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# Carbon clathrates $C_{24}$, $C_{28}$ and CA6: Structure formation and properties

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**Abstract:** The theoretical research of the potential existence and synthesizability of novel nanostructured diamond-like carbon clathrates has been carried out. Within the framework of density functional theory calculations, two previously unknown orthorhombic clathrate structures, $C_{24}$ and $C_{28}$, have been identified. The crystal lattices of these diamond-like compounds belong to the space group *Pmmm* and are characterized by five crystallographically inequivalent atomic positions. The $C_{24}$ clathrate, composed of polyhedral blocks $C_{20}$, $C_{24}$, and $C_{28}$, should be stable up to at least 500 K, whereas the $C_{28}$ clathrate is stable only at low temperatures or high pressure. The cohesive energy of the most stable clathrate ($C_{24}$) is less than the corresponding energy of diamond by 0.299 eV/atom. The densities of the new clathrates and their bulk modulus are lower than those of diamond by at least 14% and 24%, respectively. The orthorhombic clathrates are expected to be wide-bandgap semiconductors with bandgap in the range from 3.7 to 4.0 eV. The research has revealed that ultrathin hybrid carbon layers, consisting of $sp^2$ and $sp^3$ hybridized atoms, are the most plausible clathrate precursors. For the first time, it has been established that the structural variant of clathrate CA6 (carbon sodalite) can be obtained via high-pressure compression of crystals composed of layered or molecular precursors. In particular, CA6 clathrate can be formed by the process of strong compression of graphite consisting of $L_{4\text{-}6\text{-}12}$ graphene perpendicular to the planes of the graphene layers when the pressure reaches ≈29 GPa. The pressure required for complete structural transformation of precursors into this diamond-like phase can be significantly reduced to 1.1 GPa if hydrostatic compression of dense fullerite composed of $C_{24}$ clusters is applied. The experimental identification of the new carbon clathrates can be accomplished using calculated powder X-ray diffraction patterns and Raman spectra.

**Keywords:** carbon clathrates, crystal structure, Raman spectra, X-ray diffraction patterns, *ab initio* calculations

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## 1. Introduction

Carbon-based compounds receive special attention in the search for materials with unique beneficial properties, resistance to various types of impacts, and homogeneous composition. Of these compounds, diamond-like phases exhibit the highest strength characteristics and high stability [1–5]. The structural features of diamond-like compounds can also lead to a change in electronic conductivity from dielectric to semiconducting, without altering the elemental composition [1–3, 5], as well as the manifestation of auxetic properties [6, 7]. One of the groups of diamond-like phases that has retained research interest over the past decades is the group of carbon clathrates — materials consisting of a porous carbon framework [8–10], capable of hosting atoms of another chemical element within their cavities. The wide range of possible structural types of diamond-like clathrates results in strong variability of their properties [5, 8–10]. Similar to theoretically studied diamond-like phases [1–5], high-symmetry clathrates containing polyhedral blocks of four-, five-, and six-membered carbon cycles in their structures should exhibit the most desirable properties. Furthermore, the feasibility of synthesis and structural stability of these phases are intrinsically linked to the energy of interatomic bonds, which is ultimately dictated by the existence of particular polyhedral structural units and their spatial arrangement. Therefore, it is necessary to conduct a theoretical search for new forms of carbon clathrates with properties that significantly differ from those of diamond. It is also worth noting that, as of now, research has only covered certain clathrate precursors [11], while no computational modelling of their formation processes has been performed even for the most symmetrical and stable clathrate structures. Therefore, within the framework of this theoretical study, it is necessary to address the issue of possible clathrate synthesis methods using the well-studied bcc $C_6$ phase, also referred to as CA6 or carbon sodalite [5,11–13], as an example.

