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Graphene-based and graphene-like materials

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Abstract. The review generalizes information on methods for modification of graphene-based carbon materials through creation of structural defects, introduction of substitutional impurities, adsorption of impurity atoms and mechanical deformations. Graphene ribbons and nanoflakes, graphene allotropes, as well as multi-layer graphenes and graphene-containing hybrid carbon structures are considered. Methods of synthesis and the results of studies on the properties and simulation of graphene derivatives (graphane, graphone and fluorographene) are discussed. The results obtained in studies of related non-carbon graphene-like materials including silicon-, germanium- and tin-based structural analogues of graphene, graphene-like binary phases SiC, GeC, SiGe, SiSn, *etc*., as well as compounds $A^{III}B^{V}$ (white graphene, *etc*.) and $A^{II}B^{VI}$ (BeO, ZnO, ZnS) are generalized. Other graphene-like materials including metal dichalcogenides, oxides and carbides are briefly outlined. The bibliography includes 605 references.

I. Introduction

Graphene is a quasi-two-dimensional (2D) crystal comprised of carbon atoms that form an ordered hexagonal network. Intensive research of this material began in 2004 after a relatively simple 'scotch tape method' (micromechanical exfoliation) technique was proposed.[1,2]

The properties of graphene appeared to be very interesting. From the materials science viewpoint, the most remarkable features of graphene, the thinnest crystal known to date, include a combination of extremely high stiffness with elasticity and an abnormally high thermal conductivity. Graphene exhibits a number of unique physical properties which are determined by its electronic structure, namely, it is a zero band gap semimetal with massless Dirac fermions being the charge carriers. The chemical properties of graphene are due to its 2D structure and a very large specific surface area of about 2675 $m^2\ g^{-1}$; they also attract considerable attention of researchers. Unlike 3D crystals, all atoms in graphene are surface atoms, *i.e*., they are chemically reactive and can be involved in various interactions, which offers great prospects for the chemical modification of graphene.

Such a combination of the properties predetermined high research activity as well as the attractiveness of graphene as material for various technological applications. Impressive results obtained to date in the studies of graphene have been reported in numerous original communications and generalized in reviews (Fig. 1).

The authors of the early reviews[3–8] published in 2006 – 2008 compared the available information on the

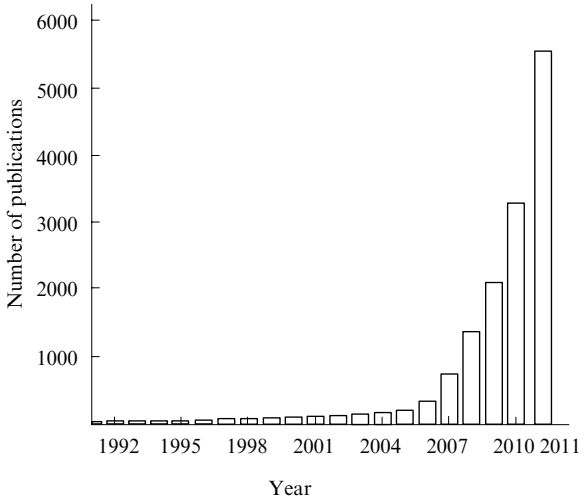


Figure 1. Number of publications on graphene since 1992 (according to the ISI Web of Knowledge data).[13]

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methods of synthesis and properties of graphene with the corresponding data for other carbon nanostructures.

General problems concerned with the synthesis and studies of the properties of graphene as well as possible fields of its application have been discussed in recent reviews.[9–17] Modern views of the 'problem of graphene' have been presented in the Nobel lectures by K S Novoselov [18] and A K Geim.[19]

Intensive studies on graphene (see Fig. 1) led to accumulation of a huge amount of new experimental data and theoretical results which are discussed in a set of modern reviews. In particular, chemical methods of graphene synthesis,[20] specific features of epitaxial synthesis of single-layer and multi-layer graphenes [21] and the synthesis of graphene and graphene ribbons on metallic substrates [22] was analyzed. The magnetic,[23–25] electronic [26,27] and electrochemical [28] properties of graphene were considered; considerable attention has been given to the formation and properties of quantum dots in graphene.[29] The results of studies on graphene oxides,[30–32] methods of graphene functionalization [33,34] and fabrication of various graphene-containing composite materials (and possible fields of their application), graphene–polymer composites,[35–37] inorganic composites [38] and graphene–carbon nanotube composites [39] were generalized on a new level. Also, graphene-based materials for solar energy conversion,[40,41] photocatalysis,[42] lithium cell electrodes,[43] quantum electronics [44] as well as electrochemical and biological sensors [45] were analyzed. A description of graphene-based nanotechnologies is available.[46] Distinctive features of graphene ribbons [47,48] and some inorganic graphene analogues including BN, WS_2 and MoS_2 were reported.[49]

Finally, mention should be made that Russian researchers also published the first reviews devoted to the chemical methods of synthesis and modification of graphene [50] and to the methods of synthesis and thermophysical properties of this material.[51]

Having noted impressive advances in the research on graphene, it is appropriate to say that, despite the uniqueness of the material (this is often emphasized by different authors), it belongs to a large family of sp^2 carbon allotropes, such as graphite, fullerenes, nanocones, nanotoroids, nanotubes, nanofoam and some other carbon structures of different dimensionality (0D–3D) (Fig. 2). Obviously, progress in the studies on the properties of graphene are due to colossal experience accumulated in comprehensive investigations of other nanoforms of carbon, first of all, fullerenes (synthesized in 1985, see Ref. 52) and carbon nanotubes (CNTs, synthesized in 1991, see Ref. 53). This follows from, *e.g.*, the reviews on fullerenes [54–74] and CNTs (see Refs 75–97) reported by Russian authors.

At the same, it was emphasized [98] that 'graphene is not the end of the road!' Currently, physical chemistry, materials science and technology of novel materials that can conditionally be called graphene-like ones are being developed intensively. The term 'graphene-like materials' is often used in the literature as a common name to two groups of

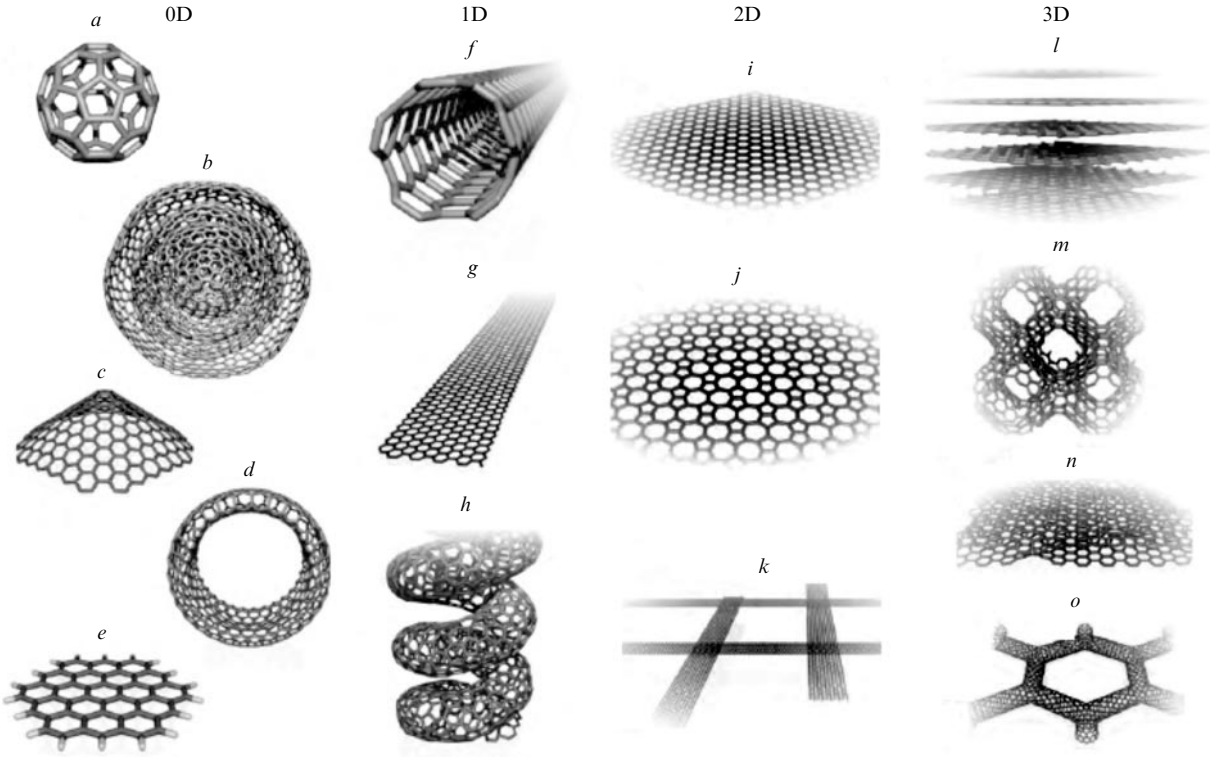


Figure 2. 0D–3D allotropes of sp^2 carbon.[47]
Fullerene (*a*), onion (*b*), nanocone (nanohorn) (*c*), nanotoroid (*d*), graphene nano-flake (*e*), carbon nanotube (*f*), graphene nanoribbon (*g*), helicoidal carbon nanotube (*h*), graphene (*i*), Haeckelite network (*j*), graphene nanoribbons 2D network (*k*), graphite (*l*), Schwarzite (*m*), carbon nanofoam (3D structure comprised of interconnected graphene nanoribbons) (*n*) and 3D nanotube network (*o*).

quasi-2D systems with significantly different chemical compositions and properties.

One group of materials (from this point on, graphene-based materials) includes systems based on or containing the 0D–2D forms of graphene. These are 2D graphene modified in different manner (by introducing structural vacancies and/or impurities, by adsorption of atoms or molecules of by mechanical deformation), as well as various hybrid structures formed by graphene with other carbon nanostructures (*e.g.*, graphene–fullerene or graphene–CNT), graphene derivatives (graphene oxide, graphane, fluorographene) or graphene-containing composites. This group also includes graphene ribbons (1D), graphene nanoflakes (0D) and multi-layer graphenes, which can either be modified or used as components of various composites.

Considering the second group of materials, graphene is treated as a prototype of the desired 2D crystals and the emphasis is placed on the synthesis and properties of such graphene-like systems. Usually, these materials are structurally similar to hexagonal graphene network and/or contain carbon as a constituent (*e.g.*, BC_x, CN_z, $B_xC_yN_z$, SiC, GeC, SnC), but they can also have other chemical compositions (*e.g.*, silicene, germanene, boron nitride network called 'white graphene', graphene-like AlN, GaN, *etc.*). This family of materials includes more complex 2D inorganic systems comprised of a number of atomic networks, *e.g.*, quasi-2D transition metal dichalcogenides. In turn, studies on further modification of the properties of these novel graphene-like materials are now in progress.

This review reports the state of the art in studies of the two groups of materials, graphene-based and graphene-like ones, and the methods for modification of their properties. Note that whereas most graphene-based materials mentioned above have been synthesized and intensively studied by various experimental methods,[21–48] in the case of graphene-like quasi-2D crystals, a significant (sometimes, leading) role is played by theoretical approaches including quantum chemistry and molecular dynamics (MD). In particular, silicene (silicon analogue of graphene) was first studied theoretically[99–102] and only then monatomic silicon layers and silicon nanoribbons a few hundred nanometres long were synthesized by molecular beam epitaxy on a silver substrate.[103–106] Many inorganic analogues of graphene (*e.g.*, germanene[107–110] or 2D zinc sulfide[111,112]) still remain hypothetical systems despite intensive research efforts made. Quantum chemistry methods and MD play an important role in the development of methods for controlling the properties of graphene and graphene-like materials; therefore, considerable attention will be paid to the results of theoretical simulations.

II. Graphene and methods for modification of its properties

At present, the focus in studies of graphene[1,2] and determination of its key physicochemical properties (for the properties of structurally perfect graphene, see reviews[3–19]) is placed on targeted control of the properties. To this end, a variety of physical and chemical methods have been developed. One of the most efficient methods involves the introduction of structural defects into the graphene network.

1. Structural defects and their influence on the properties of graphene

Structural defects in the graphene network can be divided into three main groups:

— point defects (vacancies);

— topological defects (TDs), either local and non-local ones; (the latter also include dislocations and grain boundaries, *i.e.*, the coupling lines of fragments of a graphene sheet with different orientations of hexagons or involving other carbon rings C_n with $n \neq 6$;

— edge (linear) defects, *i.e.*, edges of graphene ribbons (chains of atoms with dangling bonds) or graphene nanoflakes; this type of defects also includes perforations (up to a few hundred nanometres in size) in graphene nanomesh.

Structural defects in graphene that appeared without changing its chemical composition are often referred to as intrinsic defects[113] in contrast to extrinsic defects that are caused by the presence of foreign (non-carbon) atoms.

a. Point defects (vacancies)

Atomic vacancies arising upon removal of a carbon atom from the graphene network represent the simplest type of intrinsic defects in this material. They can be created upon exposing graphene to electron or ion irradiation (radiation-induced defects)[113–119] or by treating graphene with plasma.[113,120] Vacancy formation can be accompanied by partial amorphization and deformation of specimens. Experimental and theoretical studies[113–129] showed that vacancy formation is accompanied by rearrangement of the nearest C–C bonds and the formation of a nonagon and a pentagon to minimize the number of dangling bonds (Fig. 3). Double vacancies (created by coalescence of two single vacancies or by removal of two neighbouring carbon atoms[113,129]) are also known; in this case, the local environment is also reconstructed to form various polygons C_n with $n \neq 6$ (Table 1). It should be emphasized that the vacancy

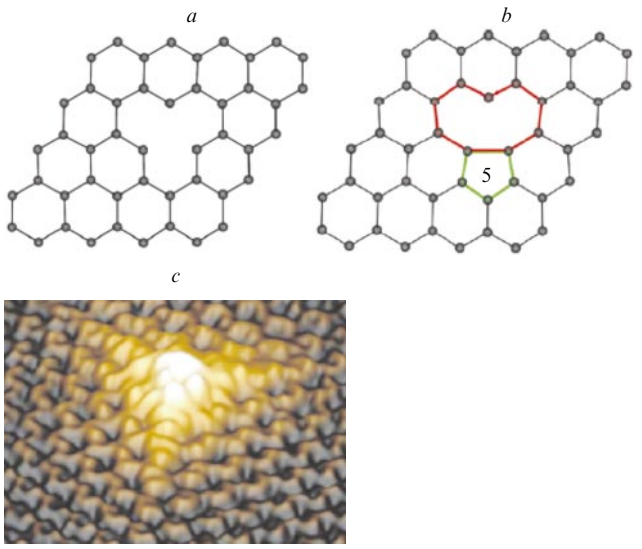


Figure 3. Models for 'ideal' single vacancies in graphene: removal of carbon atom from the graphene network (*a*), atomic structure of the vacancy after energy optimization with local reconstruction of bonds and the formation of a pentagon (*b*);[127] an STM image of a single vacancy visible as an increase in the electron density in the region of dangling bonds (*c*).[128]

Table 1. Formation and migration energies (E_f and E_m, respectively) of main structural defects in graphene.[113]

Defect	Configuration [a]	E_f/eV	E_m/eV
Single vacancy	C_5-C_9	7.3–7.5	1.2–1.4
Double vacancy	$C_5-C_8-C_5$	7.2–7.9	7
	$C_{5,5,5}-C_{7,7,7}$	6.4–7.5	6
	$C_{5,5,5}-C_6-C_{7,7,7}$	7	6
Stone–Wales defect	$C_{5,5}-C_{7,7}$	4.5–5.3	10
Inverse Stone–Wales defect	$C_{5,7}-C_{5,7}$	5.8	—

[a] Carbon rings.

formation energy (*i.e.*, the energy needed to remove a carbon atom from the network) is very high ($E_f > 7$ eV, see Ref. 113), which makes the formation of another type of intrinsic defects in graphene, *viz.*, topological defects, much more probable.

b. Topological defects

A 'structural' approach to modification of the properties of graphene involves the introduction of TDs (see above) into the hexagonal network; *i.e.*, some hexagons are replaced by other carbon polygons $C_{n\neq 6}$ or by combinations of different polygons, so that the number of atoms in the system remains unchanged. The role of TDs in the modification of the properties of carbon nanostructures has been well studied taking CNTs as examples (see reviews [87, 130, 131]).

Two main types of TDs include a single TD (or a 'cluster' of single TDs) and a chain of single TDs (linear defect).[132–141] In the former case, local changes in the graphene properties in the TD region are possible, while in the latter case, one deals with 1D modulation of the properties of the material. Figure 4 presents examples of a single Stone–Wales topological defect [132] created in the graphene network upon rotation of a C–C bond by an angle of $\pi/2$ (here, four adjacent hexagons are transformed into two pentagons and two heptagons: $4C_6 \rightarrow 2C_5 + 2C_7$), and an extended chain of defects (coupled $C_5 + C_7$ pairs). A theory of dislocations in graphene containing $C_5 + C_7$ pairs was developed.[133] Topological defects also include grain boundaries, *i.e.*, the coupling lines of two fragments of a graphene sheet with different orientations of hexagons. In the presence of TDs, the conducting properties of graphene change significantly [139] and its reactivity enhances,[140] but the stiffness decreases.[137]

Linear TDs formed by $2C_5 + C_8$ rings in epitaxial graphene on a Ni(111) substrate (see Fig. 4) were reported.[134] According to scanning tunneling microscopy (STM) data, such a TD is characterized by an increased density of electronic states and can be considered as 'nanowire' implanted into the graphene network. The formation of extended TDs of specified configuration is still a problem to be solved.

The Stone–Wales defects cause local wave-like distortions of the graphene network structure, which travel distances of the order of a few nanometres from the defect site due to displacements of carbon atoms from the plane of the network.[135] The formation of TDs of, *e.g.*, the Stone–Wales type, is characteristic [141] of graphene ribbon edges (see below).

