New van der Waals Heterostructures Based on Borophene and Rhenium Sulfide/Selenide for Photovoltaics: An Ab Initio Study

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Abstract: One of the urgent tasks of modern materials science is the search for new materials with improved optoelectronic properties for various applications of optoelectronics and photovoltaics. In this paper, using ab initio methods, we investigate the possibility of forming new types of van der Waals heterostructures based on monolayers of triangulated borophene, and monolayers of rhenium sulfide (ReS), and rhenium selenide (ReSe$_2$), and predict their optoelectronic properties. Energy stable atomic configurations of borophene/ReS$_2$ and borophene/ReSe$_2$ van der Waals heterostructures were obtained using density functional theory (DFT) calculations in the Siesta software package. The results of calculating the density of electronic states of the obtained supercells showed that the proposed types of heterostructures are characterized by a metallic type of conductivity. Based on the calculated optical absorption and photocurrent spectra in the wavelength range of 200 to 2000 nm, it is found that borophene/ReS$_2$ and borophene/ReSe$_2$ heterostructures demonstrate a high absorption coefficient in the near- and far-UV-ultraviolet) ranges, as well as the presence of high-intensity photocurrent peaks in the visible range of electromagnetic radiation. Based on the obtained data of ab initio calculations, it is predicted that the proposed borophene/ReS$_2$ and borophene/ReSe$_2$ heterostructures can be promising materials for UV detectors and photosensitive materials for generating charge carriers upon absorption of light.

Keywords: van der Waals heterostructures; ab initio methods; density functional theory; triangulated borophene; rhenium sulfide; rhenium selenide; density of electronic states; absorption coefficient; photocurrent spectra; UV radiation

1. Introduction

The discovery of graphene and the identification of its unique properties stimulated the search for other 2D materials of atomic thickness with controllable properties, capable of overcoming the limitations inherent in graphene; in particular, providing an opening of the forbidden gap in the electronic structure of the material. Thus, the attention of researchers was drawn to isolated monolayers and multilayer crystals of hexagonal boron nitride (hBN), molybdenum disulfide (MoS$_2$), other transition metal dichalcogenides (TMD), layered oxides, and elements of IV and V groups [1–5]. The interest in atomically thin two-dimensional (2D) layered structures has recently increased, in connection with their potential application in photonics, electronics, energy conversion, and storage, with the possibility of replacing traditional materials [6,7]. Along with the study of graphene-like 2D materials, the research field related to the design of vertical heterostructures, by stacking different 2D crystals on top of each other in a precisely selected sequence, has actively developed [8–10]. Strong covalent bonds ensure the stability of 2D crystals in the plane, and the action of van der Waals forces is sufficient to hold the stack of layers together.
Such structures, called van der Waals heterostructures, are obtained in practice using the technique of direct mechanical assembly (micromechanical superposition) [11], as well as chemical vapor deposition (CVD) [12] and physical epitaxy [13] methods. The created van der Waals heterostructures find their application in the development of nano- and optoelectronic devices, including field-effect tunneling transistors [14], memory devices [15], photodetectors [16], solar cells [17], and rechargeable batteries [18]. Photovoltaics is considered one of the most promising fields of application for van der Waals heterostructures. Certain successes have already been achieved in the field of creating solar cells based on TMD heterostructures, built mainly on the basis of well-studied molybdenum disulfide (MoS$_2$) and molybdenum diselenide (MoSe$_2$), as well as tungsten disulfide (WS$_2$) and tungsten diselenide (WSe$_2$) [19–23]. However, the photoelectric cells created on the basis of MoS$_2$ and WS$_2$ are mainly focused on operating in a narrow region of the visible range of the electromagnetic spectrum, and only slightly cover the region of the near-infrared range [24–27]. At the same time, the emergence of new representatives of TMD, such as ReS$_2$, ReSe$_2$, TiS$_2$, TiSe$_2$, and HfS$_2$ [28,29], exhibiting pronounced semiconductor properties, opens new possibilities in the direction of creating broadband photoelectric cells based on TMD.

