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# Novamene: A new class of carbon allotropes

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## Abstract

We announce a new class of carbon allotropes. The basis of this new classification resides on the concept of combining hexagonal diamond ( $sp^3$  bonded carbon – lonsdaleite) and ring carbon ( $sp^2$  bonded carbon – graphene). Since hexagonal diamond acts as an insulator and  $sp^2$  bonded rings act as conductors, these predicted materials have potential applications for transistors and other electronic components. We describe the structure of a proposed series of carbon allotropes, *novamene*, and carry out a detailed computational analysis of the structural and electronic properties of the simplest compound in this class: the single-ring novamene. In addition, we suggest how hundreds of different allotropes of carbon could be constructed within this class.

Keywords: Chemistry, Materials science

## 1. Introduction

Elemental carbon occurs throughout nature in a wide variety of allotropic forms. This variety of allotropic forms is attributed to carbon being the only element in the periodic table known to have stable isomers with 1, 2, or 3 dimensions. The carbon atom can hybridize electronic states forming different but mutually compatible binding geometries leading to a rich range of binding topologies and electrical properties. Schematically, carbon can function either as a conductor, in  $sp$  chains –

carbynes – and  $sp^2$  planar structures – graphene and graphite, or as a wide-gap insulator in  $sp^3$  tetrahedral coordination – e.g. diamond and alkanes. The origin of these properties can be traced directly to the type of hybridization:  $sp$ ,  $sp^2$ , or  $sp^3$ . The first two have the potential to form bonds that are electrically conducting while  $sp^3$  has insulating properties.

In 1985 Richard Smalley et al. at Rice University discovered a new class of carbon allotrope – fullerenes. Since then no other new class has been identified, although in the quest for new materials, extended research addressed a broad range of new arrangements of carbon [1, 2, 3, 4, 5, 6]. The arrangement of carbon allotropes crosses an astonishing range of extremes, yet they are all merely structural formations of the same element. What distinguishes carbon in this plethora of allotropy is not only the structure but also the bond types.

Hexagonal diamond, also called lonsdaleite, is an allotrope of carbon with a hexagonal structure. Lonsdaleite was first identified in 1967 from the Diablo Canyon meteorite, where it occurs as microscopic crystals alternating with cubic diamond [7]. Hexagonal diamond has also been synthesized in the laboratory [8] by compressing and heating graphite either in a static press or using explosives [9]. Lonsdaleite has also been produced by the thermal decomposition of a polymer, poly(hydridocarbyne), at atmospheric pressure, under argon atmosphere, at 1,000 °C [10, 11], or by chemical vapor deposition [12, 13, 14]. The hardness of lonsdaleite is theoretically superior to that of cubic diamond (up to 58% more) according to computational simulations [15]. However natural specimens exhibit significantly lower hardness through a large range of values (from 7 to 8 on Mohs hardness scale). The cause of the lower hardness is speculated to be due to significant lattice defects and impurities in the samples [16].

This speculation led the first named author of the present paper to a simple idea in September 2014: What would an allotrope of carbon resemble that combines both *hexagonal diamond* and *graphene*? It is this speculation that led to this simple concept – that hexagonal diamond has the ability to be “stitched together” with graphene to form hundreds of carbon allotropes. A substantial percentage of  $sp^2$  defects of the kind discussed in the presently proposed structures could also explain the lower hardness of lonsdaleite samples.

Due to its unique chemical and physical properties graphene is starting to find applications for electronic components including, but not limited to, integrated circuits, optoelectronics, Hall effect sensors, quantum dots, optical absorption/modulation, infrared-light detection, photovoltaic cells, conductive electrodes, fuel cells, supercapacitors, molecular absorption sensors, and piezoelectric devices.

The variety of structures of the presently disclosed novamene allotropes, combining an electron conducting graphene core surrounded by an insulating

[17] outer lonsdaleite, may prove useful for several of the above mentioned applications. Different allotropes would serve as an ideal platform providing flexibility for the desired application. For example, in the production of integrated circuits, the incorporation of the presently disclosed carbon allotrope would provide high carrier mobility due to the central graphene core, together with stiff mechanical properties.

