pentahexoctite: A new two-dimensional allotrope of carbon

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The ability of carbon to exist in many forms across dimensions has spawned search in exploring newer allotropes consisting of either, different networks of polygons or rings. While research on various 3D phases of carbon has been extensive, 2D allotropes formed from stable rings are yet to be unearthed. Here, we report a new $sp^2$ hybridized two-dimensional allotrope consisting of continuous 5-6-8 rings of carbon atoms, named as “pentahexoctite”. The absence of unstable modes in the phonon spectra ensures the stability of the planar sheet. Furthermore, this sheet has mechanical strength comparable to graphene. Electronically, the sheet is metallic with direction-dependent flat and dispersive bands at the Fermi level ensuring highly anisotropic transport properties. This sheet serves as a precursor for stable 1D nanotubes with chirality-dependent electronic and mechanical properties. With these unique properties, this sheet becomes another exciting addition to the family of robust novel 2D allotropes of carbon.

Carbon has been known to form many allotropes because of its ability to exist in different hybridizations. Among these, the most extensively studied, is graphene, a monolayer of $sp^2$ hybridized carbon atoms. It is a building block for carbon materials such as the three-dimensional (3D) graphite, one-dimensional (1D) carbon nanotubes, and zero-dimensional (0D) fullerenes, all of them exhibiting unique properties. Success of graphene has motivated the search for newer forms of 2D materials. This resulted into finding of various 2D allotropes such as graphyne6–12, graphdiyne13,14, graphenylene15, biphenylene16, radialenes17–19, pentahexite20 and haeckelites21. The carbon atoms in these allotropes are either $sp^2$ and/or $sp^3$ hybridized. Graphyne (graphdiyne) consists of a network of carbon atoms with one (two) acetylenic linkages between hexagons4,5,13,14. In graphenylene and biphenylene, the arrangement is in the form of squares, hexagons, and octagons (biphenylene)15,16. Radialenes are formed by inserting acetylenic linkages between methylene pairs17. On the other hand, sheets consisting of 5–7 defects such as, pentahexite and haeckelite are formed by the Stone-Wales transformation22 of bonds in a certain sequence20,21. Interestingly, all these allotropes are planar and exhibit unique electronic as well as mechanical properties.

In addition to the geometric stability of 5–7 rings, 5–8 rings have also been proved to be stable. 1D metallic wires made out of a 5–8 chain in graphene23 have been shown to be promising for valleytronics devices24. Motivated by the unique nature of this 5–8 line defect in graphene, we explored the possibility of its 2D analog. Here, we report “pentahexoctite”, a sheet consisting of a network of pentagons, hexagons and octagons. The planar stability of the sheet is ensured through the absence of unstable modes in the phonon spectra. The mechanical strength of the sheet is comparable to graphene. Electronic structure shows this sheet to be metallic with a combination of flat and dispersive bands at the Fermi level. The sheet can be rolled into stable nanotubes with chirality-dependent mechanical and electronic properties. These novel properties of the pentahexoctite sheet make it a potential candidate for nanoelectronics devices.

Results and Discussion

Pentahexoctite sheet. The pentahexoctite sheet has two pentagons that are mirror images of each other, surrounded by four octagons and two hexagons as shown in Fig. 1(a). This 2D lattice has a space group of $C_{mn}$, (two mirror planes represented by the purple-dashed lines in Fig. 1(a)) with no inversion symmetry. The reduction in symmetry compared to graphene results in anisotropy, which plays a role in determining physical properties. The optimized lattice parameters are $a_1 = 5.85$ Å and $a_2 = 3.78$ Å (thick green arrows in Fig. 1(a)). The hexagons in this sheet are not regular and contain two types of angles, i.e. $\alpha = 138.8^\circ$ and $\beta = 110.6^\circ$ (Fig. 1(a)). However, the bond lengths ($a = 1.43$ Å, $b = 1.37$ Å, $c = 1.49$ Å, $d = 1.41$ Å, and $e = 1.39$ Å, in the order specified in Fig. 1(a)) of the neighboring C atoms do not deviate significantly from the $sp^2$ hybridized bond length of
graphene (1.42 Å), more or less preserving the sp² hybridization in this sheet. The structure of this sheet can also be derived from graphene by the SW transformation of one of the bonds (blue-colored) in a rectangular unit cell as shown in Fig. 1(b), followed by a complete relaxation of the unit cell including the lattice vectors.

