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Accepted Manuscript

International Journal of Nanoscience

Article Title:	Electronic Properties of WS_2/WSe_2 Heterostructure Containing Te Impurity: The Role of Substituting Position
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DOI:	10.1142/S0219581X19400076
Received:	22 December 2018
Accepted:	08 February 2019
To be cited as:	A. V. Krivosheeva *et al.*, Electronic Properties of WS_2/WSe_2 Heterostructure Containing Te Impurity: The Role of Substituting Position, *International Journal of Nanoscience*, doi: 10.1142/S0219581X19400076
Link to final version:	https://doi.org/10.1142/S0219581X19400076

World Scientific
www.worldscientific.com

International Journal of Nanoscience
Vol. 1, No. 1 (2019) 1–4

ELECTRONIC PROPERTIES OF WS_2/WSe_2 HETEROSTRUCTURE CONTAINING Te IMPURITY: THE ROLE OF SUBSTITUTING POSITION

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Received 22 December 2018; accepted 8 February 2019

An impact of the positions of Te atoms substituting W atoms in two-dimensional WS_2/WSe_2 heterostructures on their electronic properties is investigated by theoretical simulation. The substitution of W by Te tends to reduce the energy band gap and can lead to metallic properties depending on the impurity position and concentration.

Keywords: 2D heterostructure, dichalcogenide, electronic property, impurity, substituting position.

1. Introduction

Individual layers of transition metal dichalcogenides, contrary to their bulk form, are known to possess direct-gap properties.[1-4] Analogously, stacking of two monolayers (MLs) of different dichalcogenides may also provide the direct nature of the gap. Moreover, doping may change band gap values and related characteristics of such heterostructures. In order to investigate how Te atoms can influence on electronic properties of a two-dimensional heterostructure made of WS_2 and WSe_2 MLs, we have calculated electronic energy band structures of different variants of the Te atoms substituting metal atoms in such structures and compared with our previous results for the case when Te atoms substituted the chalcogen ones.[5] An impact of Te atomic positions was analyzed.

2. Method

The heterostructure considered was composed of MLs of two different materials, namely WS_2 and WSe_2. We analyzed 2H phase with the space group $P6_3/mmc$ as the most stable polymorphic modification for this class of hexagonal layered two-dimensional crystals.[6] The layers were arranged in accordance with the bulk material. Electronic energy band structure and densities of states (DOSs) for WS_2/WSe_2 heterostructure were calculated using the PAW-LDA approximation[7] within the density functional theory realized in the VASP code.[8] Characteristics of the heterostructures were modeled using optB86b-vdW optimized exchange functional of J. Klimeš,[9] describing the van der Waals interaction between the monolayers, implemented in VASP code, which gives the structural parameters very close to experimental values.

We used 2×2 translational cell. The thickness of the vacuum spacer between the repeating layers was 15 Å. Three different positions of Te atoms were considered as illustrated in Fig. 1: 1) one Te atom in WS_2 layer; 2) one Te atom in WSe_2 layer; 3) Te atoms in both layers. These compositions correspond to 25 at.%, 25 at.%, and 50 at.% of Te concentrations, respectively.