## 2. Models and computational methods

Generation of target compound structures was performed by combining polyhedral precursors using the method described

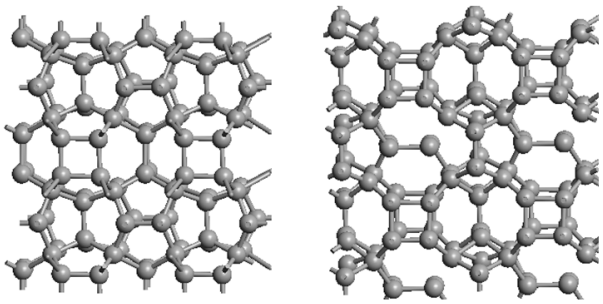
in the paper [14]. The structural and energetic characteristics of carbon nanostructures and three-dimensional crystals were modeled using the density functional theory (DFT) method implemented in the Quantum ESPRESSO [15] software package. The DFT calculations were performed using the Perdew-Burke-Ernzerhof (PBE) [16] exchange-correlation functional, which accurately describes the structure and properties of various carbon compounds [17,18]. The norm-conserving pseudopotential of Troullier and Martins was used to account for the influence of ionic cores. For calculations in the Brillouin zone of primitive lattices, *k*-point grids ranging from 6×6×6 to 12×12×12 were used, with a kinetic energy cutoff of 60 Rydberg. The relaxation of the initial structure was carried out until the force acting on each atom became less than 0.005 eV/Å and the value of stress dropped below 0.4 kbar. Elastic constants were calculated in the process of small deformations of the initial unit cells of the crystalline phases. The stability assessment of the structures of the new phases was performed using the *ab initio* variable cell molecular dynamics (vc-md) method implemented in the Quantum ESPRESSO software package [15]. The calculations were performed using simulation cells containing from 24 to 28 atoms, 4×4×4 *k*-point grids determined by the Monkhorst-Pack method and energy cutoff of 60 Rydberg. The annealing simulation time was 7 ps with a time step of 1 fs. Powder X-ray diffraction patterns of diamond-like compounds were calculated using a standard method that accounts for the Cu-Kα1 radiation wavelength (1.5405 Å) and the average coherent scattering domain size ≈500 Å. The calculation of Raman spectra was carried out using the approach presented in [19]. Theoretical calculations of phase transformations of structural modifications of graphite and cluster fullerite into diamond-like phases under high compression were performed using the method described in [20,21]. The electronic structure was studied using the SIESTA software package [22], employing the aforementioned approximation and computational parameters (the cutoff energy was set to 200 Rydberg).

## 3. Results and discussion

The first stage of the research involved modelling the structure and assessing the stability of new carbon clathrates formed by combining close-packed fullerene-like precursors ranging from $C_8$ to $C_{32}$. The analysis shows that, to date, the possibility of existence of two porous diamond-like phases composed of four polyhedral blocks has not been established. The first diamond-like phase — the $C_{24}$ clathrate — is formed from fullerene-like blocks: $C_{20}$, $C_{28}$, and two isomers of $C_{24}$ (Fig. 1a). The second phase — the $C_{28}$ clathrate — can be obtained by close packing of $C_8$, $C_{20}$, $C_{24}$ and $C_{32}$ blocks (Fig. 2b).

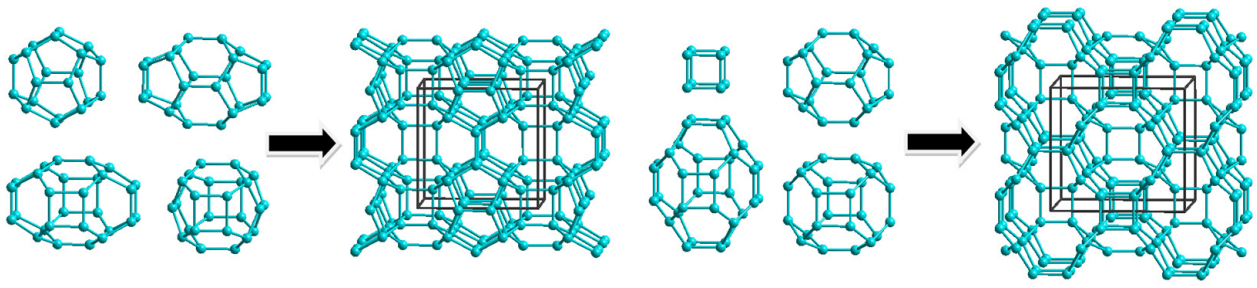
The crystal lattices of the two new clathrates belong to the space group *Pmmm* (№47) and are characterized by 5 crystallographically non-equivalent atomic positions. The unit cells of the clathrates shown in Fig. 1 have the following parameters: $a = 5.672$ Å, $b = 5.620$ Å, $c = 5.093$ Å for the $C_{24}$ clathrate; $a = 6.367$ Å, $b = 5.826$ Å, $c = 5.531$ Å for the $C_{28}$ clathrate. The studied clathrates contain nanopores, the size and shape of which are determined by the geometry of the polyhedra that form their structure (see Fig. 1). The smallest linear dimensions of the nanopores in clathrates $C_{24}$ and $C_{28}$ are 3.522 and 1.538 Å, respectively, while the largest dimensions are equal to the *a* parameters of the corresponding unit cells.

