II INTERNATIONAL WORKSHOP
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ADVANCES in Materials Science

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«II International Workshop on Advances in Materials Science – AMS-II - 2021»

«Ab initio calculations of new α-$L_{5\text{-}7a}$ and β-$L_{5\text{-}7a}$ graphyne polymorphic varieties»

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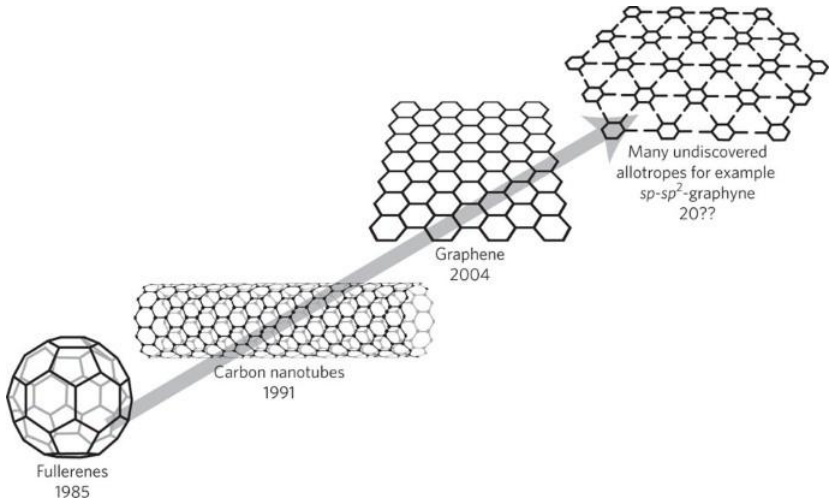
Problem statement

