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Structure and Properties of Pseudo-Graphenes. Review

N.D. Abramenko[1], M.A. Rozhkov[1], A.L. Kolesnikova[1,2] and A.E. Romanov[1,3]

[1]ITMO University, Kronverksky pr. 49, 197101, St. Petersburg, Russia
[2] Institute for Problems in Mechanical Engineering, RAS, Bolshoj pr. 61, Vas. Ostrov, 199178, St. Petersburg, Russia
[3] Ioffe Physical-Technical Institute, RAS, Polytechnicheskaya 26, 194021, St. Petersburg, Russia

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Abstract. In this review, we consider structure and properties of pseudo-graphenes – graphene-like crystals with high density of non-hexagonal (defective or improper) carbon atomic rings. As an introduction, graphene and its properties are briefly described and disclination defects in graphene are considered. Then, numerous articles presenting *graphene allotropes* and *carbon allotropes* are analyzed. As a result, a term *pseudo-graphene* for description of materials with high density of improper carbon atomic rings arranged periodically is proposed and a unified classification of pseudo-graphenes regarding the materials from available articles is suggested. The materials chart is created based on proposed classification and materials properties. In this chart, two categories are reviewed separately: sp^2 pseudo-graphenes and non-sp^2 pseudo-graphenes. The analyzed materials are subdivided into semiconductors, metals, semimetals, and superconductors.

1. INTRODUCTION

Carbon is capable to form many allotropes – solids made of the same chemical element, different in atomic arrangement of this element. Several widely known carbon allotropes are: diamond – the hardest natural material [1]; graphite, which has a wide variety of usage (for example, as a dry lubricant [2] and an electric conductor [3]), fullerenes that can be used in creation of optical devices [4], carbon nanotubes [5], which, have promising applications in biomedicine [6], and graphene– material that can be used in electronics [7].

Depending on the internal atomic arrangement, these allotropes can demonstrate different behavior of electrons of the outer electron shells that are responsible for bonding of carbon atoms [8]. It is known that a carbon atom has 4 valence electrons. Interatomic bond “carbon-carbon” (C – C) can be sp^1-, sp^2- or even sp^3-hybridized. For example, diamond has a face centered cubic crystal lattice, where all atoms are connected by sp^3 bonds.In this case, all four valence electrons participate in forming strong covalent bonds with neighboring atoms. This is what allows a diamond to be one of the most durable materials [9]. Graphite has sp^2-hybridization, in which three valence electrons form covalent bonds between carbon atoms in the plane, which form a hexagonal lattice. The remaining electron is in a free state. The described structure leads to anisotropy of properties in graphite for directions parallel or perpendicular to the atomic layers [8]. If we take one isolated atomic layer of graphite, then we get graphene – two-dimensional atomic pattern with hexagonal carbon rings, in which sp^2- hybridization is also realized [10]. Nanotubes [5,11] and fullerenes [4,12] also possess sp^2-hybridization. In addition, cases are possible when several types of bond hybridization are observed in a single carbon allotrope [13,14].

Graphene is a two-dimensional carbon allotrope, which has a variety of promising application properties: it has remarkable electronic characteristics [10,15,16], thermal conductivity [17-19] and a unique set of mechanical characteristics [20]. Its successful synthesis [21] attracted great attention and marked an active growth of interest in the study of two-dimensional crystals.

The physical and mechanical properties of graphene can be controlled by external influences: mechanical [22], electrical [23], magnetic [24], and / or by changing the local crystalline perfection of graphene [25-28]. For ex-

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Corresponding author: M.A. Rozhkov, e-mail: marozhkov@itmo.ru

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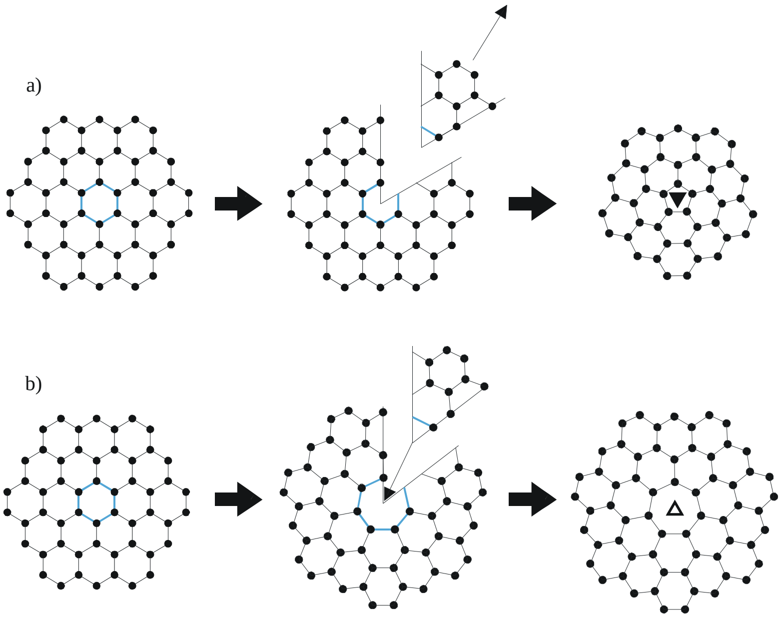

Fig. 1 – Procedure for wedge disclination formation in graphene crystals: a) for a positive wedge disclination with a strength of ω = + π/3; b) for a negative wedge disclination with a strength of ω = -π/3; positive and negative disclinations are designated with black and white triangles, respectively.

ample, calculations of the electronic band structure of graphene show that tensile deformation allows one to obtain a band gap that is absent for graphene in its natural state [22]. Graphene lattice defects, in turn, alter the mechanical properties (that is analogous to the effects observed in the conventional three-dimensional crystals) [25,26], promoting at the same time an increase in electrical conductivity [27] and thermal conductivity of graphene [25,28]. In a graphene crystal, embedded carbon atoms or vacancies that "capture" or rearrange interatomic bonds [29] lead to the appearance of carbon rings with locally broken axial hexagonal symmetry – improper rings [29-31]. Improper rings, as well as their ensembles, which form grain boundaries and interfaces between neighboring graphene crystallites [27,32], can be considered as disclination defects. Carbon rings in the form of squares, pentagons, heptagons, and octagons are then associated with cores of wedge disclinations with a strength (charge) +2π/3, +π/3, -π/3 and -2π/3, respectively [33-35].

There are numerous studies where two-dimensional carbon crystals, different from graphene, are investigated [36-39]. In such crystal one can observe high density of carbon atomic rings with defects, organized in periodic manner. These crystals are commonly called as *graphene allotropes* [40,41] *and carbon allotropes* [42,43]. However, no one has suggested a unified nomenclature for such materials yet. We propose to allocate to them a special term – *pseudo-graphene*, which we have introduced earlier, see, for example, Refs. [35,44,45].

Pseudo-graphene is a two-dimensional carbon crystal consisting mainly of improper (non-hexagonal) carbon rings, which are arranged according to a periodic law. One of the first mentions of two-dimensional carbon crystals dates back to 1987 [36], long before the experimental synthesis of pure graphene. In Ref. [36] several examples of pseudo-graphenes were given, which were called graphynes. Based on a defect structure, pseudo-graphene can possess various properties different from pristine graphene[46]. For example, a pseudo-graphene can be a semimetal [47] or a semiconductor[48] with great usage potential [42], or it can be highly thermal resistant [41],or possess enhanced mechanical characteristics [49].

The aim of this review is to analyze the current state of art of pseudo-graphene research. We start with the review of graphene lattice defects in Section 2 and modern methods of materials modeling in Section 3. In Section 4, we present the information on available pseudo-graphene studies to establish a classification of the graphene-like materials and to look for any possible consistent patterns within the classification. In Section 5, we discuss the results we reviewed in Section 4. And finally, in Section 6 we arrive to conclusions regarding the entire article.

2. DISCLINATION DEFECTS IN GRAPHENE

It is convenient to describe structural defects in graphene by accounting for the change in the local sym-

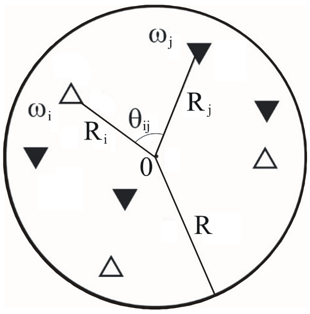

Fig. 2 – Schematics for calculating the energy of a disclination ensemble in an elastic disk of radius *R*. White and black triangles designate negative and positive disclinations, respectively; ω_i and ω_j indicates to disclination strengths.

metry of carbon rings in its two-dimensional hexagonal lattice, i.e. by the relating the defects to carbon rings with a symmetry different from the 6-th fold symmetry, see Fig. 1. The presence of improper carbon rings is unambiguously associated with defects of the rotational type – wedge disclinations [50]. An isolated 5-member carbon ring (Fig. 1b) is associated with a wedge disclination with a strength (charge) $\omega = +\pi/3$, and a 7-member ring (Fig. 1b) – with a disclination with a strength $\omega = -\pi/3$. Similarly, wedge disclinations of higher strengths can be obtained. Defects of this type can be designated by the number of atoms in the improper rings, for example, defect 5-7 is a configuration of 5- and 7-member rings being in direct contact.

Any structural defect in graphene can be described using disclinations if sp^2 hybridization is preserved. For example, the 5-8-5 defect is a configuration of three disclinations: two positive and one negative disclinations. In the same time, this configuration can be considered as divacancy or as a dislocation dipole [35].

To estimate the energy of graphene crystals with isolated disclinated carbon rings or with their ensembles, and pseudo-graphenes consisting of periodic distributions of such rings, one can utilize the formulas given by the theory of elastic continuum with disclinations. It is known that the energy of a single wedge disclination in an elastic disk is proportional to the square of its radius [51,52]. This means that radius *R* serves as the external screening parameter. From the point of view of its energy, disclination can exist either in a limited in size solids, e.g., nano-objects, or in vicinity the body boundary, or in a self-screened ensemble of disclinations of opposite sign [51,52].

In a flat crystal, the condition for self-screening of a disclination configuration is its zero total charge and dipole moment:

$$\sum_i \omega_i = 0, \qquad (1)$$

$$\sum_i \omega_i \boldsymbol{r}_i = 0, \qquad (2)$$

where ω_i is the strength (charge) and $\boldsymbol{r}_i$ is the radius vector of the *i*-the disclination position in the ensemble, respectively.