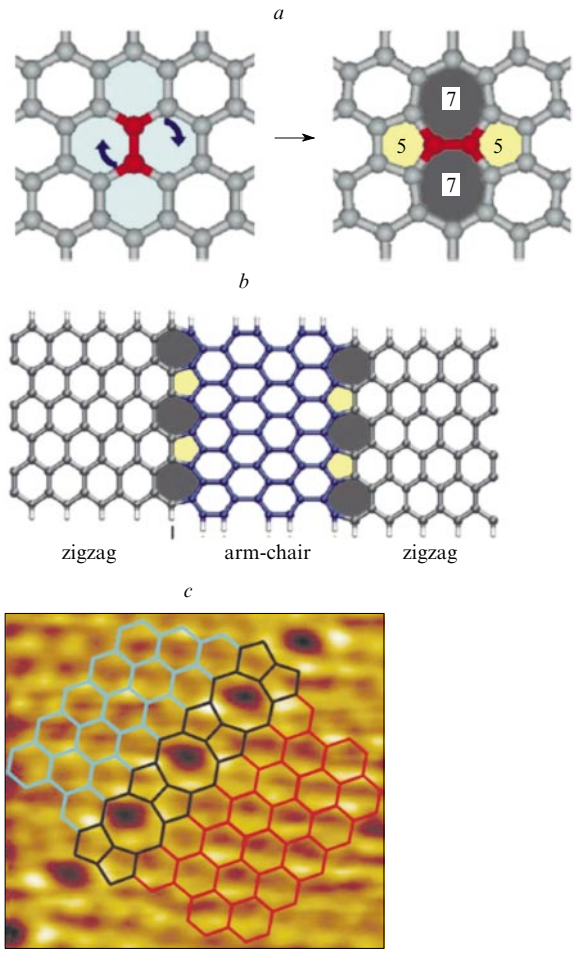


Figure 4. Topological defects in graphene.
Single Stone–Wales defect:[132] pairs of rings $2C_5 + 2C_7$ formed upon rotation of a C–C bond by an angle of $\pi/2$ (*a*); linear defect: a chain of 'coupled' rings ($C_5 + C_7$) (*b*);[47] a STM image of a linear defect (chain of rings $2C_5 + C_8$) formed in graphene epitaxial layer on Ni(111) substrate (*c*).[134]

c. Graphene allotropes

Another possible method for modification of the properties of a planar monatomic network of carbon atoms is to construct the network from C_n rings with $n \neq 6$ (see above). The search for corresponding graphene allotropes began more than two decades ago.[87, 130, 142–146] Structural fragments of graphene allotropes proposed to date are shown in Fig. 5. Among them, there are the flat networks *1* and *2* known as pentaheptites because they comprise regularly alternating pentagons and heptagons.[148, 149] The network *3* containing a combination of C_6, C_5 and C_8 rings can be considered as intermediate case between the structures of graphene and pentaheptite. Structures similar to *3* are known as Haeckelites.[150] The next group of networks, *4* and *5*, respectively includes graphynes [142, 146] and graphdiynes [145] built of C_6 rings connected by different-length chains of carbon atoms. Network *6* is composed of equal numbers of tetragons and octagons,[143] while network *7* comprises tetragons and dodecagons. Replacement of 2/3 of the total number of C–C bonds in the graphene network by carbyne-like chains leads to structure *8* formed by distorted hexagons. Replacement of all C–C bonds in

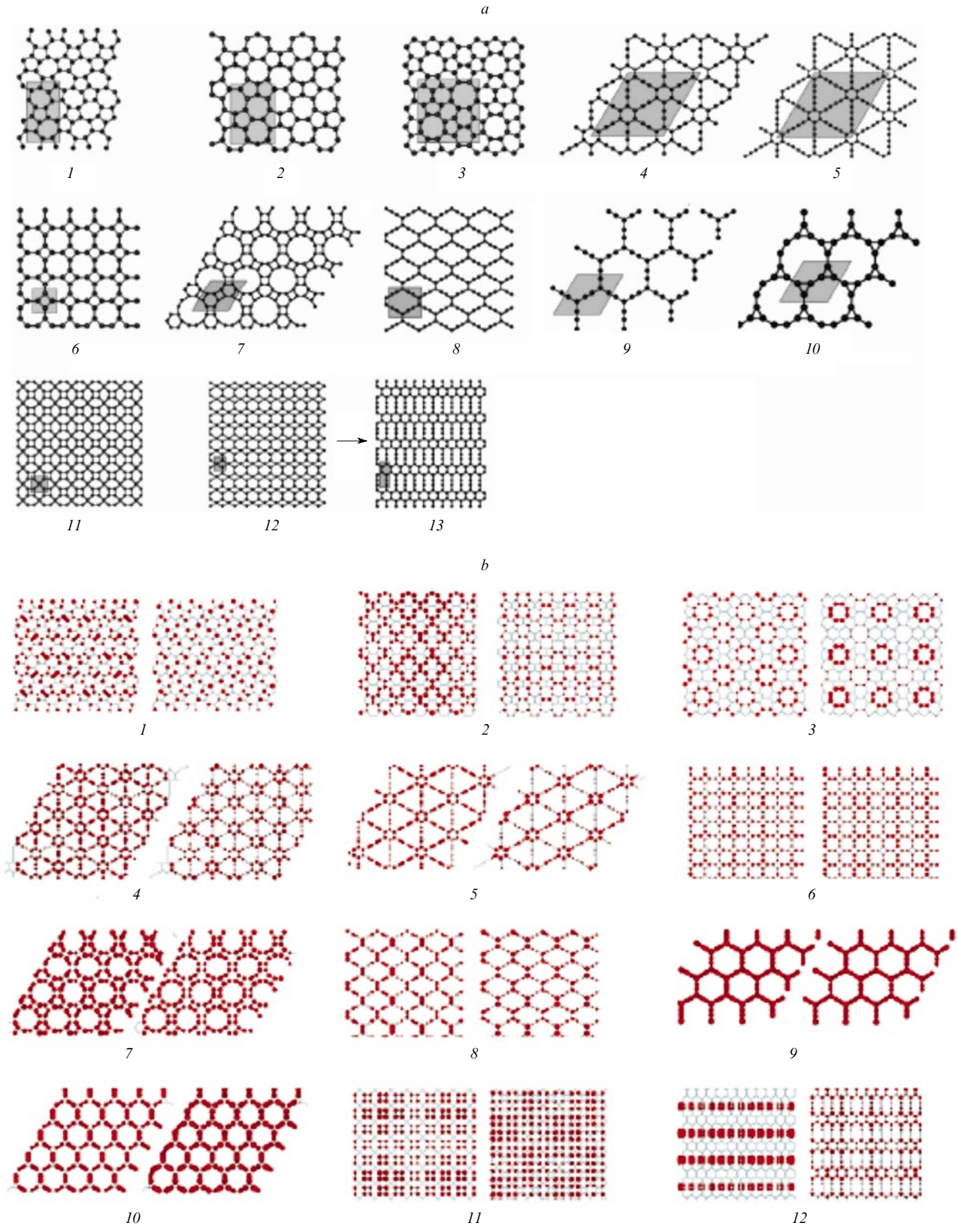


Figure 5. Optimized atomic structures of graphene allotropes (*a*) and the electron density distribution (ψ^2) at the Γ point of the Brillouin zone for the top of the valence band (on the left) and for the bottom of the conduction band (on the right) (*b*).[147]
For notations *1–13*, see text; the unit cells are given in grey.

graphene by carbyne-like chains produces the structure *9* which can be called supergraphene. The hypothetical network *10* comprises C_3 and C_{12} rings. Eventually, the networks *11* and *12*, or the so-called squarographenes,[151] are formed by distorted hexagons and regular tetragons or by regular hexagons and rhombi, respectively.

Geometry optimization of the networks *1–12* showed[147] that systems *1–11* retain their initial flat structures, whereas structure *12* is unstable and transforms to a more stable structure *13* formed by hexagons whose vertices are connected by carbyne-like atomic chains.

Using a classification of carbon structures,[152] the flat networks *1–13* can be divided into three groups depending on the hybridization (n) of carbon atoms. The first group includes conventional graphene and most networks considered (systems *1–3*, *6*, *7* and *10*) containing sp^2 carbon atoms ($n = 2$). The second group comprises the networks *4*, *5*, *8* and *9* containing fragments of carbyne chains. These structures are characterized by a mixed ($sp^2 + sp^1$) type of hybridization of carbon atoms ($1 < n < 2$). The relaxed structure *13* also falls in this group. Finally, the squarographene networks *11* and *12* contain three-coordinate (sp^2) and four-coordinate (sp^3) carbon atoms and belong to another mixed ($sp^2 + sp^3$) type of hybridization ($2 < n < 3$).

A stability analysis[147] of the allotropes *1–13 vs.* graphene (from their total energy differences)

$$\delta E = E_{\text{tot}}^{\text{al}} - E_{\text{tot}}^{\text{gr}}$$

revealed (Table 2) the lowest probability of formation for the planar networks *11* and *12* with the $sp^2 + sp^3$ hybridization type, allotropes *8* and *9* containing carbyne chains and allotrope *10* comprising strained rings C_3 and C_{12}. The networks *4*, *5* and *13* built of hexagons and carbyne chain segments are energetically more favourable; however, the network stability decreases as the carbyne chain segment length increases (*4* → *5*). The most stable structures *1–3* ('pure' sp^2 hybridization) formed by combining C_n rings with $n = 5–8$ seem to be synthetically accessible. Possible methods of preparation of graphene allotropes have been discussed.[142–151]

Table 2. Lattice types and constants (a and b), relative energies (δE), band gap (BG) widths and hybridization type (HT) of 13 graphene allotropes.[147]

Allotrope[a]	Lattice type	a/Å	b/Å	δE/eV	BG/eV	HT
1	rectangular	4.87	8.84	0.308	0	sp^2
2	"	5.70	7.56	0.323	0	sp^2
3	square	8.71	–	0.397	0.76	sp^2
4	hexagonal	11.99	–	0.695	1.32	$sp^2 + sp^1$
5	"	16.52	–	0.867	1.47	$sp^2 + sp^1$
6	square	3.47	–	0.707	0	sp^2
7	hexagonal	6.83	–	0.828	1.14	sp^2
8	rectangular	7.03	6.91	0.928	0	$sp^2 + sp^1$
9	hexagonal	7.02	–	1.035	0	$sp^2 + sp^1$
10	"	5.24	–	1.386	0	sp^2
11	square	3.62	–	2.077	0	$sp^2 + sp^3$
12	rectangular	2.72	2.92	2.914	0	$sp^2 + sp^3$
13		2.51	6.96	0.537	0.70	$sp^2 + sp^1$

[a] For notations *1–13*, see Fig. 5.

According to electronic structure calculations,[147] all the networks *1–13* can be divided into three groups:

— semimetals (graphene *1* and supergraphene *9*);
— metal-like (*1*, *2*, *6*, *8*, *10*, *11* and *12*); and
— semiconductors (*3–5*, *7* and *13*).

Haeckelites (*3*), graphyne-like (*4*, *5*) and polycyclic networks (*7*, *13*) have a semiconductor type conductivity. Therefore, the appearance of a band gap in the energy spectrum of planar carbon networks requires the presence of the following structural units: ring combinations $C_5 + C_6 + C_8$ and $C_4 + C_5$ in systems *3* and *7*, respectively, or carbyne chain segments and hexagons in systems *4*, *5* and *13*. All other networks are expected to have a metallic type conductivity or be zero band gap semimetals. In addition, an analysis of the charge density distribution near the Fermi (E_F) showed that all graphene allotropes fall in two groups, *viz.*, those with symmetric and asymmetric electron density distribution. For instance, for semiconducting allotropes (*3–5*, *7* and *13*) the top of the valence π-band and the bottom of the conduction π*-band are composed of contributions of the same atoms (for *5*, *6* and *8*) or atomic groups (for *4*). Contrary to this, for network *13* the top of the valence band is composed of the contributions of the sp^1 carbon atoms from the carbyne chains while the bottom of the conduction band is determined by the contributions of the sp^2 carbon atoms from hexagons. Some other hypothetical flat carbon networks were also reported.[153]

d. Carbon atoms adsorbed on graphene

Intrinsic defects in graphene also include carbon adatoms. Main effects in the adsorption are the formation of C–C bonds between the graphene network atoms and adatoms and local distortions of the network. The binding energy of an adatom is about 1.5–2.0 eV.[113] Diffusion of carbon adatoms across the graphene network and pairing of these atoms is possible; in the latter case, one deals with significant rearrangement of the network structure with the formation of an inverse Stone–Wales defect.[154, 155]

e. Graphene nanomesh

Yet another type of graphene systems with intrinsic defects is represented by graphene nanomeshes.[156–167] In this case, periodically ordered holes (pores) of finite size in the range from a few to a hundred nanometres are created in graphene sheet by electron beam lithography (or using various templates).[156–163] Rearrangement of the edge states favours local reconstruction of the network structure and specifies a number of interesting quantum effects related to the conductivity, magnetism and optical properties of materials.[156–167] These properties can be controlled by, *e.g.*, varying the pore shape or size, the pore–pore distance and the type of ordering in the network, as well as by adsorbing various atoms, in particular hydrogen atoms, on pore edges (Fig. 6). For instance, hydrogen-passivated graphene nanomesh prepared on porous aluminium exhibits the properties of a ferromagnetic[163] due to localization of the spin density at zigzag pore edges. This effect was theoretically interpreted[167] within the Lieb theorem,[168] which treats the rise of sp (or d^0) magnetism as a consequence of site occupation imbalance in the sublattices. Theoretical search for 'magic numbers' describing the size of the most stable nanopores in graphene and thus enabling control of the magnetic and conducting properties of graphene nanomeshes was reported.[169]

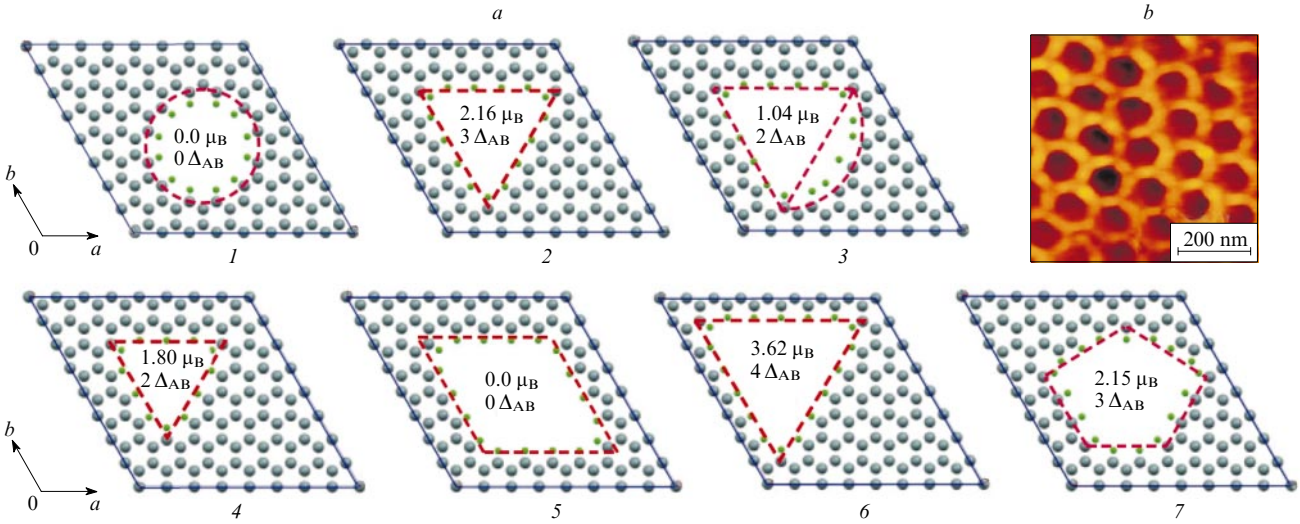


Figure 6. Possible configurations (*1*–*7*) of pores in graphene nanomesh (*a*)[165] and an STM image of a specimen of graphene nanomesh prepared on porous aluminium (*b*).[163]
Pore edge atoms are hydrogen passivated. For each structure, shown are the calculated magnetic moments (in Bohr magnetons, μ_B) and the difference (n) between the numbers of occupied sites in two sublattices ($n\,\Delta_{AB}$).[165]

2. Graphene ribbons and nano-flakes

Particular groups of graphene materials include 1D graphenes (graphene ribbons) and 0D graphenes (graphene nanosheets known as graphene nano-flakes or nano-dots). Owing to natural size confinement, graphene nano-flakes (nano-sized fragments of the graphene network, which can be either single-layer or multi-layer) have been studied much poorer than, *e.g.*, long graphene ribbons. A main feature of graphene nano-flakes consists in a large number of dangling bonds of edge atoms. Therefore, such systems are rather unstable; they have a variety of configurational degrees of freedom and can convert into various forms. In addition, the size of graphene nano-flakes can vary over a wide range from molecular sizes to, in the limiting case, something of the size of atomic ribbons, which ensures a very wide range of changes in their properties.

Potential applications of graphene nano-flakes are determined by (i) the extent to which we know how the desired properties of graphene nano-flakes depend on their size and configurations and (ii) the development of reliable methods of synthesis of graphene nano-flakes with preset functional properties. It was established that the structure stability of graphene nano-flakes depends on many factors (size, shape, temperature, charge)[170–172] and on the interaction with the environment (substrate and/or medium).[173] Recently, pioneering attempts have been made to carry out large-scale synthesis of graphene nano-flakes[174] and to isolate graphene nano-flakes of specified size (~1 μm) by controlled centrifugation (Fig. 7).[175] The variety of possible types of graphene nano-flakes significantly hampers theoretical search for the regularities of changes in their properties depending on the factors mentioned above. At present, a rather small number of types of graphene nano-flakes was simulated (see Refs 176–179). For instance, calculations of a series of single-layer hexagonal graphene nano-flakes with both zigzag and arm-chair edges (either carbon-terminated or stabilized by hydrogen atoms or molecules) predicted the highest stability for H_2-passivated graphene nano-flakes with arm-chair edges built of sp^3 terminal carbon

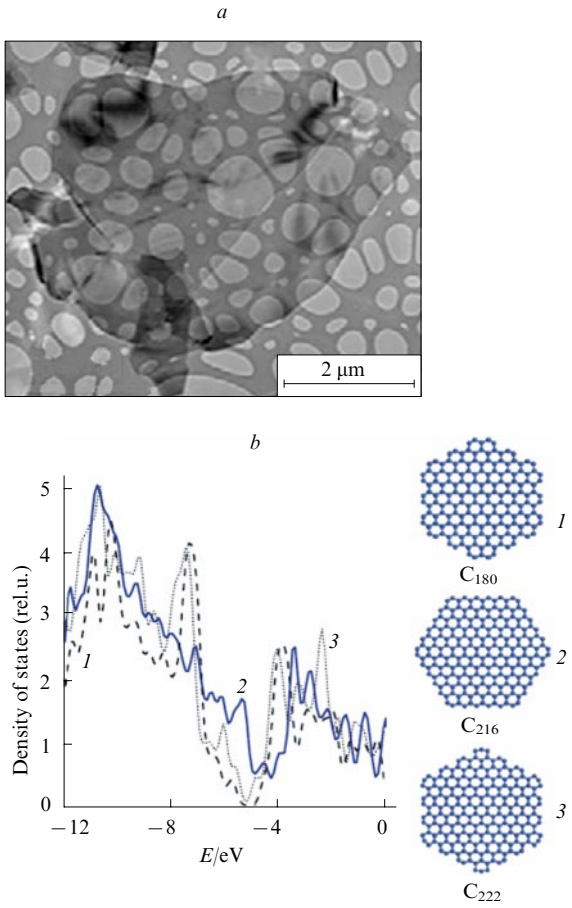


Figure 7. A TEM image of an ensemble of graphene nano-flakes separated by centrifugation (*a*)[175] and the densities of electronic states of hexagonal graphene nano-flakes with similar sizes ($C_{180-222}$) and different types of edges (*1*–*3*) (*b*).[176]

atoms.[176] At the same time, the electronic spectra of hexagonal graphene nano-flakes differ appreciably (see Fig. 7) even for specimens with close sizes ($C_{180}-C_{222}$).

a. Graphene ribbons

Recently, the structure and properties of graphene ribbons (extended graphene strips of width from a few tens to a few hundred nanometres) have attracted considerable attention of researchers. Their interest was, in particular, stimulated by advances in the studies of these quasi-1D materials by atomic-resolution microscopy methods.[180, 181] Of course, main distinctions between the properties of graphene ribbons and those of perfect 2D graphene sheet are first of all due to the states of edge atoms.[29, 47, 98, 122, 182–196] Depending on the edge type, ribbons can exhibit the properties of metals, semiconductors, semimetals, ferro- or antiferromagnets (see review [47]).