In order to verify the integrity of the planar structure, it was distorted by moving the atoms out of plane in a larger supercell. Upon complete relaxation, the atoms returned to their original positions and the sheet remained planar. Stability of the sheet was further confirmed by calculating the phonon dispersion curve along the high symmetry directions as shown in the inset. There were no negative frequencies observed in the phonon spectra (Fig. 1(c)) and vibrational density of states (VDOS) (Fig. 1(d)). In addition, there is a phononic gap in the neighborhood of 40 THz suggesting its possible application in phononic devices.

Based on the phonon spectra, we also analyze the thermal transport of this sheet. The trends in the lattice thermal conductivity can be found by calculating the group velocities of the longitudinal and transverse acoustical (LA and TA) modes and comparing these with graphene. The LA group velocity \( v_{\text{LA}} \approx 17400 \text{ m s}^{-1} \) is higher compared to the TA velocity \( v_{\text{TA}} \approx 5600 \text{ m s}^{-1} \). In addition, \( v_{\text{LA}} \) of the sheet has comparable magnitude with \( v_{\text{LA}} \) of graphene \((-21300 \text{ m s}^{-1})^{25}\), whereas, \( v_{\text{TA}} \) is lower than graphene’s \((-13600 \text{ m s}^{-1})^{25}\). The out-of-plane modes (ZA) do not contribute significantly to the lattice thermal conductivity, due to negligibly small group velocities, similar to graphene\(^{26}\).

We estimate the lattice thermal conductivity at room temperature assuming the transport to be ballistic in nature. This assumption was based on two observations: i) The temperature considered is much lower than the calculated Debye temperature of this sheet (1229 K). ii) The sheet is highly symmetric having phonon group velocities comparable to graphene. Therefore, the sheet is expected to have long mean-free paths. We employed the Landauer’s formalism as implemented in the BallTran code\(^{27}\) to obtain the lattice thermal conductivity of pentahexoctite sheet at room temperature. Due to the inherent structural anisotropy in the sheet, thermal transport is anisotropic. The thermal conductivities along x- and y-directions were 0.741\(K_0\) and 0.598\(K_0\), where \(K_0\) is the thermal conductivity of graphene. This difference arises from the higher value of the LA group velocity compared to that of the TA mode. The overall thermal conductivity of the sheet is lower than that of graphene due to reduced symmetry compared to graphene and increased mixing of the acoustical and optical modes (Fig. 1(c)).

Next, we estimate the mechanical strength of this sheet by calculating the in-plane stiffness \(C_\text{s}\), which is the double derivative of total energy \(E\) with respect to atomic displacement \(u_\alpha\), along \(\alpha\)th direction in the following second-order Taylor series expansion around equilibrium:

\[
E = E_0 + \sum_\alpha \frac{\partial^2 E}{\partial u_\alpha^2} u_\alpha + \frac{1}{2} \sum_{\alpha,\beta} \frac{\partial^2 E}{\partial u_\alpha \partial u_\beta} u_\alpha u_\beta + O(u^3)
\]

where, \(E_0\) is the equilibrium energy per atom. This expansion is written in terms of applied strain:

\[
\varepsilon = \frac{a - a_0}{a_0}
\]

with \(a\) and \(a_0\), the lattice parameters with and without strain, respectively, to obtain the equation of \(C_\text{s}\):

\[
C_\text{s} = \frac{1}{A_0} \frac{\partial^2 E(\varepsilon)}{\partial \varepsilon^2}
\]

where, \(A_0\) is the equilibrium area of the sheet per atom and \(E(\varepsilon)\) is the strain energy per atom.

The \(C_\text{s}\) value is computed by plotting the strain energy per atom \((E(\varepsilon))\) vs. applied strain \((\varepsilon)\), and fitting this curve to a second-order polynomial of the form:

\[
E(\varepsilon) = E_0 + \ddot{C}_2 \varepsilon + \ddot{C}_0 \varepsilon^2
\]

where, \(E_0\) is the equilibrium energy. Using the value of \(\ddot{C}_2\), \(C_\text{s}\) is calculated by substituting \(\ddot{C}_2\) with \(\ddot{C}_2\) in equation 3.