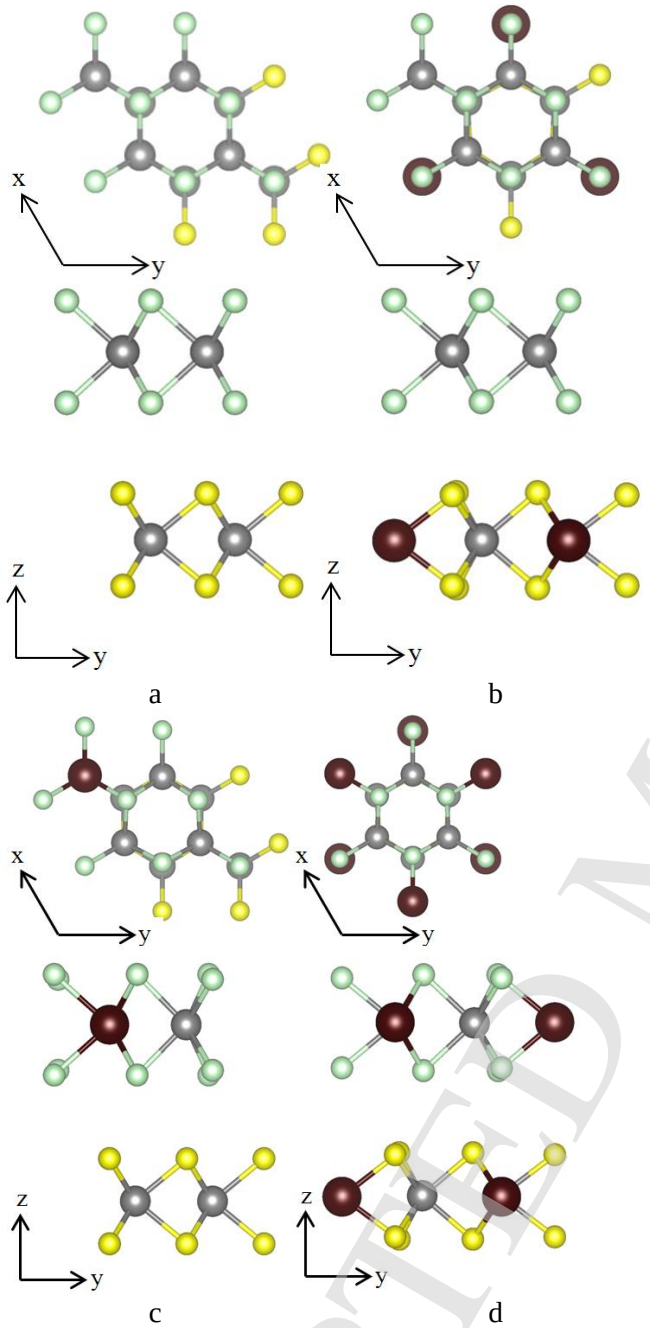

Fig. 1. Top and side view of WS_2/WSe_2 heterostructure (a) and the heterostructure with three different positions of Te atoms (b-d). Dark small balls represent W atoms, light small balls stand for chalcogen atoms (S atoms in bottom layer, Se atoms in top layer), large dark balls represent Te atoms.

Atomic relaxation via minimization of the total energy of the heterostructures was stopped when the forces acting on atoms became less than 0.01 eV/Å. The energy cutoff was fixed at 380 eV. The 9×9×2 Γ-centered grid of k-points was used.

3. Results and Discussion

The electronic band structures of WS_2/WSe_2 heterostructure and total DOSs for all the cases considered are presented in Fig. 2 and Fig. 3, respectively. It is obvious, that substitution of W atoms by Te ones strictly reduces the band gap, leading to an appearance of the electronic states at the Fermi level when Te substitutes Se and, thus, to a metallic behavior. This differs from the variant, when chalcogen atom was substituted, as described in our previous paper.[5] In that case the gap was reduced as well, but the heterostructure preserved its semiconductor properties.

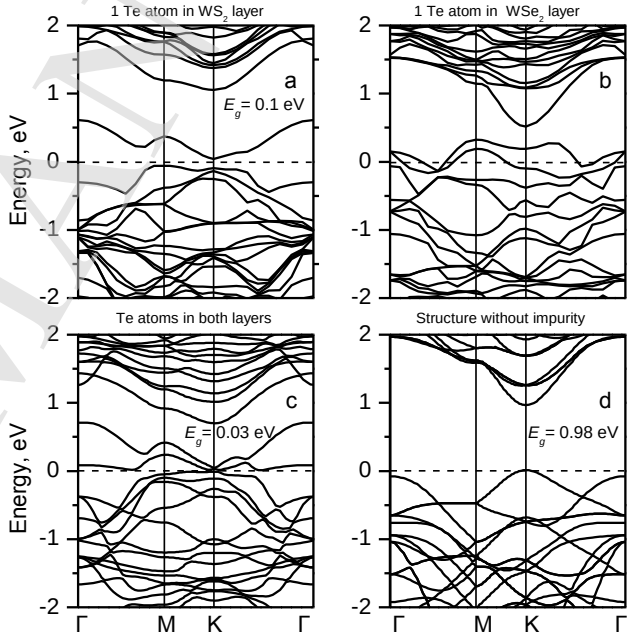

Fig. 2. Electronic energy bands in WS_2/WSe_2 heterostructures with (a,b,c) and without (d) Te atoms substituting W ones. Zero on the energy scale corresponds to the Fermi level.

The partial DOSs of undoped WS_2/WSe_2 heterostructures are presented in Fig. 3. The main impact on the band forming states is determined by *d*-states of W and *p*-states of chalcogen atoms (*s*-states are not shown).

Calculation of partial DOSs (not shown here) gave us a detailed information how the states are redistributed upon the substitution of W atoms by Te ones. When Te atom is located in WS_2 layer, the states near the Fermi level are determined by *d*-electrons of W and *p*-electrons of S. The substitution of W atom by Te one in WSe_2 layer leads to an appearance of *p*-electrons of Se and *d*-electrons of W at the Fermi

level and, thus, to transformation of the semiconducting material to a metal.

