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«MIP: Engineering-III 2021: Modernization, Innovations, Progress: Advanced Technologies in Material Science, Mechanical and Automation Engineering»

«New structural type of layered boron nitride BN-$L_{4\text{-}6\text{-}8e}$»

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Problem statement

Boron nitride compounds can have a structure similar to that of carbon compounds. Graphene-like boron nitride layers, in contrast to graphene layers, show semiconducting properties, which makes them a promising material for nanoelectronics. Graphene layers can have different structures, theoretically predicted the possibility of the existence of a number of polymorphic graphene varieties: L_6, L_{4-8}, L_{3-12}, L_{4-6-12}, L_{5-7}, etc.. Similar structural types can exist for boron nitride. Various polymorphs of graphene and boron nitride differ in structure, properties, and stability. A comparative analysis of polymorphs performed for graphene showed that one of the most stable structural varieties of graphene is the L_{4-6-8e} layer. The possibility of the existence of boron nitride layers with a structure similar to that of this graphene polymorph has not been previously investigated. Therefore, in this work, we performed ab initio calculations of the crystal structure, band structure, and densities of electronic states of the new BN-L_{4-6-8e} polymorph.

Solution methods

The structure of the new boron nitride layer was simulated by replacing carbon atoms in the $L_{4\text{-}6\text{-}8e}$ graphene layer with boron and nitrogen atoms. Atomic substitution was performed so that each boron atom in the structure formed three covalent bonds with neighboring nitrogen atoms (figure 1). Optimization of the primary structure was performed by the density functional theory method (DFT). The calculations used the generalized gradient approximation (GGA). Simulation was performed using the Quantum ESPRESSO software package. The k-point grid was 12 × 12 × 12. The cutoff energy (E_{cutoff}) for the plane wave basis was 70 Ry. In the calculations, we considered BN layers packed in stacks. The distance between the layers in the stack was taken to be 1 nm, so that adjacent layers practically did not affect each other. Therefore, the calculation results can be considered as corresponding to isolated 4-6-8e boron nitride layers.