Ribbons with arm-chair and zigzag edges as well as, *e.g.*, the Klein edges (Fig. 8) have been best studied.[122, 192, 193] However, these 'perfect' edges are usually metastable. They can be stabilized through various structural reconstructions [with the formation of, *e.g.*, pentagon–heptagon edge pairs ($2\,C_6 \rightarrow C_5 + C_7$)],[122, 194–196] folding or spontaneous rolling of the ribbon edge into a small-diameter nanotube [191] (see Fig. 8) or by passivating the dangling bonds with adatoms (*e.g.*, hydrogen atoms). The most stable ribbon edge configurations obtained from systematic theoretical analysis [187] are shown in Fig. 9. Clearly, the stability of an edge should also depend on the chemical environment of ribbons and on the substrate type.[47]

Considering the electronic structure of ribbon edges, the zigzag and Klein edges give rise to quasi-flat near-Fermi bands (so-called edge states), which are prone to spontaneous spin polarizarion and formation of magnetic moments on the edge atoms. For instance, ribbons with zigzag edges, which exhibit edge ferromagnetism, may possess the properties of semiconductors and go to the state of magnetic semimetals upon edge passivation with hydrogen atoms. Ribbons with arm-chair edges show the properties of semiconductors, while their band gaps are

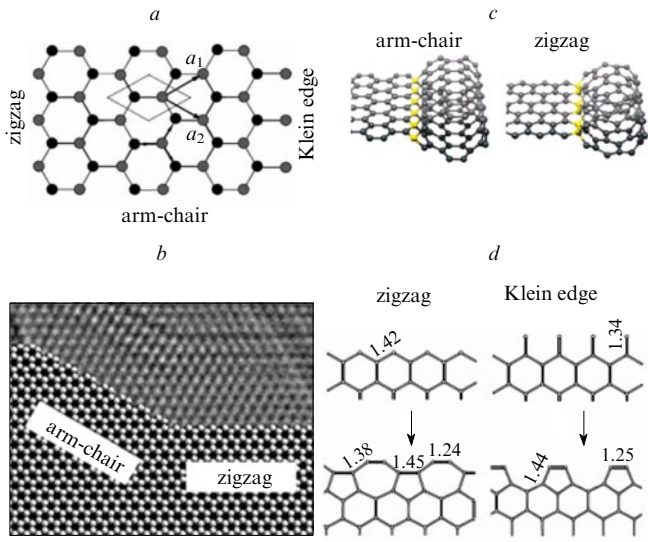


Figure 8. Graphene nanoribbon edge configurations: zigzag, arm-chair and Klein edge (*a*); a HRTEM image of overlapping zigzag and arm-chair nanoribbon edges (bottom: hexagonal atomic models presented for clarity) (*b*);[47] scheme illustrating stabilization of zigzag and arm-chair nanoribbon edges through their spontaneous rolling in small-diameter nanotubes,[191] and models for reconstruction of zigzag and Klein edges with the formation of pentagons and heptagons (numbers denote the C–C interatomic distances in Å) (*d*).[122]

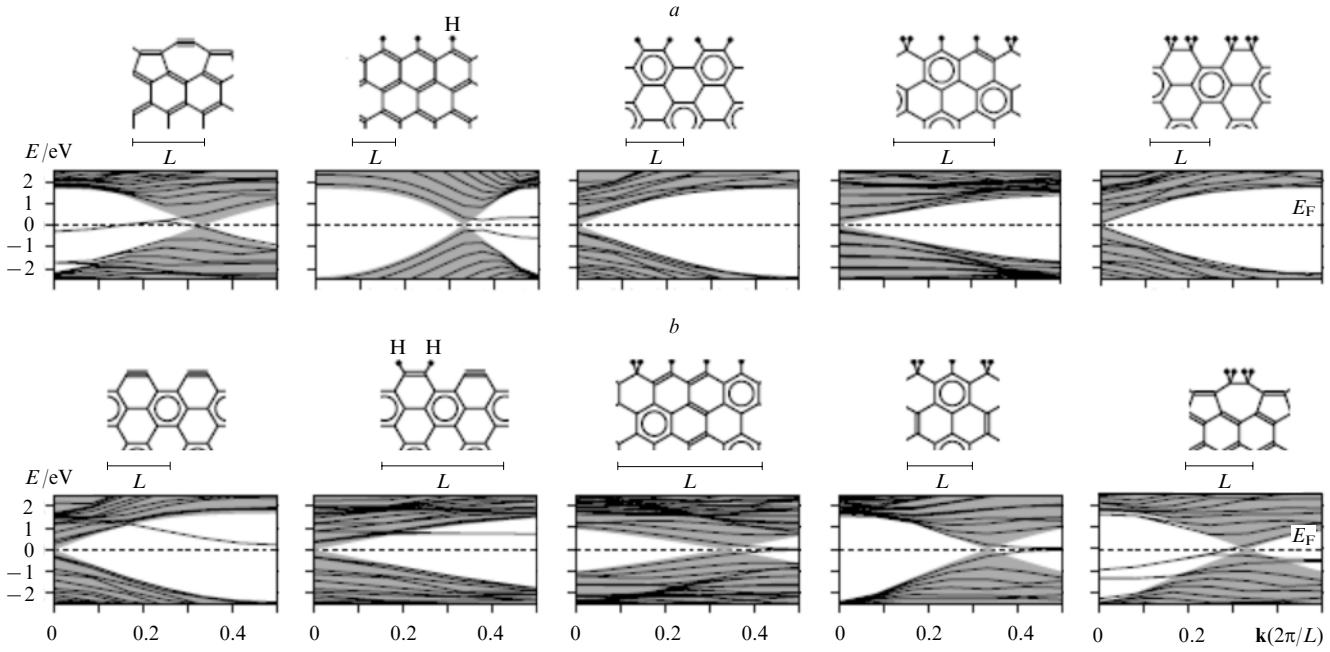


Figure 9. The most (*a*) and the least (*b*) stable configurations of graphene nanoribbon edges (both unstabilized and stabilized by hydrogen adatoms) and their electronic energy bands near the Fermi level;[187]
k is the wave vector and *L* is the periodicity of the nanoribbon along its edge.

narrowed as the ribbons become wider. These issues have been considered in more detail in reviews,[29,47] as well as the applications of graphene ribbons as functional elements in various carbon electronics devices.

b. Deformations of graphene and graphene ribbons

Up to this point, we have considered 2D–0D planar graphene materials. Their properties can be changed significantly by distorting their structures in different manner. Consider the most typical deformation-induced effects in 2D and 1D graphenes.

Folding and twisting of graphene ribbons. The properties of graphene ribbons can be changed by folding (either single or multiple) or twisting (Fig. 10). These types of deformations may arise [197,198] during the synthesis of ribbons, be a result of functionalization of ribbons or be attained by specific methods (*e.g.*, formation of folded ribbons using a metallic template [199] illustrated in Fig. 11). The first experiments on the synthesis and simulation of multiply folded ribbons [199] demonstrated their interesting mechanical, chemical and electronic properties, which can be adjusted by varying the number and orientation of folds, the type of folding and by functionalization of the folded ribbons, *e.g.*, by intercalation of folds or by adding particles to the highly curved ribbon edge (see Fig. 10). The possibility of spontaneous twisting of a graphene ribbon about an iron nanorod was reported.[200] The effect was explained by the onset of rather strong $\pi-\pi$-interactions between the ribbon and the nanorod; as follows from the results of MD simulation, the character of twisting depends on the mutual orientation of the ribbon and the rod.

Mechanical deformations of graphene and graphene ribbons. Graphene structures can be deformed under the action of external stress. Mechanical deformations represent yet another method of control of the transport, electronic, optical and magnetic properties of these systems.[98,201–216] Homogeneous deformations cause insignificant changes in the graphene conductivity type.[203] Inhomogeneous deformations, *e.g.*, uniaxial stretching, can significantly change the electronic system of the graphene sheet and give rise to a band gap of up to 1 eV.[203,212] Changes in the electronic system and conducting properties of graphene ribbons caused by stretching depend [210] on the ribbon edge type, being minor for ribbons with zigzag edges and significant for ribbons with arm-chair edges; also, they show a nonmonotonic behaviour depending on the degree of stretching.[201–204]

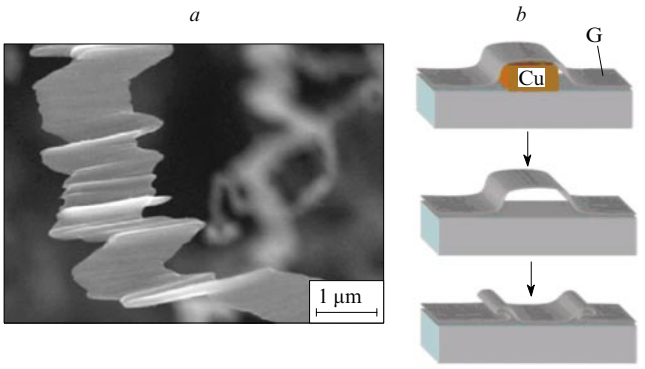


Figure 11. Deformations of graphene ribbons.
A STEM image of a multiply folded, multi-layer graphene ribbon obtained by gas-phase synthesis [196] (*a*) and an illustration of a method to produce folded ribbons [graphene ribbon (G) is transferred onto a metallic (Cu) substrate, the substrate is removed and the ribbon spontaneously folds itself][199] (*b*).

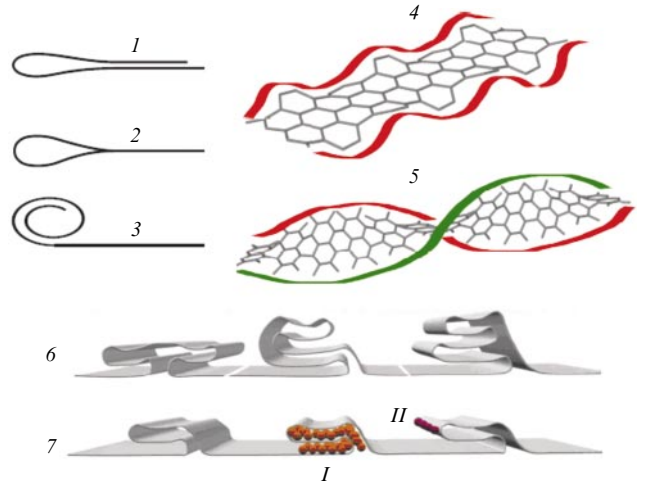


Figure 10. Deformation of graphene ribbons.[199]
Folding (*1*), folding with junction (*2*), helical folding (*3*), static ripples on the ribbon (*4*), twisting graphene ribbon (*5*), various complex folding structures (*6*), and functionalization of complex-folded ribbon by intercalation of folds (*I*) or by adding particles to the highly curved ribbon edge (*II*) (*7*).

Local variations of bond angles and bond lengths in the graphene sheet (ribbon) accompanied by corresponding perturbations of the electronic and magnetic subsystems can be used to fabricate graphene 'nanowires', electromechanical sensors, *etc*.[98] A number of possible methods for creation of heterojunctions in a graphene ribbon upon its local deformation by stretching and bending are shown in Fig. 12. In the former case,[98,204] a ribbon is placed onto a combined substrate having different thermal expansion coefficients (TEC) in different regions; for clarity, $\alpha_2 > \alpha_1$ (Fig. 12 *a*). On heating, anisotropic stretching of the ribbon (it is maximum in the substrate region with the high TEC) will give rise to a band gap in the energy spectrum of this ribbon segment. A semiconductor–metal junction in the ribbon can be created [212] by forming a step (local bending, see Fig. 12 *b*) and by varying the bending angle θ.

Of course, mechanical action (deformation) can be combined with chemical modification of graphene structures. For instance, a mechanically induced ferromagnet–

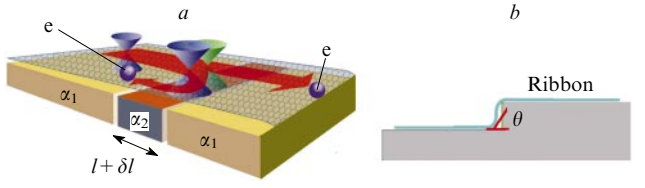


Figure 12. Creation of a metal–semiconductor heterojunction in graphene ribbon upon its local deformation by stretching upon heating a combined substrate with different thermal expansion coefficients ($\alpha_2 > \alpha_1$) (*a*) [98,204] and by bending by the angle θ when producing a step (*b*).[212]

antiferromagnet transition of the graphene sheet upon partial fluorination was substantiated.[215] Deformation-induced changes in the properties of graphene with various defects should be characterized by specific features.[216, 217]

c. The Möbius strips. Crumbled graphene

Consider two more interesting deformed graphene systems, namely, the Möbius strips and crumbled graphene. Interest in Möbius strips us due to unique properties of various classes of micro- and nanostructured systems; their properties are both size- and shape-dependent. The shape-dependent properties can be classified using the boundary conditions: the number of sides (L) and the number of edges (N) in the system. For instance, for the known families of carbon nanotubes and fullerenes the boundary conditions are respectively as follows: $L = N = 2$ and $L = 2$, $N = 0$. These boundary conditions are also typical of some related structures, *e.g.*, polygonal helicoidal nanotubes ($L = N = 2$) or ellipsoidal and toroidal cage nanoforms ($L = 2$, $N = 0$). Systems with the shape of a Möbius strip ($L = 1$, $N = 1$; the surface with only one side) or a Klein bottle ($L = 1$, $N = 0$; the surface with no edge) may possess essentially different properties.

The first 'single-sided' macromolecules, namely, organic Möbius strips, were synthesized in 1982.[218] More recently, studies on the first inorganic systems [Group V metal trisulfides and triselenides $M(S,Se)_3$, where M = Nb or Ta] in the form of Möbius strips began.[219–221] Möbius strips were constructed theoretically[222–225] from segments of graphene ribbons and some properties of these systems were predicted. In particular, it was reported that graphene Möbius strips with zigzag edges behave as topological insulators, a promising group of materials for spintronics (see reviews[226, 227]). Obviously, the Möbius strip is not the only form of 'twisted rings' which can be constructed based on graphene; examples of related systems are presented in Fig. 13.

Crumpled graphene is yet another interesting form of deformed graphene sheet. It has a very large specific surface area of about 2675 $m^2\ g^{-1}$ and has attracted attention as potential material for ultracapacitors.[228–231] Crumpled graphene retains its shape due to 'adhesion' of fragments of graphene sheets through van der Waals interactions (Fig. 14). A molecular dynamics simulation[232] showed

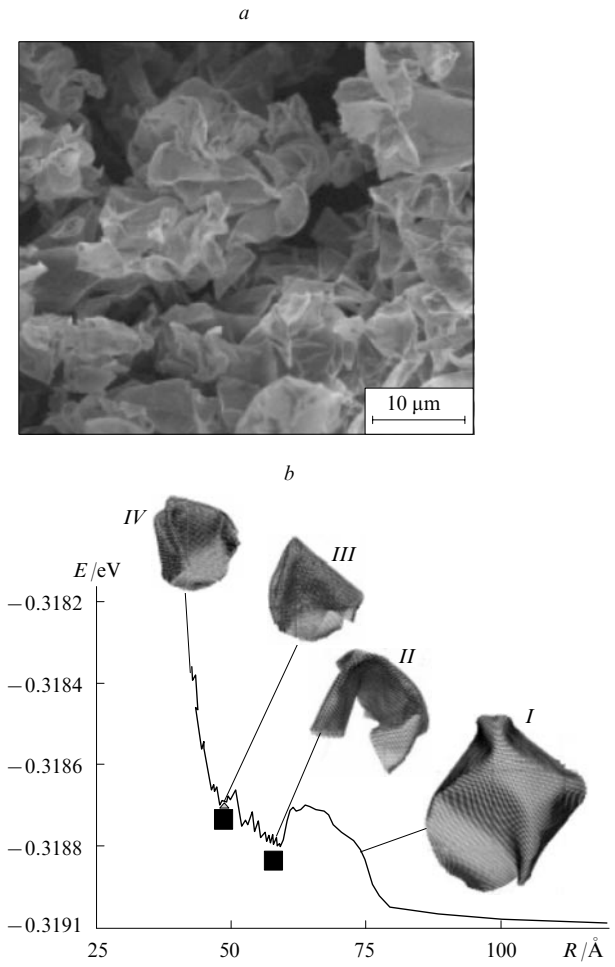


Figure 14. A SEM image of a curved graphene sheet (*a*)[231] and the potential energy of the graphene sheet in different stages ($I \rightarrow IV$) of its deformation (*b*).[232]
R is the effective radius of the crumpled graphene sheet; configurations *II* and *III* correspond to local potential energy minima (filled squares) attained due to the balance between the elastic strain energy and the adhesive energy of fragments of the crumpled graphene sheet.

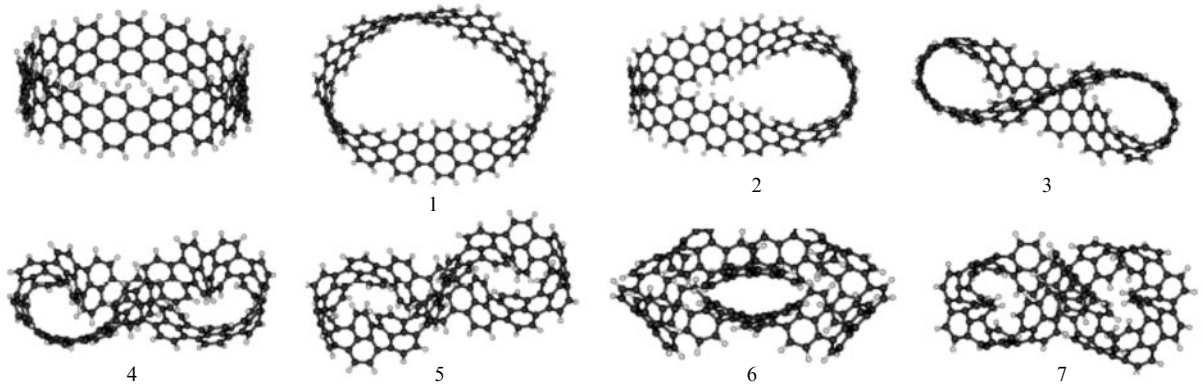


Figure 13. Atomic models for twisted rings obtained from a graphene nanoribbon with hydrogen-passivated arm-chair edges.[224]
Upper left: untwisted nanoring, 1 – 7 are twisted nanorings; numbers 1 – 7 denote the number of twists; No. 1 is a Möbius strip.

that the introduction of defects into the graphene sheet favours efficient 3D packing of crumpled graphene, which allows a maximum portion of its surface area to be used for fabrication of capacitors.