The strains were applied along the x- (x-axial strain) and y-axes (y-axial strain) and their corresponding \(C_\text{s}\) values were found to be 299.4 \text{ N m}^{-1} and 338.79 \text{ N m}^{-1}, respectively. They differ along these directions due to anisotropy in the sheet. Surprisingly, despite the presence of the pentagonal and octagonal rings, these values are similar to that of graphene\(^{26}\). Hence, the overall mechanical strength of this sheet is comparable with graphene.

To explore the feasibility of the experimental synthesis of this sheet, we compare its energy with the existing 2D allotropes. Fig. 2 shows the relative energy \((E_\text{rel})\) of various 2D sheets, with respect to graphene. Incidentally, an interesting trend in energy is observed
with respect to the average bond angle deviation ($\delta_{\text{avg}}$) from that of graphene (120°). With the increase in $\delta_{\text{avg}}$, $E_F$ increases, albeit in a non-linear fashion. This is due to the increased amount of energy required to distort the angles from $sp^2$ hybridization. The relative energy of pentahexoctite (marked in blue in Fig. 2) is comparable with that of the haeckelite and pentaheptite structures, while it is remarkably lower than graphenylene, graphene (magenta bonds), and graphdiyne (cyan bonds). Despite the high energies of graphyne and graphenylene, they have been successfully synthesized. Furthermore, graphene containing high concentrations of haeckelite rings, and 4–8 rings, have been synthesized using electron irradiation techniques. Recent experimental studies have also reported that irradiation of the graphene sheet by an electron beam of 80 keV (during TEM imaging of the sheet) transfers a maximum energy of 15.6 eV to a carbon atom which is below the threshold knock-on voltage of 18–20 eV. This transfer of high energy facilitates the formation of multiple Stone-Wales (SW) defects, surmounting the SW barrier of 10 eV. However, an exposure of this electron beam for very short durations concentrated over a small area (electron dosage of the order of 1 × 10^{10} e^-/nm^2) can lead to immediate (few seconds) relaxation to the unperturbed graphene sheet. A strategy of controlled exposure of the pristine graphene sheet to the 80 keV electron beam, along a particular direction for a longer duration over a large area may be employed to obtain the sheet.

Next, we calculate the electronic properties of this sheet. Fig. 3(a) shows the band structure along with the angular momentum resolved density of states (LDOS). The atomic quadruple (1,3,6,8), shows the band structure along with the angular momentum techniques. The electronic structure shows a combination of flat and dispersive bands. Overall, electronically, there are 3 non-equivalent atoms, therefore, two mirror planes. Similar is the case with the doubles (2,7) and (4,5).

Pentahexoctite nanotubes. This sheet can also serve as a precursor for materials of different dimensions such as quasi-1D nanotubes.

Figure 2 | Relative energy ($E_F$) of the various 2D allotropes of carbon with respect to pristine graphene as a function of average bond angle deviation ($\delta_{\text{avg}}$). The colors indicate the different rings present in each structure.

Figure 3 | Electronic properties of the pentahexoctite sheet. (a) Band structure of the pentahexoctite sheet with the angular momentum resolved density of states (LDOS). Fermi level $E_F$ is set to 0 (red-dashed line), (b) and (c) The band decomposed charge densities at $\Delta$ (blue-colored circle in (a)) and X (magenta-colored circle in (a)) points, respectively. The isosurface value was set at 0.005 e/$\text{Å}^3$.

We generate the nanotubes by rolling the pentahexoctite sheet. The chiral vector, $C_h$ and its corresponding translation vector, $T_h$ are shown in Fig. 1(a). Unlike graphene, the chiral vectors span from 0° to 90°. The chirality of a tube is defined by:

\[ C_h = ma_1 + na_2 \]  

where, $m$ and $n$ are the chiral indices. We restrict our study to achiral tubes, $(m,0)$ and $(0,n)$, formed by rolling the sheet along $a_1$ and $a_2$, respectively.