As is known, when constructing a layered heterostructure, the key point is the matching of the crystal lattices of the combined 2D materials. Borophene, which is currently being successfully synthesized, can be considered a promising material for creating new 2D heterostructures [30,31]. Due to borophene polymorphism, various configurations of bonds between the boron atoms should relax the crystallographic lattice matching requirements for the combined 2D materials. In addition, the unique combination of properties of borophene, such as lightness, flexibility, mechanical strength, high conductivity, and optical transparency, makes it one of the most promising single-element 2D materials for nano- and optoelectronic purposes [32]. The first successes have already been achieved in the field of creating and studying borophene-based heterostructures. Liu and Hersam [33] reported on the successful experimental implementation of vertical borophene/graphene heterostructures. During synthesis in an ultrahigh vacuum chamber, graphene was first grown on a Ag (111) metal substrate at a higher temperature, and then boron was deposited on the same substrate. Despite the imperfect crystallographic lattice and symmetry matching, the created graphene/borophene heterostructures have almost perfect atomic consistency. An alternative approach to obtaining vertical heterostructures based on borophene and graphene was proposed by Hou et al. [34]. A new borophene/graphene heterostructure was obtained by heating a mixture of sodium borohydride and multilayer graphene, with the subsequent stepwise thermal decomposition of sodium borohydride, in situ in a high-purity hydrogen medium. Testing the humidity sensing behavior of the heterostructure under ambient conditions has shown that the borophene/graphene heterostructure exhibits high sensitivity (4200%) and a fast response/recovery time (10.5 s/8.3 s), with long-term stability and flexibility, which makes it suitable for creating highly efficient humidity sensors. Based on the results of ab initio calculations, Yu et al. [35] predicted that borophene/graphene heterostructures are a promising anode material, demonstrating a high adsorption energy of lithium (−2.959 eV) and a high theoretical specific capacity (1469.35 mA h/g). At the same time, the assessment of the prospects for the use of borophene-based van der Waals heterostructures for the creation of photovoltaic devices is only just beginning to be carried out. In 2020, Katoch et al. presented the results of an ab initio study of the prospects for using borophene in combination with MX$_2$ (M = Mo, W and X = S, Se) to form metal-semiconductor contact. Scientists have shown that compressively strained borophene $\beta_{12}$/MX$_2$ heterostructures can be used to implement tunable Schottky barriers [36]. However, this topic needs further development.

In this paper, using ab initio methods, we study the possibility of constructing new types of van der Waals heterostructures based on 2D sheets of borophene and rhenium sulfide/selenide, and give a preliminary estimate of their optoelectronic properties.
2. Methods and Approaches

2.1. Calculation Details

The ab initio study of van der Waals heterostructures was carried out within the framework of the density functional theory (DFT) implemented in the Siesta 4.1.5 software package [37–39]. To describe exchange-correlation effects, generalized gradient approximation (GGA) was used in the parametrization of Perdew, Burke and Ernzerhof (PBE) [40]. To describe the van der Waals interaction (vdW) between heterostructure layers, we used the correction scheme proposed by Grimme, where vdW interactions are represented by a pair force field DFT + D2 [41]. When optimizing the geometry of the structure, we used the basis set of split valence orbitals DZ2P (double zeta 2 polarization), which includes polarization functions. The integration of the Brillouin zone was carried out using the Monkhorst-Pack scheme [42] with a $12 \times 6 \times 1$ k-points mesh. The relaxation of the structure was carried out until the maximum interatomic force was less than 0.025 eV/Å. The effective Broyden-Pulay mixing scheme was used to minimize the energy of the electronic subsystem [43]. In order to avoid interaction between neighboring structures in calculations with periodic boundary conditions, the translation vector along the z-axis of the supercell was set to be greater than 20 Å. The real space mesh cutoff was chosen to be 300 Ry throughout the calculations.