The structure of clathrate $C_{24}$ is less strained than the structure of clathrate $C_{28}$, as the maximum interatomic bond lengths in their structures are 1.654 and 1.714 Å, and the minimum bond angles are 90.0° and 85.9°, respectively. Under such internal stresses, the cohesive energies of the $C_{24}$ and $C_{28}$ phases are lower than that of diamond by 0.299 and 0.554 eV/atom, respectively, but are comparable to that of clathrate CA6 (carbon sodalite), which has been thoroughly studied in papers [5,11–14]. Therefore, an assessment of the thermal stability of the novel diamond-like phases is required. The thermal treatment of clathrates was simulated at 500 K for a duration of 7 ps. The results of molecular dynamics simulations demonstrate that when subjected to thermal treatment, the crystalline lattice of the orthorhombic $C_{24}$ clathrate exhibits only minor structural distortions (Fig. 2a). In contrast, the $C_{28}$ clathrate undergoes progressive structural degradation (Fig. 2b). It should be noted that the $C_{28}$ phase remains stable at relatively low temperatures (<300 K).



a b

**Fig. 2.** Structures of clathrates $C_{24}$ (a) and $C_{28}$ (b) after 7 ps of annealing simulation at 500 K.



a b

**Fig. 1.** (Color online) The formation process of the new $C_{24}$ (a) and $C_{28}$ (b) clathrate structures from clusters.

In the second stage of the research, the properties of new diamond-like compounds were investigated. The most stable clathrate phase ($C_{24}$) has a density of 2.949 g/cm$^3$, which is 14.3% lower than the corresponding value for cubic diamond. The density of the $C_{28}$ clathrate is 2.722 g/cm$^3$. The mechanical stability of the clathrates was studied under strong uniform compression and strong uniaxial tension within experimentally achievable stress ranges. Under strong hydrostatic compression of the new phases to 20 GPa (Fig. 3 a), the structures of the new clathrates were found to be stable. Based on the data in Fig. 3 a, the bulk moduli $B_0$ for the $C_{24}$ and $C_{28}$ clathrates were calculated to be 339.5 and 298.6 GPa, respectively, which are only 24 – 30% smaller than the $B_0$ for diamond. The values of the bulk modulus derivatives with respect to pressure, $B'$, range from 2.76 to 2.80. Further study of the clathrate stability was performed by stretching the structure along the main crystallographic axes, since the most strained interatomic bonds are most closely oriented relative to these axes. As a result of the relaxation of the crystal lattices under uniaxial deformations of up to 3% (and maximum stresses of 17 – 23 GPa), the clathrates do not degrade, as indicated by the nearly parabolic behavior of the $\Delta E_{total} = f(\varepsilon)$ dependence (see Fig. 3 b). Calculations of structure stretching along the main crystallographic directions also showed that for the $C_{24}$ clathrate, the ranges of Young's modulus ($Y$) and Poisson's ratio (μ) are 741 – 796 GPa and 0.03 – 0.14, respectively. These values are close to those for diamond ($Y$ = 989 GPa, μ = 0.1). For the clathrate $C_{28}$, the values of $Y$ and μ lie within the ranges of 570 – 584 GPa and 0.13 – 0.17, respectively. The calculated values of the shear moduli of diamond, phases $C_{24}$ and $C_{28}$ are 544, ≈338 and ≈298 GPa, respectively.