Results

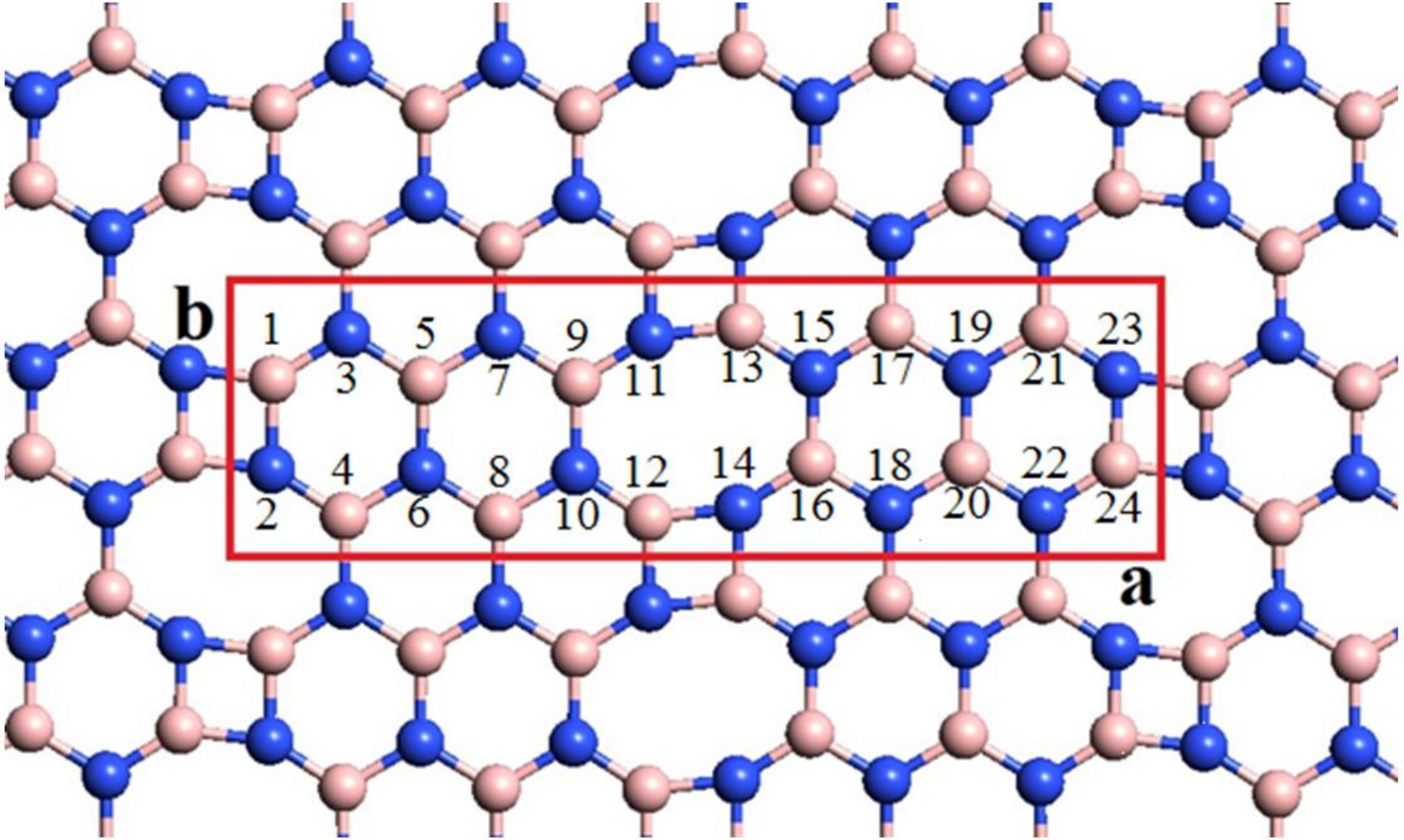


Figure 1. Geometrically optimized structure of 4-6-8e boron nitride layer and its unit cell with indication of atomic numbering (boron atoms are shown in beige, nitrogen - in blue).

Results

Table 1. Structure parameters, electronic and energy characteristics of polymorphic varieties of boron nitride (* - values of structural parameters of parameters from works are given for comparison).

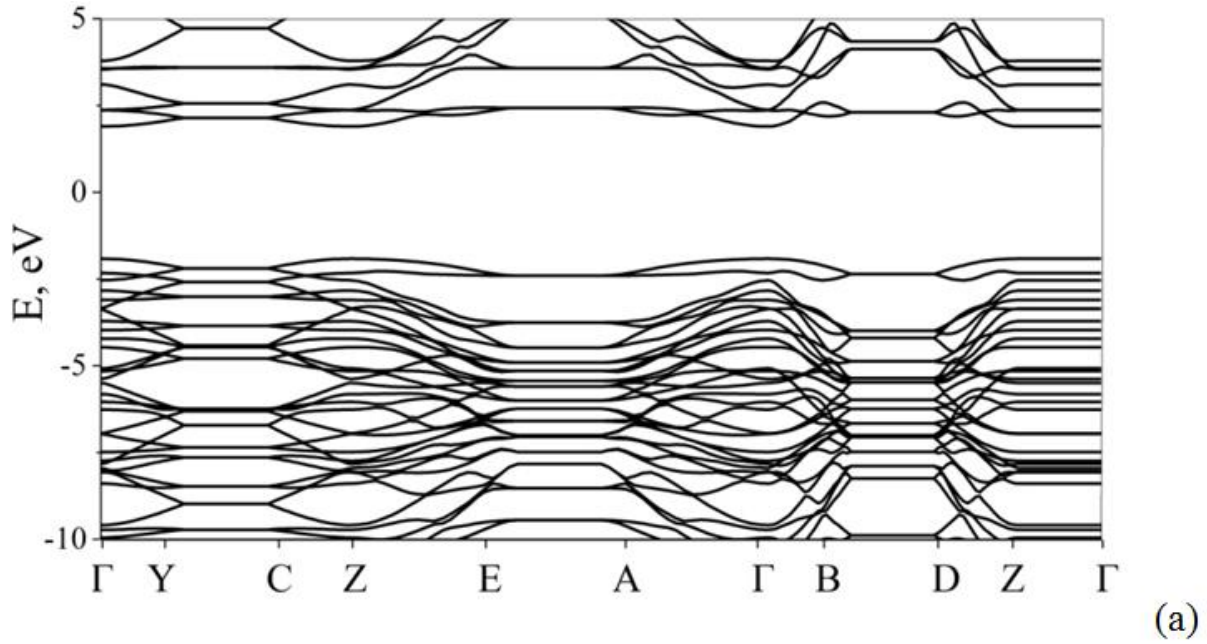
Parameters	BN-$L_{4\text{-}6\text{-}8e}$	BN-L_6*	BN-$L_{4\text{-}6\text{-}8b}$
Crystal family	Tetragonal	Hexagonal	Tetragonal
a (nm)	1.523	0.251	1.019
b (nm)	0.443	0.251	0.449
Rng_1	$4^1 6^1 8^1$	6^3	$4^1 6^1 8^1$
Rng_2	$6^2 8^1$	-	$6^2 8^1$
Rng_3	6^3	-	-
N (atom)	24	2	16
ρ (mg $(m)^{-2}$)	0,732	0.754	0.7204
E_{total} (eV $(u.c.)^{-1}$)	-4236.82	-353.43	-2823.23
E_{total} (eV $(BN)^{-1}$)	-353.07	-353.43	-353.90
E_{subl} (eV $(BN)^{-1}$)	17.78	18.14	17.61
Δ (eV)	3.8332	4.686	3.896
E_F (eV)	-3.8807	-3.764	-3.9399