To study the optical properties of van der Waals heterostructures, the complex frequency-dependent dielectric function was calculated in SIESTA software package. The calculations were carried out in the framework of the first-order time-dependent perturbation theory [44]. For this purpose, the self-consistent ground state energies and eigenfunctions were first calculated, and then they were used to calculate the transition dipole moment matrix elements. The imaginary part of the dielectric function determined the optical absorption, which was calculated from the transition rate between valance and conduction band states. The equation for calculating the absorption coefficient is as follows:

$$\alpha(\omega) = \frac{\omega}{c n(\omega)} \varepsilon_2(\omega),$$  \hspace{1cm} (1)

where $\varepsilon_2(\omega)$ is the imaginary part of the complex dielectric function, $n(\omega)$ is the refractive index, $c$ is the speed of light. The calculation of $\varepsilon_2(\omega)$ was carried out according to the following equation:

$$\varepsilon_2(\omega) = \frac{e^2}{\pi m c^3 \omega^2} \sum_{\nu,\nu'} \int_{BZ} \hat{e} \cdot \hat{p} \left| \psi_{\nu,k} \right| \left\langle \psi_{\nu',k} \right| \left( E_{\nu,k} - E_{\nu',k} - \hbar \omega \right) \delta,$$  \hspace{1cm} (2)

where the summation was carried out over each pair of states in the valence band (filled) and the conduction band (unoccupied), and integration was performed over all k-points in the Brillouin zone; the indices $\nu$ and $\nu'$ refer to the states in the conduction and valence bands, respectively, $E_{\nu,k}$ and $\psi_{\nu,k}$ are the energy and eigenfunction of these states, respectively. The electronic dipole transition matrix element is between the occupied and unoccupied states, where $\hat{e}$ is the polarization vector and $\hat{p}$ is the momentum operator. The optical characteristics of the van der Waals heterostructures were calculated for two different directions of light polarization (vector $\mathbf{E}$ is parallel to the x-axis; vector $\mathbf{E}$ is perpendicular to the x-axis) for the energy range from 0.6 eV to 20 eV using optical broadening of 0.05 eV. The optical characteristics of the heterostructures under study were calculated by integrating the Brillouin zone with a $114 \times 65 \times 1$ k-points mesh.

Based on the absorption spectrum, the photocurrent spectrum was calculated. The maximum value of the photocurrent is calculated by the following equation:

$$I_{max} = e \int_{\omega_1}^{\omega_2} \frac{\alpha(\omega) \text{Power}_{\text{solar}}(\omega)}{h\nu} d\omega,$$  \hspace{1cm} (3)

where $e$ is the electron charge; $\alpha(\omega)$ is the absorption coefficient; $\text{Power}_{\text{solar}}(\omega)$ is the solar radiation power; $h\nu$ is the energy of a quantum of solar radiation. Equation (3) is applicable
for the case of an internal quantum yield of 100%, when each absorbed photon generates an electron.