The total energy of the disclination ensemble is the sum of the self-energies of disclinations E_k^s and the energies of their pair interactions E_{ij}^{pair}:

$$E = \sum_k E_k^s + \frac{1}{2}\sum_i \sum_j E_{ij}^{pair}, \quad i \neq j. \qquad (3)$$

To calculate the energies included in the sum (3), it is convenient to use the formulas for the disclination energy and the energy of disclination pair interaction in an elastic disk, see Fig. 2, [52,53]:

$$E_i^s = \frac{G\omega_i^2 R^2 (1+\nu)}{16\pi}\left(1 - \frac{R_i^2}{R^2}\right)^2, \qquad (4)$$

$$E_{ij}^{pair} = \frac{G\omega_i\omega_j(1+\nu)}{8\pi} \times \Bigg[\left(R_i^2 + R_j^2 - 2R_iR_j\cos\theta_{ij}\right) \times \ln\frac{R^2\left(R_i^2 + R_j^2 - 2R_iR_j\cos\theta_{ij}\right)}{R_i^2R_j^2 - 2R^2R_iR_j\cos\theta_{ij} + R^4} + R^2 - R_i^2 - R_j^2 + \frac{R_i^2R_j^2}{R^2}\Bigg], \qquad (5)$$

where *G* is the shear modulus of graphene (note that graphene is elastically isotropic material); ν is its Poisson's ratio; ω_i is the charge of the *i*-th disclination; *R* is the radius of the disc; R_i is the distance of disclination to the center of the disc. θ_{ij} is the angle between the radial directions for the *i*-th and *j*-th disclinations.

Improper carbon rings in flat crystals other than those having sp^2 hybridization of carbon atom bonds cannot be modeled in this way. This is due to the fact that the "original" defect-free lattice should demonstrate the same type of hybridization as the defective one to operate with effective elastic properties of graphene. In this case, the introduction of disclinations will occur in a flat carbon crystal that is not graphene. And since the "initial" crystal lattice is unknown, it will be impossible to reveal the disclination structure.

A theoretical analysis of the crystal lattice of flat carbon crystals with sp^2-hybridization makes it possible to visually reveal the disclination structure and carry out analytical calculations of strain and stress maps in the crystal, as well as estimate the energy of defects. Ref. [44] considers the application of disclination approach to graphene with defects, where a comparison has been made between the calculations obtained analytically and by the molecular dynamics method for a limited number of pseudo-graphene configurations. The effect of the density of defects and ensembles of defects on the final energy of the crystal has been demonstrated. In Ref. [54], using analytical formulas, energies and strain maps of interfaces in graphene have been found.

3. APPROACHES TO MODELING CARBON ALLOTROPES AND GRAPHENE CRYSTALS WITH DEFECTS

In most cases, the density functional theory [55] is used to study the properties of pseudo-graphenes. This method is based on the fact that the most important properties of a system of interacting particles can be expressed using the electron density functional. Calculations are often done in VASP [56] or Quantum Espresso [57] software packages. In addition, various types of functionals are used for calculations, such as, for example, Perdew - Burke - Ernzerhofone [58]. The authors of Ref. [59] investigated the effect of deformation of graphene on its electronic band structure. The simulation was carried out using the Perdew-Wang (PW91) functional in the VASP software package. The applied method allows not only to optimize the geometry of the crystal by minimizing the potential energy, but also to calculate the physical properties of the material: electronic structure [59], elastic constants [60], and electronic characteristics [61]. The main limitation of this method is the requirement for computational resources.

The method of molecular dynamics allows one to carry out atomistic modeling of crystals using the laws of classical physics as a basis, representing atoms in the form of material points. This method makes it possible to trace the dynamics of changes in the crystal structure in time, while spending much less computer time compared to the density functional theory approach. In addition to optimizing the geometry of the crystal lattice, it is possible to calculate elastic constants, find mechanical stresses, elastic strains, and temperature fields, as well as observe physical processes over time, for example, analyzing mechanical loading of a crystal and the corresponding tension diagram. To correctly conclude on the geometry of the lattice and the physical properties of crystals, it is important to choose properly the interatomic interaction potential, which describes the nature of the interaction between atoms in the crystal. For carbon materials, the most widespread potentials are AIREBO [62], Tersoff [63] and REAXFF [64]. One of the most commonly used molecular dynamics software packages is LAMMPS [65]. Each potential has its own areas of application, and this must be considered before starting the simulation. Ref. [66] presents the results of molecular dynamics simulation of the energy of point and linear defects in graphene, its elastic constants, as well as theoretical strength and critical strain. To obtain these results, the AIREBO potential was used, which gives good agreement between the results for graphene. However, to model pseudo-graphenes, it is necessary to select the interatomic interaction potential more carefully, as it is discussed in Ref. [67].

4. PSEUDO-GRAPHENES

4.1. Classification of pseudo-graphenes

In this section we propose a classification for all existing in models pseudo-graphene crystals. According to the information in analyzed articles, one can separate pseudo-graphenes basing on several characteristics:

- *Form factor*. While several materials listed below in this review possess non-monotonous structure (materials are composed with several types of carbon rings – like cyclicgraphene [68] (3 and 12 atom rings) and graphyne [36] (6 and 12 atom rings), there are materials which have single typed atom ring in their structure – the examples are pentagraphyne [42] (15 atom ring), PCF-graphene [48] (10 atom ring), and α-graphyne [69] (18 atom ring). Graphene itself is a material which can be put into the second group.

Several pseudo-graphene crystals can be characterized as graphene-like, possessing hexagonal carbon rings within their structure.

- *Electronic structure type*. Within reviewed materials list, we can select ones with properties of a semiconductor, semimetal, metal, and superconductor (a single material – T-graphene[70]).
- *Hybridization*. Depending on interatomic bonds, all modeled pseudo-graphenes can be divided into “pure”sp^2-materials (like C65-sheet [71] and ψ-graphene [72]) and non-sp^2-materials (like penta-graphene [43] and R-graphyne [73]).

In addition, there is a separate group of pseudo-graphenes, which properties are waiting for to be investigated in the future. Their further classification will be possible with the discovery of their characteristics.

Among the reviewed articles, we have found several pseudo-graphene crystals, which consist of two atomic layers [48,74-76]. These materials are semiconductors, which coincides with the presence of a band gap in bilayer graphene [77]. We did not consider this

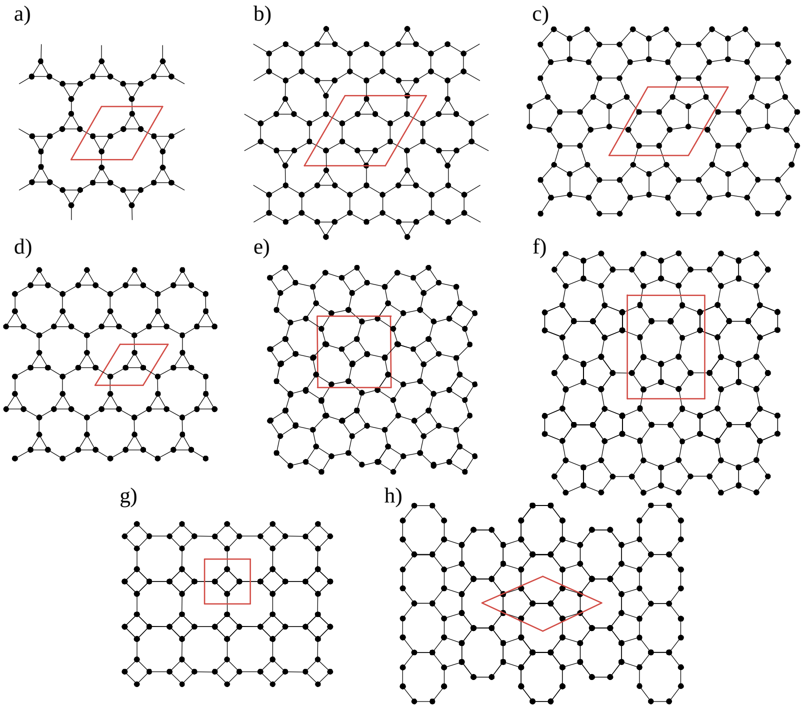

Fig. 3 – Pseudo-graphene crystals: a) cyclicgraphene reported in [69] (C312-sheet [37]),b) C65-sheet reported in [71], c) C63-sheet, d) C31-sheet reported in [71], e) C41-sheet reported in [71], f) pentaheptite reported in [78] (M-graphene [79], haeckelite [39], PeHe-B [80]),g) C48-sheet reported in [37] (T-graphene [70],octagraphene [81]), h) PO-graphene reported in [82]. Red rhombs or rectangles mark the borders of the primitive cells in pseudo-graphene crystal lattice.

type of crystals in this review, focusing only on single-layer carbon crystals.

4.2. Sp^2 pseudo-graphenes and their properties

For sp^2-hybridized pseudo-graphenes, quite a lot of of materials was theoretically investigated and, based on the data presented in the articles, we created a materials chart, splitting them on electronic band structure basis.

4.2.1. Pseudo-graphene crystals with metallic electronic band structure

In Fig. 3, metallic pseudo-graphenes, i.e. two-dimensional configurations of carbon atoms demonstrating properties of metals, with two types of carbon rings are shown.

Pentaheptite [78] is a metallic material that was predicted in 1996. At that time, only lattice structure and thermal stability were investigated and later, in 2011 [37] and 2014 [83], its electronic band structure was analyzed. In 2020, M-graphene was described by another research team [79], and this material appears to be the same as pentaheptite. In 2018, pseudo-graphene crystal 5-7B was investigated in Ref. [45], which is identical to pentaheptite. The band structure of this crystal has been revealed, and the effect of the density of defects of this kind (5- and 7-member rings) on the band structure was investigated. Hexagonal carbon rings were embedded in the crystal lattice of pseudographene 5-7B. Thus, instead of a tight contact of defect rings, they were separated by one or more hexagonal rings, thus reducing the density of defects in the crystal. This led to a change in the band structure: the Dirac cone disappeared and the valence and conduction bands overlap. If, instead of individual improper rings, the density of ensembles of four such rings (defect 7-55-7) was changed, this led to a displacement of the Dirac cone below the Fermi level by a value of about 0.25 eV.