For a detailed study of the electronic characteristics of nanostructured phases, the band structures were calculated. The energies of valence electrons were calculated in the Brillouin zones of simple orthorhombic lattices between the following high-symmetry points: G, R, S, T, U, X, Y and Z. The calculated band structures are shown in Fig. 4. The smallest band gap in clathrate $C_{24}$ is 3.73 eV and is observed at point Y, while the minimum band gap (4.03 eV) in clathrate $C_{28}$ is observed at point T. Furthermore, a computational analysis of electronic state spectra in Brillouin zones was carried out. The analysis of these spectra demonstrated that the energy gap between the valence band maximum and the conduction band minimum amounts to 3.62 eV and 3.87 eV for the $C_{24}$ and $C_{28}$ clathrates, respectively. Notably, these values

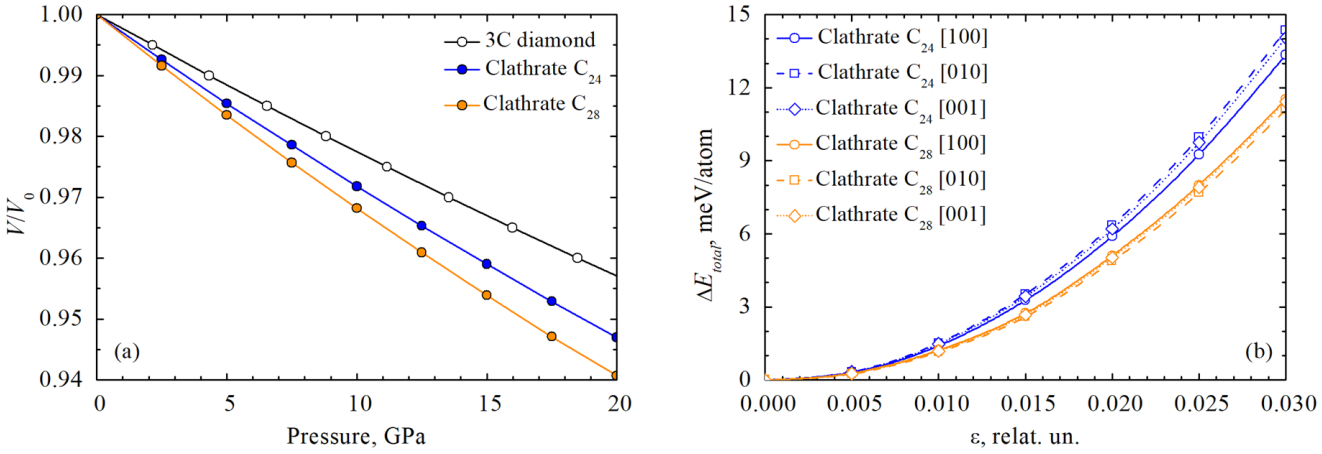



**Fig. 3.** (Color online) Dependences of the relative volume on the pressure during hydrostatic compression of diamond, clathrates $C_{24}$ and $C_{28}$ (a). Dependences of the difference total energy on the relative deformation during uniaxial tension of clathrates $C_{24}$ and $C_{28}$ (b).

