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# «Graphene polymorphs»

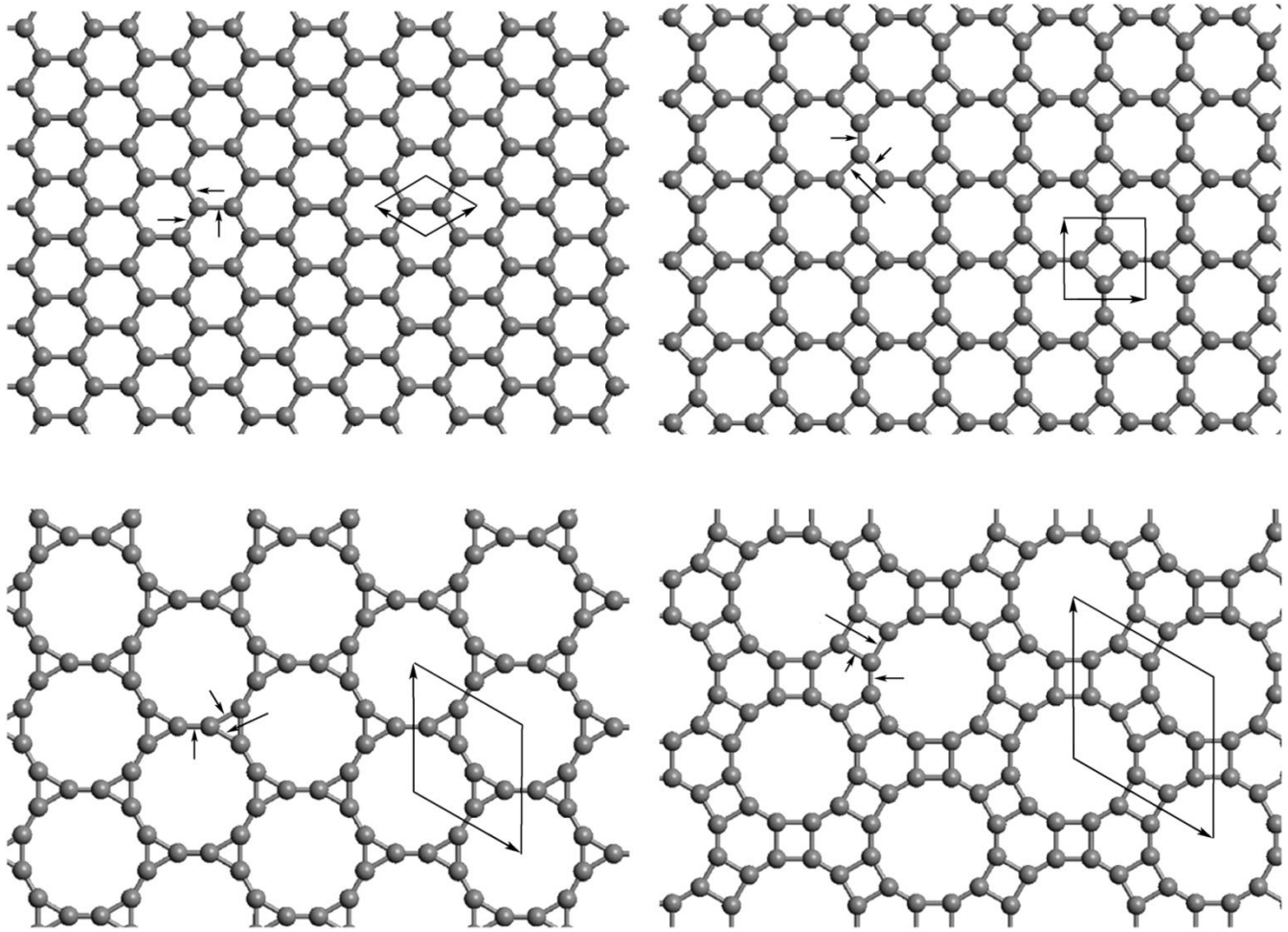
**Maxim Belenkov[1], Andrey Kochengin[2], Vladimir Chernov[1], Evgeny Belenkov[1]**

[1]Department of Physics, Chelyabinsk State University, Chelyabinsk 454001, Russia
[2]Chelyabinsk Regional Clinical Center of Oncology and Nuclear Medicine, Chelyabinsk 454087, Russia

# Problem statement

Task:

- Hexagonal graphene is a conductor, and graphene with semiconductor properties is required for use in electronics. Some polymorphs of graphene can probably be semiconductors. Therefore, it is necessary to search for new stable graphene polymorphs with such properties.



Graphene layers of four main structural modifications: (a) $L_6$, (b) $L_{4–8}$, (c) $L_{3–12}$, and (d) $L_{4–6–12}$ [1].

