A Superhard Direct Band Gap Carbon Allotrope Composed of Carbon Pentagon

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Abstract: A metastable $sp^3$-bonded carbon allotrope, Penta-C$_{20}$, consisting entirely of carbon pentagons linked through bridge-like bonds, was proposed and studied in this work for the first time. Its structure, stability, and electronic and mechanical properties were investigated based on first-principles calculations. Penta-C$_{20}$ is thermodynamically and mechanically stable, with equilibrium total energy of 0.718 and 0.184 eV/atom lower than those of the synthesized T-carbon and supercubane, respectively. Penta-C$_{20}$ can also maintain dynamic stability under a high pressure of 100 GPa. Ab initio molecular dynamics (AIMD) simulations indicates that this new carbon allotrope can maintain thermal stability at 800 K. Its Young’s modulus exhibits mechanical anisotropy. The calculated ideal tensile and shear strengths confirmed that Penta-C$_{20}$ is a superhard material with a promising application prospect. Furthermore, Penta-C$_{20}$ is a direct band gap carbon based semiconducting material with band gap of 2.89 eV.

Keywords: carbon allotrope; superhard materials; direct band gap; mechanical property; stability

1. Introduction

Carbon science is one of the most dynamic and competitive research fields. The rapid development of carbon science has extensively and deeply affected many disciplines and various fields of high technology. Carbon science also shows strong vitality as an interdisciplinary field and has formed a research field with a wide range of subject contents and potential application prospects. Carbon atoms have $sp$, $sp^2$, and $sp^3$ hybridization, which enables carbon to form a variety of structures and to exist in nature in the forms of diamond, graphite, graphene, fullerenes, and nanotubes among others. In 1985, Kroto et al. [1] succeeded in synthesizing the buckminsterfullerene (C$_{60}$) molecule by vaporizing graphite, which promoted a considerable amount of research on fullerenes. Soon after, carbon nanotubes were discovered by Iijima [2], pushing the study of carbon science to the world of one-dimensional materials. Currently, the recent discovery of layered carbon material (including graphdiyne [3], graphyne [4], and graphene [5]) is promoting carbon science to a two-dimensional (2D) field. The unique structures give fullerenes, graphene, and nanotubes a wide application prospect in nanoelectronics, biomedicine, gas detection, military defense, and so on [6,7]. To our credit, fundamental theory has improved in recent years, making it possible to predict these carbon structures. In particular, computational material science, consisting of first-principle calculations, has enabled great achievements in material design and property prediction [8–17].
To date, rich and varied kinds of carbon allotropes have been theoretically predicted or experimentally synthesized, such as C_{96} [18], carbon foam [19], P2/m C_{54} [20], M-carbon [21], W-carbon [22], C_{20}-T [23], T-carbon [24], supercubane [25], and other materials [26]. The database SACADA [27] contains about 500 examples up to May 2017. After a topology-based multiscale theoretical study, Baburin et al. [28] reported six carbon allotropes with low energy from about six hundred thousand zeolite nets. These new allotropes are superhard and transparent, and they are at most 0.12 eV/atom more energetic than diamond. In 2016, Wang et al. [23] discovered a superhard all-sp^3 hybridized carbon allotrope, C_{20}-T, which has large cavities and porous structure. C_{20}-T is a superhard carbon allotrope with a calculated Vickers hardness of about 72.76 GPa. In 2019, Zhang et al. [29] designed two superhard three-dimensional (3D) carbon allotropes, P6/mmm-C_{54} and Cmmm-C_{32}, which consist of sp^3 hybridized carbon atom. They found that Cmmm-C_{32} exhibits wide direct band gap semiconducting property. Using first-principle calculations, four 3D C_{60} polymers with ordered binary-alloy-type structures were investigated by Laranjeira et al. [30]. In these polymers, each molecule is in one of the two standard orientations and analogous to four kinds of ordered binary-alloy-type structures. The calculated band structures show that all four polymers exhibit metallic properties. After cold compression of C_{70} peapods, Yang et al. [31] obtained an all-sp^3 hybridized carbon allotrope with monoclinic unit cell, named V-carbon. V-carbon consists of five-, six-, and seven-numbered carbon rings and exhibits a honeycomb structure. The calculation shows that it is a superhard and ultraincompressible material, with a bulk modulus and hardness of 411 and 89.4 GPa, respectively. In order to predict superhard materials, Avery et al. [32] applied machine learning towards the carbon allotropes family and successfully identified 43 potential superhard carbon materials. Through topological analysis of these superhard materials, they found that phases with hardness slightly harder than the diamond phase contain a large number of diamond and/or lonsdaleite in their structures. Recently, Zhang et al. [33] proposed a cyclooctatetraene- and butadiene-based 2D fully sp^2-bonded carbon allotrope, PBCF-graphene. This 2D material has a direct band gap and has higher carrier mobility than monolayer MoS_2. Theoretical studies have shown that it can withstand equibiaxial tensile strains of 17.6% and a high temperature of 1000 K.