3. Bi-, tri- and multi-layer graphenes

In addition to single-layer graphene sheets, ribbons and nano-flakes, graphene materials comprising two, three or a few layers (or fragments) located at a distance equal to the van der Waals separation are studied (see, *e.g.*, Refs 233–245). These systems called bilayer, trilayer and multi-layer graphenes, respectively, exhibit a number of interesting features due to inter-layer interactions, separation of electronic and hole states, and the packing type of adjacent layers (Fig. 15). Particular attention is attracted to anomalies in quantum Hall effect in bilayer graphene [243, 244] and to prospects for application of these materials in microelectronics, because their band gaps can be varied by applying an electric field.[236, 237]

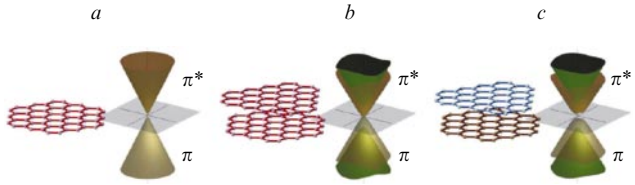


Figure 15. Schematic of near-Fermi bands for single-layer (*a*) and bilayer graphene (*b*, *c*) with symmetric (*b*) and asymmetric (*c*) network packing types.[240]

Bilayer graphene has been a subject of numerous theoretical studies concerning simulation of its electronic structure [246–248] and possible methods of targeted modification of its electronic and transport properties. For instance, the role of the layer packing type (*AB* and *AA*),[249, 250] the influence of deformation (uniaxial stretching [251]) and relative displacement of layers,[252] as well as disordering in one or both layers [253, 254] have been studied. The role of defects (vacancies and topological defects) [255, 256] and the effect of pressure on the magnetic properties of bilayer graphene with topological defects were investigated.[257] The appearance of Landau levels (energy states of electrons in external field) in bilayer graphene was simulated.[258] The role of impurities and adatoms in tuning the properties of bilayer graphene was disclosed.[259–264] The mechanical properties of bilayer graphene with additional inter-layer C—C bonds [265] and the optical properties [266] were assessed; a nonmonotonic temperature behaviour of the compressibility of bilayer graphene was predicted.[267]

In addition, the formation of quantum dots in bilayer graphene with periodic Coulomb oscillations and the temperature dependences of the potential barriers produced by them were discussed.[268] Pioneering studies on heterostructures involving bilayer graphene have been reported. In particular, the possibility of band gap variation by placing bilayer graphene between BN networks and in electric field has attracted the attention of researchers.[269] The influence of intercalation of transition metal atoms (V, Co, Fe and Ni) between two adjacent bilayer graphene pieces in the bilayer graphene–BN heterosystem was analyzed.[270] It was shown that all intercalated structures will behave as ferromagnetic metals except the bilayer graphene–V–bilayer graphene and bilayer graphene–V–BN structures.

A series of studies [271–276] was aimed to develop models for bilayer graphene ribbons and to determine the most energetically favourable packing types and corresponding electronic spectra, magnetic structure [271] and transport properties.[272, 273] The influence of stretching of bilayer graphene ribbons [274] and edge type variation [275, 276] on the electronic properties of ribbons was investigated. One can expect very interesting phenomena in the vicinity of the 'interface' (atomic step) [276] between single-layer and bilayer graphenes (Fig. 16).

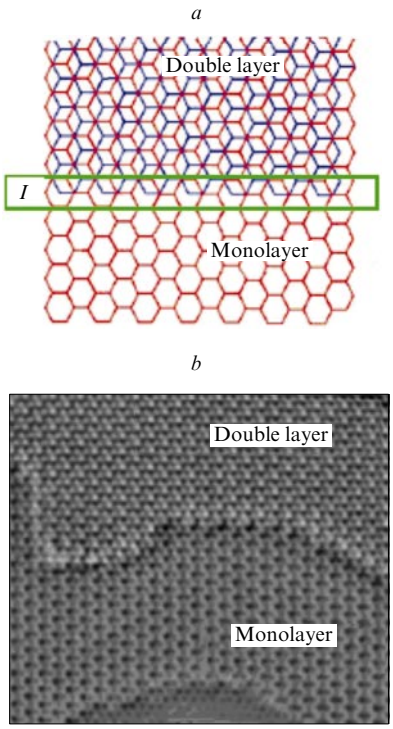


Figure 16. Atomic model (*a*) and a micrograph (*b*) of 'interface' (atomic step *I*) between single-layer and bilayer graphenes.[276]

The properties of trilayer graphene [277–280] and multilayer graphene [281–285] were studied. The electronic structure of trilayer graphene and conditions for the onset of magnetism were established.[277, 278] It was found [279] that the packing type of the layered structure is critical to the appearance of a band gap in the spectrum of trilayer graphene upon application of electric field oriented normal to the layer; namely, no band gap exists for the *ABA* packing, but a field-induced band gap appears if the packing type is *ABC*. A method for fabrication of bilayer and trilayer graphenes with controlled packing type was proposed.[280]

The electronic structure of multilayer graphene,[281–283] optical absorption spectra [283] and multi-layer graphene ribbons with H_2- or OH-passivated edges [284] were studied. Theoretical calculations showed [285] that hydrogenation of multilayer graphene is expected to be followed by a phase transition with structural rearrangement to a diamond-like phase.

4. Hybrid structures containing graphene

A particular group of graphene materials includes hybrid carbon nanostructures [33, 286–303] which combine graphene sheets (or their fragments) with other carbon nanoforms, *e.g.*, CNTs or fullerenes. Among them, various forms of carbon nanofoams [286–290] and more exotic structures, *e.g.*, pillared graphene [291–296] and some other (Fig. 17) have been best known and synthesized. Of course, the properties of these structures are significantly different from those of graphene sheet; these systems are usually considered as potential gas accumulators or materials for catalysis.[291–296] Examples of such structures are provided by, *e.g.*, nanotubes coated with multi-layer graphene sheets [299–301] or carbon nano-flowers [302] (nanospheres 200 to 600 nm in diameter, composed of a variety of graphene nano-flakes 'cross-linked' with one another).

Recently,[303] studies on the properties of yet another type of hybrid structures, diamond-decorated graphene (for nanodiamonds, see reviews [87, 304–306]), began. It was shown that at the graphene–nanodiamond interface, atoms of the graphene sheet become sp^3 hybridized which leads to changes in the conductivity type of the graphene sheet in the contact region.

5. Impurities and adatoms

The introduction of impurities into the crystal lattice is one of the most efficient methods of controlling the properties of crystals. To date, a series of experimental and theoretical studies on the introduction of various impurity atoms into the lattices of 2D–0D graphenes and investigation of their influence on the properties of these materials have been reported. For instance, substitutional impurities, *e.g.*, nitrogen and boron atoms, are the best donors of electrons and holes [307–314] for graphene. However, the introduction of a controlled amount of impurities including B and N atoms faces considerable difficulties while replacement of carbon atoms by, in particular, boron (or nitrogen) atoms is often accompanied by the formation of topological defects. At the same time, experiments showed that for many atoms including N,[315] O,[316] F,[317] Co,[318] Fe, Gd,[319] Au, Pt,[320] adsorption on the carbon sheet (or on graphene ribbon edges) is more characteristic than insertion into the graphene lattice.

A series of studies [321–332] were aimed to describe the microscopic properties of adatom–graphene (graphene ribbon) systems. In particular, they involved estimation of the energies and determination of the types of chemical bonds in these systems, simulation of the most energetically favourable adsorption sites, studies of local structural distortions in the vicinity of adatoms, description of the structure and prediction of the magnetic, mechanical, *etc.*, properties. As an illustration, Fig. 18 summarizes the results [321] of investigations on the adsorption and surface diffusion of single metal atoms on graphene and hexagonal boron nitride; also it presents the magnetic moments and effective charges of adatoms.

Clearly, many conclusions drawn in systematic studies of adatom–CNT systems (see a review [94]) will be valid for the adatom–graphene systems. For instance, one should

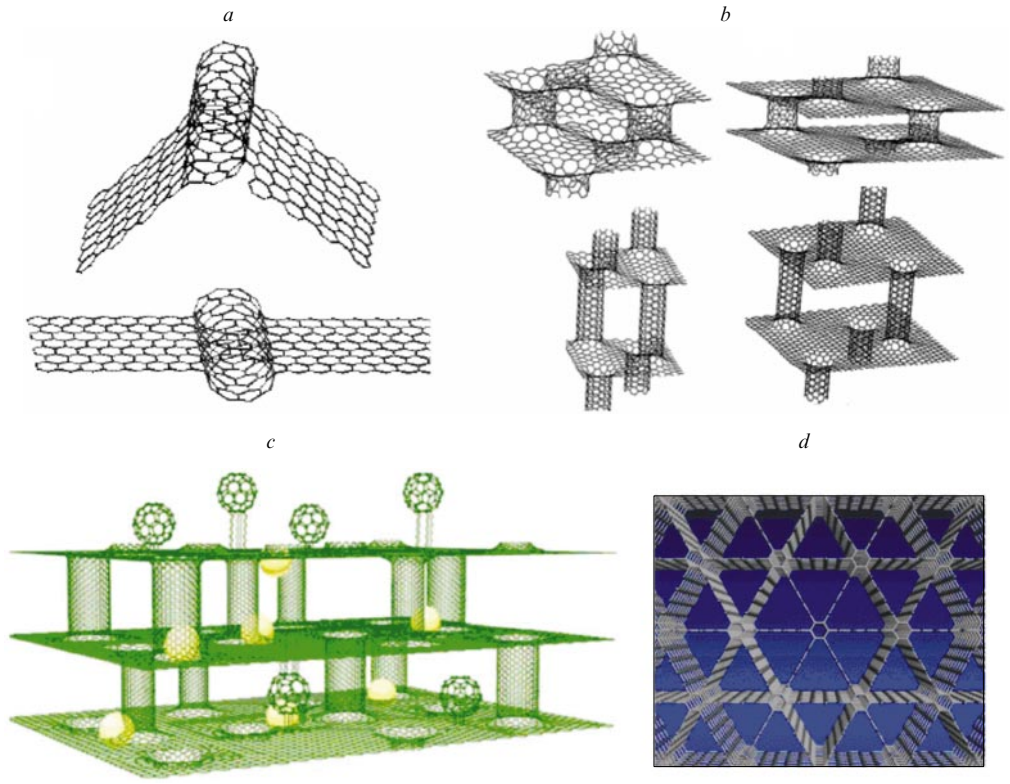


Figure 17. Atomic models for hybrid carbon structures involving graphene.
Quasi-2D graphene + CNT structures (*a*),[297] 3D structures comprising graphene sheets interconnected by nanotubes (pillared graphene) (*b*),[297] graphene + fullerene + CNT hybrid structure (*c*),[33] and a 3D crystalline network with triangular lattice containing only three-coordinate sp^2 carbon atoms (*d*).[298]

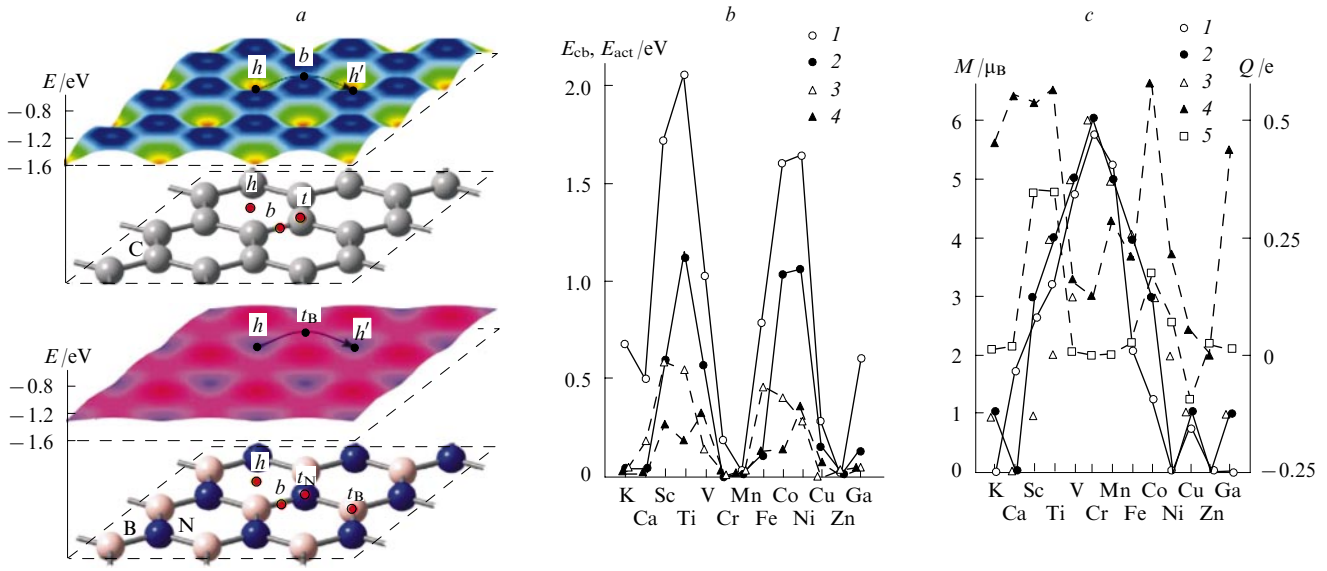


Figure 18. Adsorption and surface diffusion of some metal atoms on graphene and hexagonal boron nitride (h-BN).[321]
Potential energy surfaces of graphene–h-BN–Co systems. Shown are highly symmetric adsorption sites *h*, *b*, *t*, t_B and t_N; arrows denote the most energetically favourable trajectory of Co surface diffusion between two adjacent positions corresponding to energy minima ($h \rightarrow b \rightarrow h'$ and $h \rightarrow t_B \rightarrow h'$) (*a*); binding energies (E_b) of metal adatom to graphene (*1*) and h-BN (*2*) and activation energies (E_a) of the adatom surface diffusion on graphene (*3*) and h-BN (*4*) (*b*); and the magnetic moments (*M*) of the metal adatoms on graphene (*1*), h-BN (*2*) and free atoms (*3*), the effective charges (*Q*) of metal adatoms on graphene (*4*) and h-BN (*5*) (*c*).

expect aggregation of the transition metals with low binding energies to graphene on the surface of graphene to form 'intrinsic' metal clusters. Contrary to this, hydrogen atoms, as well as oxygen and fluorine atoms forming the strongest bonds with the graphene sheet can form 2D ordered crystal structures also known as graphene derivatives.

III. Graphene derivatives

These include three main 2D systems formed upon chemisorption of hydrogen, oxygen or fluorine atoms on the surface of graphene:

— hydrogenated graphene also known as graphane;

— graphene oxide;

— graphene fluoride or fluorographene (fluorographene).

Carbon atoms in these graphene derivatives change their hybridization from sp^2 to sp^3 owing to the formation of C–(H,O,F) bonds.[30, 333, 334]

Graphene oxide is known since 1859.[30, 334] Usually, it is obtained by treating graphite flakes with some oxidizing agent. At present, a method proposed in 1958 [335] is widely used. It is based on the reaction of graphite with anhydrous sulfuric acid, sodium nitrate and potassium permanganate. According to the experimental and theoretical studies on the structural, electronic and physicochemical properties of graphene oxide,[30, 336–344] it represents an essentially inhomogeneous system. Both chemical inhomogeneity (oxidized and unoxidized regions randomly alternate; in the oxidized regions, oxygen can react with graphene to form C–O–C or C–O–O–C bonds and OH groups can also be present) and structural inhomogeneity (local puckering of graphene sheets in the oxidized regions) are possible. Recently, calculations of some properties of perfect graphene hydroxide were reported.[345]

Conversely, graphane and fluorographene, have much more homogeneous structures. Recently, they have attracted considerable attention of researchers.

1. Graphane and graphone

The existence of graphane in the form of a 2D crystal with the chemical formula CH was predicted theoretically in 2007.[346] In 2009, graphane was synthesized by exposing graphene to cold hydrogen plasma.[347, 348] It is noteworthy that graphene interacts with hydrogen reversibly, *i.e.*, graphane can again be converted into graphene by annealing in inert atmosphere at a sufficiently low temperature (~450 °C). This allows one to vary the degree of coverage of the graphene sheet with hydrogen and thus obtain non-stoichiometric graphanes CH_{1-x} with variable properties. An essential drawback of graphane consists in its thermal instability, *viz.*, the material rapidly looses hydrogen atoms at temperatures slightly above ambient temperature and this loss is hard to control.

Perfect graphane is represented as a graphene sheet uniformly covered on both sides with hydrogen adatoms bonded to carbon atoms (Fig. 19).[346, 349–353] A hypothetical related 2D crystal in which all hydrogen adatoms are on one side of the graphene sheet is called graphone.[350] Adsorption of fluorine atoms on graphone makes this system more stable and can lead to the onset of ferro- or antiferromagnetism.[351]

The most interesting features of graphane compared to graphene are as follows:[352] the hybridization of carbon atoms (sp^3 instead of sp^2), nonuniform lattice compression (by 5% on the average), transition of graphane to the state of a wide band gap semiconductor (~3.5 eV, direct transition to the Γ point of the Brillouin zone [346]). Graphane sheets exhibit the semiconductor type conductivity irrespective of the edge type (arm-chair or zigzag).[353, 354] A series of

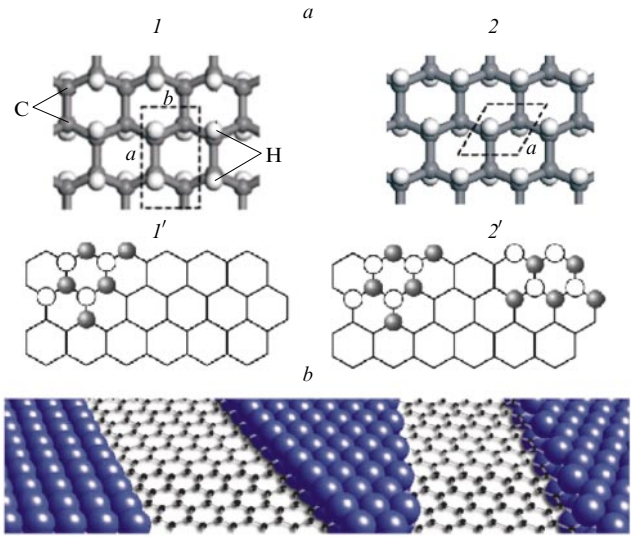


Figure 19. Structural fragments for two possible conformations of perfect graphane (*a*) and a hypothetical graphene + graphane hybrid structure combining graphene and graphane nanoribbons with different (arm-chair or zigzag) junction types (*b*).[360]
(*a*) The graphene sheet covered with hydrogen adatoms on both sides; shown are the unit cells containing eight (4H + 4C, conformation *1*) and four atoms (2H + 2C, conformation *2*); (*1′* and *2′*) illustration of the 'domain' mechanism of graphane growth from MD simulation data; filled and open circles denote hydrogen atoms located above and below the graphene sheet, respectively.[349]

theoretical studies of the structural and electronic properties of defect graphane[352, 355] as well as fluorinated[356] and partially dehydrogenated[357, 358] graphane were carried out. In the last-mentioned case, an almost linear correlation between the width of the energy gap and the degree of coverage of the graphene sheet by hydrogen atoms (H : C ratio) was established.[358] Removal of a single hydrogen atom induces a local magnetic moment ($M \approx 1\ \mu_B$) on the nearest carbon atom. Another method for inducing magnetism in graphane is to replace some hydrogen atoms by transition metal atoms.[359]

The possibility of controlling the conducting properties of graphane-like systems by creating graphene + graphane hybrid structures (see Fig. 19) was discussed. These structures can be obtained by hydrogenation of specified regions of the graphene sheet, which share a boundary with pristine graphene areas.[360]

Estimates[360–363] predict a lower in-plane stiffness but a higher bending strength of graphane compared to graphene (Young's modulus of graphane[360] is about 60% lower compared to graphene[364, 365]). Some other distinctive features of graphane nanomechanics were studied by the molecular dynamics method.[373] Deformation of graphane sheet considerably influences its electronic properties, in particular, the width of the band gap.[362]

2. Fluorographene

Fluorinated graphene CF (also known as fluorographene) represents yet another type of chemically modified graphene. Here, the band gap of the graphene sheet can be controlled through involvement of C $2p_z$-orbitals in the formation of covalent bonds C–F. As for graphane, information on CF_x was for the first time obtained from theoretical calculations.[366, 367] At that time, fluorographene was a hypothetical system.