[1] Belenkov E A and Kochengin A E 2015 *Phys. Solid State* **57** 2126

# Solution method

- Package: Quantum ESPRESSO
- Method: Density Functional Theory (DFT)
- Generalized Gradient Approximation (GGA)

# Graphene polymorphs

**Table 1**. The structural positions of atoms in graphene polymorphs (n is the number of different atomic positions; M is the relative number of different structural positions; $Rng_i$ is the value of the Wales ring parameter, where i is the number of the atomic position).

| Layer | Fig.1 | n | $Rng_1$ | $Rng_2$ | $Rng_3$ | $Rng_4$ | M | Topological defects per unit cell | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | 3 | 4 | 5 | 7 | 8 | 10 | 12 | Σ |
| $L_6$ | (a) | 1 | $6^3$ | - | - | - | 1 | - | - | - | - | - | - | - | 0 |
| $L_{4\text{-}8}$ | (b) | | $4^1 8^2$ | - | - | - | 1 | - | 1 | - | - | 1 | - | - | 2 |
| $L_{3\text{-}12}$ | (c) | | $3^1 12^2$ | - | - | - | 1 | 2 | - | - | - | - | - | 1 | 3 |
| $L_{4\text{-}6\text{-}12}$ | (d) | | $4^1 6^1 12^1$ | - | - | - | 1 | - | 3 | - | - | - | - | 1 | 4 |
| $L_{4\text{-}6\text{-}8a}$ | (e) | 2 | $4^1 6^1 8^1$ | $6^1 8^2$ | - | - | 2:1 | - | 1 | - | - | 1 | - | - | 2 |
| $L_{4\text{-}10}$ | (f) | | $4^1 10^2$ | $4^2 10^1$ | - | - | 2:1 | - | 2 | - | - | - | 1 | - | 3 |
| $L_{4\text{-}12}$ | (g) | | $4^1 12^2$ | $4^2 12^1$ | - | - | 1:1 | - | 3 | - | - | - | - | 1 | 4 |
| $L_{4\text{-}6\text{-}8b}$ | (h) | | $4^1 6^1 8^1$ | $6^2 8^1$ | - | - | 1:1 | - | 1 | - | - | 1 | - | - | 2 |
| $L_{5\text{-}7a}$ | (i) | 3 | $5^1 7^2$ | $5^1 7^2$ | $5^2 7^1$ | - | 1:2:1 | - | - | 2 | 2 | - | - | - | 4 |
| $L_{5\text{-}7b}$ | (j) | | $5^1 7^2$ | $5^1 7^2$ | $5^2 7^1$ | - | 1:2:1 | - | - | 4 | 4 | - | - | - | 8 |
| $L_{4\text{-}6\text{-}8e}$ | (k) | | $6^3$ | $4^1 6^1 8^1$ | $6^2 8^1$ | - | 1:1:1 | - | 1 | - | - | 1 | - | - | 2 |
| $L_{5\text{-}7c}$ | (l) | 4 | $5^3$ | $5^2 7^1$ | $5^1 7^2$ | $7^3$ | 1:3:6:2 | - | - | 3 | 3 | - | - | - | 6 |