The tubes are stable upon complete relaxation, as shown in Figs. 4(a) (0,8) and (b) (8,0) tubes. The relaxation of the tubes is chirality-dependent. While in the $(0,n)$ nanotubes, the buckling is observed at the pentagonal sites, the $(m,0)$ tubes are seamless. The buckling in the $(0,n)$ tubes originates from two factors: higher curvature of $(0,n)$ tubes as well as larger $\delta_{\text{avg}}$ ($\approx 1.119^\circ$ for (0,8)) in $(0,n)$ compared to the $(m,0)$ ($\approx 0.107^\circ$ for (8,0)) ones. We study the implications of the difference in the geometry on the stability of these tubes. Figs. 4(c) and (d), show the phonon dispersion of the $(0,n)$ and $(m,0)$ tubes, respectively. As a consequence of the local buckling in $(0,n)$ tubes, the TA1 and TA2 modes (right insets of Fig. 4(c)) get softened (zoomed-in version in the left inset of Fig. 4(c)). However, for the $(m,0)$ tubes, due to the seamless geometry, there is no mode-softerning (Fig. 4(d)). With the decrease (increase) in the $(0,n)$ tube’s curvature (diameter), the mode softening decreases eventually vanishing at the zero curvature (infinite diameter) limit, i.e., the sheet.

In order to further assess the mechanical stability, we calculate the in-plane stiffness ($C_l$) and the Poisson’s ratio ($\nu$). $C_l$ for $(0,n)$ tubes (Table 1) are lower than the $(m,0)$ ones (Table 2), as a direct consequence of the mode softening. The increase in $C_l$ with decrease in curvature (Table 1) reflects the trend obtained for the phonon mode-softening. On the contrary, there is no significant variation in $C_l$ with increase in $(m,0)$ tube diameters (Table 2). The Poisson ratio ($\nu$) was evaluated from the negative ratio of the radial strain ($e_{\text{radial}}$) to the axial strain ($e_{\text{axial}}$). The variation of $\nu$ with diameter, is the same for both the cases (Tables 1 and 2).

Flexural rigidity ($D$) is a very important mechanical parameter that provides a measure of the resistance of the sheet to bending to form a tube. It establishes the relationship between the tube’s equilibrium energy ($E_{\text{eq}}$) and its curvature ($1/\hat{D}$) via the following equation:

\[ E_{\text{eq}} = A + \frac{2D}{\hat{D}^2} \]  

where $A$ is the energy required to create a unit area in the sheet.

Figure 4 | Mechanical properties of various nanotubes. (a) In-plane stiffness ($C_l$) and (b) Poisson’s ratio ($\nu$) of various pentahexoctite nanotubes. $C_l$ for (0,8) tubes (Table 1) are lower than the (8,0) ones (Table 2), a direct consequence of the mode softening. The increase in $C_l$ with decrease in curvature (Table 1) reflects the trend obtained for the phonon mode-softening. On the contrary, there is no significant variation in $C_l$ with increase in (m,0) tube diameters (Table 2). The Poisson ratio ($\nu$) was evaluated from the negative ratio of the radial strain ($e_{\text{radial}}$) to the axial strain ($e_{\text{axial}}$). The variation of $\nu$ with diameter, is the same for both the cases (Tables 1 and 2).
$E_{\text{eq}}$ is plotted against the curvature as shown in Fig. 5(a). The intercept $A$ gives the energy per atom of the pentahexoctite sheet, whereas half of the slope gives the value of flexural rigidity ($D$). The $D$ values for the $(m,0)$ and $(0,n)$ tubes, are 2.82 eVÅ$^2$/atom and 1.56 eVÅ$^2$/atom, which are within a range of 30–61% of CNTs$^{37}$. Hence, despite the presence of anisotropy in the sheet, the sheet still shows a high resistance to bending.