This paper is organized as follows: the Background section sketches the idea for the new allotropy called novamene; the Results section describes this class of allotropes, focusing on the simplest novamene structure, the one based on one hexagonal ring, for which a detailed investigation based on the density-functional theory (DFT) is provided; in the Conclusions section we compare the present structures with experimental evidence about a recently synthesized material, Q carbon, and discuss the obtained results.

## 2. Background

In the present paper, we propose the concept of various  $sp^2$  hexagonal carbon rings surrounded by hexagonal diamond. Each combination of rings and additional enveloping lonsdaleite layer leads to a different allotrope of carbon.

A parallel to this allotropy was demonstrated with the fullerenes: their study began with the pursuit of identifying the structure of  $C_{60}$ . This concept grew rapidly with other allotropes such as  $C_{70}$ , carbon nano-onions, and so on. In turn, this led to the idea and discovery of single-walled carbon nanotubes, multi-walled ones, and numerous other fullerene-type allotropes of carbon.

### 2.1. Mathematical combinations of hexagonal rings

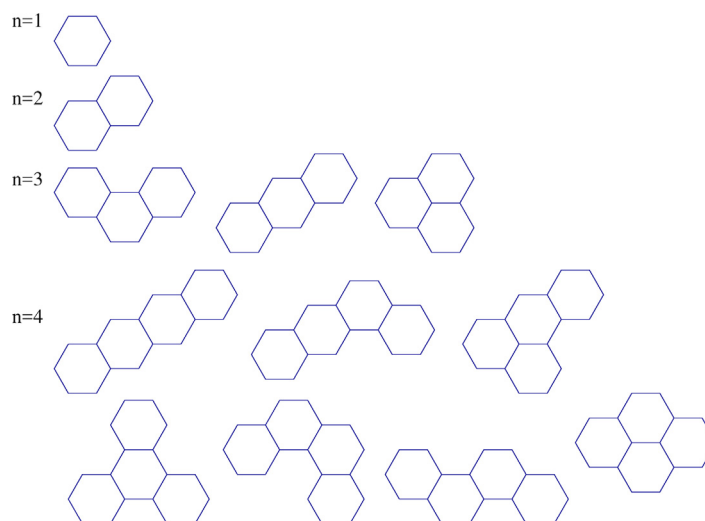
The geometric arrangements of adjacent hexagonal rings are called fusenes. Fusenes are mathematical combinations of joined hexagonal rings within a plane [18, 19], as sketched in Fig. 1, and numbered in Table 1.

This classification provides a “menu” for the configurations of the hexagonal rings forming the  $sp^2$  carbon core of the novamene compounds that we introduce in the following.

## 3. Results

### 3.1. The single-ringed novamene: concept

The simplest unit of graphene is a single six-carbon ring. When this ring is surrounded by hexagonal diamond, this  $sp^3$  carbon arranges in 3 five-carbon rings and 3 seven-carbon rings, which assemble together as illustrated in Fig. 2. A physical, three-dimensional (3D), ball-and-stick model was built and investigated



**Fig. 1.** A sketch of all possible inequivalent combinations of one to four hexagonal rings in a plane. carefully. Then the repeated unit and its symmetries were identified, and computer renderings were generated.

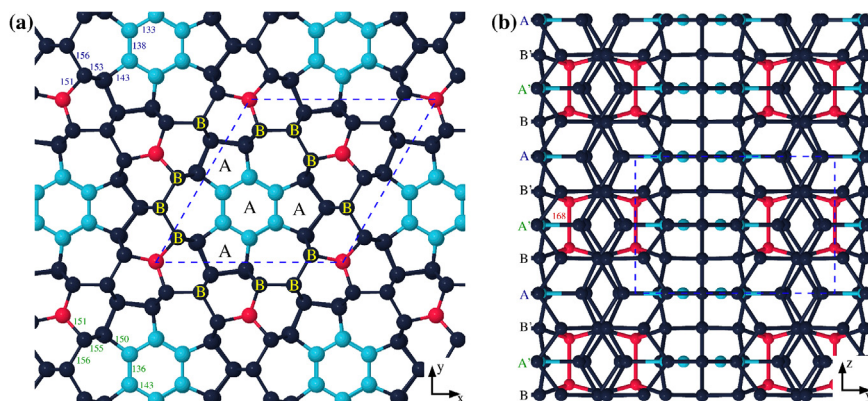
One of the key features about this proposed carbon allotrope is that a simple repeat-unit, highlighted in Fig. 2, can be translated periodically to construct an extended 3D structure. More details about the number of layers needed to fully describe the smallest repeating unit of the structure are given in the next section.