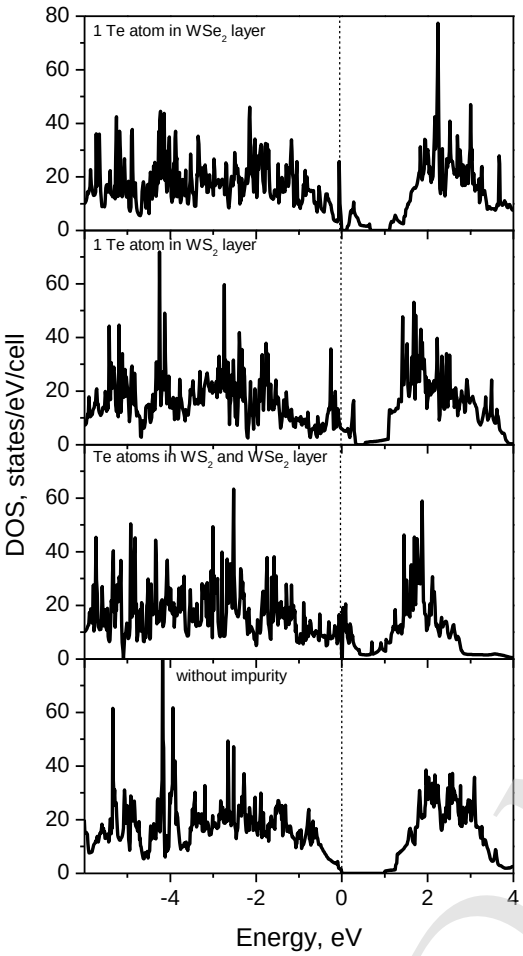

Fig. 3. Total DOSs of WS_2/WSe_2 heterostructures with (a,b,c) and without (d) Te impurity. Zero on the energy scale corresponds to the Fermi level.

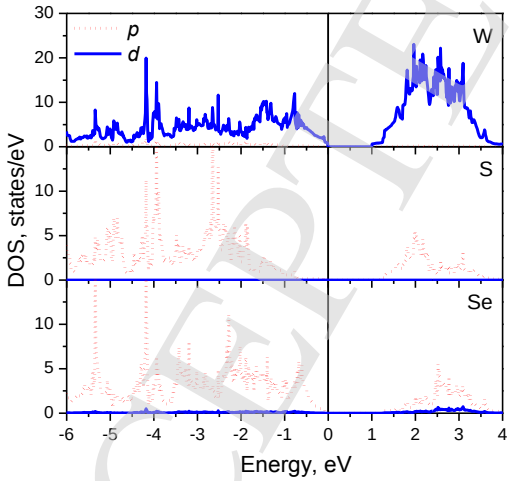

Fig. 4. Partial DOSs of undoped WS_2/WSe_2 heterostructures. Zero on the energy scale corresponds to the Fermi level.

However, the most interesting thing occurs, when Te atoms are located in both layers. We observe the appearance of the energy gap and recovery of semiconducting properties (Fig. 2c), whereas the states near the Fermi level are determined by *p*-electrons of both S and Se atoms. Contribution of Te atoms in the gap forming states is quite negligible in all the cases and is well-observed only for far-lying states.

4. Conclusion

Substitution of W atoms by Te ones in WS_2 layer in WS_2/WSe_2 heterostructure strictly reduces its energy band gap, but preserves the semiconducting properties. Analogously, the heterostructure with Te atoms both in WS_2 and WSe_2 layers possesses a small band gap, whereas the substitution of W atoms by Te ones only in WSe_2 layer leads to an appearance of new states at the Fermi level and to metallic properties.

Acknowledgments

This work was supported by the project No F17MC-017 of BRFFR and Belarusian State Scientific Program “Functional and Engineering Materials, Nanomaterials”.

References

1. K. F. Mak, C. Lee, J. Hone, J. Shan, T. F. Heinz, *Phys. Rev. Lett.* **105**, 136805 (2010).
2. A. Splendiani, L.Sun, Y. Zhang, Y. Li, J. Kim, C. Y. Chim, G. Galli, F. Wang, *Nano Letters* **10**, 1271 (2010).
3. A. V. Krivosheeva, V. L. Shaposhnikov, V. E. Borisenko, J.-L. Lazzari, N. V. Skorodumova, B. K. Tay, *Int. J. Nanotechnol.* **12**, 654 (2015).
4. A. V. Krivosheeva, V. L. Shaposhnikov, V. E. Borisenko, J.-L. Lazzari, C. Waileong, J. Gusakova, B. K. Tay, *J. Semicond.* **36**, 122002 (2015).
5. V. L. Shaposhnikov, A. V. Krivosheeva, V. E. Borisenko, *Phys. Stat. Sol. B*, 1800355 (2019).
6. R. Evarestov, A. Bandura, V. Porsev, A. Kovalenko, *J. Comput. Chem.* **38**, 2581 (2017).
7. D. M. Ceperley, B. J. Alder, *Phys. Rev. Lett.* **45**, 566 (1980).
8. G. Kresse, J. Furthmüller, *Phys. Rev. B* **54**, 11169 (1996).
9. J. Klimeš, D. R. Bowler, A. Michaelides, *Phys. Rev. B* **83**, 195131 (2011).