Later in 2013, researchers modelled cyclicgraphene [68] and calculated its electronic and mechanical characteristics, for example Young's modulus was found as 198.9±1.0 GPa and Poisson's ratio – as 0.457±0.01, ultimate tensile strength (UTS) – as 13.7 GPa, and shear module – as 47.5±1.3 GPa. Its predecessor, C312-sheet, was described in 2011 in Ref. [37] with electronic band structure calculation only.

At the same year, in Ref. [71] four new metallic materials were discovered: C65-sheet, C63-sheet, C31-sheet, and C41-sheet. For these materials,their electronic band structure has been also predicted. However, the mechanical properties for listed materials were discussed neither in Ref. [72] nor in other studies.

In 2011, in Ref. [37], C48-sheet was described as a metallic material. In 2012 [81], 2013 [84], and 2015 [80], identical material, octagraphene was investigated, and

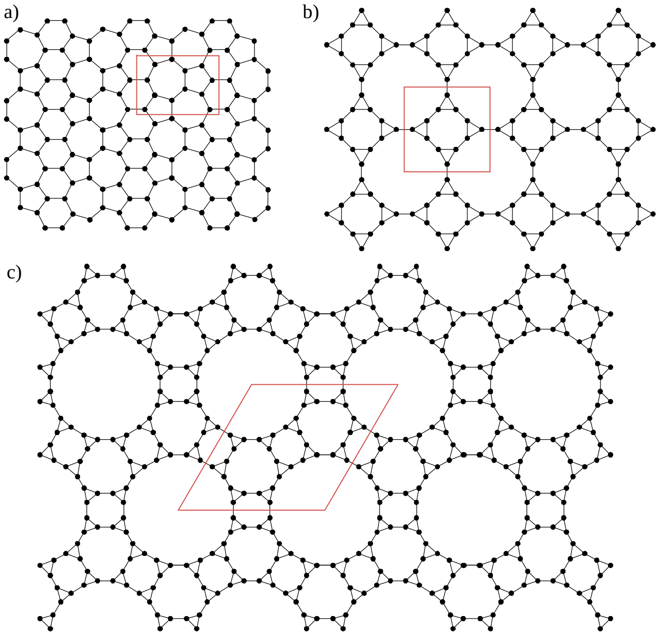

Fig. 4–Pseudo-graphene crystals:a) ψ-graphene reported in [72], b) tilene reported in [86], c) reported in flakene [86]. Red rectangle, square, or rhomb mark the borders of the primitive cells in pseudo-graphene crystal lattice.

in 2017 [70] and 2019 [85], the same material known as T-graphene was introduced. According to these studies, the material Poisson's ratio is 0.24 (in T-graphene research [70]) and 0.13 (in octagrapehene research [81]) and Young's module is 900.5 GPa [81]. In Ref. [85] octagraphene was recognized as a semiconductor with band gap -4.03 eV and UTS 101.18 GPa, and T-graphene was identified as a superconductor at 20.8 K. Octagraphene remains stable below 500 K (by this, a thermal stability of the crystal lattice is meant).

Little is known about PO-graphene [82] that was discovered in 2012. This material is viewed as sp^2-hybridized metal and its characteristics are to be described in more details.

In Fig.4, metallic materials with three types of carbon rings are presented.

In 2017, researchers predicted ψ-graphene [72] - a metal pseudo-graphene with Young's module of 833.79 GPa and Poisson's ratio of 0.275. This material is predicted to remain stable below 1000 K. Later in 2019, in Ref. [86] – tilene and flakene were described as metals thermal stability up to 500 K. Tilene's Young's module and Poisson's ratio are 0.235 TPa and 0.607, respectively, and UTS is 44.8 GPa. Flakene's Young's module and Poisson's ratio are 0.115 TPa and 0.746, respectively, and UTS is 23.6 GPa.

4.2.2. Pseudo-graphene crystals with semiconductor electronic band structure

In Fig.5, semiconducting sp2 pseudo-graphene crystals are presented.

In 2020, C3-8 [47] was modelled as a semiconducting pseudo-graphene with a band gap of 1.04 eV,which material structure remains stable below 1799 K.

In 2011, both haeckelite-like [37] and C4612-sheet [37] (also known as cyclotrimerizatedgraphyne [36]) were discovered by several research teams. These materials are expected to have band gap values of 0.76 and 1.14 eV, respectively. Their thermal and mechanical characteristics were not predicted.

In Ref. [86], where two metallic materials were predicted– tilene and flakene – two more materials were described as semiconductors – liskene and liskene-daughter.

Liskene posess band gap of 0.36 eV. It remains stable below 500 K; its Young's module is 0.412 TPa and Poisson's ratio is 0.51. Its UTS is 63.2 GPa.

Liskene-daughter material has a band gap of 0.46 eV, remaining stable below the same temperature as liskene. Its Young's module and Poisson's ratio are 0.278 TPa and 0.52. Its UTS is 27.8 GPa

4.2.3. Pseudo-graphene crystals with semi-metal electronic band structure

In Fig.6, semi-metallic sp2 materials are presented.

Little is known about S-graphene[87], which was discovered at 2014. It has no predicted values to present other than its electronic band structure. A year later after the discovery of S-graphene, phagraphene[40] was advanced. It remains stable at temperatures below 1000 K. Phagraphene mechanical characteristics were calculated a year later in Refs. [88] and [89]. Phagraphene

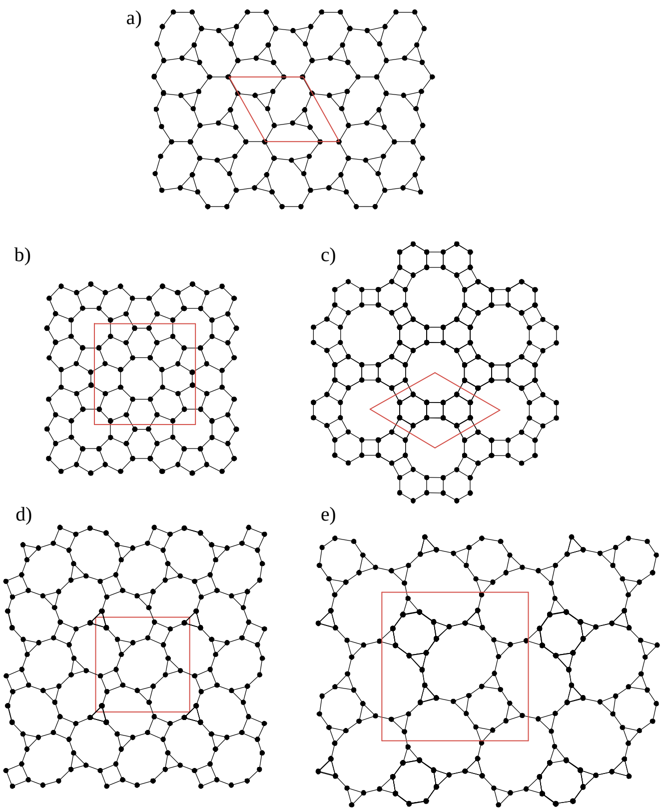

Fig. 5. Pseudo-graphene crystals: a) C3-8 reported in [47], b) haeckelite-like reported in [37], c) C4612-sheet reported in [37] (cyclotrimerizatedgraphyne[30]), d) liskene [86], e) liskene-daughter reported in [86]. Red rhombs or squares mark the borders of the primitive cells in pseudo-graphene crystal lattice.

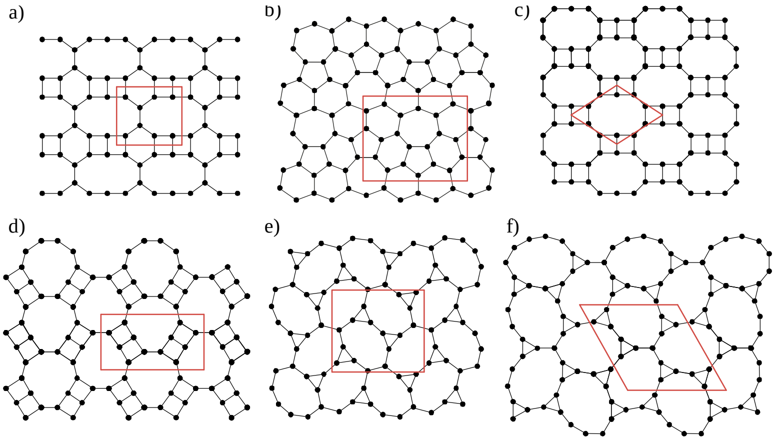

Fig. 6. Pseudo-graphene crystals: a) S-graphene reported in [87], b) phagraphene reported in [40], c) C4-10-I reported in [47], d) C4-10-II reported in [47], e) C3-9-R reported in [47], f) C3-11 reported in [47]. Red rectangles or rhombs mark the borders of the primitive cells in pseudo-graphene crystal lattice.

Young's module is expected to be 960 ± 20 GPa [88]; its Poisson's ratio is 0.255 and its UTS is 24.8 GPa[88] (132 ± 3 GPa [89]).

In 2020, in Ref.[47], C4-10-I, C4-10-II, C3-9-R and C3-11 were modelled as a semi-metallic pseudo-graphenes with thermal stability up to 1628 K, 1558 K, 1559 K, and 1192K. Their mechanical properties are to be analyzed. In addition, the phonon spectra of these crystals and the dependenced of free energy per atom as a function of temperature were plotted in Ref. [47].

4.2.4. Remaining sp^2 pseudo-graphene crystals

In Figs. 7 and 8, pseudo-graphene crystals with yet unspecified properties are displayed. This set of sp^2 pseudo-graphenes was only proposed in terms of crystal lattice geometry. Neither their electronic band structure, nor their mechanical characteristics have been researched yet. They are expected to be structurally stable, and thus they are listed in our review.