2.2. Atomistic Models of van der Waals Heterostructures

In the framework of this study, the following new atomic configurations of van der Waals heterostructures were considered: (1) the configuration based on monolayers of borophene and rhenium sulfide; (2) the configuration based on monolayers of borophene and rhenium selenide. The formation of heterostructures was carried out with the following considerations: (1) the combined layers of the heterostructure should have a small discrepancy in the vectors of the crystal lattice and differ in the type of conductivity; (2) the atomic configuration of the formed heterostructure must be energetically stable. It is known that borophene is a conductor regardless of the type of allotropic modification [45]. On the contrary, rhenium sulfide (ReS$_2$) and rhenium selenide (ReSe$_2$), depending on the type of crystal system, can exhibit either a metallic character of conductivity, both in the case of a hexagonal crystal system in ReSe$_2$ and a trigonal crystal system in ReS$_2$, and also a semiconducting character of conductivity in the case of a triclinic crystal system for both ReSe$_2$ and ReS$_2$ [46]. In this regard, the unit cells of the ReSe$_2$ and ReS$_2$ of 12 atoms with a triclinic crystal system were chosen to construct the heterostructures. They were taken from the Materials Project open-source database [47]. Among the allotropic forms of borophene, we chose borophene with a triangulated configuration. The triangulated borophene has high energy stability and geometric features that allow it to be combined with ReSe$_2$ and ReS$_2$ layers. The unit cell of triangulated borophene consists of two atoms and has optimized translation vectors, $L_x = 1.619$ Å; $L_y = 2.879$ Å, which is in good agreement with the known data [45]. Since triangulated borophene has a crystalline structure with a rectangular unit cell, for its successful combination with the ReSe$_2$ and ReS$_2$ structures, it was necessary to construct rectangular unit cells for them. Such cells, each consisting of 24 atoms, were obtained from the initial unit cells with the triclinic system by the way clearly illustrated in Figure 1. The equilibrium configurations of the obtained unit cells have the following translation vectors: $L_x = 6.411$ Å; $L_y = 11.359$ Å for ReS$_2$, and $L_x = 6.646$ Å; $L_y = 11.824$ Å for ReSe$_2$. The performed calculations of the density of electronic states (DOS) of the triclinic and rectangular unit cells showed that when passing to a rectangular cell, the features of the electronic structure of ReS$_2$ and ReSe$_2$, primarily the presence of an energy gap, remain.

In order to minimize the lattice mismatch between the combined monolayers of borophene and ReS$_2$/ReSe$_2$, the sizes of the unit cells of each monolayer were increased until the difference in the parameters of the lattice vectors was no more than 2–3%. To build borophene/ReSe$_2$ and borophene/ReS$_2$ heterostructures, the initial unit cell of borophene $1 \times 2$ (the number of atoms along the X and Y axes) was increased 16 times to a size commensurate with rectangular supercells ReSe$_2$ and ReS$_2$. The final unit cell of borophene $8 \times 32$ was already 32 atoms. When a borophene monolayer was overlaid to a rectangular cell of ReSe$_2$, the difference between the lengths of the translation vectors of the stacked monolayers was ~2.63% for the translation vector $L_x$ and ~2.67% for translation vector $L_y$. When a borophene monolayer was overlaid to a rectangular cell of ReS$_2$, the difference between the lengths of the translation vectors was even smaller, as follows: ~1% for $L_x$; ~1.38% for $L_y$. Figures 2 and 3 show the process of stacking up monolayers during the formation of the borophene/ReS$_2$ and borophene/ReSe$_2$ heterostructures.
In order to minimize the lattice mismatch between the combined monolayers of borophene and rhenium chalcogenides, the equilibrium configurations of the obtained unit cells were chosen to construct the heterostructures. They were taken from the Materials Project database [47]. Among the allotropic forms of borophene, we chose borophene with a triangulated configuration. The triangulated borophene has high energy stability and geometric features that allow it to be combined with rhenium chalcogenides.

2.2. Atomistic Models of van der Waals Heterostructures

In order to construct the supercell of van der Waals heterostructures: (a) top view; (b) side view.

Figure 1. Method for obtaining rectangular supercells of ReS$_2$ (a) and ReSe$_2$ (b) 2D structures. (Sulfur atoms are marked in yellow. Selenium atoms are marked in orange).

Figure 2. The process of constructing a supercell of van der Waals borophene/ReS$_2$ heterostructures: (a) top view; (b) side view.
Figure 3. The process of constructing a supercell of van der Waals borophene/ReSe$_2$ heterostructures: (a) top view; (b) side view.

The optimized values of the translation vectors of the borophene/ReS$_2$ heterostructure supercell were $L_x = 6.485 \, \text{Å}$ and $L_y = 11.404 \, \text{Å}$; for the borophene/ReSe$_2$ heterostructure supercell, $L_x = 6.553 \, \text{Å}$ and $L_y = 11.669 \, \text{Å}$. The distance between the borophene and ReS$_2$ layers along the $z$-axis was 2.969 Å, between the borophene and ReSe$_2$ layers it was 3.028 Å.