In this work, we obtained a new stable, semiconductor and superhard carbon allotrope Penta-C_{20}, which was obtained by using the random sampling strategy combined with space group and graph theory (RG2) [34,35] to search for structures in orthorhombic systems. After analyzing its underlying topology [36], we found that it is a known net observed in the database of hypothetical zeolites collected by Deem and called PCOD8045750 [37]. Its physical properties have been systematically calculated by applying first-principle calculations. The calculated results illustrate that this novel carbon allotrope is mechanically, thermodynamically, dynamically, and thermal stable. In addition, this material exhibits a wide direct band gap.

2. Calculation Methods

This work was performed with first-principle calculations. Most calculations were implemented within the Vienna ab initio simulation package (VASP, 5.4.4) [38–40], with the projector augmented wave (PAW) [41] method applied to provide pseudopotentials. The Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation (GGA) [42] was employed for the exchange correlation. To expand the valence electron wavefunctions, the plane–wave cutoff energy was set as 500 eV. The Brillouin zone was sampled with 7 × 7 × 7 Monkhorst-Pack (MP) [43] special k-point grids. The convergence criteria for the total energy and the atom force calculations were taken as 1 × 10^{-5} eV and 0.01 eV/Å, respectively. Phonon frequency calculations were performed in the PHONOPY code [44], with forces calculated by density functional perturbation theory (DFPT) [45], as implemented in VASP. Based on the optimized geometry of the structure obtained from the GGA-PBE functional, the hybrid HSE06 functional [46] was used for high-accuracy electronic property calculations. The elastic constants were calculated by the Cambridge Serial Total Energy Package (CASTEP) code [47] using the GGA-PBE functional.
3. Results and Discussion