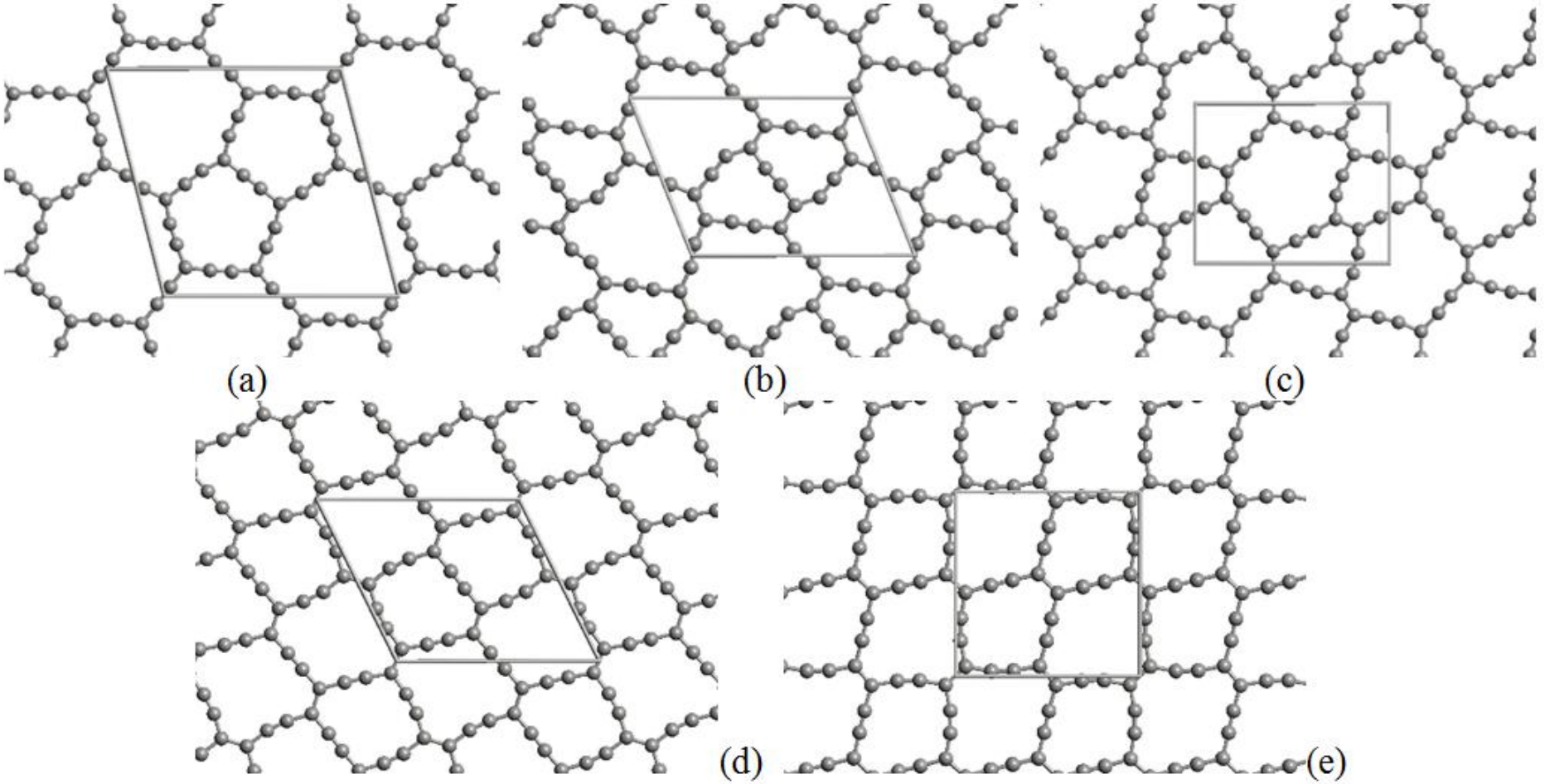


The best known two-dimensional monolayer is graphene. Based on graphene layers it is possible to design various nanoelectronic devices, which can provide the transition from microelectronics to nanoelectronics and increase the density of information storage in electronic devices and their speed. The obstacle to the use of graphene layers in electronics is that their conductivity is metallic, and electronic devices require layered nanostructures with semiconductor properties. It is possible to change the properties of carbon monolayers by forming them from atoms in different hybridized states. This work is studies $sp+sp^2$ carbon compounds (graphyne layers) based on 5-7a graphene layer was investigated, and the their structural and energy parameters and electronic properties were calculated.

Solution methods

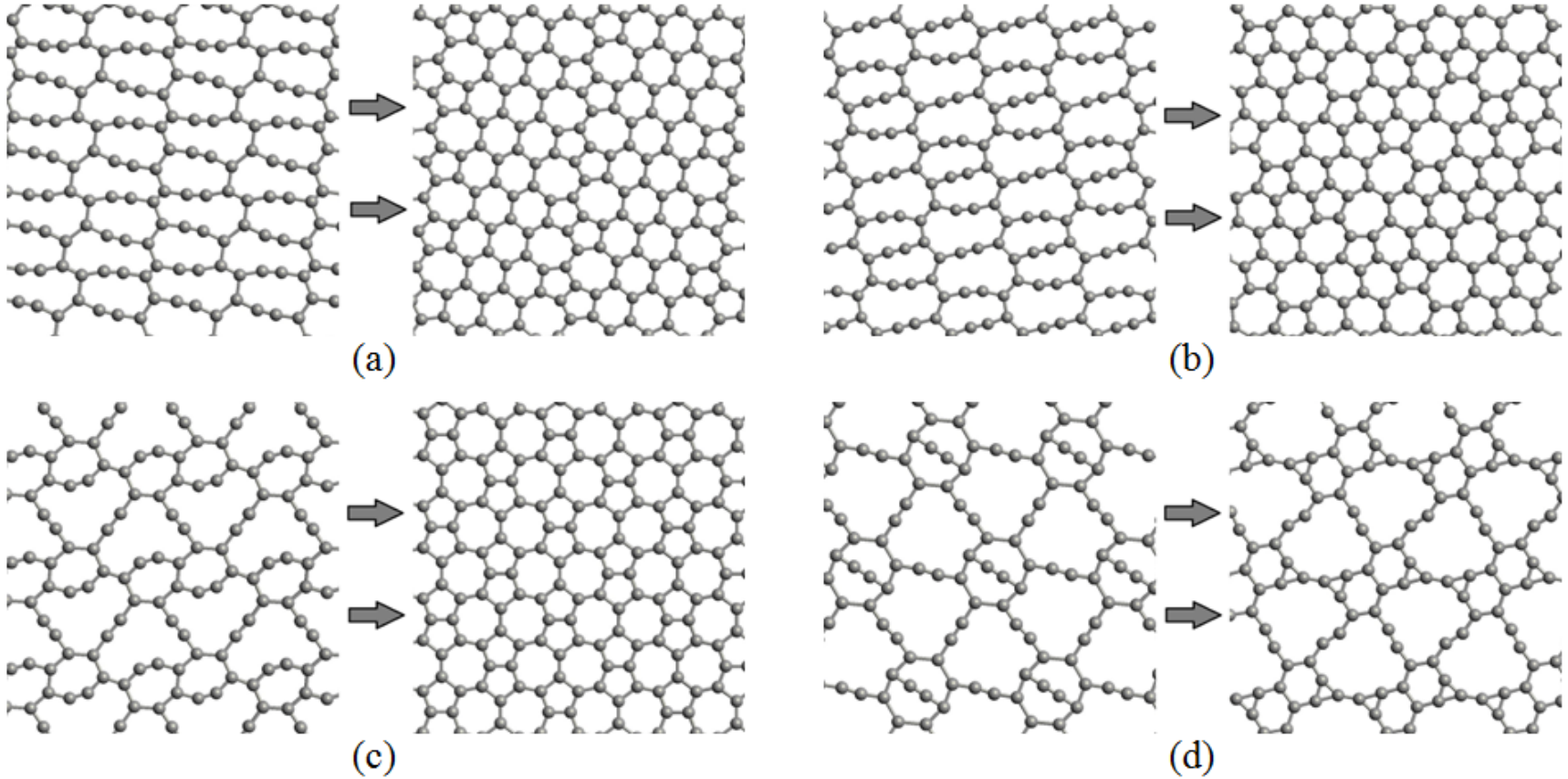
The model of construction of the sp+sp^2 graphyne layers was performed by replacing the carbon-carbon bonds in the graphene layers (the atoms in which are in three-coordinated, sp^2-hybridized states) with two-atom fragments of the carbyne chains (the atoms in which are two-coordinated, sp-hybridized). When one bond at each atom of the graphene layer is replaced with a carbyne chain, four structural varieties of γ-graphyne layers are obtained. Replacing two bonds are results in four β varieties of graphyne layers. If we replace all the bonds at each atom with carbyne chains, we obtain only one layer with an α structure. The structural parameters obtained at this stage were used as inputs for further calculations by Density Functional Theory (DFT) in Generalized Gradient Approximations (GGA). DFT-GGA calculations were performed using the Quantum ESPRESSO software package