To estimate the energy stability of the constructed supercells of the borophene/ReS$_2$ and borophene/ReSe$_2$ heterostructures, the binding energies $E_b$ were calculated. The calculation was carried out according to the following equation:

$$ E_b = \frac{[E_{B-tr}/\text{ReS}_2(\text{ReSe}_2) - E_{B-tr} - E_{\text{ReS}_2}(\text{ReSe}_2)]}{N}, $$

where $E_{B-tr}/\text{ReS}_2(\text{ReSe}_2)$ is the total energy of the borophene/ReS$_2$ (borophene/ReSe$_2$) heterostructure, $E_{B-tr}$ is the total energy of the isolated layer of triangulated borophene, $E_{\text{ReS}_2}(\text{ReSe}_2)$ is the total energy of the isolated ReS$_2$(ReSe$_2$) layer, $N$ is the number of atoms in the heterostructure. According to the calculation results, the binding energy for both heterostructures is $\sim -0.05 \, \text{eV/atom}$. A small value of $E_b$ indicates that the layers in the heterostructure are bound by van der Waals forces. The negative value of the binding energy indicates that the structures are stable in energy, which means that they can be implemented in practice.
3. Results and Discussion

3.1. Electronic Structure of Borophene/ReS$_2$ and Borophene/ReSe$_2$ van der Waals Heterostructures

The next step in our study was the analysis of the electronic structure of the formed borophene/ReS$_2$ and borophene/ReSe$_2$ van der Waals heterostructures. To this end, calculations of the band structure were carried out, and the DOS distributions were constructed based on these calculation results. Figure 4 shows the calculated DOS distributions for both borophene/ReS$_2$ (Figure 4a) and borophene/ReSe$_2$ (Figure 4b) heterostructures, and for isolated monolayers, in order to reveal the regularities in the formation of the DOS profile for van der Waals heterostructures. As can be observed from the graphs in Figure 4, the contours of the DOS profiles of the borophene/ReS$_2$ and borophene/ReSe$_2$ heterostructures largely repeat the contours of the DOS profiles of the ReS$_2$ and ReSe$_2$ isolated monolayers, respectively. At the same time, both heterostructures demonstrate a metallic type of conductivity, as evidenced by the absence of an energy gap between the valence band and conduction band.

![Figure 4. DOS of borophene/ReS$_2$ (a) and borophene/ReSe$_2$ (b) van der Waals heterostructures.](image)

Therefore, we can say that borophene makes a decisive contribution to the type of conductivity of both heterostructures. In order to explain the obtained result, we calculated the distribution of the electron charge density over the atoms of the borophene/ReS$_2$ and borophene/ReSe$_2$ supercells according to the Mulliken procedure [48]. Based on the obtained distributions, it was revealed that a charge transfer occurred from borophene to ReS$_2$/ReSe$_2$. The total value of the transferred charge to the ReS$_2$ layer was 0.76$e$, and to the ReSe$_2$ layer, it was 0.11$e$. The difference in the value of the charge transferred by borophene is explained, on the one hand, by the difference in the distance between the borophene and ReS$_2$/ReSe$_2$ layers along the z-axis. In the case of the borophene/ReS$_2$ heterostructure, the layers are closer to each other (2.96 Å), which means that the charge transfer is more intense. In the case of the borophene/ReSe$_2$ heterostructure, the layers are farther apart (3.03 Å). On the other hand, the difference in the value of the charge transferred by borophene can be caused by the fact that sulfur has higher electronegativity, according to Mulliken (6.22 eV), as compared to selenium (5.89 eV).
3.2. Optoelectronic Properties of Borophene/ReS$_2$ and Borophene/ReSe$_2$ van der Waals Heterostructures

Next, we analyze the optoelectronic properties of borophene/ReS$_2$ and borophene/ReSe$_2$ van der Waals heterostructures. This analysis was carried out on the basis of the calculated absorption spectra in the wavelength range of electromagnetic radiation, from 200 to 2000 nm, and spectra of the photocurrent. The calculated absorption spectra are shown in Figure 5. To reveal the regularities in the formation of the profile of the absorption spectra of the heterostructures, the absorption spectra of isolated monolayers of borophene and ReS$_2$/ReSe$_2$ were calculated, which are also shown in Figure 5.