3.1. Structural Properties

The equilibrium crystal structure of this novel structure is depicted in Figure 1. The equilibrium structure information, including space group, lattice parameters, and density of this novel carbon allotrope are listed in Table 1, together with those of TY-carbon [48], Y-carbon, T-carbon [49], C_{20}^-T [23], and diamond [50] for comparison. In this work, the calculated crystal structure information of TY-carbon, C_{20}^-T, Y-carbon, T-carbon, and diamond are in line with previous work, proving the reliability of our theoretical work. This novel structure belongs to the orthorhombic system and has Cmcm (No. 63) symmetry with \( a = 5.595 \text{ Å}, b = 9.168 \text{ Å}, \) and \( c = 2.577 \text{ Å}. \) As shown in Figure 1a, its orthorhombic unit cell consists of 20 \( sp^3 \) hybridized carbon atoms. Within its unit cell, three inequivalent carbon atoms occupy the Wyckoff positions \( 8g (0.28168, 0.84609, 0.75), \) \( 8g (0.63477, 0.68028, 0.75), \) and \( 4c (0, 0.54828, 0.25), \) which are represented as pastel cyan (C1), light brown (C2), and pastel magenta (C3) spheres in Figure 1. This novel structure consists entirely of carbon pentagons linked through bridge-like bonds and is named Penta-C_{20}, as shown in Figure 2a. In a unit cell, each C1 atom is covalently bonded with one C2 atom and three C3 atoms, while two neighboring C2 atoms and two neighboring C3 atoms are covalently bonded. Penta-C_{20} has five distinct bond lengths. Its basic carbon pentagon building block contains three distinct bond lengths, \( 1.557 \text{ Å} \) (C1-C2), \( 1.589 \text{ Å} \) (C1-C3) and \( 1.505 \text{ Å} \) (C3-C3), while its bridge-like bonds have two different bond lengths: \( 1.545 \text{ Å} \) (C1-C3) and \( 1.561 \text{ Å} \) (C2-C2). The average bond length is \( 1.552 \text{ Å}, \) slightly longer than that of diamond (1.54 Å). Additionally, Penta-C_{20} has eight different bond angles, namely, \( 89.630^\circ, 90.370^\circ, 103.126^\circ, 107.077^\circ, 110.961^\circ, 111.360^\circ, 112.747^\circ, \) and \( 120.887^\circ. \) Penta-C_{20} has a honeycomb structure along the c-axis. Its largest pore is an ellipse of twelve atoms with a short axis of 3.31 Å. In addition to the ellipse, there are also pentagons and quadrilaterals on the c-axis projection. The honeycomb structure causes the density of Penta-C_{20} (3.031 g/cm\(^3\)) to be lower than the density of diamond (3.518 g/cm\(^3\)).

![Figure 1](image-url)

**Table 1.** The lattice parameters and mass density for Penta-C_{20} and other carbon allotropes.

| Structures  | Methods | Space Group | \( \rho \) (g/cm\(^3\)) | \( a \) (Å) | \( b \) (Å) | \( c \) (Å) | \( E_{tot} \) (eV) |
|-------------|---------|-------------|----------------|------------|------------|------------|----------------|
| Penta-C_{20} | PBE     | Cmcm        | 3.031          | 5.595      | 9.168      | 2.577      | −8.639        |
| T-carbon     | PBE     | Fd-3m       | 1.503          | 7.516      | -          | -          | −7.921        |
| -            | PBE [b] | Fd-3m       | 1.503          | 7.517      | -          | -          | −7.922        |
| -            | Exp. [b] | Fd-3m       | -             | 7.80       | -          | -          | -             |
with the coordinates of the high symmetry points as follows: Y: (0.5, 0.5, 0), S: (0, 0.5, 0), and R: (0, 0.5, 0.5). As shown in Figure 3a and (b), the phonon spectra at 0

To examine the lattice dynamic stability of Penta-C20, we calculated the total energy of Penta-C20 in comparison with several other previous carbon allotropes. Energetically more

The equilibrium total energy of Penta-C20 is 0.134, 0.568, 0.184, and 0.718 eV/atom lower than those of C20-T, T-carbon, diamond, and Y-carbon, respectively. Notably, T-carbon and supercubane have been synthesized experimentally by Zhang et al. [24] and Liu et al. [25], respectively. Energetically more

- PBE [c]
  - PBE [c]
- PBE [c]
- Exp. [c]
  - Exp. [c]

Table 1. Cont.

| Structures | Methods  | Space Group | ρ (g/cm³) | a (Å) | b (Å) | c (Å) | $E_{\text{tot}}$ (eV) |
|------------|----------|-------------|----------|-------|-------|-------|---------------------|
| Y-carbon   | PBE      | Fd-3m       | 0.892    | 9.636 | -     | -     | -8.071             |
| -          | PBE [c]  | Fd-3m       | 0.894    | 9.636 | -     | -     | -8.074             |
| TY-carbon  | PBE      | Fd-3m       | 0.524    | 13.459| -     | -     | -8.038             |
| -          | PBE [c]  | Fd-3m       | 0.523    | 13.460| -     | -     | -8.034             |
| C20-T      | PBE      | P2/13       | 3.293    | 4.948 | -     | -     | -8.505             |
| -          | PBE [d]  | P2/13       | 3.298    | 4.945 | -     | -     | -             |
| Diamond    | PBE      | Fd-3m       | 3.518    | 3.567 | -     | -     | -9.093             |
| -          | Exp. [c] | Fd-3m       | 3.516    | 3.567 | -     | -     | -             |