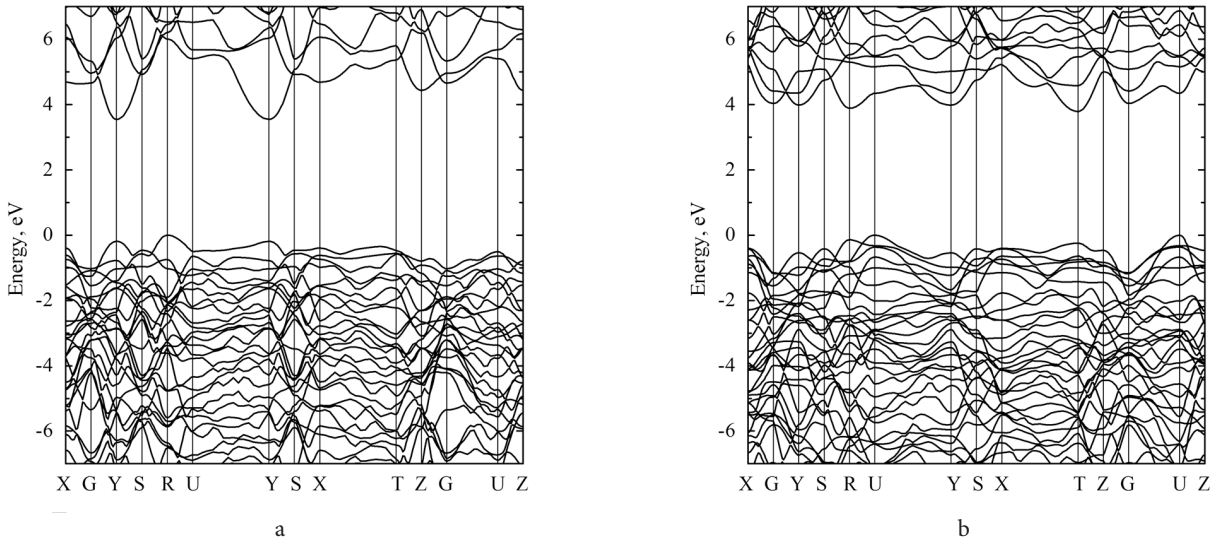



**Fig. 4.** Electronic band structures of clathrates $C_{24}$ (a) and $C_{28}$ (b).

are lower by 0.09 – 0.34 eV compared to the value $\Delta_{bandgap}$ of the highly symmetric CA6 clathrate [14]. The obtained values of indirect energy gaps are in very good agreement with the results of band structure calculations shown in Fig. 4. The calculated value of the indirect band gap in cubic diamond is 5.44 eV, so the studied orthorhombic phases should be wide-bandgap semiconductors.

At the next stage of the research, methods for the possible synthesis of the most stable carbon clathrates, such as the new orthorhombic $C_{24}$ and CA6 (bcc $C_6$), were studied. One of the possible methods of synthesizing new clathrates might involve the formation of a clathrate layer and its subsequent growth, for example, through the process of carbon deposition from the gas phase onto a substrate with a specific morphology. When examining various precursors of the $C_{24}$ clathrate, it was found that the most stable smallest structural units necessarily containing $sp^3$ hybridized atoms are exclusively layered nanostructures (Fig. 5 a, b). Among them, the hybrid rhombic layer shown in Fig. 5 a has a total energy that is 0.178 eV/atom lower than the corresponding energy of the final phase. In turn, the CA6 clathrate has a corrugated layer of minimum thickness (Fig. 5 c) as its precursor, which is similar to pentagraphene [23], with an energy difference $\Delta E_{CA6} = 0.348$ eV/atom. Based on this precursor, a stable clathrate-like layer shown in Fig. 5 d ($\Delta E_{CA6} = 0.147$ eV/atom) can be formed, and its total energy approaches that of the CA6 phase as the layer grows along [110].

Another method for obtaining diamond-like compounds may involve high-pressure compression of precursor associates composed of $sp^2$-hybridized carbon atoms [20, 21, 24]. Since the structure of the CA6 phase, unlike other clathrates, is characterized by only one Wyckoff position [12], there is a high probability of finding uniform precursors for its synthesis. One of the 0D precursors is a $C_{24}$ fullerene isomer in the form of a truncated octahedron [14, 25]. In the article [26] it was shown that this isomer can be stable at 300 K, however, this temperature may indicate a low probability of synthesis of the molecule under standard conditions. Therefore, an additional molecular dynamics study of the stability of the precursor molecule $C_{24}$ from 350 to 600 K with a step of 50 K was performed. It was found that the $C_{24}$ cluster begins to decompose only after 6.5 ps of annealing at 600 K (Fig. 6). The destruction is expressed in the rupture of the most strained C-C bond in the tetragonal unit (see Fig. 6). Therefore, the $C_{24}$ cluster is stable at least up to 550 K, and the condensate based on it is a good candidate for a precursor for obtaining the CA6 clathrate.

In the performed phase transition modeling, the initial structures of $C_{24}$ fullerite and $L_{4\text{-}6\text{-}12}$ graphite ABC were represented by trigonal unit cells. Figure 7a shows the plot of the differential total energy of phases ($\Delta E_{total} = E_{phase} - E_{CA6}$) versus atomic volume ($V$) under uniform compression from all directions. Calculations show that the diamond-like CA6 phase forms when the volume of the parent fullerite is reduced by 13.4%, at which point the pressure reaches 1.1 GPa. As the second and more stable precursor, the graphene layer $L_{4\text{-}6\text{-}12}$ (Fig. 7b) was experimentally obtained, as reported in [27]. The structural transformation of ABC-stacked graphite $L_{4\text{-}6\text{-}12}$ into a diamond-like phase was modeled under compression along the [001] crystallographic direction (in the trigonal representation). Figure 7b presents the $\Delta E_{total} = f(V)$ dependence for graphite $L_{4\text{-}6\text{-}12}$ and clathrate CA6, illustrating the phase transitions occurring between these compounds. The structural transformation of graphite into the CA6 phase can occur at a pressure of 29.1 GPa ($P_{33}$) by overcoming a potential barrier of 0.192 eV/atom. The obtained energy