Experimental studies on fluorographene[317, 368–371] showed that it is a wide band gap semiconductor (band gap ranges from about 3.1 to 3.8 eV, see Refs 317 and 370) with high resistance and mechanical strength, *viz*., Young's modulus of fluorographene (~0.3 TPa)[317] is much lower than that of pristine graphene, although being 1.5 times higher than that of steel. It was emphasized that fluorographene, which can be produced on a large scale in the form of 'paper',[317] combines its properties with good structural, chemical and thermal stability up to 400 °C.[317] This makes fluorographene (in addition to possible applications in carbon microelectronics[317, 368–370]) a candidate to replace Teflon in various protective coatings. Also, the luminescent and optical properties of fluorographene are similar to those of diamond and make it an attractive material for optoelectronics.[370] A number of specimens of formal stoichiometry C_2F_x ($x \leqslant 1$) exhibited magnetism.[371]

The authors of a series of theoretical studies[366, 367, 372–380] calculated the electronic and phonon spectra of fluorographene with equiatomic composition C : F = 1 at different possible coverage patterns of fluorine adatoms on both sides of graphene sheet[373, 375] and at partial coverage of the graphene sheet with fluorine atoms.[372, 378] Prospects for the formation of quantum dots were discussed[373] and the specific features of the magnetic and electronic states of CF_x nanoribbons were established.[377] The electronic and structural properties of fluorographene upon adsorption of various metal atoms (K, Li, Au) were assessed[376] and models for a hypothetical graphane–fluorographene (CH_xF_y) hybrid material, *i.e*., the graphene sheet with fluorine and hydrogen adatoms, were proposed.[376, 379] Estimates predict that fluorographane is the most stable system among the possible isoelectronic analogues, namely, graphene bromide, chloride and iodide.[380]

IV. Structural analogues of graphene

Up to this point, we have discussed graphene materials based on the 0D–2D forms of graphene. Below we will consider graphene-like materials. Most of them differ from graphene in chemical compositions but are structurally similar to the hexagonal graphene sheet.

1. Silicene

Silicene (hexagonal network of silicon atoms), a silicon analogue of graphene, recently has attracted considerable attention of researchers. Research on silicene began with the theoretical studies[99–102] concerning silicon nanotubes (Si-NT) and their fabrication from hexagonal ribbons of silicon atoms. More recently, the synthesis of Si-NT was indeed reported.[381–383] Even at that time, it was established that, unlike perfect cylindrical walls of CNTs, the Si-NT walls will be buckled (Fig. 20). Buckling can be explained by instability of 'pure' π-bonds in silicon (as is characteristic of sp^2 carbon) and by the energy preferableness of the sp^3 configurations of silicon atoms.[384]

The first attempt to obtain silicene *per se* by chemical isolation of silicon monolayer sheets from $CaSi_2$ was undertaken by Nakano *et al*.[385] Recently, the synthesis of silicon monolayers and silicon nanoribbons (a few hundred nanometres long) on a silver substrate (see Fig. 20) by molecular

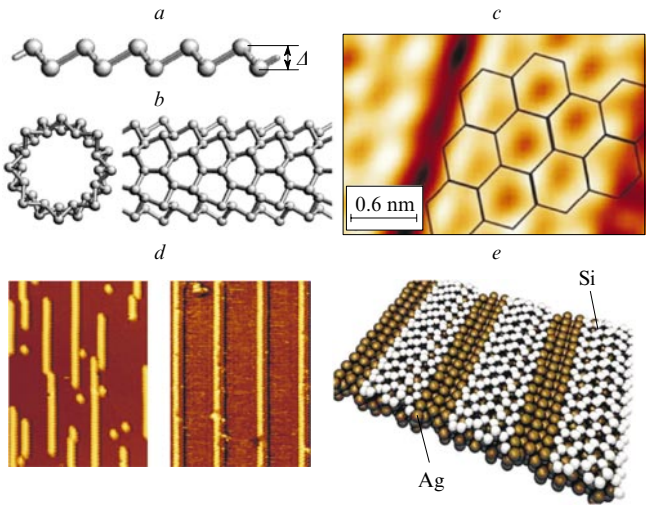


Figure 20. Atomic models for monoatomic silicon sheet (*a*) and single-walled silicon nanotube (*b*);[99] STM images of silicene sheet (*c*) and silicene nanoribbons (*d*);[387] and an atomic model for silicene nanoribbon on silver substrate (*e*).[105]
(*a*) Shown is the buckling distance *Δ*; (*b*) top view and side view; (*c*) the honeycomb structure is depicted.

beam epitaxy was proposed and implemented in practice.[103–106] The structures obtained were substantiated by the results of quantum chemical calculations.[386] These results were summarized in a review.[387] There is number of methods to obtain silicene.[388–390] Preliminary experimental data suggest that silicene is stable towards oxidation;[380] according to X-ray photoelectron spectroscopy, the edges of silicene nanoribbons can have different electronic structures.[387, 391]

Silicene, silicene nanoribbons and silicene nano-flakes have been studied theoretically in considerable detail.[392–421] Similarly to graphene, silicene is a zero band gap semimetal (Fig. 21); this provides high mobility of charge carriers.[393, 394, 400, 407, 409, 410] Conditions for the appearance of the quantum Hall effect were discussed.[412] The buckling distance for the silicene sheet (*Δ*) is ~0.44–0.46 Å (Table 3). The silicene network remains stable upon the introduction of some substitutional impurities[413, 414] and vacancies.[405]

Hydrogenation of silicene with the formation of the SiH phase called silicane leads[400, 408, 411, 416] to the appearance of a band gap in the energy spectrum (see Fig. 21). In this case, the type of hydrogenation plays an important role because it determines a uniform or 'island'-like pattern of hydrogen chemisorption atoms on the silicon sheet. In the case of uniform distribution of adatoms on the silicon sheet, the

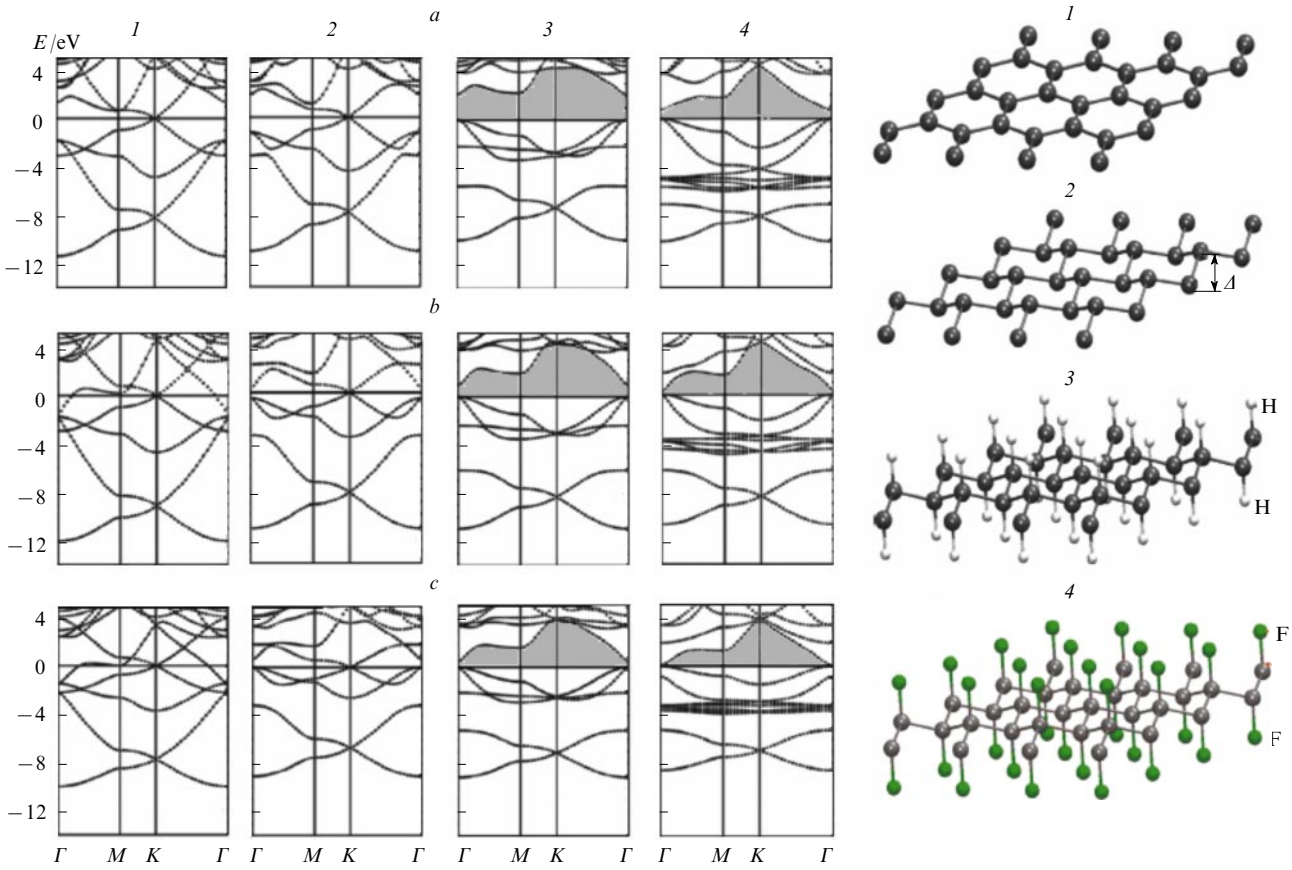


Figure 21. Energy band structures (calculated) of graphene-like planar (*1*) and buckled (*2*) (shown is the buckling distance *Δ*) networks of silicene (*a*), germanene (*b*), tin (*c*) and their hydrides (*3*) and fluorides (*4*).
The band gaps are shown in grey. The structural models for systems (*1–4*) are shown on the right.[396]

Table 3. Lattice constants (a), interatomic distances (d), buckling distances (Δ), cohesive energies (E_{coh}), band gap widths for graphene-like planar (α), buckled (β) atomic networks of Group IV elements and for the corresponding hydrides and fluorides (according to calculations [396]).

Material	a /Å	d /Å	Δ /Å	E_{coh} /eV (see [a])	BG /eV
α-Si	3.897	2.250	0	3.89	0
β-Si	3.867	2.279	0.459	3.91	0
SiH	3.968	2.392	0.687	3.38	2.11
SiF	3.968	2.395	0.697	4.66	0.70
α-Ge	4.127	2.383	0	3.11	0
β-Ge	4.061	2.444	0.690	3.24	0
GeH	4.091	2.473	0.730	2.88	0.95
GeF	4.182	2.492	0.627	3.89	0.19
α-Sn	4.798	2.770	0	2.58	0
β-Sn	4.639	2.841	0.947	2.72	0
SnH	4.719	2.846	0.824	2.52	0.45
SnF	5.028	2.951	0.531	3.63	0

[a] For diatomic (Si, Ge, Sn) and tetraatomic (hydrides and fluorides) unit cells.

SiH_x ($0 < x < 1$) system retains the metal-like conductivity up to $x = 0.75$, whereas at 'island' adsorption, the band gap in the spectrum of SiH_x appears at $x = 0.25$.[402] Thus, by specifically patterning the surface of the silicene sheet with SiH_x domains one can form metal–semiconductor heterostructures.[402]

Fluorination of silicene also causes a transition of the SiF network to the semiconductor state (see Fig. 21), but in this case, the band gap is smaller than for SiH. As the concentration of halogen adatoms (F, Cl, Br and I) increases, the silicene band gap changes nonmonotonically; this is assumed [415] to be due to the change in the type of states of the edge atoms involved in the formation of Si–Si or Si–halogen bonds.

The electronic properties of silicene ribbons can also be varied over a wide range.[395, 398, 405, 417, 418] This can be attained by varying the ribbon width,[398] the type of edges (arm-chair or zigzag), by adsorbing various atoms on the edges, by doping with impurities or by introducing vacancies (for instance, single or double vacancies in nanoribbons may induce a change in the type of the band gap (direct or indirect transition), while the orientation of double vacancies may lead to a semiconductor–metal transition),[405] or by mechanically stretching the nanoribbon in different directions.[410, 418] An MD simulation of thermally induced structural transformations of nanoribbons showed [395] that short ribbons can roll to form tubular structures with increasing temperature. A method of magnetization of silicene nanoribbons by decorating their edges with a chain of carbon atoms was proposed.[420] The plastic deformation parameters of silicene were estimated and an atom-based mechanism of breakage of silicene ribbons on stretching was described.[410, 419] The structural and electronic parameters of a system comprising two silicene sheets were simulated.[397, 421]

2. Germanene, graphene-like tin network

In contrast to silicene, germanene (a graphene-like network of germanium atoms) still remains a hypothetical material, although attempts to obtain epitaxial germanium monolayers on the (100), (110) and (111) surfaces of silver have been reported.[387] Information on germanene was obtained [107–110, 393, 394, 396, 401, 408, 411] within the framework of model calculations (see Table 3, Fig. 21). According to predictions,[393, 401] germanene is a 'bad metal' with low density of electronic states at the Fermi level, but biaxial stretching may induce its transition to a semimetal state similar to the graphene state.[107] This transition may also occur upon buckling of a hexagonal germanium sheet which is more stable than the flat structure.[394] Hydrogenation of germanene [396, 398, 408] gives rise to a band gap of about 1 eV in the energy spectrum;[396] a similar effect can also be attained by fluorination, but the band gap will be much narrower (~0.2 eV).[396] Interestingly, the cohesive energy of germanene decreases upon hydrogenation but increases upon fluorination as in the case of silicene.[396] Germanene nanoribbons may exhibit magnetic properties due to magnetization of edge atoms;[109, 394] magnetism of germanene sheets and nanoribbons can also be induced by adsorption of some transition metal atoms (Cr, Mn, Fe and Co).[108]

The behaviour predicted for graphene-like tin sheets (see Table 3, Fig. 21) is much like that of germanene.[396] However, fluorination of tin sheets will not influence their metal-like properties (see Fig. 21).

3. Graphene-like binary phases of Group IV elements

Investigations on graphene-like compounds of Group IV elements (Si, Ge and Sn) were logically followed by the search for corresponding binary phases, namely, SiC, GeC, SiGe, SnC, SnSi and SnGe. To date, a theoretical stability analysis was performed for them and the structural, electronic and some other properties were studied.[397, 401, 409, 422–431] Without dwelling on the description of each phase, only the key trends in changes in their properties depending on the chemical compositon will be pointed out.

From the data of Table 4 it is seen that the binary phases GeC and SnC have flat sheets; for all other phases (SiC, SiGe, SnSi and SnGe), significant structural distortions were found, *viz*., the sheets are buckled, the buckling distance Δ being in the range from 0.55 to 0.73 Å. Also, structural distortions are characteristic of the sheets with the increased lattice constants (interatomic distance d).

All graphene-like binary phases are expected to be semiconductors whose band gaps vary over a wide range from 0.230 (SnGe, SnSi) to 3.526 eV (SiC).

A number of interesting correlations between the cohesive energies (cohesive energy is defined as the difference between the energy of the crystal and the sum of the energies

Table 4. Bond lengths, buckling distances, cohesive energies and band gap widths in binary graphene-like phases of Group IV elements (according to calculations [401, 409]).

Phase	d /Å	Δ /Å	E_{coh} /eV (see [a])	BG /eV (see [b])
SiC	1.77–1.79	0.64	15.3	3.526
GeC	1.83–1.86	–	13.2	3.160
SiGe	2.28–2.31	0.55	9.6	0.257
SnC	2.05	–	11.6	1.180
SnSi	2.52	0.67	8.7	0.230
SnGe	2.57	0.73	8.3	0.230

[a] For comparison: E_{coh} of graphene is ~20 eV.[401]
[b] Calculated in the local electron density approximation.

of all isolated atoms comprising the crystal; E_{coh} is related to the energies of chemical bonds in crystals) of these phases and their structural and mechanical properties were established (Fig. 22). As the lattice constant increases, the E_{coh} value decreases, buckling of sheets being a feature of the phases with minimum cohesive energies. A decrease in E_{coh} is accompanied by a decrease in the stiffness of the crystal lattices. Unlike the sheets formed by the same-type atoms (graphene, silicene or germanene), 2D binary phases are characterized by significant charge polarization between the constituent different-type atoms and the chemical bonds acquire a mixed covalent-ionic character.[401]

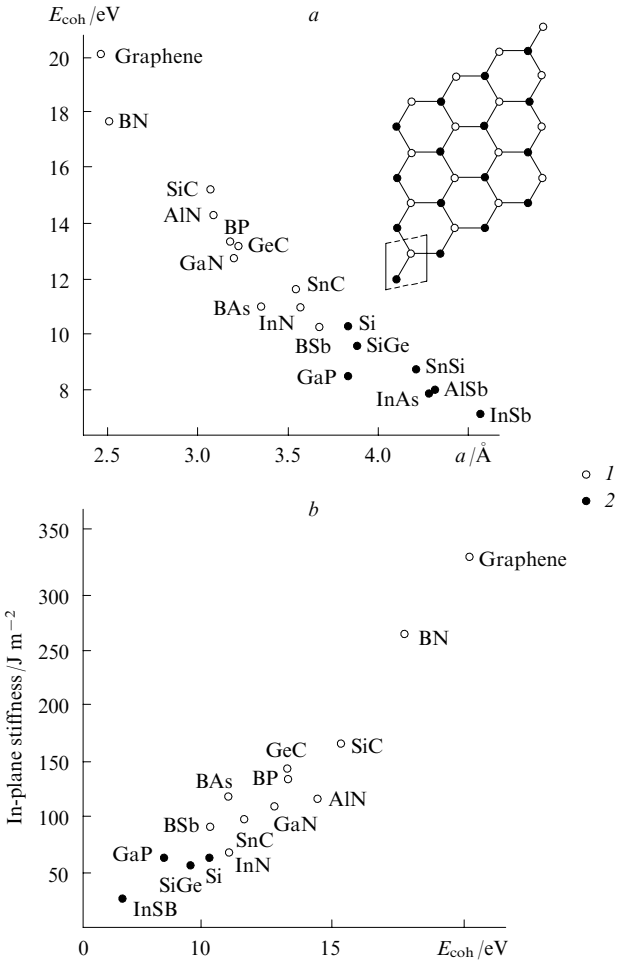


Figure 22. Correlations between cohesive energy and lattice constant (*a*) and the in-plane stiffness and cohesive energy (*b*) for hexagonal networks of silicene and binary graphene-like phases comprised of atoms of Group III – V elements.[401]
Notations: (*1*) stands for the planar networks and (*2*) stands for puckered networks. Inset: a structural model for the hexagonal networks of these phases; shown is the unit cell.

In terms of the E_{coh} energy, the phases in question can be arranged as follows

$$SiC > GeC > SnC > SiGe > SnSi \sim SnGe.$$

Judging from these data, the first three phases are expected to be the most stable, whereas the synthesis of the last three phases (they are the most unstable ones) in the form of hexagonal sheets seems to be problematic. Emphasize that pristine graphene is characterized by the smallest lattice constant and maximum cohesive energy and stiffness compared to all hexagonal sheets formed by atoms of Group IV elements.

