

Controlling the electronic properties of quasi-2D borophene/GaN and borophene/ZnO van der Waals heterostructures through deformation

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Within the framework of density functional theory, an *ab initio* study of the influence of uniaxial and biaxial compression/tension deformation on the electronic properties of two types of van der Waals quasi-2D heterostructures is carried out. The first type of heterostructures is formed by 2D monolayers of buckled triangular borophene and graphene-like gallium nitride. The second type of heterostructures is formed by 2D monolayers of buckled triangular borophene and graphene-like zinc oxide. The cases of deformation that lead to the appearance of an energy gap in the band structure of the studied heterostructures are determined. To explain the reason for the opening of the gap, calculations of the distributions of the total and partial densities of electronic states are performed. A numerical estimate of the magnitude of the *p*-type Schottky barrier for holes and the *n*-type Schottky barrier for electrons in borophene/GaN and borophene/ZnO heterostructures is given.

Keywords: density functional theory, band structure, density of states, energy gap, Schottky barrier.

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Introduction

Vertical stacking of various 2D-crystals of atomic thickness in the form of layered heterostructures with a Van der Waals type of bond between the layers makes it possible to obtain new materials with attractive properties [1,2]. Both traditional 2D-materials such as graphene, boron nitride, molybdenum and tungsten disulfides and diselenides, zinc oxide, and recently synthesized representatives of carbides, nitrides and carbonitrides of transition metals, as well as metal-organic compounds are used for the formation of vertical Van der Waals heterostructures [3–6]. Due to their promising electronic and optical properties, Van der Waals heterostructures are widely used for designing vertical field-effect transistors, photodetectors, light-emitting and photovoltaic devices [7–10]. The successful synthesis of borophene [11,12] stimulated interest in the construction of Van der Waals heterostructures based on borophene. Borophene is a two-dimensional boron crystal and its atomic structure comprises triangular and hexagonal elements [13]. Borophene is rightfully considered to be one of the most promising single-element 2D-materials for nano- and optoelectronics due to such unique properties as mechanical strength and flexibility, high thermal and electrical conductivity, as well as optical transparency [14–16]. The presence of many allotropic forms, differing in configurations of covalent bonds between boron atoms allowing it to be successfully combined with different 2D-crystals in a vertical heterostructure is one

of the main advantages of borophene. The possibility of creation of borophene/g-C₂N [17], borophene/InSe [18], borophene β_{12}/MX_2 (M = Mo, W and X = S, Se) [19] Van der Waals heterostructures and their subsequent use as metal-semiconductor contacts with an adjustable Schottky barrier height has been already demonstrated. The synthesis of vertical borophene-graphene heterostructures which are much needed for the development of humidity sensors was reported in Ref. [20]. It is predicted by *ab initio* methods that borophene/boron nitride and borophene/MoS₂ Van der Waals heterostructures are promising materials for creating molecular sensors [21,22]. Two new atomic configurations of borophene Van der Waals quasi-2D heterostructures such as borophene/GaN and borophene/ZnO are considered in this work. These configurations include buckled triangular borophene, which has the highest energy stability among other allotropic forms [23]. Graphene-like monolayers ZnO and GaN have previously been successfully used to form Van der Waals heterostructures based on graphene, which have demonstrated promising electronic and optoelectronic properties [24,25]. The close similarity of the parameters of the GaN and ZnO crystal lattice with the buckled borophene crystal lattice makes it possible to significantly reduce the size of the borophene/GaN and borophene/ZnO calculated atomic structures. The purpose of this work is to study by *ab initio* methods the possibility of controlling the electronic properties of borophene/GaN and borophene/ZnO Van der Waals heterostructures using mechanical strain.