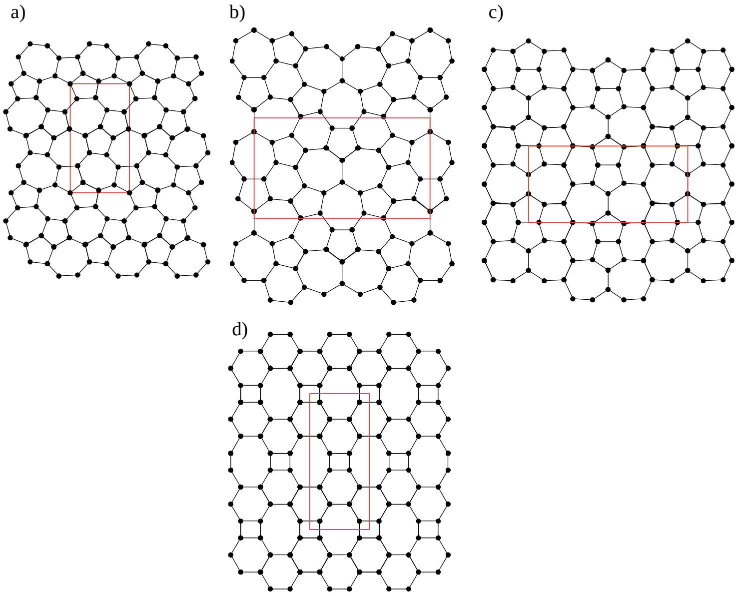

Fig. 7. Pseudo-graphene crystals: a) pentaheptite v2 reported in [37,90] (PeHe-A [80]), b) hexagonal haeckelite reported in [39], c) oblique haeckelite reported in [39], d) net-W reported in [87]. Red rectangles mark the borders of the primitive cells in pseudo-graphene crystal lattice.

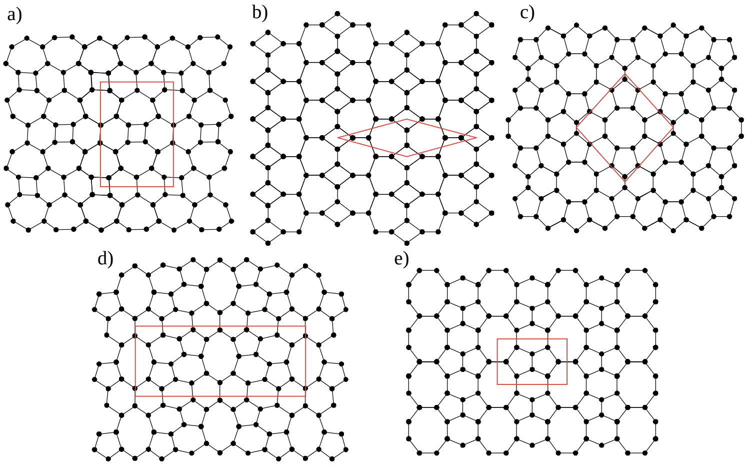

Fig. 8. Pseudo-graphene crystals: a) PGC 7-4-7A reported in [35], b) PGC 7-4-7B reported in [35], c) PGC 5-8-5A reported in [35], d) PGC 5-8-5B reported in [35], e) PGC 5-8-5C reported in [35]. Red rectangles or rhombs mark the borders of the primitive cells in pseudo-graphene crystal lattice.

4.3. Non-sp^{2}pseudo-graphenes and their properties

As for sp^2-hybridized pseudo-graphenes, we can develop the same type of chart for non-sp^2-materials.

In this section, only three materials are presented (see Fig. 9), and there were no attempts to study their mechanical properties.

According to Ref. [37], C14-sheet (also known as 14,14,14-graphyne [36]) is a sp^2-sp^1 metal. Its thermal and mechanical properties are to be analyzed. The same applies to squarographene from mentioned Ref. [37], which is sp^2-sp^3 metal without calculated properties.

4.3.1. Pseudo-graphene crystals with metallic electronic band structure

Fortunately, there is one material with calculated thermal characteristics:R-graphyne, discovered in Ref.[73]. It is a sp^2-sp^1 material, which remains stable up to 500 K.

In Fig. 10, non-sp2 pseudo-graphene crystals with semiconductor electronic band structure are displayed.

In 2020, pentagraphyne [42] was described as a sp^1-sp^2-sp^3 semiconducting material with a band gap value of 0.977 eV and thermal stability up to 1000K. Its Young's module and Poisson's ratio are 53.59 GPa and 0.47, respectively. Similar material, penta-graphene, was investigated in 2014 [43]. It is a sp^2-sp^3 pseudo-graphene with

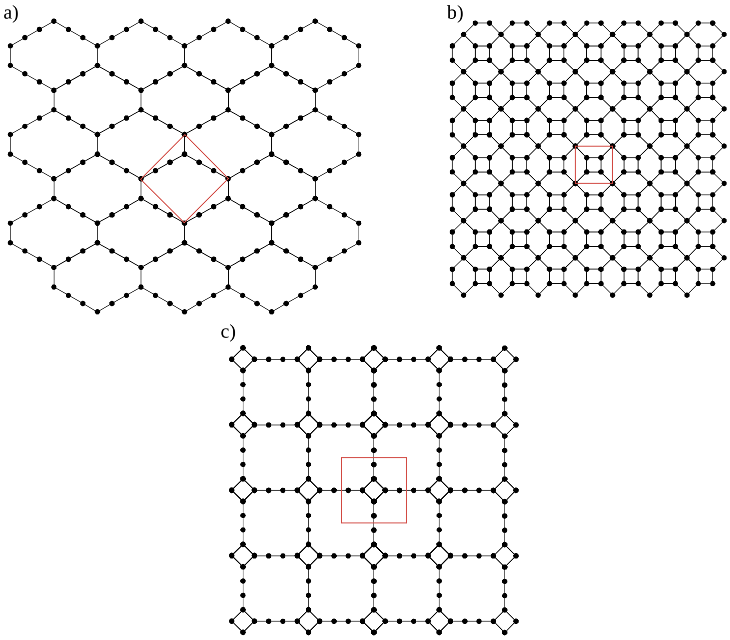

Fig. 9. Pseudo-graphene crystals: a) C14-sheet reported in [37] (14,14,14-graphyne [36]), b) squarographene reported in [37], c) R-graphyne reported in [73]. Red rhombs or squares mark the borders of the primitive cells in pseudo-graphene crystal lattice.

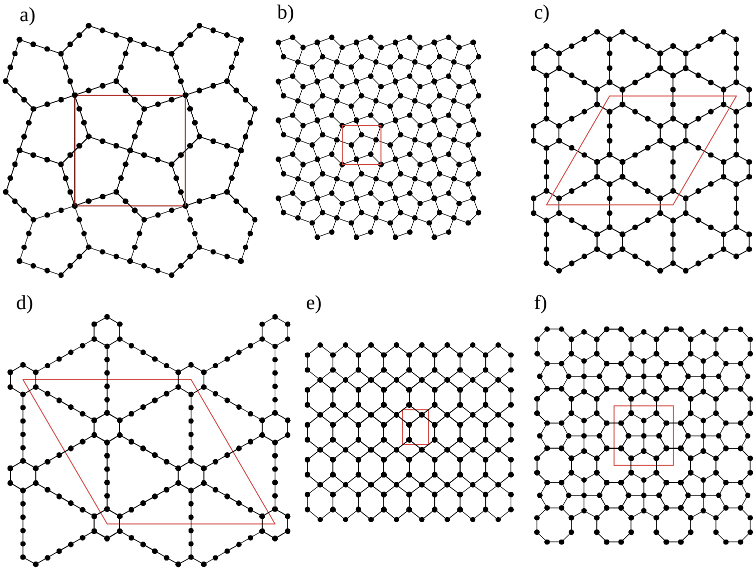

Fig. 10. Pseudo-graphene crystals: a) pentagraphyne reported in [42], b) penta-graphene reported in [43], c) graphyne reported in [36] (γ-graphyne [69]), d) graphdiyne reported in [91], e) tetrahexcarbon reported in [46] (squarographene [37]), f) Me-graphene reported in [41] (C568-sheet [92]). Red rhombs, squares, or rectangle mark the borders of the primitive cells in pseudo-graphene crystal lattice.

band gap of 3.25 eV. It remains stable below 1000K and its Young's module is 263.8 GPa*nm. Its Poisson's ratio is -0.07.

4.3.2. Pseudo-graphene crystals with semiconductor electronic band structure

Earlier predictions of graphyne (also known as γ-graphyne [69]) can be found in works done in 1987 [36] and1998 [93]. Its electronic band structure was analyzed in 2011 [37]. Its mechanical properties were described in 2013 [68] and 2016 [94]. It is a sp^2-sp^1 semiconductor with band gap value of 1.2 eV [36] (0.52 eV [93], 1.32 eV [37]). Its Young's modulus is 532.5 GPa [49] (448.53 GPa [94], 525.0±0.6 GPa [68]), Poisson's ratio is 0.172±0.01 [68] and shear modulus of 122.7±1.5 GPa [68]. The ultimate tensile strain is 8.19% [49], and UTS is 48.2 GPa [94].

Based on graphyne, graphdiyne was predicted in 1998 [91,93] and later modelled in 2011 [37]. This is a sp^2-sp^1 pseudo-graphene with band gap value of 1.47 eV [37] (or 0.53 eV [93]).

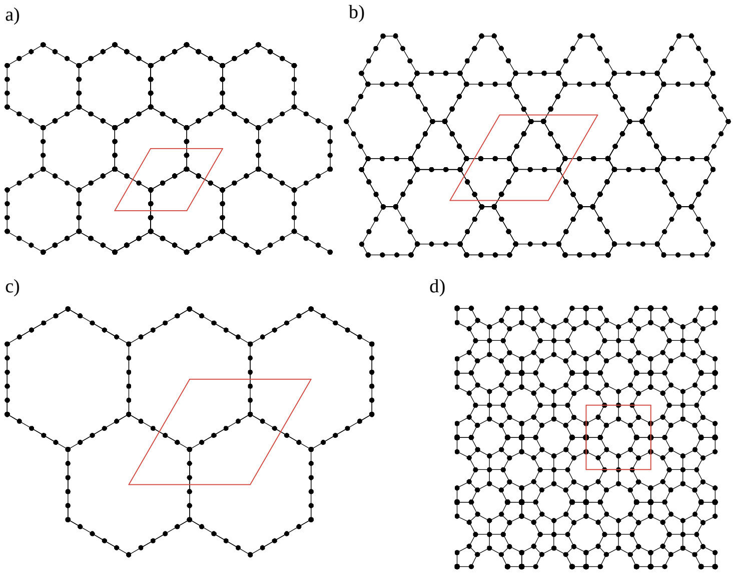

Fig. 11. Pseudo-graphene crystals: a) α-graphyne reported in [69] (supergraphene [37],18,18,18-graphyne [36]), b) β-graphyne reported in [69] (12,12,12-graphyne [36]), c) supergraphene reported in [68], d) penta-octa-graphene reported in [95]. Red rhombs or squares mark the borders of the primitive cells in pseudo-graphene crystal lattice.