Analysis of the absorption spectra profiles showed that both heterostructures are characterized by the appearance of two noticeable peaks in the UV range. In the absorption spectrum of the borophene/ReS$_2$ heterostructure, these peaks are located in the far ($\lambda = 130$ nm) and near-UV ranges ($\lambda = 268$ nm). Moreover, the peak in the near-UV region is due to the contribution of ReS$_2$, and the peak in the far-UV region is due to the contribution of borophene. Consequently, there is a synergistic effect of the combination of borophene and ReS$_2$, leading to an increase in the absorption capacity of the borophene/ReS$_2$ heterostructure in the UV range. At the same time, in the near-IR region (0.75–2 $\mu$m), the absorption coefficient is minimal and is no more than 3%. The presence of absorption in this region is due to the contribution of borophene, since there is no absorption in ReS$_2$ in the range 0.75–2 $\mu$m. A similar picture was observed for the borophene/ReSe$_2$ heterostructure. One of the characteristic absorption peaks is located in the far-UV region ($\lambda = 134$ nm) and is due to the contribution of borophene, and the other peak is located in the near-UV region ($\lambda = 300$ nm) and is explained by the contribution of ReSe$_2$. In the near-IR region (0.75–2 $\mu$m), absorption is due to the presence of borophene in the heterostructure, but the absorption coefficient is minimal and does not exceed 4%. Nevertheless, it should be noted that the borophene/ReS$_2$ and borophene/ReSe$_2$ heterostructures are characterized by greater absorption in the IR range, as compared, for example, with molybdenum disulfide MoS$_2$ and molybdenum diselenide MoSe$_2$, which absorb no more than 1% [49].

Based on the obtained absorption spectra and solar radiation spectra on the Earth’s surface (AM1.5) and outside the Earth’s atmosphere (AM0), the photocurrent spectra were calculated. The solar radiation spectra AM0 and AM1.5 were taken from the National Renewable Energy Laboratory (NREL) website [50], which shows solar spectra in the
wavelength range of 280–2000 nm. The photocurrent spectra of the borophene/ReS$_2$ and borophene/ReSe$_2$ van der Waals heterostructures are shown in Figure 6. The photocurrent values are given for a surface area of 1 cm$^2$. Figure 6 shows that the maximum value of the photocurrent for the borophene/ReS$_2$ heterostructure falls at a wavelength of 600 nm, and is 9.36 mA cm$^{-2}$ µm$^{-1}$ in the case of the spectrum AM0 and 7.81 mA cm$^{-2}$ µm$^{-1}$ in the case of the spectrum AM1.5. For the borophene/ReSe$_2$ heterostructure, the photocurrent maximum is shifted closer to the left edge of the visible range and falls at a wavelength of 480 nm. In the case of the AM0 spectrum, this value is 10.19 mA cm$^{-2}$ µm$^{-1}$, and in the case of the AM1.5 spectrum, it is 7.98 mA cm$^{-2}$ µm$^{-1}$. Thus, for both heterostructures, the peak of the photocurrent falls within the visible range of electromagnetic radiation.

![Figure 6](image-url)

**Figure 6.** Photocurrent spectra of van der Waals borophene/ReS$_2$ (a) and borophene/ReSe$_2$ (b) heterostructures on the Earth’s surface (AM1.5) and outside the Earth’s atmosphere (AM0).

One of the most important physical characteristics of optoelectronic devices is the magnitude of the integrated photocurrent or the density of the photocurrent. It is calculated as the integral of the photocurrent spectrum. Table 1 shows the calculated integral values of the photocurrent for the entire solar radiation spectrum, and for the visible range of the solar spectrum, 380–780 nm, as well as the maximum value of the photocurrent at a wavelength of 550 nm, which corresponds to the maximum power of solar radiation. For comparison, Table 1 also shows the calculated values of the above optoelectronic characteristics for graphene and borophene with the allotropic form $\beta_{12}$.