1. Research methods

The study was conducted based on the density functional theory (DFT), implemented in the SIESTA 4.1.5 software package [26]. The generalized gradient approximation (GGA) was used in the Perdew, Burke and Ernzerhof (PBE) parametrization to describe the exchange-correlation effects [27]. The Van der Waals interaction between the layers of the heterostructure was taken into account by adding a dispersion correction term to the total energy within the framework of the DFT-D2 Grimme correction scheme [28]. A basic set of split valence orbitals DZP, including polarization functions, was used for optimization of the geometric parameters of the structure. Not only the coordinates of the atoms varied during the optimization, but also the translation vectors of the supercells. Relaxation of the structure was carried out until all components of the forces acting on atoms became less than 10^{-4} eV/Å. The vacuum gap was no less than 20 Å to exclude any impact of the heterostructure layers on each other in the nonperiodic direction. The cutoff energy was set to 300 Ry. LDA/GGA+U semi-empirical scheme in the modification of Dudarev et al. was used to solve the problem of underestimation of the band gap of the material [29].

2. Atomic structure of supercells of borophene/GaN and borophene/ZnO heterostructures

The construction of rectangular supercells of borophene/GaN and borophene/ZnO quasi-2D heterostructures is described below. The unit cells of graphene-like GaN and ZnO monolayers were taken from the open access database Materials Project [30]. The initial cell translation vectors were $L_x = 3.20$ Å and $L_y = 5.55$ Å for both 2D-structures. The data from [31] were used for the construction of buckled triangular borophene lattice cell with a triangular crystal lattice. The translation vectors of the lattice cell of corrugated borophene with a triangular crystal lattice were $L_x = 1.61$ Å; $L_y = 2.86$ Å. Next, the unit cells of borophene and GaN monolayers described above were superimposed to form a rectangular supercell of the borophene/GaN heterostructure and unit cells of borophene and ZnO monolayers to form a rectangular supercell of the borophene/ZnO heterostructure. It was followed by the optimization of supercell atomic structure during which not only the coordinates of the atoms, but also the translation vectors were varied. The total energy was the target function. The atomic configurations of the supercells obtained as a result of optimization are shown in Fig. 1. $L_x = 3.35$ Å and $L_y = 6.10$ Å were the translation vectors of the borophene/GaN supercells, $L_x = 3.28$ Å and $L_y = 5.83$ Å were translation vectors of borophene/ZnO supercells. The distance between the borophene and GaN

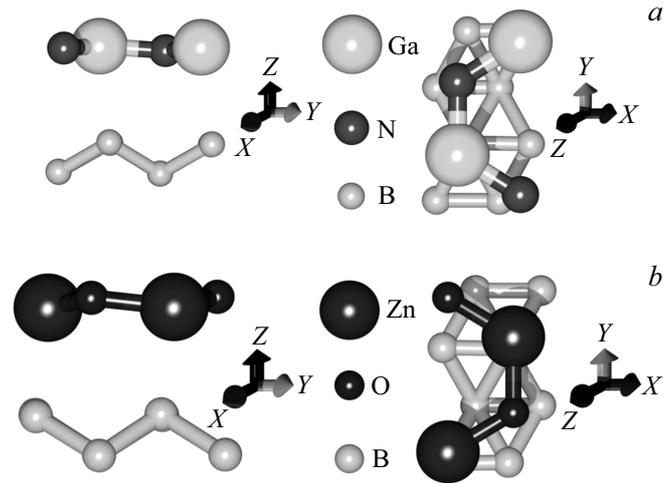


Figure 1. Atomic structure of rectangular supercells of borophene/GaN (a) and borophene/ZnO (b) Van der Waals quasi-2D heterostructures. The figure on the left shows the view of supercells in the plane YZ, the figure on the right shows the view of supercells in the plane XY. The supercells were broadcast along the axes X and Y.

layers along the Z axis was 2.91 Å, the distance between the layers of borophene and ZnO was 2.51 Å.

The constructed supercells were tested for thermodynamic stability, which was estimated by the magnitude of the binding energy (the difference between the total energy of the heterostructure and the total energy of its constituent monolayers). The binding energy is ~ -50 meV/atom for the borophene/GaN heterostructure, the binding energy is ~ -80 meV/atom for the borophene/ZnO heterostructure. Negative values of the binding energy indicate that the studied heterostructures are stable in terms of energy. The binding energy of the borophene/GaN and borophene/ZnO heterostructures exceed the binding energy of Janus-like MoSSe/GaN heterostructures by 2 times [32] and exceed the binding energy of the ZnO/GeC heterostructures by 6 times [33].