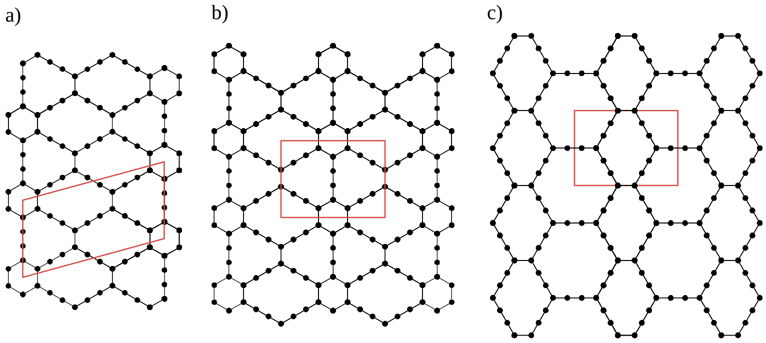

Fig. 12. Pseudo-graphene crystals: a) 6,6,14-graphyne reported in [36], b) 6,6,12-graphyne reported in [36], c) 14,14,18-graphyne reported in [36]. Red parallelogram or rectangles mark the borders of the primitive cells in pseudo-graphene crystal lattice.

In 2018, Ref. [46] advanced tetrahexcarbon (also known as 6-4 squarographene [37]) as a sp^2-sp^3 semiconductor with band gap value of 3.7 eV and thermal stability up to 1000 K. In 2019, the same research team discovered C568-sheet [92] (also known as Me-graphene [41]). This material is a sp^2-sp^3 semiconductor with band gap value of 1.13 eV. It remains stable below 800 K. Its Young's modulus, Poisson's ratio, and ultimate tensile strain are 619.18 GPa, 0.0045, and 11.2%, respectively.

4.3.3. Pseudo-graphene crystals with semi-metal electronic band structure

This section presents two pseudo-graphenes from graphyne group, another two from supergraphene group and a single groupless material (see Fig. 11).

Both α-graphyne[69] (also known as supergraphene [37] or 18,18,18-graphyne [36]) and β-graphyne [69] (also known as 12,12,12-graphyne [36]), are sp^2-sp^1 semi-metallic pseudo-graphenes with predicted electronic band structure. However, their other parameters have not been found yet. Supergraphene [68] first described in 2011 is a similar sp^2-sp^1 modification of graphene sheets. For supergraphene, Young's modulus is 124.1±1.5 GPa [68] (84.81 GPa [94]), Poisson's ratio is 0.454±0.01. UTS and shear moduli are 5.5 GPa·nm and 19.6±0.6 GPa, respectively.

The last material in chart, penta-octa-graphene[95], modelled in 2020, is a sp^2-sp^3 gapless semi-metal with predicted thermal stability up to 1000 K. Its Poisson's ratio is 0.44.

4.3.4. Remaining pseudo-graphene crystals with mixed hybridization

In Fig. 12, one can see non-sp^2 pseudo-graphene crystals with unknown characteristics. This set of non-sp^2

Table 1. Pseudo-graphenes and their characteristics**.**

Proposed nomenclature	Used nomenclature and references	Material property	Bond hybridization
G3-12v1	cyclicgraphene [68,94] C312-sheet[37]	metal	sp2
G3-6-8v1	C65-sheet[71]	metal	sp2
G5-6-9v1	C63-sheet[71]	metal	sp2
G3-9v1	C31-sheet[71]	metal	sp2
G4-7v1	C41-sheet[71]	metal	sp2
G5-7v1	pentaheptite[37,78,83,90] haeckelite[37, 97] M-graphene[79] PGC 5-7B [45] PeHe-B[80]	metal[37] n/a metal [79] semimetal [45] n/a	sp2
G5-6-7v1	ψ-graphene[72]	metal	sp2
G4-8v1	C48-sheet[37] T-graphene[70, 85] octagraphene[80,81,84] PGC 4-8 [98]	metall [37] superconductor(at 20.8K) [85] semimetal [81] metal [98]	sp2
G3-8-16v1	tilene[86]	metal	sp2
G5-8v1	PO-graphene[82] PGC 5-8D [45]	metal	sp2
G3-8-12-24v1	flakene[86]	metal	sp2
G5-6-8v1	haeckelite-like[37]	semiconductor	sp2
G4-6-12v1	C4612-sheet[37] cyclotrimerizatedgraphyne[36]	semiconductor	sp2
G3-4-10v1	liskene[86]	semiconductor	sp2
G3-8-14v1	liskene-daughter [86]	semiconductor	sp2
G3-8v1 C3-8 [47]		semiconductor	sp2
G5-6-7v2	phagraphene [40,88,89] PGC 5-7A [45]	semimetal	sp2
G4-6-10v1	S-graphene [87]	semimetal	sp2
G4-10v1	C4-10-I [47]	semimetal	sp2
G4-10v2	C4-10-II [47]	semimetal	sp2
G3-9v2 C3-9-R [47]		semimetallic	sp2
G3-11v1	C3-11 [47]	semimetallic	sp2
G4-6-8v1	net-W [87]	n/a	sp2
G5-7v2	pentaheptite v2 [37,90] PeHe-A [80]	n/a	sp2
G5-6-7v3	hexagonalhaeckelite [39]	n/a	sp2
G5-6-7v4	obliquehaeckelite [39]	n/a	sp2
G4-6-7v1	PGC 7-4-7A [35]	n/a	sp2
G4-7v2	PGC 7-4-7B [35]	n/a	sp2
G5-6-8v2	PGC 5-8-5A [35]	n/a	sp2
G5-6-8v3	PGC 5-8-5B [35]	n/a	sp2
G5-6-8v4	PGC 5-8-5C [35]	n/a	sp2
C14v1	C14-sheet [37] 14,14,14-graphyne [36]	metal	sp2sp1
C4-6v1	squarographene [37]	metal	sp2sp3
C4-16v1	R-graphyne [73]	metal	sp2sp1
C15v1	pentagraphyne [42]	semiconductor	sp1sp2sp3
C6-12v1	graphyne [36,37,49,68,93,94]	semiconductor	sp2sp1

	γ-graphyne [69]		
C6-18v1	graphdiyne [37,91,93]	semiconductor	sp2sp1
C5-6-8v1	Me-graphene [41]	semiconductor	sp2sp3
	C568-sheet [92]		
C5v1	penta-graphene [43,88.99]	semiconductor	sp2sp3
C4-6v2	squarographene [37]	semiconductor	sp2sp3
	tetrahexcarbon [46]		
C30v1	supergraphene [68,94]	semimetal	sp2sp1
C18v1	α-graphyne [69]	semimetal	sp2sp1
	supergraphene [37,96]	semimetal	
	18,18,18-graphyne [36]	n/a	
C5-8v1	penta-octa-graphene [95]	semimetal	sp2sp3
C12-18v1	β-graphyne [69]	semimetal	sp2sp1
	12,12,12-graphyne (12-18) [36]	n/a	
C6-14v1	6,6,14-graphyne [36]	n/a	sp2sp1
C6-14v2	6,6,12-graphyne [36]	n/a	sp2sp1
C14-18v1	14,14,18-graphyne [36]	n/a	sp2sp1

pseudo-graphenes was only proposed in terms of crystal lattice geometry. As for sp^2 materials, neither their electronic band structure, nor their mechanical characteristics have been analyzed yet.

5. DISCUSSION

One of the most important messages in this review is the proposed materials classification. The majority of articles regarding graphene-like carbon allotrope prediction are not standardized; there is no unite database and nomenclature for the described materials. This leads to repeated studies on a single material and workload increase for all the background study that research teams must do. The proposed materials classification provides a basis, which can be used in further pseudo-graphene investigations. Moreover, the classification is also suitable for the analysis of materials different from graphene-based, e.g. MoS_2, phosphorene, and other two-dimensional crystals.

Among the materials considered in this review, we did not find any connection between their electronic structure, crystal lattice structure, and crystal hybridization.

As for the form-factor, it is clearly seen that there is no connection between monotonous and non-monotonous lattice structure and hybridization/electronic band structure.Within each chart section, we can find all types of material – single ringed, multi-ringed, and those with hexagonal carbon rings. There is only one exception – non-sp^2 semi-metallic materials, where no two-dimensional crystals with hexagonal carbon rings were reported.

Table 1 summarizes all the materials and their characteristics that were considered in the review. Sections of the table, shaded in gray, denote pseudo-graphene crystals, on which several studies were carried out, in which these crystals had different designations. In the Table, we introduce a new nomenclature (naming convention) for pseudo-graphenes. In our opinion, the name for a material should contain the information regarding the carbon atomic ring types, on which the material is based on. If a duplicate material is encountered (it has a similar basis carbon atomic rings), the material should have a “newer” variation. For example, we propose to name phagraphene [40] as“G5-6-7v2”, where “G” is for graphene-like (sp2-hybridization), “5-6-7” is for types of carbon rings present in the material and “v2” is for the second variation of such material (the first one is ř-graphene [72]). In addition, supergraphene [37,96] can be named as C18v1, where “C” is for “carbon” (all materials that are not “graphene-like”), “18” is for a single atomic ring type within the material and “v1” is for the first variation of this material.

As for future possible applications of the pseudo-graphenes – there is a large variety of options. Several pseudo-graphene crystals possess high thermal conductivity which makes them good candidates for use in thermal applications (for example, cooling hardware). Most of the present materials in this chart have promising properties for use in optoelectronics and electronics.

We have plans to explore the content of the review in our future work:

- To supplement the currently existing Table with other low-energy pseudographenes. For this, it is planned to use the USPEX software package [100], which specializes in predicting the crystal structure from the specified chemical composition.
- Many of the pseudo-graphenes considered in this review have not been studied in sufficient details, i.e. not all of their physical characteristics have been determined.