Results



Geometrically optimized by the DFT-GGA method stable structures of the graphyne layers modeled on the graphene layer $L_{5\text{-}7a}$: (a) α-$L_{5\text{-}7a}$; (b) β1- $L_{5\text{-}7a}$; (c) β2- $L_{5\text{-}7a}$; (d) β3- $L_{5\text{-}7a}$; (e) β4-$L_{5\text{-}7a}$.

Results



Transformation of the structure of γ-$L_{5\text{-}7a}$ graphyne layers during geometric optimization: (a) γ1-$L_{5\text{-}7a}$ graphyne layer is transformed to $L_{5\text{-}6\text{-}7a}$ graphene layer; (b) γ2-$L_{5\text{-}7a}$ graphyne layer is transformed to $L_{5\text{-}6\text{-}7b}$ graphene layer; (c) γ3-$L_{5\text{-}7a}$ graphyne layer is transformed to $L_{5\text{-}7a}$ graphene layer; (d) γ4-$L_{5\text{-}7a}$ graphyne layer is transformed to $L_{3\text{-}6\text{-}13}$ graphyne layer.

Results

Table 1. Structural characteristics and some properties of the graphyne layers modeled on the graphene layer $L_{5\text{-}7a}$.

Graphyne layer	α-$L_{5\text{-}7a}$	β1-$L_{5\text{-}7a}$	β2-$L_{5\text{-}7a}$	β3-$L_{5\text{-}7a}$	β4-$L_{5\text{-}7a}$
a, Å	13.4	12.1	11.2	10	10
b, Å	13.4	9.2	9.3	11.1	10
γ, °	104.2	111.6	90	116.0	90
N, atom	32	24	24	24	24
P	10	12	12	12	7
ρ, mg/m^2	0.37	0.46	0.46	0.48	0.48
L(sp-sp), Å	1.215	1.249	1.255	1.243	1.241
L(sp-sp^2), Å	1.424	1.414	1.412	1.412	1.416
L(sp^2-sp^2), Å	-	1.474	1.459	1.452	1.443
E_{total}, eV/atom	-156.22	-156.22	-156.27	-156.34	-156.34
ΔE, eV/atom	1.10	1.10	1.05	0.98	0.98
E_{sub}, eV/atom	6.66	6.66	6.71	6.78	6.78
E_F, eV	-4.69	-4.71	-4.64	-4.84	-4.83