### 3.2. The single-ringed novamene: crystal structure

Since the study of the proposed carbon allotrope starts from a qualitative 3D model, it is important to propose physical constraints to the bond-lengths in this arrangement. As such, the proposed structure is better understood by making comparisons to known carbon allotropes, including diamond, graphite (where

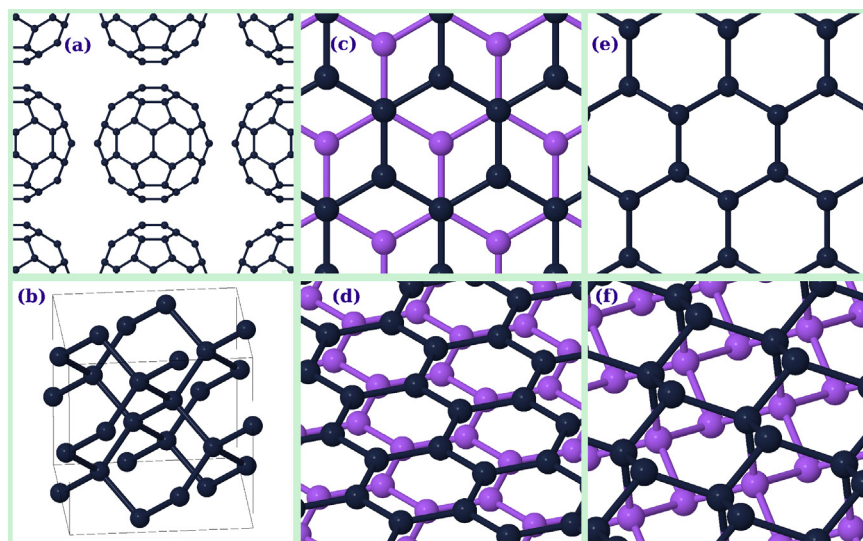
**Table 1.** The number of combinations of inequivalent hexagonal ring placements as a function of the number of rings in the plane.

No. of Rings	No. of Combinations	No. of Rings	No. of Combinations
1	1	9	7,036
2	1	10	33,836
3	3	11	166,246
4	7	12	829,987
5	22	13	4,197,273
6	82	14	21,456,444
7	339	15	110,716,585
8	1,505	16	576,027,737



**Fig. 2.** The structure of single-ring novamene crystal; (a): top view; (b): side view. Atoms in the rings surrounding A letters belong to the A or A' planes. Atoms marked by a B letter belong to B or B' planes. Red “switching” atoms move out of the B and B' planes to form a bond. All atoms are carbon; most are bonded to four other atoms, except for the cyan ones in the A hexagonal rings which are  $sp^2$  and bonded to three other atoms. Blue/green bond lengths (in pm) refer to bonds in the A/A' plane and with adjacent B or B' planes. Dashed line: the boundary of the periodic unit cell.

graphene is a single layer of graphite), lonsdaleite, and fullerene, see Fig. 3. Indeed, the proposed structure draws on elements of each of these compounds. For example, the motif of single hexagonal rings of carbon surrounded by three carbon pentagons is similar to the fundamental repeating pattern in “bucky-balls” (Fig. 3a). In that structure, C-C distances in the hexagonal rings surrounded by a total of six alternating pentagons and hexagons are on the order of 1.45–1.49 Å [20]. It is the folding up of these alternating hexagons and pentagons surrounding a



**Fig. 3.** Structures of common carbon allotropes used for comparison in this study: (a) fullerene; (b) diamond; graphite, (c) top view looking down the  $z$ -axis, and (d) tilted side view below; lonsdaleite, (e) top view looking down the  $z$ -axis, and (f) tilted side view. All balls represent carbon atoms, different colors are used purely to distinguish alternating layers in hexagonal structures (c-f).

central hexagonal carbon ring that leads to the classic soccer-ball shape of fullerenes. In contrast, in the present novamene the grouping of 3 pentagons surrounding a central hexagonal ring remains “in plane”, thanks to 7-atom carbon rings popping up from the A to the nearing B plane. For the AB interplanar distance we initially take a tentative 2.5 Å.