In addition, performing calculations by the same method in the same software package under the same conditions will make it possible to more correctly compare the results and avoid inconsistencies in the data that were found, e.g. for the G4-8v1 or G5-7v1 crystals.
- It is necessary to conduct an analytical study of graphene-like pseudographenes (with sp^2-hybridization) using the theory of disclinations. Perhaps this will allow us to clarify relationships between the crystal structure and the final properties of pseudographenes that we could not find.

6. SUMMARY AND CONCLUSIONS

The main purpose of the review was to advance a novel pseudo-graphene classification and to list various patterns within this classification. In the review, 47 materials from various sources were described. Among them, 6 materials were investigated in parallel by independent research teams, while others were discovered once in single publications. According to this materials set, we proposed a classification that we think is the best fitting for the area of research. With given classification, we created the chart splitting materials into classification categories.

Based on the result we got, the materials distribution among the proposed classification is roughly equal – we have a rich variety of materials, starting from sp^2-hybridized metallic materials to non-sp^2 semi-metallic pseudo-graphenes.

Although all the discussed pseudo-graphene materials have not been synthesized yet, we hope that this will change in the future. With further synthesis of these proposed materials researchers will be able to compare the materials actual parameters against calculation models and thus, improve this modelsto a higher precision and result quality.

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REFERENCES

[1] W. Taylor, *Structure and Properties of Diamond*, Nature, 1947, vol. 159, no. 1947, pp. 729–731. https://doi.org/10.1038/159729a0

[2] J. Suparno, D.A. Halim, A. Setiawan, M. Effendy and J. Jamari, *Graphite as Dry Lubricant to Reduce Rail Wheels Wear Level*, Mater. Sci. Forum, 2019, vol. 961, pp. 126–133. https://doi.org/10.4028/www.scientific.net/msf.961.126

[3] P. Qian, H. Zhang, J. Chen, Y. Wen, Q. Luo, Z. Liu, D. You and B. Yi, *A Novel Electrode-bipolar Plate Assembly for Vanadium Redox Flow Battery Applications*, J. Power Sources, 2008, vol. 175, no. 1, pp. 613–620. https://doi.org/10.1016/j.jpowsour.2007.09.006

[4] M.S. Dresselhaus and G. Dresslhaus, *Fullerenes and Fullerene Derived Solids as Electronic Materials*, Annu. Rev. Mater. Sci., 1995, vol. 25, no. 1, pp. 487–523. https://doi.org/10.1146/annurev.ms.25.080195.002415

[5] N. Gupta, S.M. Gupta and S.K. Sharma, *Carbon Nanotubes: Synthesis, Properties and Engineering Applications*, Carbon Letters, 2019, vol. 29, no. 5. pp. 419–447. https://doi.org/10.1007/s42823-019-00068-2

[6] N. Anzar, R. Hasan, M. Tyagi, N. Yadav and J. Narang, *Carbon Nanotube - A Review on Synthesis, Properties and Plethora of Applications in the Field of Biomedical Science*, Sensors International, 2020, vol. 1, art. 100003. https://doi.org/10.1016/j.sintl.2020.100003

[7] M.J. Allen, V.C. Tung and R.B. Kaner, *Honeycomb Carbon: A Review of Graphene*, Chem. Rev., 2010, vol. 110, no. 1, pp. 132–145. https://doi.org/10.1021/cr900070d

[8] P. Bhattacharya, R. Fornari and H. Kamimura, *Comprehensive Semiconductor Science and Technology* (Elsevier Science, 2011).

[9] C.A. Brookes and E.J. Brookes, *Diamond in Perspective: aReview of Mechanical Properties of Natural Diamond*, Diam. Relat. Mater., 1991, vol. 1, no. 1, pp. 13–17. https://doi.org/10.1016/0925-9635(91)90006-V

[10] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, M.I. Katsnelson, I.V. Grigorieva, S.V. Dubonos and A.A. Firsov, *Two-Dimensional Gas of Massless Dirac Fermions in Graphene*, Nature, 2005, vol. 438, no. 7065, pp. 197–200. https://doi.org/10.1038/nature04233

[11] S. Iijima, *Helical Microtubules of Graphitic Carbon*, Nature, 1991, vol. 354, no. 6348, pp. 56–58. https://doi.org/10.1038/354056a0

[12] H.W. Kroto, J.R. Heath, S.C. O'Brien, R.F. Curl and R.E. Smalley, *C_{60}: Buckminsterfullerene*, Nature, 1985, vol. 318, pp. 162–163. https://doi.org/10.1038/318162a0

[13] F.L. Coffman, R. Cao, P.A. Pianetta, S. Kapoor, M. Kelly and L.J. Terminello, *Near Edge X ray Absorption of Carbon Materials for Determining Bond Hybridization in Mixed sp2/sp3 Bonded Materials*, Appl. Phys. Lett., 1996, vol. 69, no. 4, pp. 568–570. https://doi.org/10.1063/1.117789

[14] H. Kabir, H. Zhu, J. May, K. Hamal, Y. Kan, T. Williams, E. Echeverria, D.N. McIlroy, D. Estrada, P.H. Davis, T. Pandhi, K. Yocham, K. Higginbotham, A. Clearfield and I.F. Cheng,

The sp2-sp3 Carbon Hybridization Content of Nanocrystalline Graphite from Pyrolyzed Vegetable Oil, Comparison of Electrochemistry and Physical Properties with Other Carbon Forms and Allotropes, Carbon, 2019, vol. 144, pp. 831–840. https://doi.org/10.1016/j.carbon.2018.12.058

[15] A.H. Castro Neto, F. Guinea, N.M.R. Peres, K.S. Novoselov and A.K. Geim, *The Electronic Properties of Graphene*, Rev. Mod. Phys., 2009, vol. 81, pp. 109–162. https://doi.org/10.1103/RevModPhys.81.109

[16] A.K. Geim and K.S. Novoselov, *The Rise of Graphene*, Nat. Mater., 2007, vol. 6, no. 3, pp. 183–191. https://doi.org/10.1038/nmat1849

[17] S. Chen, A.L. Moore, W. Cai, J. W. Suk, J. An, C. Mishra, C. Amos, C.W. Magnuson, J. Kang, L. Shi and R.S. Ruoff, *Raman Measurements of Thermal Transport in Suspended Monolayer Graphene of Variable Sizes in Vacuum and Gaseous Environments*, ACS Nano, 2010, vol. 5, no. 1, pp. 321–328. https://doi.org/10.1021/nn102915x

[18] A.A. Balandin, *Thermal Properties of Graphene and Nanostructured Carbon Materials*, Nat. Mater., 2011, vol. 10, no. 8, pp. 569–581. https://doi.org/10.1038/nmat3064

[19] S. Chen, Q. Wu, C. Mishra, J. Kang, H. Zhang, K. Cho, W. Cai, A.A. Balandin and R.S. Ruoff, *Thermal Conductivity of Isotopically Modified Graphene*, Nat. Mater., 2012, vol. 11, no. 3, pp. 203–207. https://doi.org/10.1038/nmat3207

[20] C. Lee, X. Wei, J.W. Kysar and J. Hone, *Measurement of the Elastic Properties and Intrinsic Strength of Monolayer Graphene*, Science, 2008, vol. 321, no. 5887, pp. 385–388. https://doi.org/10.1126/science.1157996

[21] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V. Grigorieva and A.A. Firsov, *Electric Field Effect in Atomically Thin Carbon Films*, Science, 2004, vol. 306, no. 5696. pp. 666–669. https://doi.org/10.1126/science.1102896

[22] Z.H. Ni, T. Yu, Y.H. Lu, Y.Y. Wang, Y.P. Feng and Z.X. Shen, *Uniaxial Strain on Graphene: Raman Spectroscopy Study and Band-Gap Opening*, ACS Nano, 2008, vol. 2, no. 11, pp. 2301–2305. https://doi.org/10.1021/nn800459e

[23] Y.-J. Yu, Y. Zhao, S. Ryu, L.E. Brus, K.S. Kim and P. Kim, *Tuning the Graphene Work Function by Electric Field Effect*, Nano Lett., 2009, vol. 9, no. 10, pp. 3430–3434. https://doi.org/10.1021/nl901572a

[24] M.O. Goerbig, *Electronic Properties of Graphene in a Strong Magnetic Field*, Rev. Mod. Phys., 2011, vol. 83, no. 4, pp. 1193–1243. https://doi.org/10.1103/RevModPhys.83.1193

[25] F. Hao, D. Fang and Z. Xu, *Mechanical and Thermal Transport Properties of Graphene with Defects*, Appl. Phys. Lett., 2011, vol. 99, no. 4, art. 041901. https://doi.org/10.1063/1.3615290

[26] Y. Wei, J. Wu, H. Yin, X. Shi, R. Yang and M. Dresselhaus, *The Nature of Strength Enhancement and Weakening by Pentagon–Heptagon Defects in Graphene*, Nat. Mater., 2012, vol. 11, no. 9, pp. 759–763. https://doi.org/10.1038/nmat3370

[27] S.H.M. Jafri, K. Carva, E. Widenkvist, T. Blom, B. Sanyal, J. Fransson, O. Eriksson, U. Jansson, H. Grennberg, O. Karis, R. A. Quinlan, B. C. Holloway and K. Leifer, *Conductivity Engineering of Graphene by Defect Formation, J. Phys. D: Appl. Phys., 2010, vol. 43, no. 4, art.* 045404. https://doi.org/10.1088/0022-3727/43/4/045404

[28] A. Bagri, S.-P. Kim, R.S. Ruoff and V.B. Shenoy, *Thermal Transport Across Twin Grain Boundaries in Polycrystalline Graphene from Nonequilibrium Molecular Dynamics Simulations*, Nano Lett., 2011, vol. 11, no. 9, pp. 3917–3921. https://doi.org/10.1021/nl202118d

[29] F. Banhart, J. Kotakoski and A.V. Krasheninnikov, *Structural Defects in Graphene*, ACS Nano, 2010, vol.5, no. 1, pp. 26–41. https://doi.org/10.1021/nn102598m

[30] L. Liu, M. Qing, Y. Wang and S. Chen, *Defects in Graphene: Generation, Healing, and Their Effects on the Properties of Graphene: A Review*, J. Mater. Sci. Technol., 2015, vol. 31, no. 6, pp. 599–606. https://doi.org/10.1016/j.jmst.2014.11.019

[31] J. Kotakoski, A. V. Krasheninnikov, U. Kaiser and J.C. Meyer, *From Point Defects in Graphene to Two-Dimensional Amorphous Carbon*, Phys. Rev. Lett., 2011, vol. 106, no. 10, art. 105505. https://doi.org/10.1103/PhysRevLett.106.105505

[32] K. Kim, Z. Lee, W. Regan, C. Kisielowski, M.F. Crommie and A. Zettl, *Grain Boundary Mapping in Polycrystalline Graphene*, ACS Nano, 2011, vol. 5, no. 3, pp. 2142–2146. https://doi.org/10.1021/nn1033423

[33] W.F. Harris, *Disclinations*, Scientific American, 1977, vol. 237, no. 6, pp. 130-145.