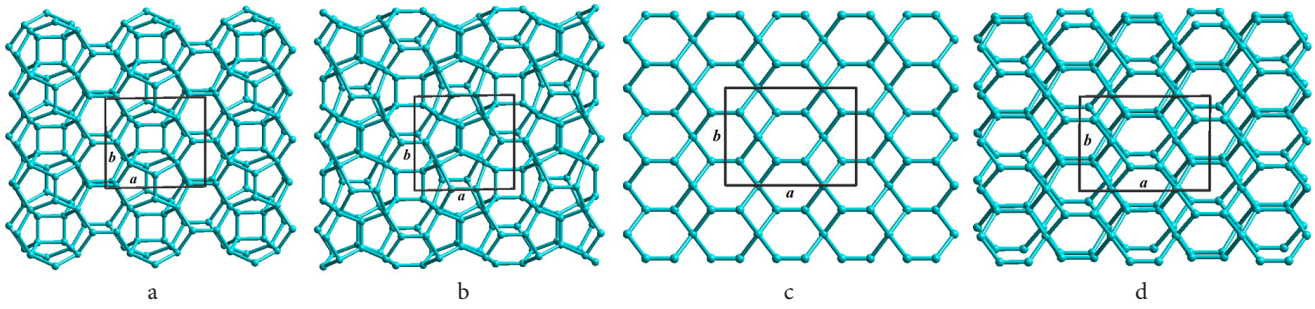



**Fig. 5.** (Color online) Hybrid layered precursors of clathrates $C_{24}$ (a, b) and CA6 (c, d).

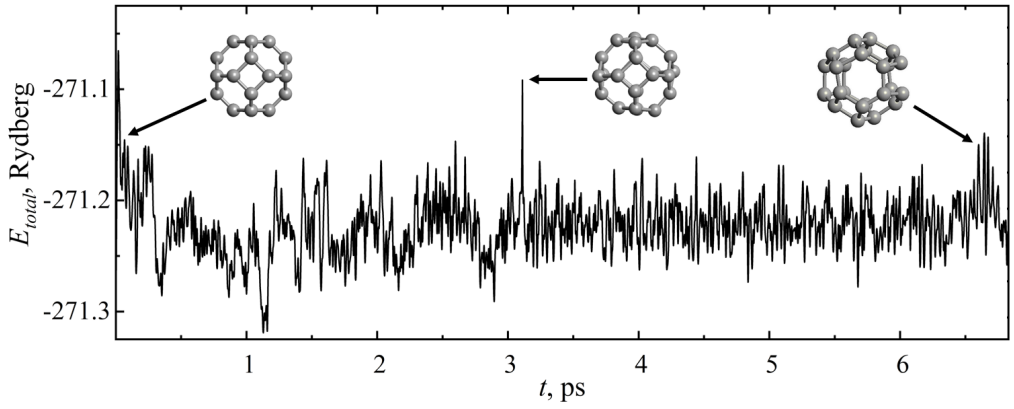



**Fig. 6.** Dependence of the total energy on time for the carbon cluster $C_{24}$, obtained as a result of simulating annealing at 600 K.