Pioneering studies on the interaction of sheets formed by binary phases [399] and on their hydrogenation and fluorination reactions have been reported.[426, 427, 429] It was found that interactions of monolayers in a bilayer can strongly influence the electronic properties (band gap) and phonon characteristics (type of dispersion of phonon frequencies) of the SiC, GeC and SiGe phases and cause distortions of their flat sheets.[399] Decoration of flat hexagonal SiC, GeC and SiGe sheets with hydrogen or fluorine atoms leads to transition of these systems to the ferromagnetic or antiferromagnetic semiconductor state, respectively, and the hybridized orbitals of carbon and hydrogen (fluorine) atoms participate in spin polarization.[427] Also, local magnetic moments can be induced in SiC sheets on the atoms adjacent to silicon vacancies.[109] Some feasible methods of synthesis of the graphene-like sheets under study have been discussed.[431]

4. White graphene (graphene-like BN)

A monolayer-thick, hexagonal boron nitride (h-BN) sheet (Fig. 23) is the nearest isostructural and isoelectronic heteroatomic analogue of graphene. Taking into account this fact as well as the optical properties of a wide band gap semiconductor graphene-like boron nitride, this 2D polymorph of BN is often called white graphene (WG) (sometimes, it is also called boronitrene).[432]

The key structural and electronic properties of an infinite isolated h-BN sheet (as 'precursor' of boron-nitride nanotubes) were studied theoretically in the 1990s.[433 – 435] At the same time, research on the synthesis of BN sheets on the surface of transition metals began [436 – 440] and a number of possible structural modifications of hexagonal BN sheet (BN-graphynes and BN-Haeckelites) and various nanostructures based on them were proposed.[87]

A new round of studies on white graphene began soon after publication of pioneering communications [1, 2] on the preparation of graphene. Investigations aimed to develop methods of synthesis of white graphene and composites containing this compound were continued.[432, 441 – 455] Some results obtained in these studies are summarized in a review.[49] Theoretical research is mainly focused on the search for methods of controlling the properties of white graphene by introducing various B_nN_n rings ($n \neq 3$) and other structural defects into the white graphene sheet, by changing the type of white graphene nanoribbon edge structures or by chemically modifying it.

Prior to considering these results, we will briefly outline the key properties of perfect white graphene (see Fig. 23, Table 5). White graphene is a nonmagnetic, wide band gap semiconductor with a $\pi - \pi^*$ inter-band transition. The top of the valence band is composed of $N2p_z$ orbitals while the bottom of the conduction band is composed of $B2p_z$ orbitals. All atoms are sp^2 hybridized (N2p – B2p orbital overlap); chemical bonds are covalent with some contribution of ionic component due to partial polarization of the charge density along the B → N direction. The degree of charge transfer was estimated as about 0.43 e per atom.[456] The phonon spectrum of white graphene includes three acoustic and three optical modes.[456, 457] Theoretical estimates of mechanical parameters showed that white graphene is a softer material than graphene.[401]

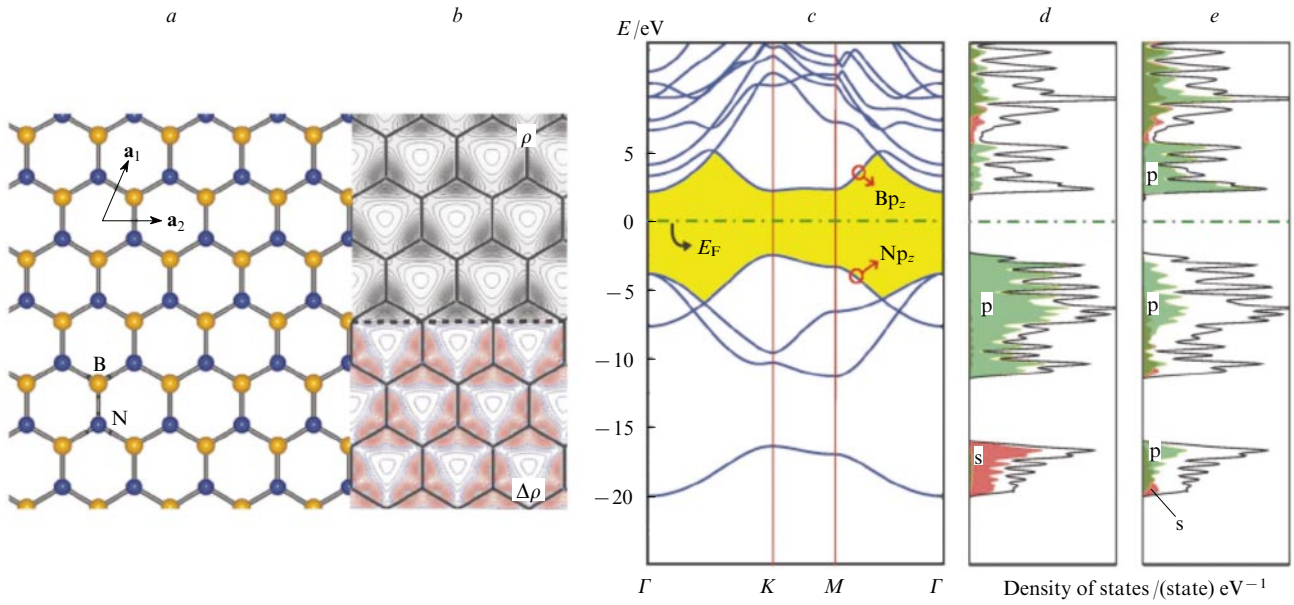


Figure 23. Fragment of the crystal structure of white graphene (*a*) (shown are the translation vectors $\mathbf{a}_1$ and $\mathbf{a}_2$); the total (ρ) and differential ($\Delta\rho = \rho - S\rho_{at}$) charge density distributions in the plane of the network (*b*); the energy band structure (shown are the main orbital contributions to the top of the valence band and to the bottom of the conduction band) (*c*); the total (solid line) and partial (shown in grey) densities of states of nitrogen (*d*) and boron (*e*) atoms.[456]

Table 5. Lattice constants, interatomic distances, bond angle (θ), cohesive energy, band gap widths and Poisson ratios (ν) for h-BN atomic network and graphene (according to calculations[401,456]).

Parameter	h-BN	Graphene	Parameter	h-BN	Graphene
a/Å	2.51	2.46	E_{coh}/eV	14.65	20.08
d/Å	1.45	1.42	BG/eV	4.61	see [a]
θ/deg	120.0	120.0	ν	0.21	0.16

[a] Semimetal.

White graphene polymorphs. White graphene polymorphs formed by introducing B_nN_n rings ($n = 2$, 4, 6, *etc.*) into the network composed of B_3N_3 hexagons were studied theoretically.[458–462] Fragments of the atomic structures of some polymorphs are shown in Fig. 24. The white graphene polymorphs can be divided into several groups. The first group includes polymorphs *1* and *2* in which all B and N atoms have a coordination number (CN) of 3 and are sp^2 hybridized, as in perfect white graphene. Regular networks of these polymorphs are composed of equal numbers of tetragons B_2N_2 and octagons B_4N_4 (polymorph *1*) or periodically coupled B_2N_2, B_3N_3 and B_6N_6 rings (polymorph *2*).

The next group includes polymorphs *3*–*5* belonging to systems with mixed type of hybridization ($sp^2 + sp^1$); the sheet structures of these modifications contain boron and nitrogen atoms with CN 2 (sp^1) and CN 3 (sp^2). Polymorph *3* is obtained by inserting BN dimers between boron and nitrogen atoms in 2/3 of the total number of edges in the B_3N_3 rings forming the network structure of white graphene; this results in a rectangular lattice of distorted hexagons. Applying this procedure to all edges of B_3N_3 rings, one gets the hexagonal network structure of polymorph *4*. In the structure of polymorph *5*, the network is built of B_3N_3 hexagons whose vertices are connected by BN dimers. A series of graphyne-like polymorphs whose network structures comprise B_3N_3 rings linked by B_2N_2 and B_4N_4 chains was also considered.[461]

The structure of polymorph *6* combines rings containing B and N atoms with CN 3 (sp^2) and CN 4 (sp^3).

The results of calculations for $T = 0$ and 300 K[462] suggest that polymorphs *1*–*6* are less stable than white graphene ($\delta E > 0$, Table 6). Nevertheless, they retain their structures at 300 K, although structural distortions become more pronounced as temperature increases; in particular, the network structures are buckled (see Fig. 24). All polymorphs *1*–*6* are wide band gap semiconductors, but their energy gaps are narrower than that of white graphene. According to theoretical estimates,[462] the band gap of white graphene can be narrowed by about 1 eV by introducing non-hexagonal B_nN_n rings ($n \neq 3$) or sp^1-hybridized atoms into its network structure.

Structural defects and impurities in white graphene. The introduction of defects into white graphene can cause a fundamental rearrangement of its energy spectrum and the onset of magnetic effects.[456,463,464] This is illustrated in Fig. 25, which presents a scheme of formation of uncompensated spin density ($\Delta\rho^{\uparrow\downarrow} = \rho^{\uparrow} - \rho^{\downarrow}$) in white graphene with single vacancies (boron and nitrogen atoms) and a B + N double vacancy. In the case of single vacancies, local magnetic moments are induced on the atoms coordnating the defect, whereas in the case of the double vacancy, the system remains nonmagnetic. A general explanation for this effect is provided by a theorem[168] according to which the magnetic moment of the system (per unit cell) is determined by the difference between the number of atoms (N) in different sublattices, *i.e.*, in this case

$$M \sim (N_{B(N)} - N_{N(B)})\mu_B .$$

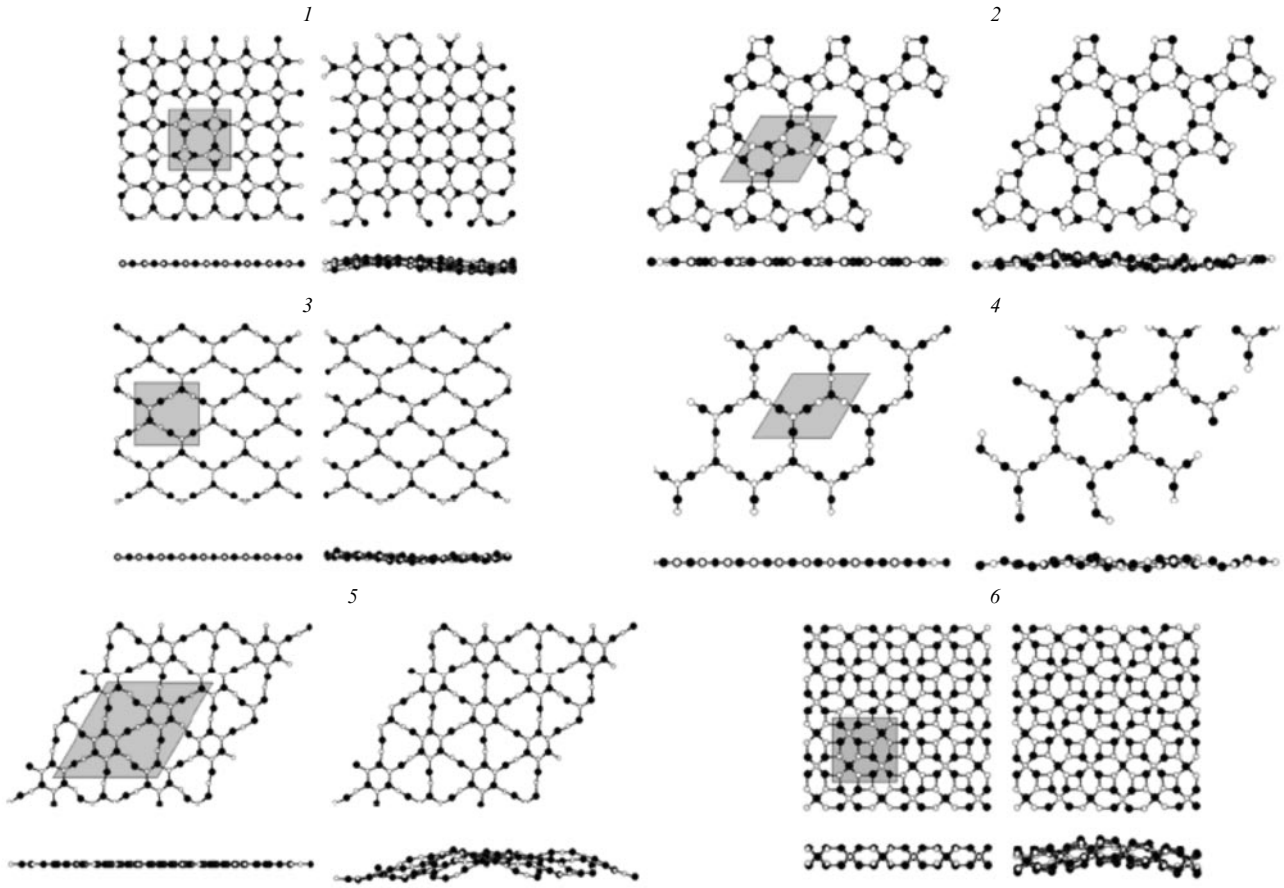


Figure 24. Fragments of atomic structures (top and side views) of white graphene polymorphs.[462]
For notations (*1–6*), see text; for each polymorph shown are the atomic structures at 0 (on the left) and at 300 K (on the right); the unit cells are marked.

Table 6. Lattice types and constants, relative energies, band gap widths and hybridization types of six possible polymorphs of white graphene.[462]

Polymorph [a]	Lattice type	a /Å	b /Å	δE /eV (see [b])	BG /eV	HT
1	square	7.08	–	0.540	3.11	sp^2
2	hexagonal	6.98		0.666	3.22	sp^2
3	rectangular	7.21	7.09	0.928	3.22	$sp^2 + sp^1$
4	hexagonal	7.21		1.043	3.31	$sp^2 + sp^1$
5	"	11.76		0.750	3.42	$sp^2 + sp^1$
6	square	6.62		0.784	2.47	$sp^2 + sp^3$

[a] For notations *1–6*, see Fig. 24.
[b] Relative to the total energy of white graphene $\delta E = E_{tot}^{polymorf} - E_{tot}^{WG}$.

Indeed, numerical calculations of white graphene with single boron or nitrogen vacancies showed that the magnetic moment of the unit cell in the defect network approaches a value of 1 μ_B. Microscopically, the formation of a magnetic moment on the atoms adjacent to the vacancy can be explained taking into account the energy states of dangling bonds (see also a review [84]). For instance, the appearance of a boron vacancy means that three bonds with the nearest nitrogen atoms are broken, and a decrease in the energies of corresponding N2p-orbitals causes their shift towards the band gap of white graphene and subsequent spontaneous spin polarization. A similar effect for B2p-orbitals occurs if a nitrogen vacancy is introduced into the white graphene sheet. As a result, the uncompensated spin density (local magnetic moments) is formed on the boron atoms for BN_{1-x} and on the nitrogen atoms for $B_{1-x}N$ (see Fig. 25). The magnetization of a system through polarization of p-states is referred to as d^0-magnetism (see above). The magnetization of white graphene can be attained by doping with other substitutional admixtures. This problem was studied taking Be, O, Al, C and Si admixtures as examples.[463, 465–467] Another method assumes adsorption of various atoms on white graphene to influence its electronic and magnetic properties.[468–470]

White graphene nanoribbons. Studies on the properties of white graphene nanoribbons are focused on how they depend on the type of terminal structures, on the width of the nanoribbon and on possible coatings of these nanoribbons.[456, 471–480] It was established that ribbons with armchair edges are the most stable, whereas ribbons with zigzag edges are metastable and their edges are prone to reconstruction with the formation of pentagons and heptagons (this is also favoured by edge passivation with hydrogen atoms).[477] Generally, the edge adsorption of various atoms extends the potential of controlling the magnetic and electronic properties of white graphene nanoribbons. For

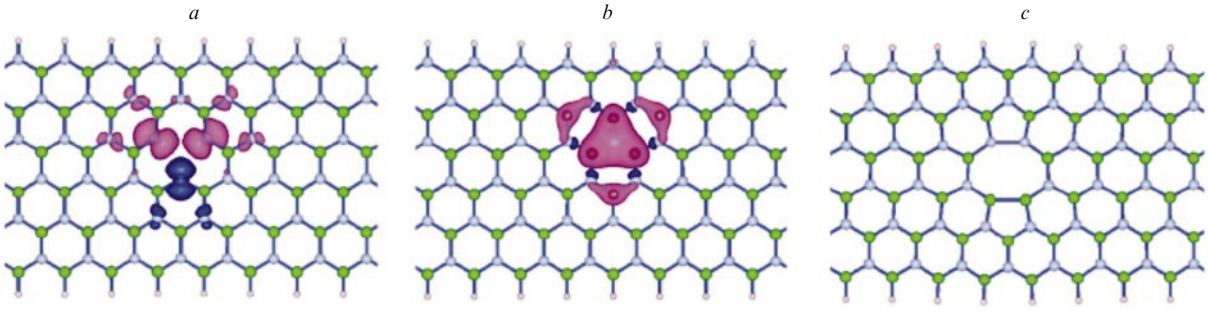


Figure 25. Defects in white graphene network.[456]
Shown is the formation of uncompensated spin density $\Delta\rho^{\uparrow\downarrow}$ on the atoms adjacent to the single boron (*a*) and nitrogen (*b*) vacancy; white graphene with double vacancy B + N (*c*) remains nonmagnetic.

instance, the system with iron-decorated arm-chair edges will exhibit the properties of an antiferromagnetic metal, whereas the system with one edge covered with hydrogen atoms and the other edge covered with iron atoms acquires the properties of a magnetic semimetal.[478]

5. Graphene-like B–C–N sheets

A large family of graphene-like sheets in the B–C–N system can be designed by partial replacement of carbon atoms in graphene by boron and(or) nitrogen atoms. However, specific features of the structure of electron shells and reactivities of atoms in this system (B, C and N) impose essential limitations on the possibility of existence of hexagonal $B_xC_yN_z$ sheets, which leads, depending on the B : C : N ratio, to different effects of atomic ordering in the network structure or to instability of flat structures. This was established in the search for flat systems containing some of these atoms and having simpler elemental compositions.

In particular, elemental boron forms buckled atomic sheets;[481] structures with triangular-hexagonal lattices (so-called α-B) are possible.[481–484] The existence of graphene-like hexagonal boron sheets on the (0001) surfaces of CrB_2 and MoB_2 was predicted.[485]

In the B–C system, models for flat BC_3 sheets were proposed[486] and more recently, these objects were actually synthesized;[487,488] simulation of more carbon-rich BC_5 sheets was reported.[489] These flat boron–carbon structures[486,489–491] contain particular motifs of mutual ordering of boron and carbon atoms.