3. Electronic properties of borophene/GaN and borophene/ZnO heterostructures

A band structure was calculated for constructed supercells of borophene/GaN and borophene/ZnO Van der Waals heterostructures, a fragment of this band structure near the Fermi level (shifted to 0 eV) is shown in Fig. 2. This energy interval was chosen for demonstration, since the electronic states near the Fermi level make a decisive contribution to the electronic properties of the material. The Brillouin zone was a rectangle. The selected path of the zone bypass was G–X–S–Y–G–S. Fig. 2 shows that both heterostructures do not have an energy gap between the valence band and the conduction band.

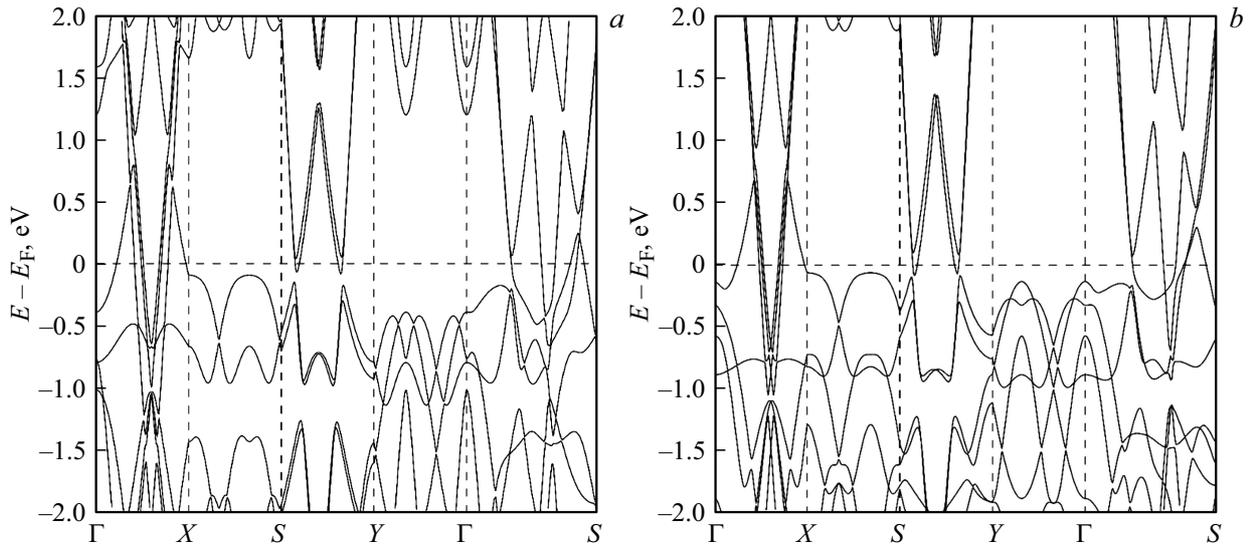


Figure 2. Fragments of the band structure near the Fermi level (shifted to 0 eV) of the borophene/GaN (a) and borophene/ZnO (b) Van der Waals heterostructures.

The distributions of total (TDOS) and partial densities of electronic states (PDOS) were analyzed for explaining the above-mentioned features of the electronic structure of the borophene/GaN and borophene/ZnO Van der Waals heterostructures. The calculated distributions of TDOS and PDOS are shown in Fig. 3. According to Fig. 3, *a*, the vacant $2p$ -orbitals of nitrogen atoms make the main contribution to the formation of electronic states in the valence band (to the left of 0 eV) for the borophene/GaN heterostructure, while the formation of electronic states in the conduction band is attributable to the contribution of vacant $2p$ -orbitals of boron atoms. Similarly, Fig. 3, *b* shows that for borophene/ZnO heterostructure, the main contribution to the formation of electronic states of the valence band is made by vacant $2p$ -orbitals of nitrogen atoms, and vacant $2p$ -orbitals of boron atoms make the main contribution to the formation of electronic states of the conduction band. Therefore, it is possible to conclude that borophene makes a decisive contribution to the formation of the conduction band of the borophene/GaN and borophene/ZnO heterostructures, explaining their gap-free nature.