[a] Ref. [48]. [b] Ref. [24]. [c] Ref. [49]. [d] Ref. [23]. [e] Ref. [50].

Figure 2. (a) The bond lengths and bridge-like bonds between carbon pentagons in the Penta-C20 structure. The bridge-like bonds are represented as bright yellow sticks. (b) The total energy vs the volume per atom for Penta-C20 in comparison with several other previous carbon allotropes.

3.2. Stability

To study the thermodynamic stability of Penta-C20, we calculated the total energy vs the volume per atom for Penta-C20 in comparison with those of supercubane, C20-T, Y-carbon, diamond, and T-carbon, as shown in Figure 2b. In this work, the equilibrium total energies per atom of Penta-C20, Y-carbon, supercubane, C20-T, T-carbon and diamond are −8.639, −8.071, −8.455, −8.505, −7.921, and −9.093 eV/atom, respectively. Although Penta-C20 is metastable with energy higher than diamond of 0.454 eV/atom, it is energetically more stable than supercubane, Y-carbon, C20-T, and T-carbon: The equilibrium total energy of Penta-C20 is 0.134, 0.568, 0.184, and 0.718 eV/atom lower than those of C20-T, Y-carbon, supercubane, and T-carbon, respectively. Notably, T-carbon and supercubane have been synthesized experimentally by Zhang et al. [24] and Liu et al. [25], respectively. Energetically more stable than supercubane and T-carbons, this novel carbon allotrope may be synthesized experimentally. To examine the lattice dynamic stability of Penta-C20, we calculated the phonon spectra for Penta-C20 at 0 and 100 GPa, as represented in Figure 3a,b. The first Brillouin zone of Penta-C20 is shown in Figure 3c with the coordinates of the high symmetry points as follows: Γ: (0, 0, 0), Z: (0, 0, 0.5), T: (0.5, 0.5, 0.5), Y: (0.5, 0.5, 0), S: (0, 0.5, 0), and R: (0, 0.5, 0.5). As shown in Figure 3a and (b), the phonon spectra at 0 and 100 GPa do not show any imaginary frequencies, indicating that Penta-C20 can maintain lattice dynamic stability under a high pressure of 100 GPa. Furthermore, the predicted highest vibrational frequency of Penta-C20 at 0 GPa is 40.40 THz, which is very similar to that of $sp^3$-bonded diamond (40.11 THz). Ab initio molecular dynamics (AIMD) simulations is a very important method to examine the thermal stability of materials. In this work, the AIMD simulations of Penta-C20 were performed...
using canonical (NVT) ensemble in a 2 × 2 × 3 supercell. The total energy fluctuations of Penta-C\textsubscript{20} during the simulation time (for 5 ps with a time step of 1 fs) under 300 and 800 K are shown in Figure 4. No dramatic change was observed in structure and the total energy is almost constant, indicating that Penta-C\textsubscript{20} is thermal stable at 300 and 800 K.

![Figure 3](image-url)  
**Figure 3.** The phonon spectra of Penta-C\textsubscript{20} under (a) 0 GPa and (b) 100 GPa, and the coordinates of the high symmetry points in the Brillouin zone of Penta-C\textsubscript{20} (c).

![Figure 4](image-url)  
**Figure 4.** The total energy fluctuations of Penta-C\textsubscript{20} as a function of the AIMD simulation at 300 K (a) and 800 K (b). The insets are the atomic configurations of 2 × 2 × 3 supercell of Penta-C\textsubscript{20} at the end of the 5 ps AIMD simulation.