In the C–N system, a layered nitride carbon polymorph C_3N_4 comprising flat sheets was proposed;[492] the synthesis of C_3N_4 was discussed in a review.[493] Models for more carbon-rich, layered carbon nitride phases CN and C_3N

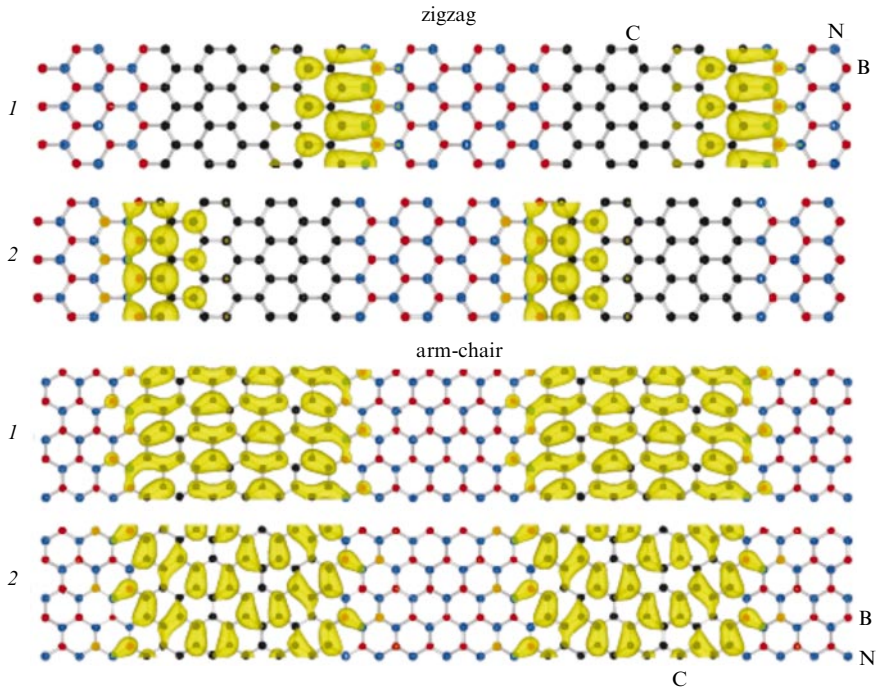


Figure 26. Charge density distribution at the top of the valence band (*1*) and at the bottom of the conduction band (*2*) for hybrid graphene BC_2N composed of the BN and graphene nanoribbons with different edge types (zigzag and arm-chair).[523]
In both cases, the edges of the energy gap are composed of the states of carbon atoms.

were reported.[494–496] All C_xN_y structures studied so far contain ordered motifs of nitrogen and carbon atoms.

Atomic sheets with ordered arrangement of B, C and N atoms are present in the crystalline, layered, ternary boron carbonitride phases $B_xC_yN_z$; the properties of, *e.g.*, the BC_4N, BC_2N and $B_3C_2N_3$ systems (and corresponding nanotubes) were predicted theoretically (see Refs 80 and 496–502). Graphene-like B–C–N sheets can be obtained by implantation of carbon atoms into white graphene.[503]

There is a number of $B_xC_yN_z$ thin films exhibiting the properties of semiconductors;[504–508] however, the degrees of their crystallinity are low, which can be associated with the tendency of boron and nitrogen atoms to 'clustering'[509] with the formation of BN domains in the B–C–N system. Spontaneous separation of boron, carbon and nitrogen atoms into the carbon and BN domains was predicted theoretically[510–513] and revealed in the walls of actually synthesized 'composite' $B_xC_yN_z$ nanotubes.[514–518] This can be explained by the fact that C–C and B–N bonds are the strongest ones (give maximum contributions to stabilization of the $B_xC_yN_z$ lattice), whereas other possible bonds (C–N, N–N, B–B and C–B) are much weaker. Thus, the most stable $B_xC_yN_z$ systems should contain a maximum possible number of C–C and B–N bonds.[507, 509]

The formation of flat C–BN sheets (called hybrid graphene[519, 520]) in which the hexagonal network includes alternating domains or strips of carbon atoms and BN was established experimentally.[520, 521] The possibility to control the width of the band gap by varying the relative content of the C and BN domains was substantiated by the results of calculations.[519, 520, 522, 523] It was found that the band gap is determined by the states of carbon atoms in the graphene domains (Fig. 26) and depends on the domain size (in extended ribbon-like domains, it depends on the width and mutual orientation of graphene and BN ribbons in the common structure).[519, 523]

Simulation of $B_xC_yN_z$ ribbons showed[524–526] that the properties of these structures depend on the type of the edge (zigzag or arm-chair) and on arrangement of different-type atoms B, C and N relative to the nanoribbon edges. In particular, ribbons with zigzag edges will exhibit metal-like properties and are prone to spontaneous magnetization. Graphene-like boron carbonitride whose stoichiometry is close to that of BCN was synthesized.[527]

6. Graphene-like $A^{III}B^{V}$ phases

In contrast to graphene-like BN and $B_xC_yN_z$ sheets that are constituents of corresponding stable layered (anisotropic) 3D phases, most known $A^{III}B^{V}$ phases (A and B are main-Group III and V elements) crystallize in the sphalerite or wurtzite diamond-like structures with 3D isotropic system of directional bonds. Therefore, the synthesis of graphene-like sheets of $A^{III}B^{V}$ phases will face significant difficulties.

Nevertheless, there is a series of computational studies[401, 427, 428] reporting prognoses of structural parameters, stability conditions, as well as the electronic and some other properties of graphene-like $A^{III}B^{V}$ phases. The key results are summarized in Table 7 and in Fig. 22. All graphene-like $A^{III}B^{V}$ phases are semiconductors whose band gaps vary from 0.4 (BSb) to 3.1 eV (AlN). As the lattice constant increases, the sheets are buckled, the cohesive energies of the phases and the stiffnesses of their lattices decrease. The most stable systems include flat hexagonal AlN, GaN, InN, BP and BAs sheets. Hydrogenation of graphene-like sheets $A^{III}B^{V}$ with the formation of $A^{III}B^{V}H_2$ phases (Fig. 27) causes the band gap to increase (see Table 7). Selective adsorption of hydrogen (fluorine) on one side of the sheet of graphene-like $A^{III}B^{V}$ phases with the formation of A^{III}–H(F) bonds may induce magnetization of these systems.[427] A number of models for semiconductor heterostructures combining two semiconductors with different band gaps are based on graphene-like $A^{III}B^{V}$ sheets.[401]

In addition, calculations of the properties of hydrogenated diamond-like (110) and (111) monolayers of $A^{III}B^{V}$ phases were carried out.[529–531] Their band gaps decrease on going from nitrides to phosphides and then to arsenides. Based on the available data,[528] for the graphene-like $A^{III}B^{V}H_2$ phases one gets

$$BG(GaNH_2) > BG(GaPH_2) > BG(GaAsH_2).$$

However, the dependence for pristine graphene-like $A^{III}B^{V}$ sheets can be different (see Table 7), *e.g.*,

$$BG(InP) > BG(InAs) > BG(InN).$$

Table 7. Bond lengths, buckling distances, cohesive energies and band gap widths for hexagonal (graphene-like) phases $A^{III}B^{V}$ (Ref. 401) and the cohesive energies and band gap widths for two possible conformations of hydrogenated phases $A^{III}B^{V}H_2$.[528]

Phase	d/Å	Δ/Å	E_{coh}/eV	BG/eV (see [a])	Phase	E_{coh}/eV (see [b])	BG/eV (see [b])
AlN	1.79	–	14.3	3.1	$AlNH_2$	5.53; 5.58	3.46; 4.99
GaN	1.85	–	12.7	2.3	$GaNH_2$	5.34; 5.37	3.60; 4.77
InN	2.06	–	10.9	0.6	–	–	–
InP	2.46	0.51	8.4	1.2	–	–	–
InAs	2.55	0.62	7.9	0.9	–	–	–
InSb	2.74	0.73	7.1	0.7	–	–	–
GaAs	2.36	0.55	8.5	1.3	$GaAsH_2$	3.90; 3.90	2.13; 2.11
BP	1.83	–	13.3	0.8	BPH_2	5.20; 5.19	3.62; 3.09
BAs	1.93	–	11.0	0.7	$BAsH_2$	4.81; 4.80	3.43; 2.90
GaP	2.25	0.40	8.5	1.9	$GaPH_2$	4.18; 4.18	2.76; 2.37
AlSb	2.57	0.60	8.0	1.5	–	–	–
BSb	2.12	–	10.3	0.4	–	–	–

[a] Calculated in the local density approximation.

[b] The first and second number represents E_{coh} for conformations *1* and *2*, respectively (see Fig. 27).

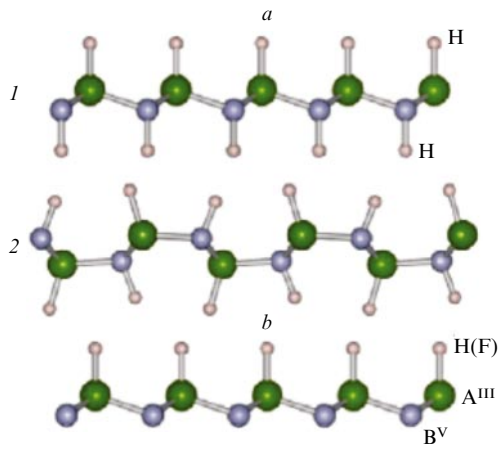


Figure 27. Structural models (side view) for hydrogenated phases $A^{III}B^{V}H_2$ (*a*) (possible conformations *1* and *2*)[528] and phases of formal stoichiometry $A^{III}B^{V}H(F)$ (so-called semidecorated phases) with chemisorbed hydrogen (fluorine) atoms only at A^{III} atoms (*b*).[427]

7. Graphene-like $A^{II}B^{VI}$ phases

Initially, graphene-like structural motifs of binary compounds of Group II and VI elements ($A^{II}B^{VI}$, *e.g.*, ZnO or BeO) have attracted the attention of researchers as 'precursors' for constructing atomic models for corresponding nanotubes or fullerene-like molecules.[532–545] A number of earlier theoretical studies were carried out to evaluate the stability of graphite-like $A^{II}B^{VI}$ crystals in regard to the stability of their most stable diamond-like polymorphs.[546–549] The lattice constants, electronic spectra and some other properties of 2D $A^{II}B^{VI}$ crystals and corresponding isolated graphene-like sheets were calculated.[546–549]

Models predicting stabilization of thin-film graphite-like $A^{II}B^{VI}$ phases are available.[549] For instance, thin polar BeO films can be stabilized by the relaxation mechanism, which implies structural transformation of wurtzite-like thin films into graphite-like ones, where each ion goes from the tetracoordinate sp^3 state to the tricoordinate sp^2 state. According to calculations,[549] a graphite-like structure which should be formed in the initial step of film growth is more favourable for BeO thin films (less than 9 layers thick). As the number of layers increases, the graphite-like structure of the film will convert to a nonpolar wurtzite-like structure. Similar conclusions were also drawn for some other $A^{II}B^{VI}$ phases.[547, 548, 550] For instance, calculations predict that ZnO films up to four monolayers thick will represent graphene-like sheets.[550] This conclusion was confirmed in recent experiments in which thin (one to four monolayers thick) graphene-like ZnO films were synthesized on the Ag(111) (Fig. 28) and Pd(111) surfaces.[552]

Consider the results of studies on graphene-like $A^{II}B^{VI}$ phases and methods of modification of their properties taking ZnO, ZnS and BeO as examples.

Zinc oxide. Structural features of isolated hexagonal ZnO sheet have been established reliably.[533, 553] The lattice constant is $a = 3.263$ Å and the interatomic distances are $d(Zn-O) = 1.895$ Å. In contrast to silicene, germanene and graphene-like $A^{III}B^{V}$ phases, the zinc oxide sheet is flat, its stability was substantiated by calculations of the phonon spectrum in which all vibrational modes have positive frequencies. Moreover, an MD simulation predicted only minor deformations of a flat ZnO sheet upon 'heating' up to 750 K.[553] The ZnO sheet on the Ag(111) surface is slightly distorted due to anisotropic interactions of zinc and oxygen atoms with silver atoms (substrate).[554]

A hexagonal ZnO sheet is a nonmagnetic semiconductor with direct inter-band transition at the Γ point. Estimates of its band gap vary over a wide range from about 1.7 to 5.6 eV depending on the computational method and on the shape of the exchange-correlation potential cho-

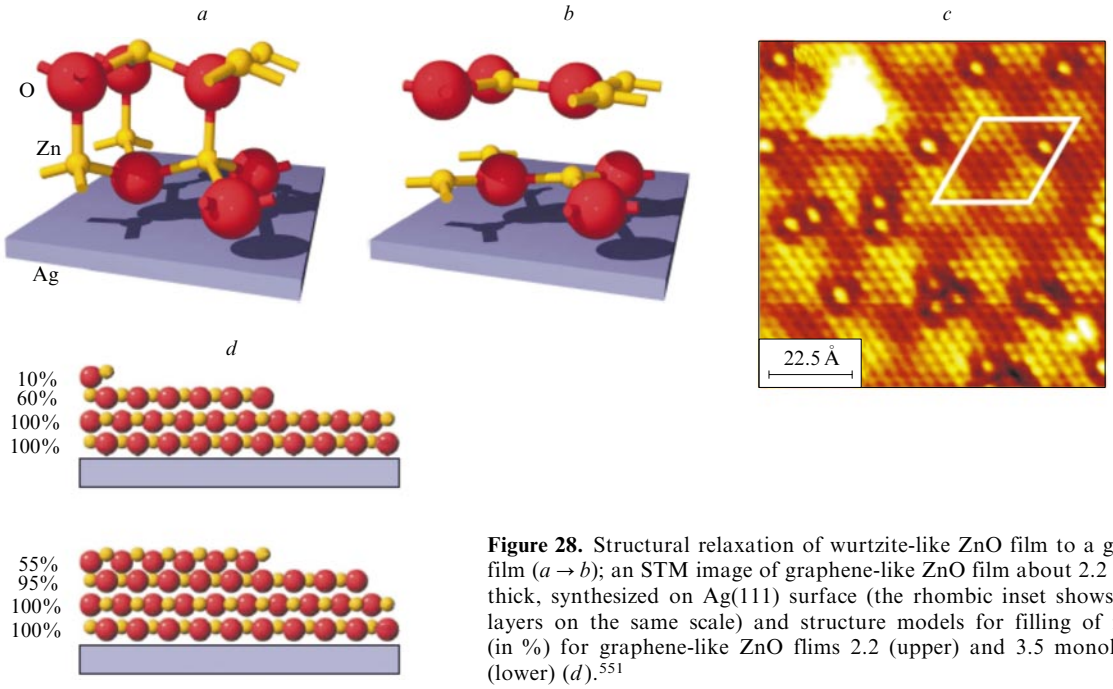


Figure 28. Structural relaxation of wurtzite-like ZnO film to a graphite-like film ($a \rightarrow b$); an STM image of graphene-like ZnO film about 2.2 monolayers thick, synthesized on Ag(111) surface (the rhombic inset shows 3.2 monolayers on the same scale) and structure models for filling of monolayers (in %) for graphene-like ZnO flims 2.2 (upper) and 3.5 monolayers thick (lower) (*d*).[551]

sen.[553, 555, 556] A graphene-like ZnO bilayer is also a semiconductor whose band gap is somewhat narrower than that of the ZnO monolayer.[553] The Poisson ratio for the ZnO sheet is much larger than for graphene, while Young's modulus is lower; *i.e.*, ZnO is a much softer material than graphene.[555, 557] Graphene-like ZnO is a piezoelectric.[555] Vacancies in the zinc sublattice of the zinc oxide sheet are responsible for induction of local magnetic moments on adjacent atoms; other types of point defects (oxygen vacancies, Zn + O double vacancies or Zn ↔ O antisite defects) cause no magnetism in the system.[553] The electronic and magnetic properties of graphene-like ZnO can be significantly changed by adsorption of transition metal atoms,[558] as well as fluorine[556, 559, 560] or hydrogen[561] atoms on its surface. For instance, adsorption of fluorine atoms on all atoms of the zinc oxide sheet will cause the $ZnOF_2$ system to exhibit the properties of a nonmagnetic semiconductor; however, partial adsorption (chemical composition ZnOF) makes the fluorine-decorated sheet a magnetic semimetal.[556, 560] Thus, the degree of coverage with adatoms is an important factor which enables targeted variation of the properties of graphene-like zinc oxide and some other graphene-like materials (see above).

Zinc oxide nanoribbons with arm-chair edges are expected to remain nonmagnetic semiconductors;[553, 562] calculations of ZnO nanoribbons with zigzag edges predict[563] the onset of ferromagnetism and subsequent loss of the ferromagnetic properties upon decoration of edges with hydrogen atoms; the magnetic properties of the nanoribbons can also vary upon mechanical deformation.[553] By stretching nanoribbons one can induce a semiconductor–metal transition.[564] As the ribbon width increases, the band gap decreases.[553]

Zinc sulfide. Studies of possible graphene-like ZnS structures began very recently.[111, 112] Unlike ZnO, the most stable zinc sulfide structure represents an essentially reconstructed network (Fig. 29) with the lattice constants $a = 14.542$ Å and $b = 13.971$ Å rather than a flat hexagonal sheet; atomic displacements from the plane of the sheet are rather large (to about 1.95 Å).[111] The effect is explained by

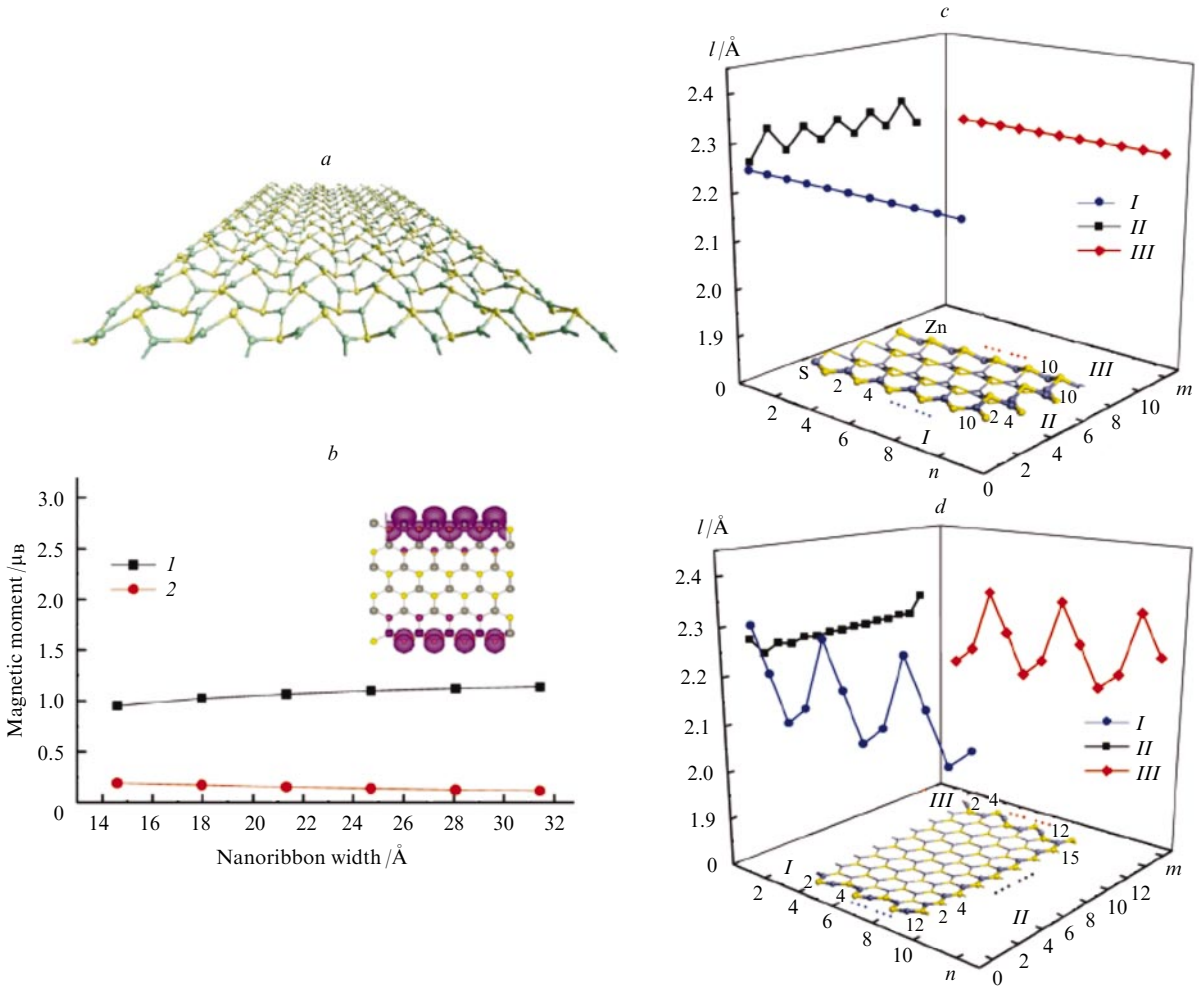


Figure 29. Structure of the most stable (reconstructed) graphene-like ZnS network (*a*);[111] the total magnetic moment of ZnS (*1*) and the magnetic moment per formula unit of ZnS (*2*) plotted *vs.* width of zigzag nanoribbon (inset: uncompensated spin density illustrating the formation of magnetic moment of the Zn and S edge atoms) (*b*); Zn–O interatomic distances (*l*) at the edges (*I*, *III*) and in the cross-section (*II*) of a reconstructed zigzag nanoribbon (*c*) and an arm-chair nanoribbon retaining its planar structure (*d*) plotted *vs.* number of bonds (*n* and *m*).[112]

the tendency of sulfur atoms to sp^3-hybridization. This was also reported for other ZnS nanostructures.[549, 565] The degr ee of Zn → O charge transfer is ~0.9 e. The ZnS network structure is a nonmagnetic semiconductor; its energy gap decreases by about 0.5 eV on going from the flat sheet to the most stable reconstructed network.