Having analyzed the data on the patterns of the electronic structure of the initial configurations of the borophene/GaN and borophene/ZnO Van der Waals heterostructures, we proceeded to identify ways to control their electronic properties, including the study of the possibility of opening an energy gap in the band structure. Various types of mechanical strains were considered as such methods, namely uniaxial and biaxial extension/compression, which are often found in a real experiment. The cases of uniaxial compression and extension strain (along the axis Y) by 0–14%, biaxial compression and extension strain (along the axes X and Y) by 1–10% were considered. The selected strain intervals are attributable to the computational

complexity of the quantum calculations performed for the studied heterostructures. At the same time, there was not task of determination of their tensile/compressive strength limits.

It was found that the energy gap between the valence band and the conduction band of the borophene/GaN heterostructure opens in cases of uniaxial compression by 14% and biaxial compression by 4%. The gap size in the first case is 0.028 eV and 0.018 eV in the second case. PDOS charts are provided on Fig. 4 to explain the reason for the opening of the energy gap in the borophene/GaN heterostructure in these strain cases. It can be seen that there are no electronic states at the Fermi level in the DOS distributions of $2s$ - and $2p$ -orbitals of boron atoms, $2s$ - and $2p$ -orbitals of nitrogen atoms and $4s$ - and $4p$ -orbitals of Ga atoms. This is the reason for the opening of the energy gap in the zone structure. The opening of an energy gap in the band structure of the borophene/ZnO heterostructure was found for cases of uniaxial extension by 10% and biaxial compression by 6%. The value of the opened energy gap is 0.063 eV in the first case. Calculated distributions of PDOS for this case (Fig. 5, *a*) showed that DOS of all orbitals of borophene atoms and ZnO atoms have zero density of states near the Fermi level. Consequently, each orbital contributes to the opening of the energy gap between the zones. The gap value is 0.012 eV in the second case. The results of the calculation of PDOS clearly demonstrated (Fig. 5, *b*) that zero DOS is present in the distributions of PDOS of s - and p -orbitals of boron and nitrogen atoms, as well as s - and d -orbitals of zinc atoms with such a magnitude of biaxial compression.

The sensitivity of the electronic structure of the studied heterostructures to deformations was also monitored by changing the position of the Fermi level. In the absence of strain, the Fermi level is -5.25 eV for the borophene/GaN

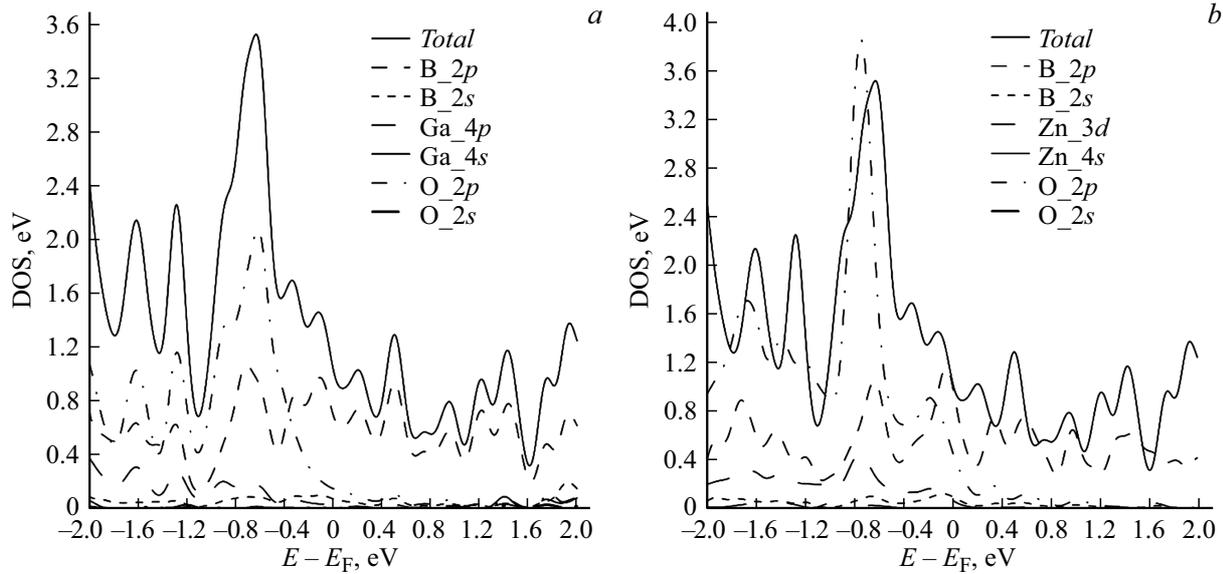


Figure 3. Graphs of the total and partial DOS of borophene/GaN (a) and borophene/ZnO Van der Waals quasi-2Dheterostructures (b) near the Fermi level (shifted to 0 eV).