[34] M.A. Rozhkov, A. L. Kolesnikova, I. S. Yasnikov and A. E. Romanov, *Disclination Ensembles in Graphene*, Low Temp. Phys., 2018, vol. 44, no. 9, pp. 918–924. https://doi.org/10.1063/1.5052677

[35] A.E. Romanov, M.A. Rozhkov and A.L. Kolesnikova, *Disclinations in Polycrystalline Graphene and Pseudo-Graphenes. Review*, Lett. Mater., 2018, vol. 8, no. 4, pp. 384–400. https://doi.org/10.22226/2410-3535-2018-4-384-400

[36] R.H. Baughman, H. Eckhardt and M. Kertesz, *Structure property Predictions for New Planar Forms of Carbon: Layered Phases Containing sp2 and sp Atoms*, J. Chem. Phys., 1987, vol. 87, no. 11, pp. 6687–6699. https://doi.org/10.1063/1.453405

[37] A.N. Enyashin and A.L. Ivanovskii, *Graphene Allotropes*, Phys. Stat. Sol. (b), 2011, vol. 248, no. 8, pp. 1879–1883. https://doi.org/10.1002/pssb.201046583

[38] Z. Gong, X. Shi, J. Li, S. Li, C. He, T. Ouyang, C. Zhang, C. Tang and J. Zhong, *Theoretical Prediction of Low-Energy Stone-Wales Graphene with an Intrinsic Type-III Dirac Cone*, Phys. Rev. B, 2020, vol. 101, no. 15, art. 155427**.** https://doi.org/10.1103/physrevb.101.155427

[39] H. Terrones, M. Terrones, E. Hernández, N. Grobert, J.-C. Charlier and P.M. Ajayan, *New Metallic Allotropes of Planar and Tubular Carbon*, Phys. Rev. Lett., 2000, vol. 84, no. 8, pp. 1716–1719. https://doi.org/10.1103/physrevlett.84.1716

[40] Z. Wang, X.-F. Zhou, X. Zhang, Q. Zhu, H. Dong, M. Zhao and A.R. Oganov, *Phagraphene: A Low-Energy Graphene Allotrope Composed of 5–6–7 Carbon Rings with Distorted Dirac Cones*, Nano Lett., 2015, vol. 15, no. 9, pp. 6182–6186. https://doi.org/10.1021/acs.nanolett.5b02512

[41] Z. Zhuo, X. Wu and J. Yang, *Me-graphene: aGraphene Allotrope with near Zero Poisson's Ratio, Sizeable Band Gap, and High Carrier Mobility*, Nanoscale, 2020, vol. 12, no. 37, pp. 19359–19366. https://doi.org/10.1039/d0nr03869e

[42] J. Deb, D. Paul and U. Sarkar, *Pentagraphyne: aNew Carbon Allotrope with Superior Electronic and Optical Property*, J. Mater. Chem. C, 2020, vol. 8, no. 45, pp. 16143–16150. https://doi.org/10.1039/d0tc04245e

[43] S. Zhang, J. Zhou, Q. Wang, X. Chen, Y. Kawazoe and P. Jena, *Penta-Graphene: A New Carbon Allotrope, Proc. Natl. Acad. Sci. U.S.A.*,2015, vol. 112, no. 8, pp. 2372–2377. https://doi.org/10.1073/pnas.1416591112

[44] M.A. Rozhkov, A.L. Kolesnikova, I.S. Yasnikov and A.E. Romanov, *Disclination Ensembles in Graphene*, Low Temp. Phys., 2018, vol. 44, no. 9, pp. 918–924. https://doi.org/10.1063/1.5052677

[45] M.A. Rozhkov, A.L. Kolesnikova, I. Hussainova, M.A. Kaliteevskii, T.S. Orlova, Yu.Yu. Smirnov, I.S. Yasnikov, L.V. Zhigilei, V.E. Bougrov and A.E. Romanov, *Evolution of Dirac Cone in Disclinated Graphene*, Rev. Adv. Mater. Sci., 2018, vol. 57, no. 2, pp. 137-142. https://doi.org/10.1515/rams-2018-0057

[46] B. Ram and H. Mizuseki, *Tetrahexcarbon: A Two-dimensional Allotrope of Carbon*, Carbon, 2018, vol. 137, pp. 266–273. https://doi.org/10.1016/j.carbon.2018.05.034

[47] Q. Xie, L. Wang, J. Li, R. Li and X.-Q. Chen, *General Principles to High-Throughput Constructing Two-Dimensional Carbon Allotropes*, Chin. Phys. B, 2020, vol. 29, no. 3, art. 037306. https://doi.org/10.1088/1674-1056/ab6c4b

[48] Y. Shen, J. Yu, J. Liu, Y. Guo, Y. Qie and Q. Wang, *PCF-Graphene: A 2D sp2-Hybridized Carbon Allotrope with a Direct Band Gap*, J. Phys. Chem. C, 2019, vol. 123, no. 7, pp. 4567–4573. https://doi.org/10.1021/acs.jpcc.8b12205

[49] S.W. Cranford and M.J. Buehler, *Mechanical Properties of Graphyne*, Carbon, 2011, vol. 49, no. 13, pp. 4111–4121. https://doi.org/10.1016/j.carbon.2011.05.024

[50] A.L. Kolesnikova, M.A. Rozhkov, I. Hussainova, T.S. Orlova, I.S. Yasnikov, L.V. Zhigilei and A.E. Romanov, *Structure and Energy of Intercrystallite Boundaries in Graphene*, Rev. Adv. Mater. Sci., 2017, vol. 52, no. 1/2, pp. 91-98. http://www.ipme.ru/e-journals/RAMS/no_15217/12_15217_kolesnikova.pdf

[51] V.I. Vladimirov and A.E. Romanov, *Disclinations in Crystals* (Nauka, Leningrad, 1986), In Russian.

[52] A.E. Romanov and V.I. Vladimirov, *Disclinations in Crystalline Solids*, In: Dislocations in Solids, vol. 9, ed. by F.R.N. Nabarro (North-Holland, Amsterdam, 1992), p. 191-402.

[53] I.S. Yasnikov, A.L. Kolesnikova and A.E. Romanov, *Multi-disclination Configurations in Pentagonal Microcrystals and Two-Dimensional Carbon Structures*, Phys. Sol. State, 2016, vol. 58, no. 6, pp. 1184–1190. https://doi.org/10.1134/S1063783416060342

[54] M.A. Rozhkov, N.D. Abramenko, A.L. Kolesnikova and A.E. Romanov, *Zero Misorientation Interfaces in Graphene*, Lett. Mater., 2020, vol. 10, no. 4s, pp. 551–557. https://doi.org/10.22226/2410-3535-2020-4-551-557

[55] W. Kohn and L.J. Sham, *Self-Consistent Equations Including Exchange and Correlation Effects*, Phys. Rev., 1965, vol. 140, no. 4A, pp. A1133–A1138. https://doi.org/10.1103/PhysRev.140.A1133

[56] https://www.vasp.at/

[57] https://www.quantum-espresso.org/

[58] J.P. Perdew, K. Burke and M. Ernzerhof, *Generalized Gradient Approximation Made Simple*, Phys. Rev. Lett., 1996, vol. 77, no. 18, pp. 3865–3868 https://doi.org/10.1103/PhysRevLett.77.3865

[59] G. Gui, J. Li and J. Zhong, *Band Structure Engineering of Graphene by Strain: First-Principles Calculations*, Phys. Rev. B, 2008, vol. 78, no. 7, art. 075435. https://doi.org/10.1103/PhysRevB.78.075435

[60] I.V. Lebedeva, A.S. Minkin, A.M. Popov and A.A. Knizhnik, *Elastic Constants of Graphene: Comparison of Empirical Potentials and DFT Calculations*, Physica E: Low Dimens. Syst. Nanostruct., 2019, vol. 108, pp. 326–338. https://doi.org/10.1016/j.physe.2018.11.025

[61] B.D. Kong, S. Paul, M.B. Nardelli and K.W. Kim, *First-principles Analysis of Lattice Thermal Conductivity in Monolayer and Bilayer Graphene*, Phys. Rev. B, 2009, vol. 80, no. 3, art. 033406. https://doi.org/10.1103/PhysRevB.80.033406

[62] S.J. Stuart, A.B. Tutein and J.A. Harrison, *A Reactive Potential for Hydrocarbons with Intermolecular Interactions*, J. Chem. Phys., 2000, vol. 112, no. 14, pp. 6472–6486. https://doi.org/10.1063/1.481208

[63] J. Tersoff, *Empirical Interatomic Potential for Silicon with Improved Elastic Properties*, Phys. Rev. B, 1988, vol. 38, no. 14, pp. 9902–9905. https://doi.org/10.1103/PhysRevB.38.9902

[64] K. Chenoweth, A.C.T. van Duin and W.A. Goddard, *ReaxFF Reactive Force Field for Molecular Dynamics Simulations of Hydrocarbon Oxidation*, J. Phys. Chem. A, 2008, vol. 112, no. 5, pp. 1040–1053. https://doi.org/10.1021/jp709896w

[65] https://lammps.sandia.gov/.