Results

Table 2. The lengths of interatomic bonds and the angles between bonds in the structure of the BN-$L_{4\text{-}6\text{-}8e}$ layer

Interatomic bond lengths	Atomic type		The angle between the bonds	Atomic type	
	N	B		N	B
L_1 (nm)	0.1455	0.1456	φ_1 (°)	122.08	121.206
L_2 (nm)	0.1467	0.1463	φ_2 (°)	121.44	121.02
L_3 (nm)	0.1471	0.1471	φ_3 (°)	116.48	117.78
L_4 (nm)	0.1416	0.1467	φ_4 (°)	121.05	123.13
L_5 (nm)	0.1467	0.1416	φ_5 (°)	120.59	119.99
L_6 (nm)	0.1454	0.1454	φ_6 (°)	118.36	116.87
L_7 (nm)	0.1416	0.1419	φ_7 (°)	83.98	122.76
L_8 (nm)	0.1471	0.1472	φ_8 (°)	121.82	96.02
L_9 (nm)	0.1467	0.14670	φ_9 (°)	154.21	141.22
			Def (°)	82.37	58.68

Results



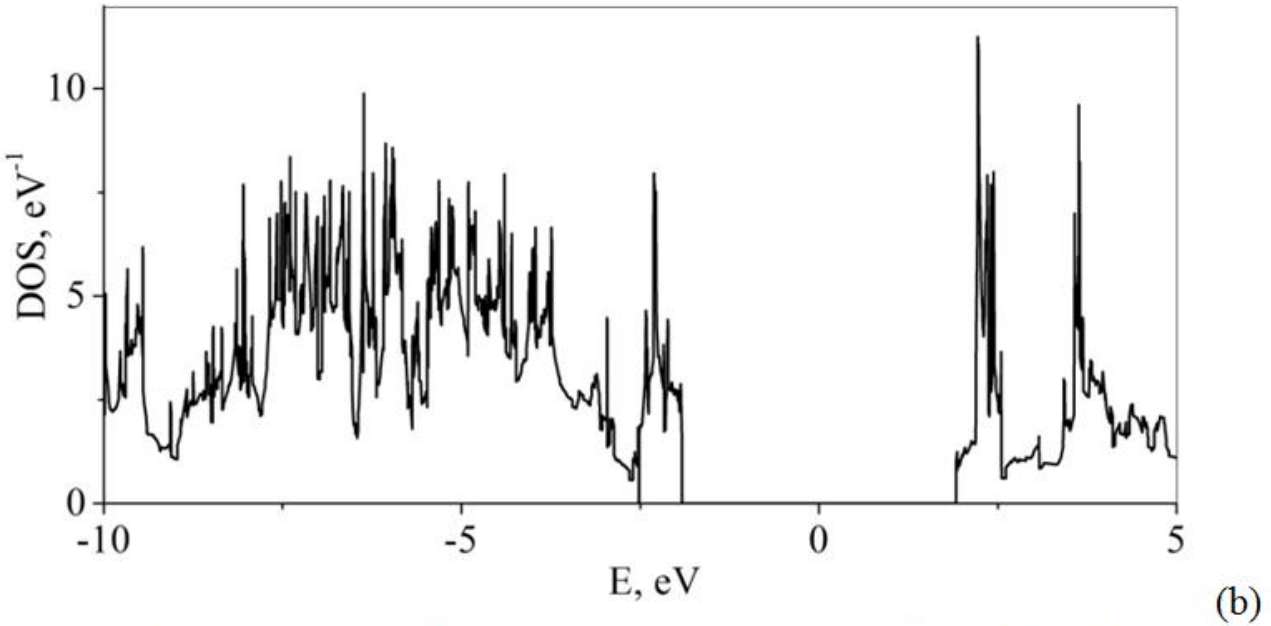


Figure 2.Band structure (a) and density of electronic states (b) of the BN-$L_{4\text{-}6\text{-}8e}$ layer.

Conclusions

In this work, the structure, electronic and energy characteristics of a new structural type of boron nitride - the BN-$L_{4\text{-}6\text{-}8e}$ layer were calculated using the first-principle DFT-GGA method. The relatively high sublimation energy of 17.78 eV $(BN)^{-1}$ compared to other boron nitride layered polymorphs indicates that the BN-$L_{4\text{-}6\text{-}8e}$ layer should have a stable structure under normal conditions. The rectangular unit cell of the layer contains 24 atoms. The values of the vectors of elementary translations are a = 1.523 nm, b = 0.443 nm. The lengths of B-N interatomic bonds vary in the range from 0.1416 to 0.1471 nm, and the angles between the bonds, in the range from 83.98° to 154.21°. The band gap for the BN-$L_{4\text{-}6\text{-}8e}$ layer is 3.83 eV. This layer must be a wide-gap semiconductor and can find practical application in the design of heterostructures for nanoelectronic devices.

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