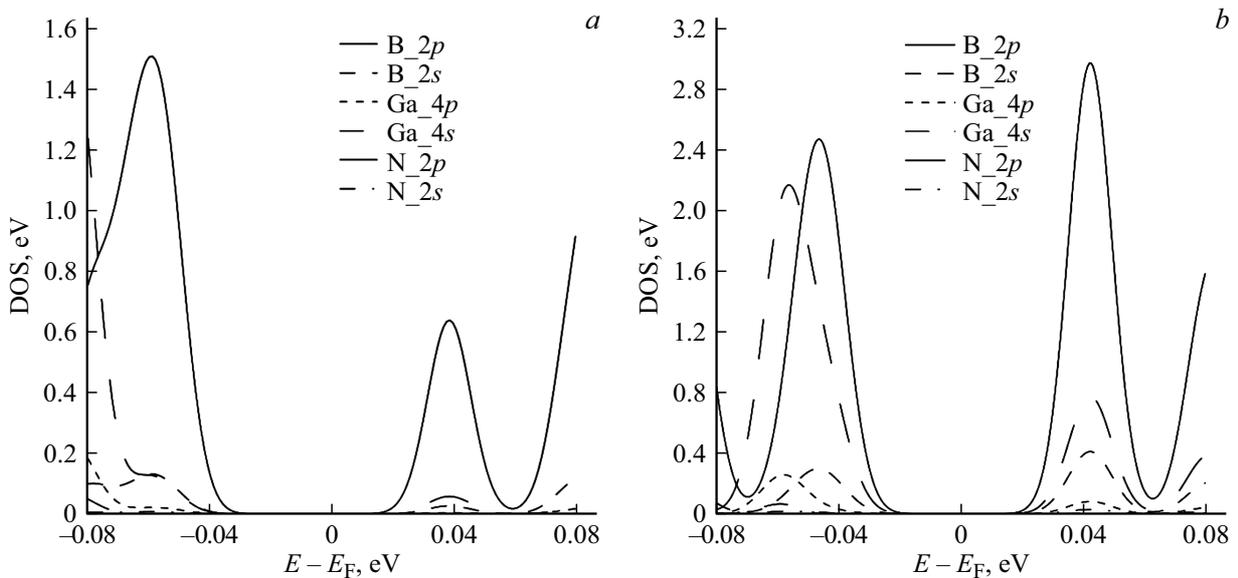


Figure 4. Graph of partial DOS near the Fermi level (shifted to 0 eV) for the borophene/GaN Van der Waals quasi-2Dheterostructure with uniaxial compression by 14% (a) and biaxial compression by 4% (b).

heterostructure and -5.90 eV for the borophene/ZnO heterostructure. The Fermi level of the borophene/GaN heterostructure changes abruptly in case of uniaxial compression: it shifts down (towards the valence band) along the energy axis by a maximum value of 0.06 eV when compressed to 8% , it shifts up (towards the conduction band) along the energy axis by a maximum the value is 0.1 eV when compressed to 14% . The Fermi level remains unchanged in the range of small deformations ($1-6\%$). The Fermi level maintains a tendency to shift upward along the energy axis, at uniaxial extension changing by 0.1 eV at 12% tension. The Fermi level shifts down the energy axis throughout

the entire considered strain interval for borophene/ZnO heterostructure under uniaxial compression, and the shift value is 0.92 eV in case of compression by 14% . In case of uniaxial tension, on the contrary, the Fermi level shifts upwards along the energy axis. The maximum shear value of 0.3 eV is achieved in case of 12% extension. The changes of the position of the Fermi level are even more noticeable in case of biaxial extension/compression strain than in case of uniaxial extension/compression. The Fermi level shifts down the energy axis in borophene/GaN heterostructure, both under biaxial extension and biaxial compression: maximum shift is 0.3 eV in case of extension,