Raman spectroscopy is a very important tool for probing the properties of CNTs. One of the most important, of the many Raman active modes, is the low-frequency radial breathing mode (RBM) or the $A_{1g}$ mode, given by the following equation$^{35–38}$:

$$\omega_{\text{RBM}} = \frac{1}{2\pi c R} \sqrt{\frac{C}{\rho_s (1 - v^2)}}$$

(7)

where, $R$, $\rho_s$, and $c$ are the radius, the mass density per cross-sectional area of the tube, and the speed of light (to convert to the spectroscopic unit of cm$^{-1}$), respectively. It is possible to characterize the tubes derived from the pentahexoctite sheet by calculating $\omega_{\text{RBM}}$. $\omega_{\text{RBM}}$ for pentahexoctite tubes were calculated and plotted against the inverse of the radius, as shown in Fig. 5(b). The inset in this figure, illustrates RBM for the $(8,0)$ tube. A linear variation in $\omega_{\text{RBM}}$ is observed which is in agreement with the results obtained for CNTs$^{36,39}$. The values of $\omega_{\text{RBM}}$ were subsequently fitted to the equation:

$$\omega_{\text{RBM}} = A_0 + \frac{A_1}{R}$$

(8)

to obtain the spectroscopic constants $A_0$ and $A_1$: 8.04 cm$^{-1}$ and 1081.97 cm$^{-1}$ Å for $(m,0)$ tubes, and 40.29 cm$^{-1}$ and 774.57 cm$^{-1}$ Å for $(0,n)$ tubes. These spectroscopic constants provide a reliable method for theoretically predicting the RBM frequency for any given diameter of the tube. $\omega_{\text{RBM}}$ values obtained from continuum mechanics were further verified by DFPT calculations for both $(0,8)$ and $(8,0)$ tubes.

Turning to the electronic properties of the tubes, we find that the $(m,0)$ and $(0,n)$ tubes exhibit different electronic properties, due to the anisotropy in the parent sheet. Figs. 6(a) and (b) show the band structures and projected DOS (PDOS) of the $(7,0)$ and $(0,7)$ nanotubes, respectively. The presence of finite number of states at $E_F$ (Figs. 6(a) and (b)), renders these tubes metallic. The flat bands of the $(0,7)$ tube resembles a portion of the band structure of the sheet along the $\Gamma$-X-M direction, whereas the highly dispersive bands of $(7,0)$, the $\Gamma$-Y-M direction. The band structure of the sheet is, therefore, ‘split’ depending on the chirality of the tubes. This unique splitting feature is not restricted to these two tubes but is observed in the entire family of $(0,n)$ and $(m,0)$ tubes. An interesting feature of the electronic structure of the $(0,n)$ tubes, is the presence of linear dispersive bands forming a Dirac cone at the X point. The band-decomposed charge densities are calculated for the flat band (colored

### Table 1 | Mechanical stiffness values for $(0,n)$ family of nanotubes

| Tube | $\frac{\varepsilon^2 E(\varepsilon)}{\varepsilon^2}$ (eV) | $C_v$ (Nm$^{-1}$) | $v$ | $\omega_{\text{RBM}}$ (cm$^{-1}$) |
|------|---------------------------------|----------------|---|------------------|
| (0,6) | 36.06                           | 208.64         | 0.203 | 251.79         |
| (0,7) | 36.72                           | 212.47         | 0.216 | 218.83         |
| (0,8) | 42.28                           | 244.59         | 0.179 | 204.24         |
| (0,9) | 41.59                           | 240.63         | 0.249 | 182.70         |
| (0,10) | 43.03                          | 248.93         | 0.182 | 164.83         |
| (0,$\infty$) | 51.75                      | 299.40         | -   | -              |

### Table 2 | Mechanical stiffness values for $(m,0)$ family of nanotubes

| Tube | $\frac{\varepsilon^2 E(\varepsilon)}{\varepsilon^2}$ (eV) | $C_v$ (Nm$^{-1}$) | $v$ | $\omega_{\text{RBM}}$ (cm$^{-1}$) |
|------|---------------------------------|----------------|---|------------------|
| (6,0) | 54.04                           | 312.69         | 0.220 | 204.47         |
| (7,0) | 54.30                           | 308.35         | 0.230 | 174.62         |
| (8,0) | 54.26                           | 313.88         | 0.156 | 152.08         |
| (9,0) | 55.31                           | 320.01         | 0.291 | 140.97         |
| (10,0) | 55.30                          | 319.92         | 0.254 | 125.31         |
| ($\infty$,0) | 58.56                      | 338.79         | -   | -              |
green in Fig. 6(c), as well as the bands constituting lower, and upper Dirac cones (colored blue and red, respectively in Fig. 6(c)). As expected, the flat band shows a localized charge density. On the other hand, lower and upper cones originate from highly delocalized charge densities leading to linearly dispersive bands at the X point. Although the tubes are metallic, the band structures of the \((m,0)\) and \((0,n)\) tubes are quite different and very rich in features, and therefore, would lead to very interesting transport properties.