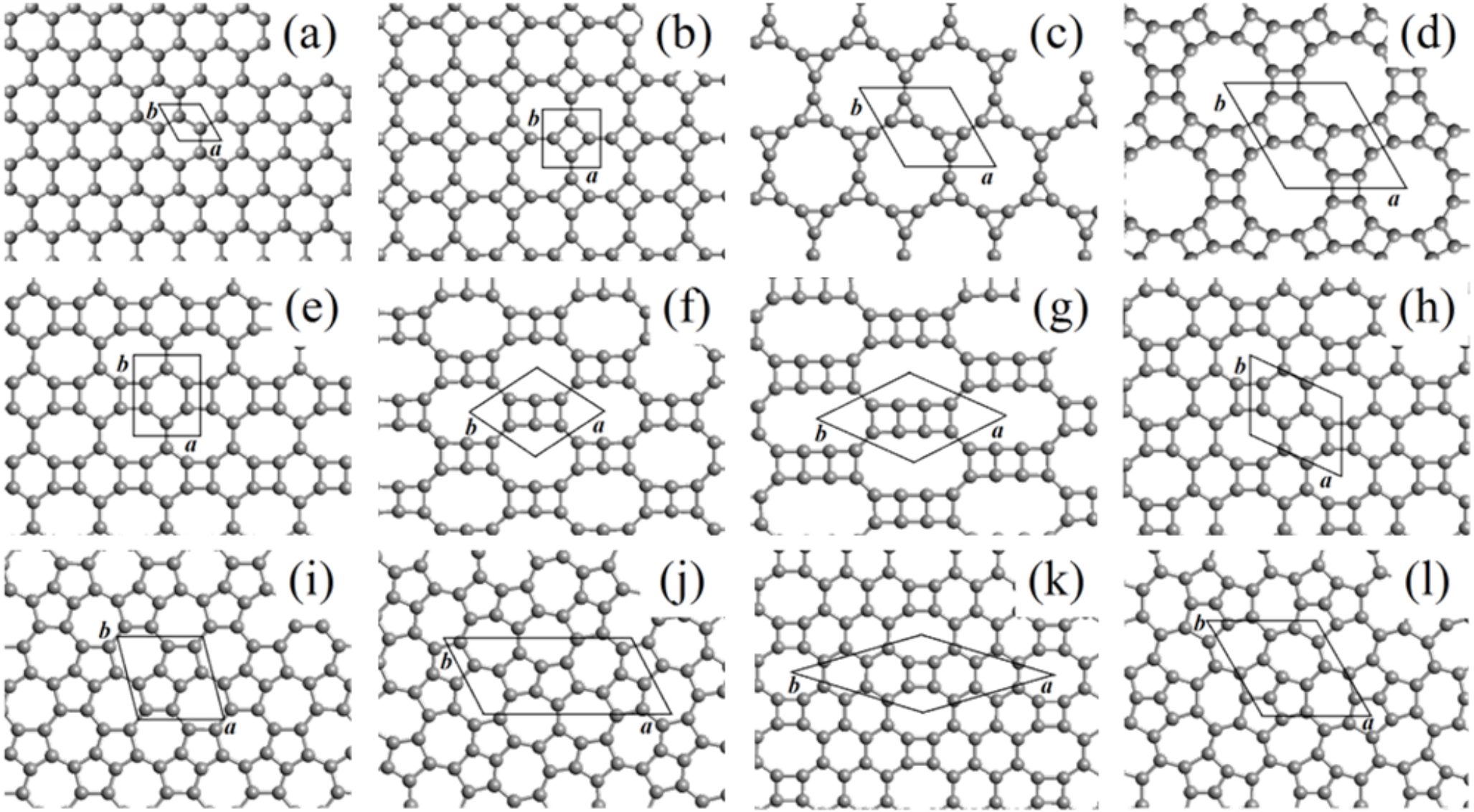



**Figure 1**. The structure of graphene polymorphs: (a) $L_6$; (b) $L_{4\text{-}8}$; (c) $L_{3\text{-}12}$; (d ) $L_{4\text{-}6\text{-}12}$; (e) $L_{4\text{-}6\text{-}8a}$; (f) $L_{4\text{-}10}$; (g) $L_{4\text{-}12}$; (h) $L_{4\text{-}6\text{-}8b}$; (i) $L_{5\text{-}7a}$; (j) $L_{5\text{-}7b}$; (k) $L_{4\text{-}6\text{-}8e}$; (l) $L_{5\text{-}7c}$.

**Table 2.** Structural characteristics and properties of graphene polymorphs (a, b are the lengths of the elementary translation vectors, γ is the angle between the translation vectors, N is the number of atoms in the unit cell, Def is the deformation parameter, $E_{total}$ is the total specific energy, $\Delta E_{total}$ is the total specific difference energy, $E_{sub}$ is the sublimation energy, $E_g$ is the band gap).

| Graphene | The lattice parameters | | | N, atom | Def, ° | Σ / N | $E_{total}$, eV/atom | $\Delta E_{total}$, eV/atom | $E_{sub}$, eV/atom | $E_g$, eV |
|---|---|---|---|---|---|---|---|---|---|---|
| | a, Å | b, Å | γ, ° | | | | | | | |
| $L_6$ | 2.471 | | 120 | 2 | 0 | 0 | -157.34 | 0 | 7.78 | 0 |
| $L_{4\text{-}8}$ | 3.429 | | 90 | 4 | 60 | 0.5 | -156.78 | 0.56 | 7.22 | 0 |
| $L_{3\text{-}12}$ | 5.130 | | 120 | 6 | 120 | 0.5 | -156.22 | 1.14 | 6.64 | 0 |
| $L_{4\text{-}6\text{-}12}$ | 6.713 | | 120 | 12 | 60 | 0.33 | -156.65 | 0.70 | 7.08 | 0 |
| $L_{4\text{-}6\text{-}8a}$ | 3.801 | 4.554 | 90 | 6 | 46.53 | 0.33 | -156.80 | 0.54 | 7.24 | 0 |
| $L_{4\text{-}10}$ | 4.642 | | 115.0 | 6 | 79.53 | 0.5 | -156.27 | 1.07 | 6.71 | 0 |
| $L_{4\text{-}12}$ | 5.914 | | 129.6 | 8 | 88.95 | 0.5 | -156.01 | 1.33 | 6.45 | 0.59 |
| $L_{4\text{-}6\text{-}8b}$ | 5.517 | 4.476 | 113.6 | 8 | 34.25 | 0.25 | -156.91 | 0.43 | 7.35 | 0 |
| $L_{5\text{-}7a}$ | 4.776 | | 104.0 | 8 | 31.3 | 0.5 | -157.05 | 0.29 | 7.49 | 0 |
| $L_{5\text{-}7b}$ | 10.413 | 4.779 | 117.5 | 16 | 28.9 | 0.5 | -157.07 | 0.27 | 7.51 | 0 |
| $L_{4\text{-}6\text{-}8e}$ | 7.879 | | 147.6 | 12 | 24.06 | 0.17 | -157.04 | 0.3 | 7.48 | 0.37 |
| $L_{5\text{-}7c}$ | 6.193 | | 120 | 12 | 66.4 | 0.5 | -156.83 | 0.51 | 7.27 | 0 |