### 3.3. Mechanical Properties

To characterize the mechanical properties of Penta-C\textsubscript{20}, we examined its single-crystal elastic constant $C_{ij}$, which is listed in Table 2. For an orthorhombic structure, there are nine independent elastic constants: $C_{11}$, $C_{12}$, $C_{13}$, $C_{22}$, $C_{23}$, $C_{33}$, $C_{44}$, $C_{55}$, and $C_{66}$. According to Born stability criteria \cite{51}, necessary and sufficient mechanical stability criteria are:

\begin{equation}
C_{11} > 0, \quad C_{11}C_{22} > C_{12}^2, \\
C_{11}C_{22}C_{33} + 2C_{12}C_{13}C_{23} - C_{11}C_{23}^2 - C_{22}C_{13}^2 - C_{33}C_{12}^2 > 0, \\
C_{44} > 0, \quad C_{55} > 0, \quad C_{66} > 0.
\end{equation}
where which are ductile materials. The Young’s modulus sphere illustrates that Penta-C has a higher Young’s modulus than HS-C48, C96, superprismane, C72, K6-carbon, and T-carbon. The 3D Young’s modulus given by the above formula is illustrated in Figure 6a. The distorted 3D Young’s modulus sphere illustrates that Penta-C has inherent mechanical anisotropy. The maximum

Table 2. The calculated elastic constants (C_ii, in GPa), elastic modulus (B and G, in GPa), and hardness (H_{USPEX}, H_{Tian} and H_{Exp}, in GPa) for Penta-C_20 and other carbon allotropes.

| Materials       | C_11 | C_12 | C_13 | C_22 | C_23 | C_33 | C_{44} | C_{55} | C_{66} | B     | G     | B/G   | H_{USPEX} | H_{Tian} | H_{Exp} |
|-----------------|------|------|------|------|------|------|--------|--------|--------|-------|-------|-------|----------|----------|---------|
| Penta-C_20      | 1020 | 76   | 97   | 539  | 59   | 905  | 289    | 332    | 299    | 313   | 327   | 0.96  | 76.23   | 58.30    | -       |
| HS-C_{48}[a]    | 656  | 137  | 266  | 151  | 94   | 777  | 112    | 92     | 323    | 287   | 178   | 1.61  | -       | -        | -       |
| C_{96}[b]      | 623  | 108  | -    | -    | -    | 194  | -      | -      | -      | 279   | 219   | 1.2   | -       | -        | -       |
| Superprismane   | 306  | 136  | 185  | -    | -    | 525  | 226    | -      | -      | 238   | 150   | 1.59  | -       | -        | -       |
| C_{72}[d]      | 273  | 139  | -    | -    | -    | 81   | -      | -      | -      | 183   | 75    | 2.46  | -       | -        | -       |
| K_6-carbon      | 203  | 136  | -    | -    | -    | 70   | -      | -      | -      | 159   | 52    | 3.08  | -       | -        | -       |
| T-carbon[e]     | 1053 | 119  | -    | -    | -    | 566  | -      | -      | -      | 431   | 524   | 0.82  | 89.77   | 96.73    | -       |
| Diamond         | 1076 | 125  | -    | -    | -    | 577  | -      | -      | -      | 442   | 634   | 0.83  | 89.72±5  | 93.6±5   | 96±5    |