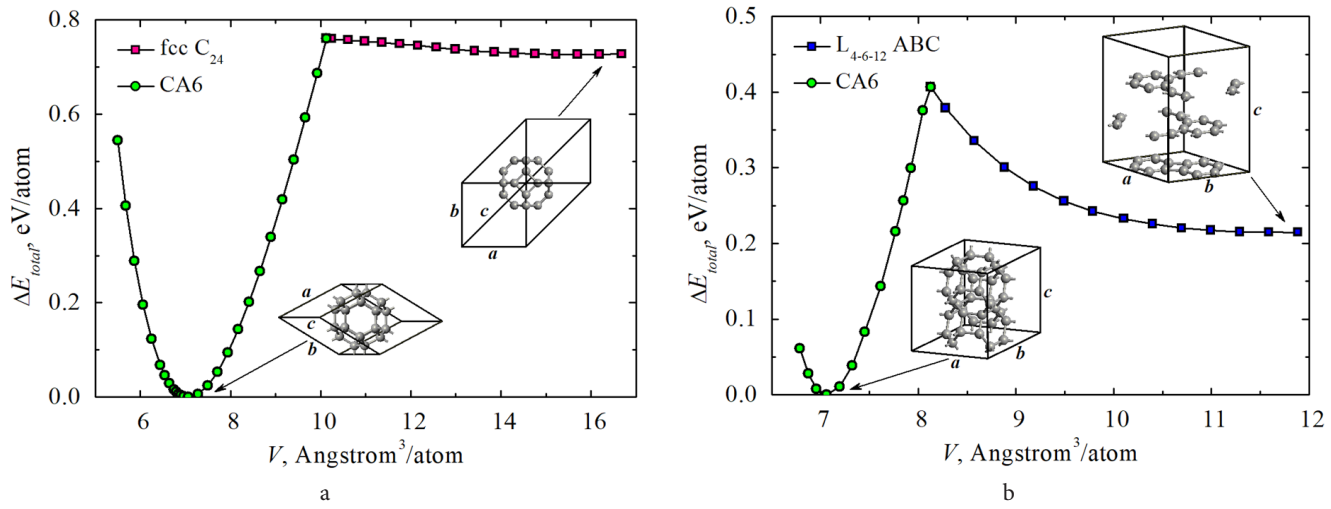



**Fig. 7.** Dependences of the differential total energy ($\Delta E_{total}$) on volume ($V$) for the phase transitions "close-packed fullerite $C_{24}$→CA6" (a) and "$L_{4\text{-}6\text{-}12}$ graphite ABC→CA6" (b).

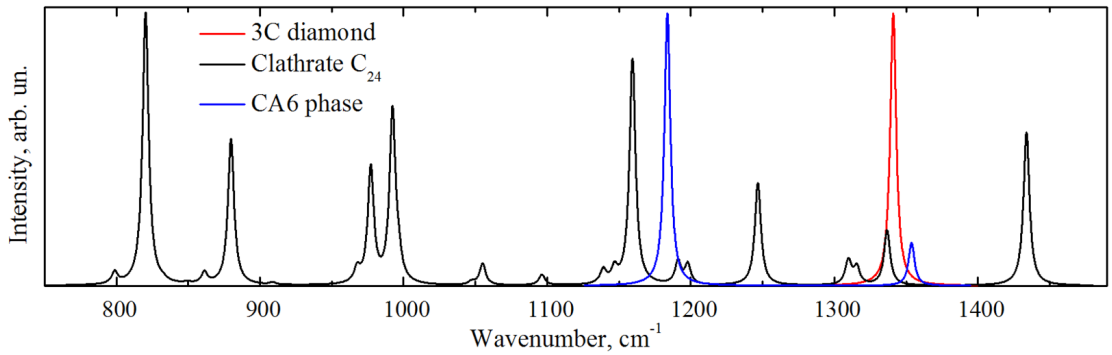



**Fig. 8.** (Color online) Calculated Raman spectra of diamond and diamond-like phases.

**Table 1.** Calculated values of diffraction angles, interplanar distances and relative intensities of X-ray diffraction maxima for carbon clathrates (λ=1.5405 Å, $L_{cryst}$ = 500 Å).