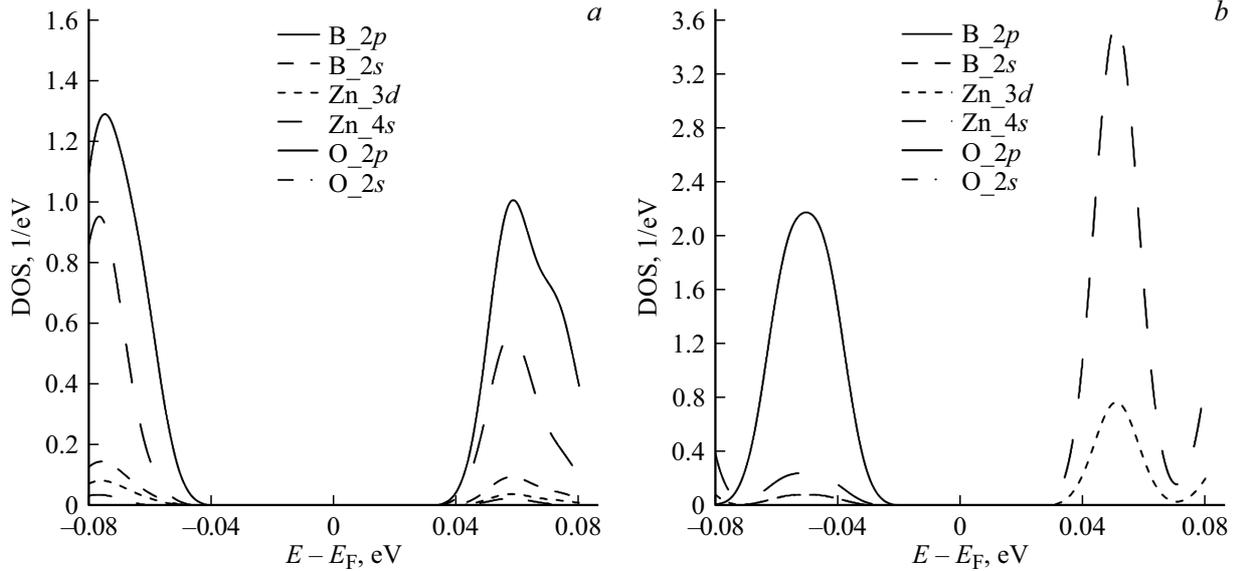


Figure 5. The graph of the partial DOS near the Fermi level (shifted to 0 eV) for borophene/ZnO Van der Waals quasi-2D heterostructure with uniaxial extension by 10% (a) and biaxial compression by 6% (b).

maximum shift is 0.2 eV in case of compression. For the borophene/ZnO heterostructure, the same patterns of changes in the position of the Fermi level are observed in biaxial strain as in the case of uniaxial strain. The Fermi level shifts to the left along the energy axis in case of biaxial compression, wherein the maximum shift is 1 eV (under 8% compression). The Fermi level shifts along the energy axis to the right by a maximum value of 0.6 eV at 10% extension in case of biaxial extension.

The different sensitivity of the electronic structure of the borophene/GaN and borophene/ZnO heterostructures to the same types of axial strain can be explained by the following reasons: 1) the difference in the distances along the Z axis between monolayers in the composition of Van der Waals heterostructures supercells; 2) differences in the characteristic features of the band structure of the monolayers GaN and ZnO. The smaller distance between borophene and ZnO causes more noticeable changes in the atomic structure of the ZnO monolayer as part of the borophene/ZnO heterostructure compared with changes in the atomic structure of the GaN monolayer as part of the borophene/GaN heterostructure. In particular, the magnitude of the dihedral angles is very different for GaN and ZnO monolayers: it is negative for GaN and amounts to -7.21 , and it is positive for ZnO and amounts to 19.18 . The band structure of graphene-like GaN has an indirect band gap, and graphene-like ZnO has a direct band gap with different values of the energy gap between the valence band and the conduction band [34].