Clearly, all nine independent elastic constants of Penta-C_20 are positive and satisfy the above criteria very well, thus proving the mechanical stability of Penta-C_20. The elastic parameters of HS-C_{48} [52], C_{96} [18], superprismane [53], C_{72} [54], K_6-carbon, T-carbon [55], and diamond [56] are also listed in Table 2. C_{11}, C_{22}, and C_{33} can be used to characterize the resistance of materials to elastic strain along the x, y, and z-axes. As listed in Table 2, for Penta-C_20, C_{11} is higher than C_{33} and C_{22}, indicating that this material is less compressible along the x-axis. Furthermore, C_{11}, C_{22}, and C_{33} values for Penta-C_20 are higher than C_{11}, C_{22}, and C_{33} values for HS-C_{48}, C_{96}, superprismane, C_{72}, K_6-carbon, and T-carbon, as listed in Table 2. We then calculated the average bulk modulus B and shear modulus G of Penta-C_20 according to the Voigt-Ruess-Hill approximation [60], as listed in Table 2. Penta-C_20 has larger bulk and shear modulus (B = 313 GPa and G = 327 GPa) than HS-C_{48}, C_{96}, superprismane, C_{72}, K_6-carbon and T-carbon, indicating that Penta-C_20 has stronger resistance to volume and shape changes than HS-C_{48}, C_{96}, superprismane, C_{72}, K_6-carbon and T-carbon. The B/G value of brittle materials is generally lower than 1.75, while that of ductile materials is greater than 1.75. [61] The B/G value of Penta-C_20 is 0.96, indicating that Penta-C_20 is a brittle material. This is different from C_{72}, K_6-carbon and T-carbon, which are ductile materials. The B/G value of Penta-C_20 is much lower than those of HS-C_{48}, C_{96} and superprismane, indicating that Penta-C_20 may be more brittle than HS-C_{48}, C_{96}, and superprismane.

Hardness is another indispensable parameter to characterize the mechanical properties of materials and has an important influence on the application of materials. In this work, we calculated the hardness of Penta-C_20 and diamond by using the Lyakhov-Oganov model (H_{USPEX}) [57] and Tian model (H_{Tian}) [60]. As listed in Table 2, the hardness calculated in this work for diamond are H_{USPEX} = 89.77 GPa and H_{Tian} = 96.73 GPa, which are consistent with the experimental [59] and previously theoretical values. The calculated hardnesses of Penta-C_20 are H_{USPEX} = 76.23 GPa and H_{Tian} = 58.30 GPa. Considering that the hardness criterion for superhard materials is 40 GPa, the theoretical results calculated by the above two hardness models all prove that Penta-C_20 is a potential superhard carbon material. To further determine the superhard property of Penta-C_20, we then calculated its ideal tensile and shear strength [62], as shown in Figure 5. The figure shows that the minimum tensile and shear strengths of Penta-C_20 reached 48.59 GP (in [111] direction) and 47.67 GP (along the (011)(0–11) slip system), respectively, which still satisfy the hardness criterion for superhard materials. Thus, it turns out that Penta-C_20 is intrinsically a superhard carbon material.

Studying the direction dependence of the Young’s modulus is an effective and intuitive method for describing the mechanical anisotropy of materials. For the orthorhombic system, the direction dependence of the Young’s modulus can be obtained as follow [63]:

$$
\frac{1}{E} = S_{11}I_1^4 + S_{22}I_2^4 + S_{33}I_3^4 + (S_{44} + 2S_{23})(I_2I_3)^2 + (S_{55} + 2S_{13})(I_1I_3)^2 + (S_{66} + 2S_{12})(I_1I_2)^2
$$

where $S_{ij}$ is the elastic compliance constant; $I_1$, $I_2$, and $I_3$ are the direction cosines of the direction vectors. The 3D Young’s modulus given by the above formula is illustrated in Figure 6a. The distorted 3D Young’s modulus sphere illustrates that Penta-C_20 has inherent mechanical anisotropy. The maximum
planes exhibit the largest and smallest mechanical anisotropy, respectively. Namely, the (001), (011), (100), (101), (010), (110), and (111) planes, in Figure 6b. All seven main planes contain the (0, 0, 0) point. The maximum Young’s modulus $E_{\text{max}}$, minimum Young’s modulus $E_{\text{min}}$, and $E_{\text{max}}/E_{\text{min}}$ ratio in the seven main planes are shown in Figure 6c. The distorted 2D Young’s modulus circles illustrate that Penta-C20 exhibits mechanical anisotropy in all seven planes. The maximum $E_{\text{max}}/E_{\text{min}}$ ratio reaches 1.405, whereas the minimum $E_{\text{max}}/E_{\text{min}}$ ratio is 1.24; thus, the (001) and (010) planes exhibit the largest and smallest mechanical anisotropy, respectively.