| $C_{24}$ clathrate | | | | | | $C_{28}$ clathrate | | | | | | CA6 | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| *h* | *k* | *l* | 2θ,° | *d*, Å | *I*, % | *h* | *k* | *l* | 2θ,° | *d*, Å | *I*, % | *h* | *k* | *l* | 2θ,° | *d*, Å | *I*, % |
| 1 | 1 | 1 | 28.41 | 3.142 | 100 | 1 | 1 | 1 | 26.26 | 3.394 | 100 | 1 | 1 | 0 | 28.62 | 3.119 | 100 |
| 1 | 0 | 0 | 15.62 | 5.672 | 50 | 1 | 0 | 0 | 13.91 | 6.367 | 32 | 2 | 1 | 1 | 50.69 | 1.801 | 19 |
| 0 | 1 | 0 | 15.77 | 5.620 | 34 | 0 | 0 | 1 | 16.02 | 5.531 | 25 | 2 | 0 | 0 | 40.92 | 2.205 | 12 |
| 1 | 0 | 2 | 38.76 | 2.323 | 24 | 2 | 0 | 0 | 28.03 | 3.184 | 18 | 2 | 2 | 2 | 74.52 | 1.273 | 12 |
| 0 | 2 | 0 | 31.84 | 2.810 | 16 | 1 | 1 | 0 | 20.66 | 4.298 | 16 | 3 | 1 | 0 | 67.10 | 1.395 | 6 |
| 2 | 0 | 0 | 31.55 | 2.836 | 13 | 1 | 1 | 2 | 38.71 | 2.326 | 11 | 3 | 2 | 1 | 81.68 | 1.179 | 6 |
| 2 | 2 | 0 | 45.44 | 1.996 | 9 | 1 | 0 | 1 | 21.28 | 4.176 | 10 | 2 | 2 | 0 | 59.25 | 1.559 | 5 |
| 0 | 1 | 3 | 56.64 | 1.625 | 9 | 3 | 1 | 1 | 48.53 | 1.876 | 7 | 4 | 0 | 0 | 88.71 | 1.103 | 5 |

barrier value is 18% lower than that for the transformation of graphite into diamond polytypes [28].

X-ray diffraction and spectroscopy are used for the experimental detection of carbon diamond-like compounds. If the studied phases are obtained in macroscopic quantities, X-ray crystallographic analysis can be applied for their structural identification. Table 1 presents data obtained from modeling the X-ray diffraction patterns of clathrates. It has been established that the new $C_{24}$ clathrate can be unambiguously identified by two high-intensity maxima and two medium-intensity maxima. Detection of the $C_{28}$ clathrate may be challenging because the position of its main maximum ($d_{111}$≈3.39 Å) is close to that of the primary graphite maximum ($d_{002}$) [29], and only two maxima exhibit medium intensity. The high symmetry of the CA6 clathrate crystal lattice causes all diffraction maxima positions on the X-ray diffraction pattern to differ significantly from those observed for the most stable carbon materials. However, these maxima, except the main one, have relatively low intensity (not exceeding 19%), which should significantly complicate the identification of the CA6 phase in synthesized carbon materials.

If clathrates are obtained as single crystals of nano- or microscopic dimensions, Raman spectroscopy can be used for their identification. The calculated Raman spectra of 3C diamond and hypothetical clathrates are presented in Fig. 8. It has been established that the vibrational spectrum of orthorhombic $C_{24}$ clathrate exhibits seven high-intensity

peaks in the wavenumber range from 820 to 1435 $cm^{-1}$, which do not overlap with the peaks of diamond, graphite, and carbon nanotubes [30]. The cubic CA6 phase exhibits only two peaks in its spectrum, with wavenumbers of 1184 and 1354 $cm^{-1}$. The latter peak has low intensity and may overlap with the 3C diamond peak. Consequently, the Raman spectra of the most stable predicted phases differ significantly from the similar spectra of the major carbon allotropes and polymorphs [30]. Therefore, $C_{24}$ and CA6 clathrates can be identified in carbon materials.

## 4. Conclusions

The first-principles study of the structure, thermal stability, electronic and mechanical characteristics, synthesis methods, and identification of carbon clathrates containing structural units in the form of polyhedra ranging from $C_8$ to $C_{32}$ has been performed. The possibility of existence of two new orthorhombic clathrates, $C_{24}$ and $C_{28}$, has been established. These compounds are expected to be wide-bandgap semiconductors with high mechanical characteristics. Even greater variation in these properties of the new clathrates, which are important from a practical point of view, can be achieved by doping their structures with boron and lithium atoms, which was demonstrated for various carbon clathrates in [31]. In addition, the most stable precursors of the predicted clathrates were identified, and the most probable methods for obtaining the cubic clathrate CA6, also known as carbon sodalite, through strong compression of fullerene-like $C_{24}$ clusters or $L_{4\text{-}6\text{-}12}$ graphites were proposed for the first time. The main experimentally controlled parameters for the realization of two proposed alternative methods for the practical production of carbon solidate, potentially feasible in high-pressure installations, have been calculated. The studied carbon clathrates can be identified using calculated powder X-ray diffraction patterns and Raman spectra.

***Conflicts of interest**: The authors declare no conflicts of interest.*

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