We construct the initial guess for the structure by enforcing threefold symmetry around the center of the  $sp^2$  hexagon, and a repeated hexagonal cell with the same symmetry. Each periodically repeated cell includes 26 carbon atoms, 15 of which in the A plane plus 11 in the B plane. It is crucial to consider the possibility that the atoms in the B layer marked in red in Fig. 2 (“switching atoms”) could move out of the plane switching from  $sp^2$  to  $sp^3$  and forming an extra bond with their partners in the next B layer. As this bonding occurs with the atoms in one plane moving toward the other, the two planes are not equivalent any more, with the result that the minimum repeated cell for the dimerized structure includes a ABA'B' alternation for a total of 52 atoms. Both structures are characterized by the same space group P-62 m (#189).

### 3.3. DFT simulations for the structure of single-ringed novamene

To obtain a reliable equilibrium structure for the single-ring novamene, we resort to DFT simulations. We describe the electronic structure in the local density approximation (LDA) using a plane-waves basis with a kinetic energy cutoff of 408 eV, with standard ultrasoft pseudopotentials to account for the 1s core electrons of carbon [21] as implemented in the Quantum Espresso [22] package. The same standard approach was adopted in similar carbon-only contexts in previous work [23, 24, 25, 26, 27, 28, 29, 30].

Starting from the tentative initial structure described in Sect. 3.1, we relax the atomic positions and cell parameters and identify a local minimum of the total DFT energy. Atomic relaxation is carried out until all forces are equal to or less than 4 pN, the residual stress less than 10 bar and the total energy converged to less than  $10^{-6}$  eV/atom. We provide the basis of fully relaxed atomic positions of the 52 atoms in the cell in the Supplementary Content. Space-group symmetries would allow one to obtain all 52 atomic positions in terms of 9 inequivalent ones.

Table 2 summarizes the properties of the resulting lowest-energy structure, which is the dimerized semiconducting one, based on the 52-atoms cell. These results are compared with other common allotropes of carbon. The tendency of LDA to overestimate binding and to underestimate energy gaps is evident in the comparison. From the thermodynamical point of view, the single-ring novamene structure is slightly less stable than graphite and diamond, but it is a sharp local energy minimum, guaranteeing its long-term stability.

**Table 2.** The main structural and electronic properties of single-ring novamene compared to selected carbon allotropes. These properties are obtained by means of DFT-LDA simulations with the same technical characteristics described in the text; \* refers to experimental figures.

Structural parameter	Single-ring novamene (hexagonal)	Graphite (hexagonal)	Diamond (face-centered cubic)	Lonsdaleite (hexagonal)
a [Å]	8.4188	2.433	3.523	2.477
		2.464*	3.56683*	2.51*
c [Å]	4.9981	5.898	–	4.126
		6.711*		4.12*
N <sub>atoms</sub> per cell	52	4	2	4
Cell volume [Å <sup>3</sup> ]	306.79	30.23	10.93	21.93
		35.29*	11.34*	22.658*
Density [kg/m <sup>3</sup> ]	3381	2639	3649	3638
		2261*	3516*	3521*
Cohesive energy [eV/atom]	9.930	10.303	10.157	10.132
		7.374*	7.346*	
Band gap [eV]	0.34	0	4.22	3.03
		0*	5.47*	4.5*

The alternative structure where the switching atoms remain in their  $sp^2$  hybridization laying flat inside equivalent B layers is metallic instead. Our simulations evaluate the total energy of the metallic structure above the ground state by 0.042 eV/atom, or 2.18 eV per cell, or, more significantly, 1.09 eV per pair of switching atoms. This energetics suggests a weak Peierls dimerization transition [31]. This energy difference is comparably small, and suggests the possibility to switch between the ground-state distorted semiconductor to the undistorted metal and back. Such switching may be driven by temperature, light, and/or uniaxial strain. We investigated also the possibility of an alternating bonding pattern with one of the pairs of the switching atoms binding inside the cell, and the other two atoms binding to like atoms in neighboring cells: the total energy is the same within our resolution, and the crystal is a small-gap semiconductor in this other