The heights of the p -type Schottky barrier for holes and the heights of n -type Schottky barrier for electrons were calculated for identification of the prospects for the potential application of the studied borophene/GaN and borophene/ZnO Van der Waals heterostructures as devices

implementing a contact of metal-semiconductor type. According to the approach described in Ref. [35,36], Schottky barriers for holes or electrons are defined as the energy difference between the Fermi level and the maximum of the valence band or minimum of the conduction band of heterostructures, respectively. The numerical evaluation performed using this approach showed that the heights of Schottky barriers for holes (ϕ_h) and electrons (ϕ_e) in case of the borophene/GaN heterostructure were 0.43 and 1.04 eV, respectively, and these values amounted to 0.15 and 0.95 eV, respectively, in case of borophene/ZnO heterostructure. The possibility of controlling the value of the Schottky barrier by strain was verified by calculating ϕ_h and ϕ_e for strained borophene/GaN and borophene/ZnO heterostructures. Calculations were performed for the considered cases of maximum and minimum extension and compression uniaxial and biaxial strains, as well as for those strain cases in which an energy gap between the valence band and the conduction band opened in the band structure of Van der Waals heterostructures. The obtained calculation results are shown in the following table.

Based on the calculated data, it was found it was possible to achieve a maximum reduction of the value of the Schottky barrier ϕ_h in borophene/GaN heterostructure to 0.19 eV in the case of biaxial compression strain by 4% and the value of the Schottky barrier ϕ_e was reduced to 0.87 eV in the case of uniaxial compression strain by 14%. It was possible to achieve a maximum reduction of the value of the Schottky barrier ϕ_h in borophene/ZnO heterostructure to 0.08 eV and the value of the Schottky barrier ϕ_e was reduced to 0.67 eV in the case of uniaxial compression strain by 12%. Comparison of the obtained values of Schottky barriers with the parameters of Van der Waals heterostructures based on borophene and transition metal dichalcogenides [19] showed

Schottky barriers for holes ϕ_h and electrons ϕ_e of Van der Waals heterostructures under uniaxial and biaxial compression and tension deformation

Type of heterostructure	Type of deformation	ϕ_h , eV	ϕ_e eV
Borophene/GaN	Uniaxial compression 14%	0.38	0.87
Borophene/GaN	Uniaxial extension 6%	0.29	1.11
Borophene/ZnO	Uniaxial compression 12%	0.08	0.67
Borophene/ZnO	Uniaxial extension 10%	0.41	1.03
Borophene/GaN	Biaxial Compression 4%	0.19	1.01
Borophene/GaN	Biaxial extension 6%	0.31	0.89
Borophene/ZnO	Biaxial extension 6%	0.47	0.84
Borophene/ZnO	Biaxial extension 10%	0.23	1.10

that the strained borophene/GaN and borophene/ZnO heterostructures are superior to such heterostructures as borophene β_{12}/MoS_2 , borophene β_{12}/MoSe_2 , borophene β_{12}/WS_2 , borophene β_{12}/WSe_2 in both parameters (ϕ_h and ϕ_e).

Conclusion

Therefore, it was found based on the results of ab initio calculations that the biaxial compression strain is more effective of the two types of biaxial strain considered for controlling the electronic properties of the studied Van der Waals heterostructures. It was found that the zero density of electronic states near the Fermi level should be present in the DOS distributions of electronic orbitals of both borophene and GaN/ZnO atoms for the occurrence of an energy gap in the electronic structure of the borophene/GaN and borophene/ZnO heterostructures. At the same time, the electronic p -orbitals of boron and nitrogen atoms make a decisive contribution to the borophene/GaN heterostructure DOS distribution, while the electronic p - orbitals of boron and oxygen atoms make the main decisive contribution to the borophene/ZnO heterostructure DOS distribution. It is possible to predict based on the obtained results of calculating the height of the Schottky barrier for holes and electrons that the considered configurations of borophene/GaN and borophene/GaN quasi-2D heterostructures with electronic properties adjustable by extension/compression strain can be a promising material for nano- and optoelectronics, including Schottky barrier devices.

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Conflict of interest

The authors declare that they have no conflict of interest.

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