Conclusions

In summary, we propose a new \(sp^2\) hybridized 2D allotrope of carbon, named as “pentahexoctite”. This sheet has a reduced \(C_{mmm}\) symmetry with mechanical strength comparable with that of graphene. The band structure of the sheet is a very unique combination of flat as well as highly dispersive bands, consequently rendering it metallic. The difference in the nature of the bands along different directions would lead to the anisotropy in the electronic transport of the sheet. The band structure of the sheet ‘splits’ when the nanotubes with \((0,n)\) and \((m,0)\) chiralities, respectively, are rolled out of these sheets. In addition to the very rich and chirality-dependent electronic properties, the mechanical properties are also chirality-dependent. The absence of the negative frequencies in the phonon spectra along with comparatively lower energy with respect to the already existing 2D allotropes, indicates a strong possibility for this sheet to be realized experimentally.

Methods

All calculations were performed using first-principles density functional theory (DFT)\(^{44}\) as implemented in the Vienna \(ab\) initio simulation package (VASP)\(^{41,42}\). Projector augmented wave (PAW)\(^{43,44}\) pseudopotentials were used to represent the electron-ion interactions. The exchange and correlation part of the total energy was approximated by the generalized gradient approximation (GGA) using Perdew-Burke-Ernzerhof (PBE) type of functional\(^{45}\). A unit cell of the sheet consists of eight atoms, with a vacuum of 15 \(\AA\) added along the \(z\) axis to avoid spurious interactions between the sheet and its periodic images. For integrations over the Brillouin zone, a well-converged Monkhorst-Pack (MP) \(k\)-point mesh\(^{46}\) of \(13 \times 21 \times 1\) (commensurating with the lattice vectors) was used. For tubes, a 15 \(\AA\) vacuum was included in both, \(x\) and \(y\) directions, and well-converged MP \(k\)-meshes of \(1 \times 1 \times 5\) and \(1 \times 1 \times 7\) were used for \((m,0)\) and \((0,n)\) chiralities, respectively. Structural relaxation was performed using the conjugate-gradient method until the absolute value of the components of the Hellman-Feynman forces were converged to within 0.005 eV/\(\AA\). The convergence with respect to the energy cut-offs were performed and the default energy cut-off value of 400 eV was found to be sufficient. Phonon dispersion were obtained by using density functional perturbation theory (DFPT)\(^{44,47}\) with a strict energy convergence criterion of \(1 \times 10^{-6}\) eV and an energy cut-off of 500 eV in order to obtain accurate forces.

![Figure 5](image5.png)

**Figure 5 | Mechanical parameters of the nanotubes.** (a) Equilibrium energy per atom \(\left(E_{eq}\right)\) of the tube vs. curvature \((1/d^2)\) for both \((m,0)\) (blue circles) and \((0,n)\) (red squares) tubes. (b) The radial breathing mode (RBM) frequency \((\omega_{RBM})\) of the \((m,0)\) (blue circles) and \((0,n)\) (red squares) tubes as a function of the inverse of their radii. The inset shows the RBM for the \((8,0)\) tube. The green- and orange-dashed lines, in both (a) and (b), correspond to the linear fits of the \((m,0)\) and \((0,n)\) tubes respectively.

![Figure 6](image6.png)

**Figure 6 | Electronic properties of the \((0,n)\) and \((m,0)\) nanotubes.** (a) and (b) Band structures and PDOS of atoms 1,2, and 4 for the \((7,0)\) and \((0,7)\) nanotubes, respectively. Fermi level \(E_F\) is set to 0 (red-dashed line). (c) Indicates the band-decomposed charge densities corresponding to flat band (green color), as well as lower and upper Dirac cones (blue and red colors, respectively) at the X point. The isosurface value was set at 0.0011 e/\(\AA^3\).
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Author contributions
B.R.S. and A.M. performed all the calculations and contributed equally. All the authors participated in writing of the manuscript. A.K.S. conceived, designed, and supervised the entire project.

Additional information
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