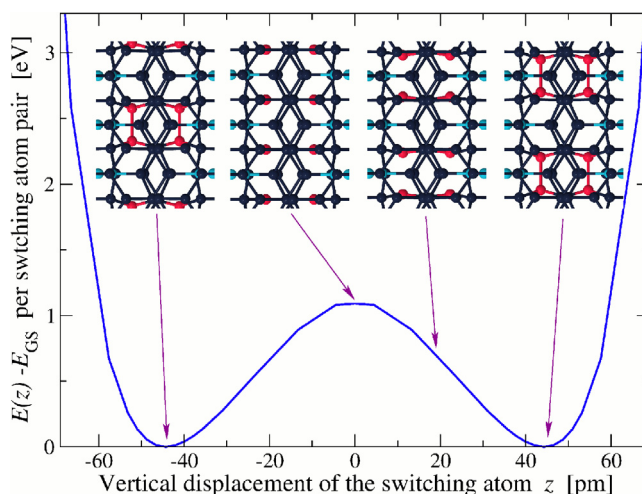
structure too. This indicates that in the actual crystal each individual vertical row of switching atoms can form dimers almost independently of the other rows. As a result, even with perfectly ordered dimerized lines, we can predict a weak lateral correlation (and therefore structural disorder) of these dimerized lines.

The switching atoms can also explore the non-dimerized configuration, crossing a relatively shallow energy barrier depicted in Fig. 4. High temperature will certainly favor the exploration of this shallow double-well potential profile, most likely leading to a metallic non-dimerized phase.

### 3.4. Electronic properties of the single-ringed novamene

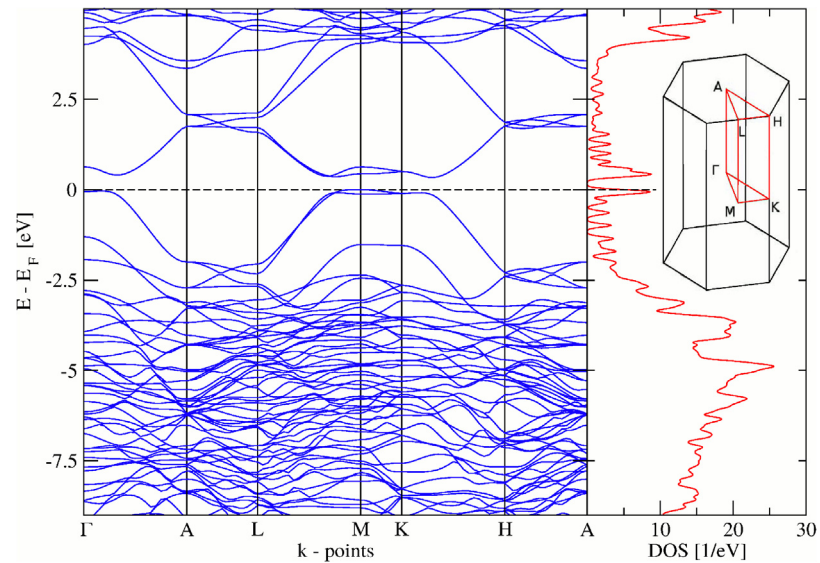
Fig. 5 reports the band structure of the relaxed crystal. The overall density of states is very much resemblant of that of hexagonal diamond [32], except for the bands near the Fermi energy, which move in very close, and remain separated by a quite small gap. These bands describe the energies of  $\pi$  orbitals localized mostly on the hexagonal rings. These bands are dispersive mostly in the  $k_z$  direction ( $\Gamma$ -A, L-M, and K-H segments), while they are quite flat in the in-plane directions, indicating strong localization around the  $sp^2$  rings and “insulation” provided by the surrounding  $sp^3$  carbons.