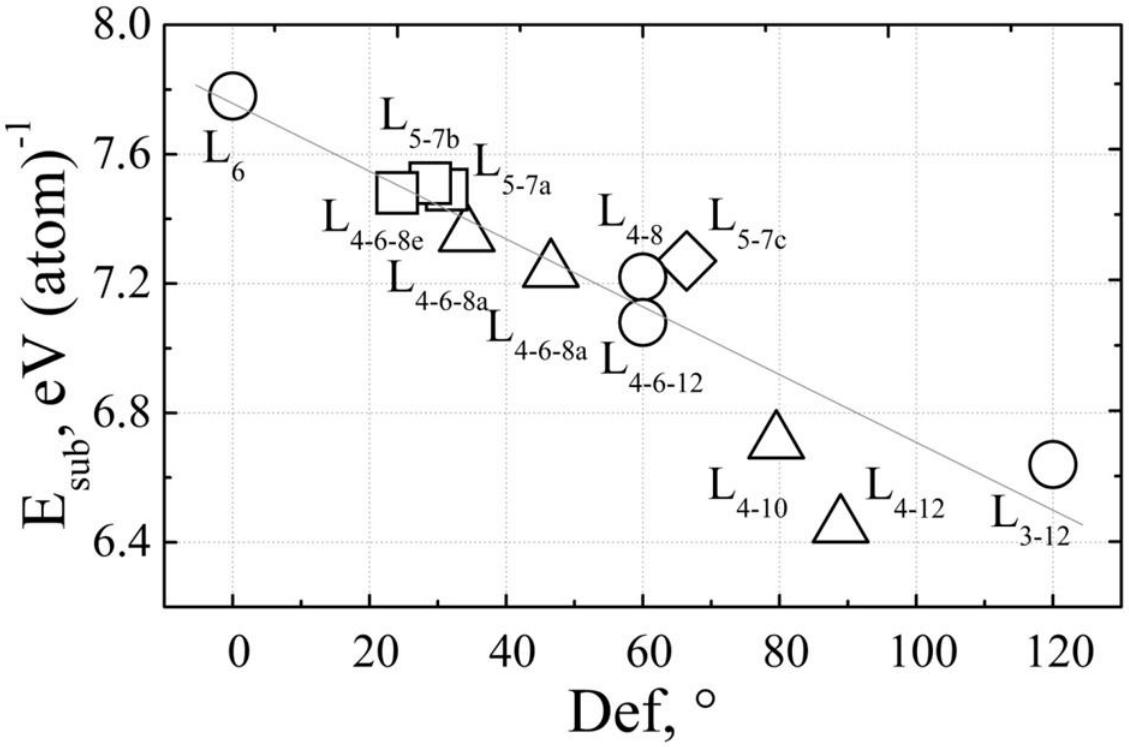



**Figure 2.** The dependency graph of the sublimation energy ($E_{sub}$) of graphene polymorphs on the deformation parameter (Def).

# Conclusions

Thus, in the course of research by the DFT-GGA method, the structure, electronic properties, and energy characteristics of twelve polymorphic graphene forms were calculated. The dependence of the sublimation energy of graphene layers on the degree of distortion of their structure is established in comparison with the structure of hexagonal graphene. Two graphene polymorphs were found, both of which should have semiconductor properties and sufficient stability to exist stably under normal conditions.

# Contacts

Maxim E. Belenkov

Chelyabinsk State University

E-mail: me.belenkov@gmail.com

Andrey E. Kochengin

Chelyabinsk Regional Clinical Center of Oncology and Nuclear Medicine

E-mail: kochengin.ae@gmail.com

Vladimir M. Chernov

Chelyabinsk State University

E-mail: chernov@csu.ru

Evgeny A. Belenkov

Chelyabinsk State University

E-mail: belenkov@csu.ru

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