[66] D. Akinwande, C.J. Brennan, J.S. Bunch, P. Egberts, J.R. Felts, H. Gao, R. Huang, J.-S. Kim, T. Li, Y. Li, K.M. Liechti, N. Lu, H.S. Park, E.J. Reed, P. Wang, B.I. Yakobson, T. Zhang, Y.-W. Zhang, Y. Zhou and Y. Zhu, *A Review on Mechanics and Mechanical Properties of 2D Materials—Graphene and Beyond*, Extreme Mech. Lett., 2017, vol. 13, pp. 42–77. https://doi.org/10.1016/j.eml.2017.01.008

[67] S. Winczewski, M.Y. Shaheen and J. Rybicki, *Interatomic Potential Suitable for the Modeling of Penta-Graphene: Molecular Statics/Molecular Dynamics Studies*, Carbon, 2018, vol. 126, pp. 165–175. https://doi.org/10.1016/j.carbon.2017.10.002

[68] J. Zhao, N. Wei, Z. Fan, J.-W. Jiang, and T. Rabczuk, *The Mechanical Properties of Three Types of Carbon Allotropes*, Nanotechnology, 2013, vol. 24, no. 9, art. 095702. https://doi.org/10.1088/0957-4484/24/9/095702

[69] B.G. Kim and H.J. Choi, *Graphyne: Hexagonal Network of Carbon with Versatile Dirac Cones*, Phys. Rev. B, 2012, vol. 86, no. 11, art. 115435. https://doi.org/10.1103/physrevb.86.115435

[70] R. Majidi, *Density Functional Theory Study on Structural and Mechanical Properties of Graphene, T-graphene, and R-graphyne*, Theor. Chem. Acc., 2017, vol. 136, no. 9, art. 109. https://doi.org/10.1007/s00214-017-2148-1

[71] H. Lu and S.-D. Li, *Two-dimensional Carbon Allotropes from Graphene to Graphyne*, J. Mater. Chem. C, 2013, vol. 1, no. 23, art. 3677. https://doi.org/10.1039/c3tc30302k

[72] X. Li, Q. Wang and P. Jena, *ψ-Graphene: A New Metallic Allotrope of Planar Carbon with Potential Applications as Anode Materials for Lithium-Ion Batteries*, J. Phys. Chem. Lett., 2017, vol. 8, no. 14, pp. 3234–3241. https://doi.org/10.1021/acs.jpclett.7b01364

[73] W.-J. Yin, Y.-E. Xie, L.-M. Liu, R.-Z. Wang, X.-L. Wei, L. Lau, J.-X. Zhong and Y.-P. Chen, *R-graphyne: a New Two-dimensional Carbon Allotrope with Versatile Dirac-like Point in Nanoribbons*, J. Mat. Chem. A, 2013, vol. 1, no. 17, art. 5341. https://doi.org/10.1039/c3ta00097d

[74] D. Bhattacharya and D. Jana, *Twin T-graphene: aNew Semiconducting 2D Carbon Allotrope*, Phys. Chem. Chem. Phys., 2020, vol. 22, no. 18, pp. 10286–10294. https://doi.org/10.1039/d0cp00263a

[75] W. Zhang, C. Chai, Q. Fan, Y. Song and Y. Yang, *PBCF Graphene: a 2D sp2 Hybridized Honeycomb Carbon Allotrope with a Direct Band Gap*, ChemNanoMat, 2019, vol. 6, no. 1, pp. 139–147. https://doi.org/10.1002/cnma.201900645

[76] J.-W. Jiang, J. Leng, J. Li, Z. Guo, T. Chang, X. Guo and T. Zhang, *Twin Graphene: A Novel Two-Dimensional Semiconducting Carbon Allotrope*, Carbon, 2017, vol. 118, pp. 370–375. https://doi.org/10.1016/j.carbon.2017.03.067

[77] Y. Zhang, T.T. Tang, C. Girit, Z. Hao, M.C. Martin, A. Zettl, M.F. Crommie, Y.R. Shen and F. Wang, *Direct Observation of a Widely Tunable Bandgap in Bilayer Graphene*, Nature, 2009, vol. 459, no. 7248, pp. 820-823. https://doi.org/10.1038/nature08105

[78] V. H. Crespi, L. X. Benedict, M. L. Cohen and S. G. Louie, *Prediction of a Pure-Carbon Planar Covalent Metal*, Phys. Rev. B., 1996, vol. 53, no. 20, pp. R13303–R13305. https://doi.org/10.1103/physrevb.53.r13303

[79] C. Kou, Y. Tian, M. Zhang, E. Zurek, X. Qu, X. Wang, K. Yin, Y. Yan, L. Gao, M. Lu and W. Yang, *M-Graphene: a Metastable Two-Dimensional Carbon Allotrope*, 2D Materials, 2020, vol. 7, no. 2, art. 025047. https://doi.org/10.1088/2053-1583/ab7977

[80] Z.G. Fthenakis and N.N. Lathiotakis, *Graphene Allotropes Under Extreme Uniaxial Strain: anAb Initio Theoretical Study*, PCCP, 2015, vol. 17, no. 25, pp. 16418–16427. https://doi.org/10.1039/c5cp02412a

[81] X.-L. Sheng, H.-J. Cui, F. Ye, Q.-B. Yan, Q.-R. Zheng and G. Su, *Octagraphene as a Versatile Carbon Atomic Sheet for Novel Nanotubes, Unconventional Fullerenes, and Hydrogen Storage*, J. Appl. Phys., 2012, vol. 112, no. 7, art. 074315. https://doi.org/10.1063/1.4757410

[82] C.-P. Tang and S.-J. Xiong, *A Graphene Composed of Pentagons And Octagons*, AIP Advances, 2012, vol. 2, no. 4, art. 042147. https://doi.org/10.1063/1.4768669

[83] M.P. Molepo, R.E. Mapasha, K.O. Obodo and N. Chetty, *First Principles Calculations of Pentaheptite Graphene and Boronitrene Derivatives*, Comput. Mater. Sci., 2014, vol. 92, pp. 395–400. https://doi.org/10.1016/j.commatsci.2014.06.004

[84] A.I. Podlivaev and L.A. Openov, *Kinetic Stability of Octagraphene*, Phys. Solid State, 2013, vol. 55, no. 12, pp. 2592–2595. https://doi.org/10.1134/s1063783413120299

[85] Q. Gu, D. Xing and J. Sun, *Superconducting Single-Layer T-Graphene and Novel Synthesis Routes*, Chinese Phys. Lett., 2019, vol. 36, no. 9, art. 097401. https://doi.org/10.1088/0256-307x/36/9/097401

[86] T. Morresi, A. Pedrielli, S.A. Beccara, R. Gabbrielli, N.M. Pugno and S. Taioli, *Structural, Electronic and Mechanical Properties of All-sp2 Carbon Allotropes with Density Lower Than Graphene*, Carbon, 2019, vol. 159, pp. 512-526. https://doi.org/10.1016/j.carbon.2019.12.024

[87] L.-C. Xu, R.-Z. Wang, M.-S. Miao, X.-L. Wei, Y.-P. Chen, H. Yan, W.-M. Lau, L.-M. Liu and Y.-M. Ma, *Two Dimensional Dirac Carbon Allotropes From Graphene*, Nanoscale, 2014, vol. 6, no. 2, pp. 1113–1118. https://doi.org/10.1039/c3nr04463g

[88] H. Sun, S. Mukherjee and C. V. Singh, *Mechanical Properties of Monolayer Penta-Graphene and Phagraphene: a First-Principles Study*, PCCP, 2016, vol. 18, no. 38, pp. 26736–26742. https://doi.org/10.1039/c6cp04595b

[89] L.F.C. Pereira, B. Mortazavi, M. Makaremi and T. Rabczuk, *Anisotropic Thermal Conductivity and Mechanical Properties of Phagraphene: a Molecular Dynamics Study*, RSC Advances, 2016, vol. 6, no. 63, pp. 57773–57779. https://doi.org/10.1039/c6ra05082d

[90] M. Deza, P.W. Fowler, M. Shtogrin and K. Vietze, *Pentaheptite Modifications of the Graphite Sheet*, J. Chem. Inf. Comput. Sci., 2000, vol. 40, no. 6, pp. 1325–1332. https://doi.org/10.1021/ci000010j

[91] U.H.F. Bunz, Y. Rubin and Y. Tobe, *Polyethynylated Cyclic π-Systems: Scaffoldings for Novel Two And Three-Dimensional Carbon Networks*, Chem. Soc. Rev., 1999, vol. 28, no. 2, pp. 107–119. https://doi.org/10.1039/a708900g

[92] B. Ram and H. Mizuseki, *C568: A New Two-Dimensional sp2-sp3 Hybridized Allotrope of Carbon*, Carbon, 2020, vol. 158, pp. 827–835. https://doi.org/10.1016/j.carbon.2019.11.062

[93] N. Narita, S. Nagai, S. Suzuki and K. Nakao, *Optimized Geometries and Electronic Structures of Graphyne and its Family*, Phys. Rev. B, 1998, vol. 58, no. 16, pp. 11009–11014. https://doi.org/10.1103/physrevb.58.11009

[94] B. Zou, J. Shen, P. Yu and J. Zhao, *The Young's Moduli of Three Types of Carbon Allotropes: a Molecular Mechanics Model and a Finite-Element Method*, Proc. Roy. Soc. A, 2016, vol. 472, no. 2186, art. 20150628. https://doi.org/10.1098/rspa.2015.0628

[95] H. Gao and W. Ren, *Emergence of Type-I and Type-II Dirac Line Nodes in Penta-Octa-Graphene*, Carbon, 2020, vol. 158, pp. 210–215. https://doi.org/10.1016/j.carbon.2019.11.083

[96] J. Hou, Z. Yin, Y. Zhang and T.C. Chang, *Structure Dependent Elastic Properties of Supergraphene*, Acta Mech.Sinica, 2016, vol. 32, no. 4, pp. 684–689. https://doi.org/10.1007/s10409-016-0560-8

[97] Y. Wang, A.J. Page, Y. Nishimoto, H.J. Qian, K. Morokuma and S. Irle, *Template Effect in the Competition Between Haeckelite and Graphene Growth on Ni(111): Quantum Chemical Molecular Dynamics Simulations*, J. Am. Chem. Soc., 2011, vol. 133, no. 46, pp. 18837–18842. https://doi.org/10.1021/ja2064654

[98] M.A. Rozhkov, *Mechanical and Electrical Properties of Graphene Crystals with Disclinations*, PhDThesis, (ITMO University, 2019), In Russian.

[99] F. Q. Wang, J. Yu, Q. Wang, Y. Kawazoe and P. Jena, *Lattice Thermal Conductivity of Penta-Graphene*, Carbon, 2016, vol. 105, pp. 424–429. https://doi.org/10.1016/j.carbon.2016.04.054

[100] https://uspex-team.org/.