Analysis of the data in Table 1 shows that the borophene/ReS$_2$ and borophene/ReSe$_2$ heterostructures are approximately 10 times higher than graphene and borophene $\beta_{12}$, in terms of the integral value of the photocurrent in the visible range for the AM0 and AM1.5 spectra. The value of the maximum photocurrent at a wavelength of 550 nm is also higher in van der Waals heterostructures. In terms of this indicator, they exceed graphene by more than 4 times, and borophene $\beta_{12}$ by more than 10 times. It should also be noted that the integral photocurrent of borophene/ReS$_2$ and borophene/ReSe$_2$ heterostructures in the visible range of radiation correlates well with the photocurrent density of the graphene/MoS$_2$ heterostructure (3 mA/cm$^2$) [51] and multilayer WS$_2$ (4.10 mA/cm$^2$) [52] obtained in a real experiment.
Table 1. Some optoelectronic characteristics of van der Waals borophene/ReS$_2$ and borophene/ReSe$_2$ heterostructures.

| Solar Spectrum AM0 | The Integral Value of the Photocurrent for the Entire Solar Radiation Spectrum, mA/cm$^2$ | Maximum Photocurrent at a Wavelength of 550 nm, mA cm$^{-2}$ μm$^{-1}$ | Integral Value of the Photocurrent for the Visible Spectrum 380–780 nm, mA/cm$^2$ |
|-------------------|------------------------------------------------------------------------------------------|-------------------------------------------------------------------|---------------------------------------------------------------------|
| borophene/ReS$_2$ | 2.26                                                                                     | 8.04                                                              | 6.3                                                                 |
| borophene/ReSe$_2$ | 2.03                                                                                     | 8.72                                                              | 6.05                                                                |
| graphene          | 2.1                                                                                      | 1.85                                                              | 0.677                                                               |
| borophene $\beta$$_{12}$ | 1.32                                                                                     | 0.733                                                             | 0.506                                                               |

| Solar Spectrum AM1.5 |
|----------------------|------------------------------------------------------------------------------------------|
| borophene/ReS$_2$    | 1.67                                                                                     |
| borophene/ReSe$_2$   | 1.53                                                                                     |
| graphene             | 1.5                                                                                      |
| borophene $\beta$$_{12}$ | 1.0                                                                                     |

4. Conclusions

Based on the results of an ab initio study, the following conclusions can be drawn. The proposed atomic configurations of van der Waals borophene/ReS$_2$ and borophene/ReSe$_2$ heterostructures are energetically stable and characterized by a metallic type of conductivity. The synergistic effect of the combination of a triangulated borophene monolayer and ReS$_2$/ReSe$_2$ monolayers leads to an increased sensitivity of borophene/ReS$_2$ and borophene/ReSe$_2$ heterostructures to radiation in the UV range, which makes them potentially promising materials for the development of UV detectors in the near- and far-UV ranges. It is predicted that the efficiency of such detectors will be high, since both heterostructures are practically insensitive to other wavelengths. Based on the calculated photocurrent spectra in the wavelength range from 200 to 2000 nm, it was predicted that the borophene/ReS$_2$ and borophene/ReSe$_2$ heterostructures have a pronounced ability to generate a photocurrent in the visible wavelength range. It was shown that the integral value of the photocurrent in the visible radiation range of borophene/rhenium sulfide and borophene/rhenium selenide heterostructures is many times higher than the indices of monolayers of graphene and borophene $\beta_{12}$, and correlates well with the data of full-scale experiments with other layered vertical 2D structures. At the same time, for the effective use of borophene/rhenium sulfide and borophene/rhenium selenide heterostructures as a material for creating solar cells, it is necessary to solve the problem of opening a band gap in their band structure. This task is the subject of further research.

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