Results

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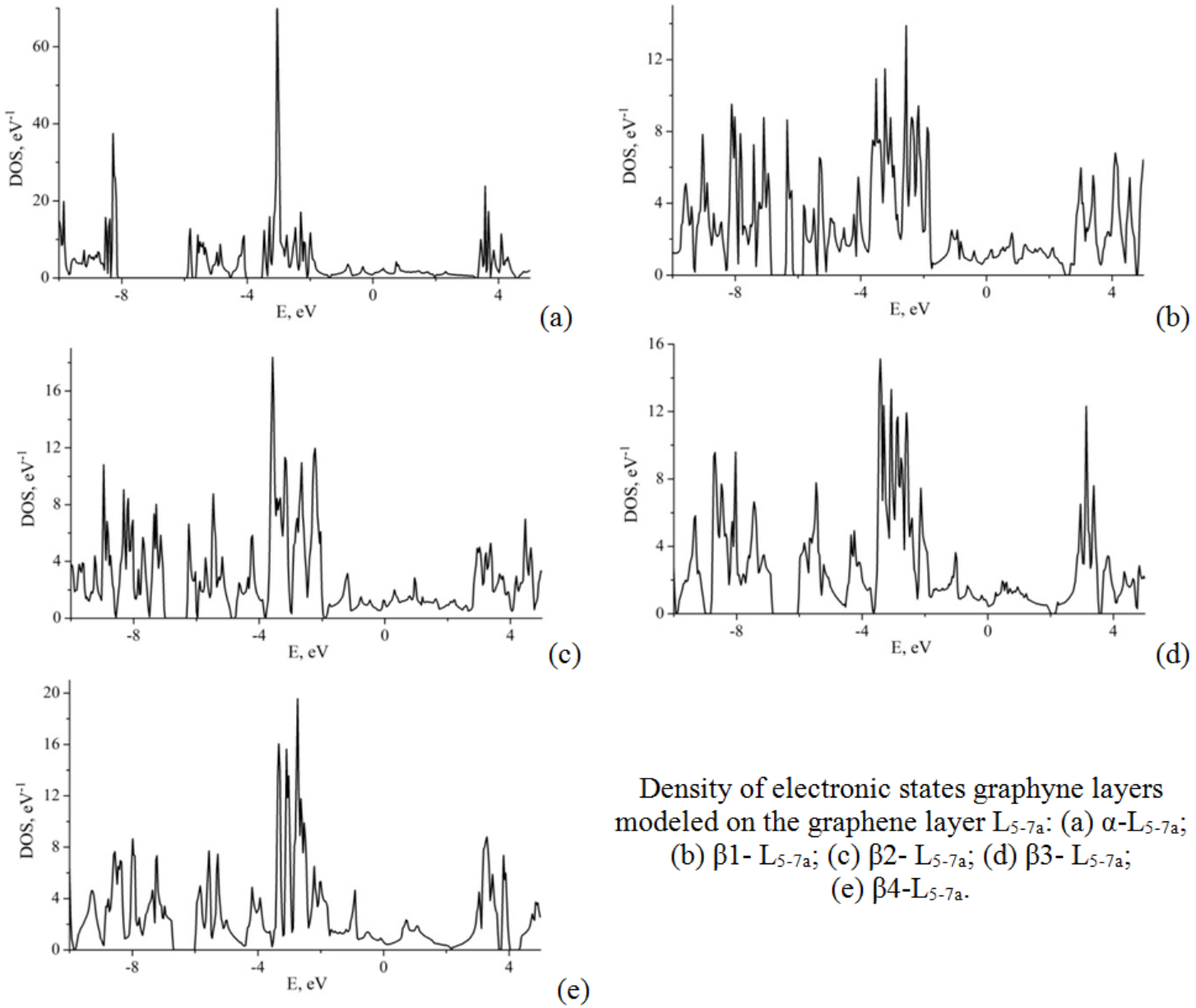

Density of electronic states graphyne layers modeled on the graphene layer $L_{5\text{-}7a}$: (a) α-$L_{5\text{-}7a}$; (b) β1- $L_{5\text{-}7a}$; (c) β2- $L_{5\text{-}7a}$; (d) β3- $L_{5\text{-}7a}$; (e) β4-$L_{5\text{-}7a}$.

Conclusions

Thus, ab initio DFT-GGA calculations have established that only α-$L_{5\text{-}7a}$ and β-$L_{5\text{-}7a}$ graphyne layers, whose sp:sp^2 atom ratio is 3:1 and 2:1, respectively, have a stable structure. Hybrid graphyne layers of γ-$L_{5\text{-}7a}$ type consisting of sp+sp^2 hybridized atoms at a ratio of 1:1 tend to transform their structure transforming into graphene layers consisting only of sp^2 hybridized atoms. Conducting properties of the investigated graphyne layers are metallic. A possible way of experimental synthesis of the new polymorphic graphyne varieties could be polymerization of the molecular structures having the structure of the carbon framework close to the structure of the corresponding graphyne layers. Practical application of new graphyne nanostructures is possible as molecular sieves, in hydrogen power engineering and in lithium batteries.

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