![Figure 5](image1.png)  
**Figure 5.** The calculated ideal tensile (a) and shear (b) strength of Penta-C20.

![Figure 6](image2.png)  
**Figure 6.** The directional dependence of the (a) 3D Young’s modulus and (b) 2D Young’s modulus for Penta-C20, and (c) the maximum Young’s modulus $E_{\text{max}}$, minimum Young’s modulus $E_{\text{min}}$, and $E_{\text{max}}/E_{\text{min}}$ in the (001), (010), (011), (100), (101), (110), and (111) planes for Penta-C20.
3.4. Electrical Properties

The density of states (DOS) and band structure are effective methods to analyze the electrical properties of crystals. Using the HSE06 hybrid function, the orbital projection band structure and the partial DOS (PDOS) of Penta-C\textsubscript{20} are calculated and shown in Figure 7. As shown in Figure 7, Penta-C\textsubscript{20} is a direct band carbon based semiconducting material with band gap of 2.89 eV, as the conduction band minimum (CBM) and valence band maximum (VBM) are both found at Y point. As the orbital projection band structure shows, both VBM and CBM of Penta-C\textsubscript{20} are composed mainly of the \(-p_x\) orbital, although other orbital contributions are not less significant. Moreover, the electrons in the \(-p_z\) orbital contribute more in VBM than in CBM. The electrons in the \(-p_x, -p_y,\) and \(-p_z\) orbitals contribute more in the valence band than in the conduction band, while the electrons in the \(-s\) orbital contribute more in the conduction band. As shown in the PDOS, C atoms contribute the least to the orbits of the considered energy range. Both VBM and CBM of Penta-C\textsubscript{20} are composed mainly of C\textsubscript{1-}\(p_x\) and C\textsubscript{3-}\(p_x\) orbitals.

![Figure 7. The calculated partial density of states (PDOS) and orbital projection band structure for Penta-C\textsubscript{20}. Cyan, magenta, olive, and orange lines correspond to the \(-s, -p_x, -p_y,\) and \(-p_z\) orbitals of electrons.](image)

4. Conclusions

Based on first-principle calculations, the physical properties (including structural properties, stability, and mechanical and electronic properties) of a novel carbon material, Penta-C\textsubscript{20}, were studied in detail. Penta-C\textsubscript{20} can be formed from carbon pentagons linked through bridge-like bonds. In the direction of the c-axis, Penta-C\textsubscript{20} presents a honeycomb structure composed of quadrilateral, pentagonal, and twelve-sided shapes, which makes its density lower than that of diamond. Under a high pressure of 100 GPa, Penta-C\textsubscript{20} can maintain lattice dynamic stability. Penta-C\textsubscript{20} is energetically more stable than supercubane and T-carbons, illustrating that it has thermodynamic stability and may be synthesized in the future. In terms of mechanical properties, Penta-C\textsubscript{20} is a potential superhard carbon material and exhibits mechanical anisotropy. In terms of the Young’s modulus, the (001) plane exhibits the largest mechanical anisotropy, while the (010) plane shows the smallest mechanical anisotropy. In addition, Penta-C\textsubscript{20} is a semiconducting material with a wide direct band gap of 2.89 eV. The low energy, high stability, superhard property, and wide direct band gap of Penta-C\textsubscript{20} suggest that it has potential value in high-power and high-voltage devices. This work not only enriches the carbon allotrope family but also provides novel superhard direct band gap carbon materials.

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