However, it was also stated [112] that graphene-like ZnS nanoribbons can have either a nearly flat arm-chair or an essentially distorted zigzag structure depending on edge configurations [zigzag or arm-chair (see Fig. 29)]. In addition, nanoribbons with zigzag edges are expected to have the properties of a ferromagnetic metal. Their magnetism is governed by the uncompensated electron density on the Zn and S edge atoms (see Fig. 29); the total magnetic moment of the nanoribbons decreases as the width of the nanoribbon increases. All ribbons with arm-chair edges are nonmagnetic semiconductors whose band gaps monotonically decrease as the ribbons become wider. According to calculations of ZnS nanoribbons with similar sizes, the stability order is as follows: wurtzite-type ribbons > graphene-like ribbons with arm-chair edges > graphene-like ribbons with zigzag edges. No reliable information on the synthesis of graphene-like ZnS structures is available at the moment.

Beryllium oxide. Although graphene-like BeO (a nonmagnetic wide band gap semiconductor) was theoretically predicted more than two decades ago,[546] it still remains a hypothetical material. A theoretical analysis of the influence of fluorination and hydrogenation on the properties of hexagonal BeO network structure and BeO ribbons was reported.[566] It is expected that hydrogenation will lead to weakening of Be–O bonds and thus make the systems less stable; the reverse effect is expected for the adsorption of fluorine atoms. Moreover, a transition to a ferromagnetic semimetal upon selective adsorption of fluorine atoms on beryllium atoms was predicted. Considering the results of a study on the effect of impurities and vacancies on graphene-like BeO nanotubes,[540] one can expect that partial replacement of oxygen atoms by boron, carbon or nitrogen atoms in the corresponding flat structures may induce local magnetic moments on these impurities; the probability of transformation of the system to a magnetic semiconductor also considerably increases. Yet another scheme of magnetization of a BeO sheet may involve creation of Be vacancies.[545]

V. Graphene-like 2D phases of inorganic compounds

As mentioned above, the term 'graphene-like phases' is applied to the actually synthesized (or simulated) quasi-2D crystals. An analogy with graphene consists in that, like graphene, these quasi-2D systems represent monolayers of corresponding layered 3D crystalline phases and are comprised of one or more atomic sheets.[567–573]

Among the graphene-like inorganic materials known to date, a high position is held by 2D oxide and hydroxide systems. Usually, they are obtained as charged flakes in colloidal solutions. Ma and Sasaki [567] have reported a 'library of oxide nanosheets', discussed their chemical properties and outlined potential fields of application.

Below we will consider oxygen-free graphene-like materials. Their best known representatives are isolated molecular layers of transition metal dichalcogenides.

1. Metal dichalcogenides

Transition metal dichalcogenides MCh_2 (Ch = S, Se and Te) have layered structures with {Ch–M–Ch} molecular monolayers stacked along the *c* axis. The layers represent hexagonal metal sheets sandwiched between two chalcogen sheets (Fig. 30). Within the monolayer, there exists the system of strong directed bonds M–Ch, whereas adjacent layers, {Ch–M–Ch}/{Ch–M–Ch}, interact through weak van der Waals bonds. Therefore, isolated MCh_2 dichalcogenide sheets were successfully prepared by the micromechanical separation technique [2] previously used to obtain graphene.[1]

Interest in 2D dichalcogenides is due to the variety of properties characteristic of the parent 3D phases. For instance, metal-like $NbSe_2$, $TaSe_2$, NbS_2 or TaS_2 are charge-density-wave crystals undergoing a transition to the superconducting state at low temperatures, while MoS_2 is a wide band gap semiconductor. Therefore, issues of common interest arise, namely, what are the changes in the properties of dichalcogenides upon reduction of their dimensionality (3D → 2D) and what are hypothetical novel properties of corresponding 2D graphene-like materials? A series of experimental and theoretical studies on 2D systems has been carried out.[49, 568–588] Experimental investigations were focused on methods of synthesis of graphene-like MCh_2 systems usually obtained as flakes of different thick-

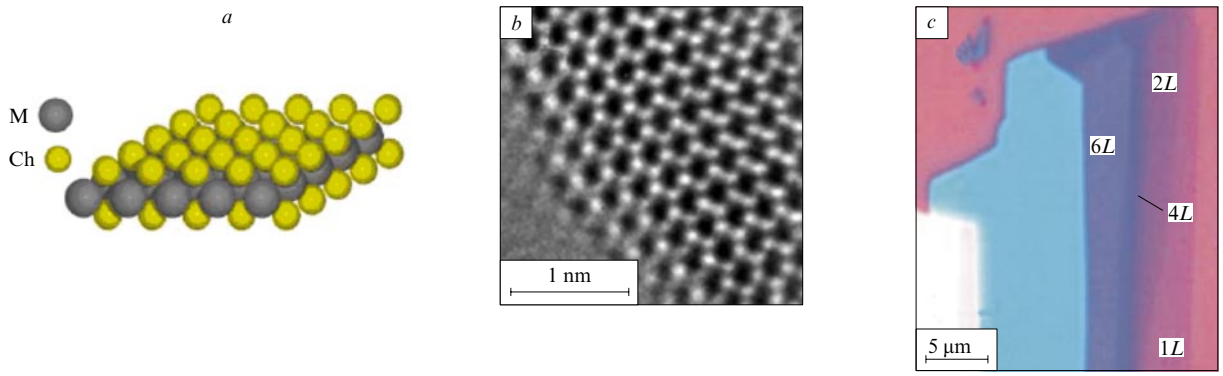


Figure 30. Atomic structure of transition metal dichalcogenide (MCh_2) monolayer (*a*); an STM image of MoS_2 layer (*b*);[571] an optical microscope image of a specimen of multi-layer MoS_2 on Si/SiO_2 substrate demonstrating different contrasts for the regions comprising one (1*L*), two (2*L*), four (4*L*) and six monolayers (6*L*) (*c*).[573]

ness on substrates (see Fig. 30); on the development of techniques for visualization of these structures,[572] on the optical, luminescent[573, 574] and conducting properties[575] and on the electronic structure.[576]

Theoretical studies were aimed to simulate structural features and the electronic structure of graphene-like dichalcogenides[393, 574, 577–579] and to discuss the lattice dynamics and features of the phonon spectra of isolated MoS_2 and WS_2 monolayers.[578, 580] Selected results of calculations[578] of geometric parameters and electron-energy data for MCh_2 monolayers (M = Mo, W, Nb, Ta; Ch = S, Se and Te) are presented in Table 8. The geometric parameters (lattice constants, interatomic distances M–Ch and the monolayer thicknesses) appreciably increase in the order $MS_2 \rightarrow MSe_2 \rightarrow MTe_2$, being close for MoS_2 and WS_2. The cohesive and formation energies and the degrees of charge transfer M → Ch (*i.e.*, the ionic component of the chemical bond) considerably decrease in the order $MS_2 \rightarrow MSe_2 \rightarrow MTe_2$, thus indcating destabilization of corresponding isolated monolayers. At the same time, the $(Nb,Ta)Ch_2$ graphene-like phases exhibit metal-like properties, whereas $(Mo,W)Ch_2$ possess semiconductor properties. Thus, the structural properties and stability of graphene-like dichalcogenides are governed by the type of the chalcogen while their electronic properties are determined by the type of the transition metal.

A number of feasible methods for controlling the properties of graphene-like dichalcogenides was repotred in a series od studies.[581–585] They include:

— mechanical methods (cutting sheets into ribbons,[581] stretching–compression[582]);

— the action of external potential;[583]

— chemical modification.[582, 584, 585]

In particular, an increase in the amplitude of external electric field applied normal to the 2D structures of MoS_2, $MoSe_2$ and $MoTe_2$ comprised of two monolayers causes their band gaps to markedly narrow.[583] Systematic calculations[584] were carried out for the effect of functionalization of MoS_2 monolayer on its electronic and magnetic properties through adsorption of atoms of one of the following sixteen elements (C, Co, Cr, Fe, Ge, Mn, Mo, Ni, O, Pt, S, Sc, Si, Ti, V, W) and in the presence of five types of defects (Mo and S single vacancies, S_2 and MoS double vacancies and a MoS_2 triple vacancy) in the layer. It was found that adsorption of transition metal, Si and Ge atoms induces a magnetic moment in the adatom–MoS_2 system (impurity-induced magnetism); vacancy-induced magnetism (due to the formation of magnetic moments on the atoms adjacent to the defect) was disclosed for the MoS_2 triple vacancy. Similar calculations[585] of how adatoms (H, B, C, N, O and F) and atomic vacancies affect the properties of graphene-like $MoSe_2$, $MoTe_2$ and WS_2 showed that, among defects, only the Mo vacancy in $MoSe_2$ induces magnetic moments, whereas all adatoms mentioned above favour the formation of magnetic moments in the $MoSe_2$, $MoTe_2$ and WS_2 monolayers.

In conclusion, it was proposed[586–588] to use MoS_2 monolayers for fabrication of transistors[586] and 2D MoS_2–amorphous carbon–graphene composites as possible materials for lithium cells.[587, 588]

2. Graphene-like metal carbides

At present, there are two types of graphene-like metal carbide materials. One of them is graphene bearing regularly arranged metal (M) adatoms. Attempts to simulate the properties of this type of materials have been undertaken. This involved solution of tasks typical of many other adatom–graphene systems including the determination of specific features of adsorption of M atoms on graphene, the character of adatom–graphene interactions, the influence of adatoms on the properties of graphene; considerable attention was paid to the description of magnetic states of these systems as potential materials for spintronics and magnetic nanodevices.[321, 331, 332, 589, 590]

Likely, in the synthesis of graphene-like carbides, researchers will face the same difficulties as in the fabrication of other carbon nanostructures (nanotubes, fullerenes) decorated with metal atoms (see review[94]). First of all, this is a tendency of many metal atoms to aggregation into intrinsic metal clusters M_n. This will lead to the formation of M_n–graphene composites.[34, 591–594]

Recently, a very interesting method for preparation of an other type of graphene-like carbides was proposed and practically implemented. The method is based on separation of single carbide layers from so-called nanolaminates also known as MAX phases.[595] These ternary phases having the

Table 8. Lattice constants, M–Ch distances, monolayer thicknesses (h), cohesive and formation energies, degrees of charge transfer M → Ch (Q) and monolayer conductivity types in isolated monolayers of metal dichalcogenides MCh_2 with M = Mo, W, Nb, Ta; Ch = S, Se and Te (according to calculations[578]).

Phase	a /Å	d_{M-Ch} /Å	h /Å	$-E_{coh}$ /eV	$-E_f$ /eV	Q /e atom^{-1}	Conductivity[a]
MoS_2	3.13	2.39	3.12	6.26	1.71	0.86	S
$MoSe_2$	3.25	2.51	3.32	5.73	1.50	0.84	S
$MoTe_2$	3.47	2.69	3.60	5.13	1.14	0.24	S
WS_2	3.13	2.39	3.13	6.90	1.65	0.98	S
WSe_2	3.25	2.51	3.34	6.31	1.38	0.58	S
WTe_2	3.47	2.70	3.61	5.63	0.95	0.24	S
NbS_2	3.29	2.46	3.12	6.45	1.81	1.04	M
$NbSe_2$	3.41	2.58	3.34	5.97	1.63	0.92	M
$NbTe_2$	3.59	2.78	3.69	5.35	1.26	0.36	M
TaS_2	3.28	2.47	3.10	6.87	1.85	1.10	M
$TaSe_2$	3.40	2.57	3.32	6.31	1.60	0.88	M
$TaTe_2$	3.61	2.77	3.64	5.62	1.15	0.34	M

[a] 'S' and 'M' stand for semiconductor and metal, respectively.

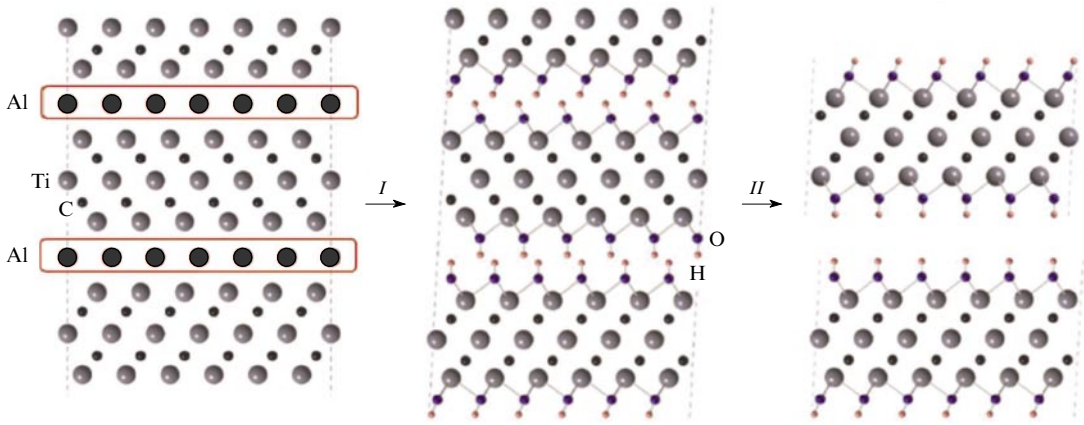


Figure 31. Preparation of graphene-like carbide Ti_3C_2.[595]
Step *I*: treatment of nanolaminate Ti_3AlC_2 with HF to replace Al atoms in the crystal by OH groups. Step *II*: breakage of hydrogen bonds and separation of $Ti_3C_2(OH)_2$ sheets upon sonication.

formal stoichiometry $M_{n+1}AX_n$ ($n = 1, 2, 3, ...$; M is the transition d-metal; A is a p-element, *e.g.*, Si, Ge, Al, S, Sn, *etc.*; X is carbon or nitrogen) form a unique class of layered materials combining the physicochemical properties of metals and ceramics.[596–601] The structures of nanolaminates $M_{n+1}AX_n$ are composed of $M_{n+1}X_n$ carbide (nitride) layers separated by flat atomic sheets of p-elements.

The method of preparation of graphene-like carbides from nanolaminate Ti_3AlC_2 is illustrated in Fig. 31.[595] Treatment of Ti_3AlC_2 with HF to remove aluminium layers was followed by sonication to separate the Ti_3C_2 carbide layers. The corresponding reactions can be written as follows:

$$2\,Ti_3AlC_2 + 6\,HF \longrightarrow 2\,AlF_3 + 3\,H_2 + 2\,Ti_3C_2$$

$$Ti_3C_2 + 2\,H_2O \longrightarrow Ti_3C_2(OH)_2 + H_2$$

$$Ti_3C_2 + 2\,HF \longrightarrow Ti_3C_2F_2 + H_2$$

This led to graphene-like carbide representing quasi-2D Ti_3C_2 sheets covered with fluorine atoms or OH groups.

Pioneering calculations[595] of graphene-like carbide Ti_3C_2, $Ti_3C_2(OH)_2$ and $Ti_3C_2F_2$ also involved the determination of their electronic structure and assessment of the elastic moduli ($\sim$300 GPa), which appeared to be higher than that of Ti_3AlC_2 ($\sim$140 GPa)[602] but comparable in magnitude with corresponding values for binary transition metal carbides (see Refs 603–605).

One can assume with ease that the method[595] can be used to obtain a large family of novel graphene-like carbides (nitrides) based on nanolaminates of different stoichiometry $M_{n+1}X_n$ ($n = 1, 2, 3, ...$).[597–601]

VI. Conclusion

Recent investigations revealed and gave knowledge about a number of very interesting properties of graphene including conducting, thermal, mechanical, optical, chemical and some other. The properties of graphene related to its quasi-2D structure, *e.g.*, the quantum Hall effect, extremely high conductivity and thermal conductivity have not been observed earlier. This gave a strong impetus to progress in fundamental physics and chemistry of graphene and made it possible, first, to propose graphene as a basis for new-generation materials for solar energy conversion,[40,41] photocatalysis,[42] lithium cell electrodes,[43] for electrochemical and biological sensors,[45] as '2D filler' for organic matrices,[35] *etc.*, and, second, to consider graphene as prototype in the search for a novel class of 2D crystals with unusual properties.[98]

In this review, we tried to generalize the results of studies on modification of the properties of graphene *per se*, on the design of graphene-based materials and on the search for novel graphene-like non-carbon materials.

In addition to impressive progress in recent basic research and a lot of predictions of technological applications of graphene (from graphene quantum electronics and nanobiology to aeronautics), the design of appropriate graphene or graphene-like materials faces many problems due to very high sensitivity of the properties of graphene to various (even minor) changes in its structure, the presence of defects, impurities, substrate type and changes in the environment.

On the one hand, this seems to be very attractive, and many theoretical calculations predict a variety of methods for fine tuning of the properties of graphene (graphene ribbons and graphene nano-flakes) including physical, chemical, mechanical, *etc.* ones. In particular, based on the model calculations, a number of methods for magnetization of graphene and graphene nanoribbons (by introducing structural defects, doping with impurities or by adsorption of various atoms) were proposed for spintronics applications. However, none of these recommendations were experimentally brought into effect up to the present. The case in point is that the high sensitivity of the functional properties of graphene to many factors creates severe difficulties in the attempts to practically implement these recommendations. For instance, there are no rigorous methods of control of, *e.g.*, selective chemical reactions on the surface of or a graphene sheet. Even for pristine graphene, many key issues related to large-scale production of homogeneous specimens with reproducible parameters are still to be solved. The available methods of synthesis (micromechanical exfoliation, chemical deposition on a substrate, electric arc synthesis, thermal decomposition of SiC, epitaxial growth on the surface of metals, *etc.*[9–17]) are unsuitable for fabrication of same-type graphene specimens

with the same morphology, structure and functional parameters, which significantly restricts the usefulness of graphene as material for production of various devices. This to even greater extent concerns novel non-carbon graphene-like materials and prospects for their applications. Solving these problems is a demanding task for near-future research.

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