The present simulation indicates that the novamene structure is a semiconductor characterized by a 335 meV indirect gap (most likely larger in reality due to the



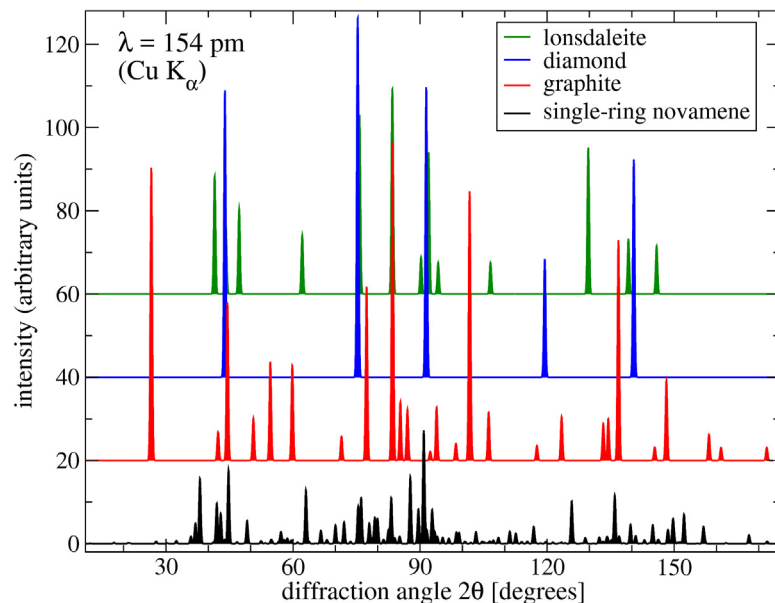
**Fig. 4.** The total energy of the single-ring novamene crystal structure as a function of the (fixed) vertical position of the switching atoms, with all other atomic positions allowed to relax. Insets display the atomic configurations corresponding to the minima, the maximum and an intermediate distortion. The minima represent equivalent relaxed configurations with the dimers forming across B-B' or B'-B planes. The reference coordinate  $z = 0$  identifies the high-symmetry non-dimerized condition where switching atoms hybridize exactly  $sp^2$  and remain in the B planes, so that planes A = A' and B = B', and the crystal can be described in terms of a 26-atoms cell.





**Fig. 5.** Left: the band structure of single-ring novamene along a path through special points in the Brillouin zone depicted as an inset. Right: the density of electronic states (DOS).

well-known tendency of the LDA to underestimate band gaps). The maximum of the valence band is at the M point and the minimum of the conduction band is along the K-H line. However the flatness of the bands determines peaks in the density of states near the band edges, which should translate into strong light absorption in the infrared immediately above the gap energy. The anisotropy of the



**Fig. 6.** Theoretical XRD pattern generated for the single-hexagon novamene structure (black). For comparison, the simulated patterns for the experimental structures of graphite (red), diamond (blue), and lonsdaleite (green).

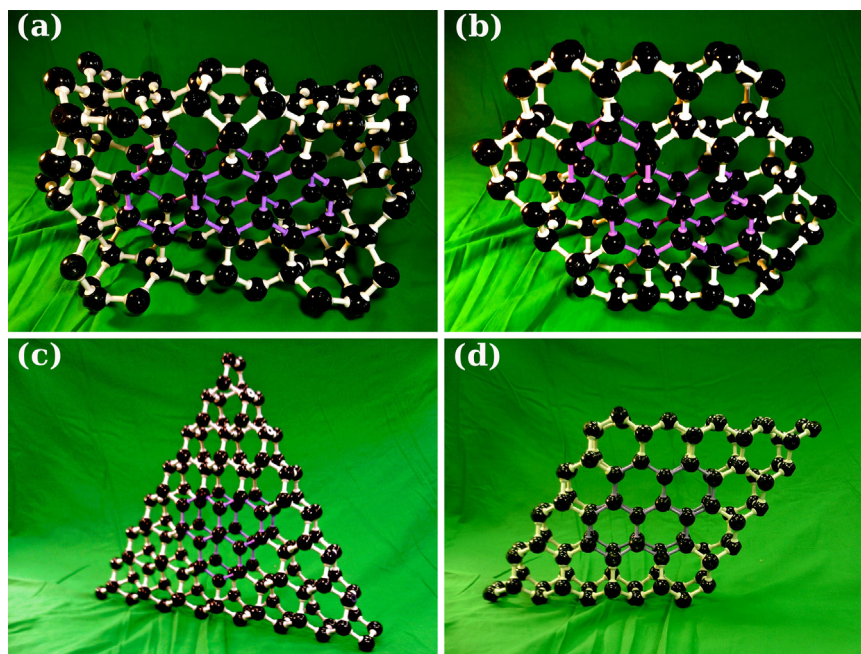


**Fig. 7.** Ball-and-stick model of a two-ringed novamene. The purple bonds connect  $sp^2$  carbon and the white bonds link  $sp^3$  carbon.

novamene structure is likely to provide a directional guide for excitons generated by absorbed light in solar-energy harvesting applications [33].

### 3.5. Single-ringed novamene: simulated diffraction pattern

The equilibrium geometry determined in this report provide enough structural data to generate a theoretical X-ray diffraction (XRD) pattern, shown in Fig. 6. While the XRD pattern of the proposed single-ring novamene structure exhibits several overlapping occurrences with experimental peaks of diamond, graphite, and



**Fig. 8.** Ball-and-stick models of (a) a "linear" three-ring novamene allotrope; (b) a "bent" three-ring novamene allotrope; (c) a "clustered" three-ring novamene allotrope; and (d) a "clustered" four-ring novamene allotrope.

lonsdaleite, the larger cell generates numerous additional peaks in between the main peaks of the more conventional allotropes. The computed XRD pattern will allow experimentalists to identify the proposed allotrope when it is synthesized.

### 3.6. Multi-ringed novamene

Based on the above analysis, it is intuitively obvious that other novamene allotropes would also be possible. This concept expands the number of rings “encased” in hexagonal diamond, tilting the  $sp^2$ – $sp^3$  balance in favor of  $sp^2$ , and leading to a number of other structures, a few examples of which are displayed in Figs. 7 and 8.

The detailed investigation of the structural and electronic properties of these higher novamenes will be the subject of future investigation.

## 4. Conclusions

We introduce a new class of allotropes of carbon. By ab-initio studies we prove the relative stability of the simplest of these compounds, single-ring novamene. We propose the structures of a few other carbon-only crystals in this class.

The structural information (space group, lattice parameters, and atomic positions) provide the necessary starting ground for future investigations of the mechanical properties, phonon spectra, and thermodynamical stability as a function of pressure and temperature. The main challenge ahead is the synthesis of actual crystals of novamene, and their experimental characterization.

Recently, J. Narayan, and A. Bhaumik [1, 34] synthesized a novel phase of carbon by nanosecond laser melting and quenching carbon from the super undercooled state in the form of thin films or filaments. They called this material “Q-carbon”, and showed that it has an amorphous structure. The Raman spectrum of Q-carbon exhibited a very large fraction of  $sp^3$  (75%–85%) bonded carbon from the relative intensity of the diamond peak at  $1333\text{ cm}^{-1}$  and the  $sp^2$ -related peaks at  $1140\text{ cm}^{-1}$  and  $1580\text{ cm}^{-1}$ . It is perhaps too early to speculate, however, our single-ring novamene has an  $sp^3$  fraction (77%) that is comparable. It is our conjecture that a detailed structural analysis could prove that Q carbon is a disordered arrangement containing a substantial percentage of single-ring novamene, plus hexagonal carbon, plus possibly multiple-ringed novamene.

On the theory side, using electronic-structure methods, the next step will be the exploration of the electronic properties of the multi-ringed novamene, including band gaps and electrical transport properties. Also the optical properties of these compounds should be investigated in depth.

Finally, we suggest that, in addition to carbon, novamene-type structures could be relevant even for silicon and germanium.

## Declarations

### Author contribution statement

Larry Burchfield: Conceived and designed the experiments; Performed the experiments; Analyzed and interpreted the data; Wrote the paper.

Mohamed Al Fahim: Contributed reagents, materials, analysis tools or data.

Richard S Wittman and Francesco Delodovici: Performed the experiments; Analyzed and interpreted the data; Wrote the paper.

Nicola Manini: Performed the experiments; Analyzed and interpreted the data; Contributed reagents, materials, analysis tools or data; Wrote the paper.

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## Competing interest statement

The authors declare no conflict of interest.

## Additional information

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