# ELECTROPHYSICAL PROPERTIES OF TRANSITION METALS CHALCOGENIDES STRUCTURES USED AS STRUCTURAL ELEMENTS OF THE NANOELECTRONICS DEVICES

M. Baranava[1], M. Najbuk[2], D. Hvazdouski[1], V. Stempitsky[1]
[1] Belarusian State University of Informatics and Radioelectronics, Minsk, Belarus
[2] University of Bialystok, Bialystok, Poland

## I. INTRODUCTION

Isolated graphene, which was successful manufactured, has a zero bandgap [1]. Two dimensional materials can be use for solve this problem. In our work the bilayered heterostructures have been studied. The energetic influence of the 2D $MoS_2$ and $WSe_2$ on the electrical properties of the graphene has been simulated. Also, electrical properties modified by effect of external electric field, so crucial in semiconductor application was simulated.

## II. COMPUTATIONAL DETAILS

Our calculations were performed based on the density functional theory (DFT). The projector-augmented wave (PAW) [2] potentials and Perdew–Burke–Ernzerhof (PBE) [3] functional have been used. The exchange–correlation potentials was described through the local density approximation (LDA) [4] and Hubard correction for 3d electrons of Mo and We (U= 5 eV) were employed. A cutoff energy of 480 eV and a 5×5×1 k-points grids determined by a fine grid of gamma-centered method [5] in the Brillouin zone. The valence electron configurations for Mo, S, We, Se and C were $4d^{10}5s^25p^2$, $3s^23p^4$, $5d^{10}6s^26p^2$ and $5s^25p^5$, respectively. The heterostructures were built by 3 unit cells of $MoS_2$ and 4 unit cells of C ($MoS_2$/G), also 3 unit cells of $WSe_2$ and 4 unit cells of C ($WSe_2$/G). The atomic structures were relaxed until the forces on all unconstrained atoms were smaller than 0.01 eV/Å. A vacuum layer of 15 Å along z direction was constructed to eliminate the interaction with spurious replica images. The DFT-D3 method of Grimme [6] was used to account for long range vdW interaction between monolayers.

All of calculations have been carried out using VASP (Vienna Ab-initio Simulation Package) [3, 7] wherein implemented methods described above.

Structural figures and charge density drawings were produced by VESTA package [8].

## III. RESULTS AND DISCUSSION

First of all the total energy optimization were performed for the unit cells relaxation of investigated materials. The lattice mismatch of created heterostructures was about 3.01 percents for $MoS_2$/G and 1.15 percents for $WSe_2$/G. The shape and volume of supercells were considered to be unchangeable at self-consistent calculations. Interlayer distances between sheets of structures have been calculated. Thereby, calculated interlayer distances are 3.50 Å and 3.45 Å for $WSe_2$/G and $MoS_2$/G respectively (Fig. 1.).

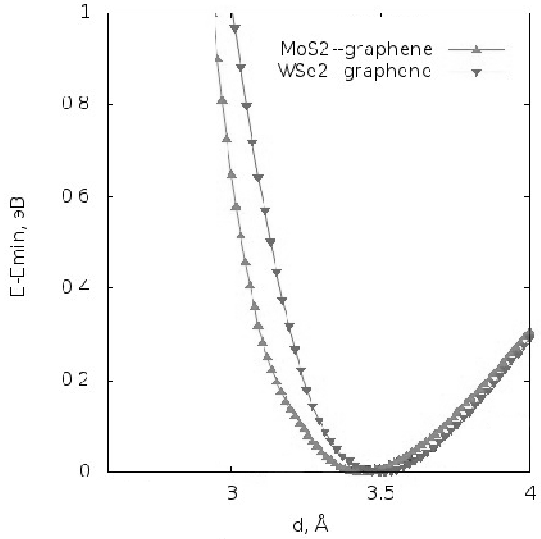


Figure 1 – Interlayer distance of heterostructures

Non-self-consistent calculations have been carried out along the lines between the high symmetry points K-Γ-M-K of the first Brillouin zone. Energy dispersion of graphene sheet in heterostructure has similar character to the pristine graphene, i.e. zero band gap remains (Fig. 2.).

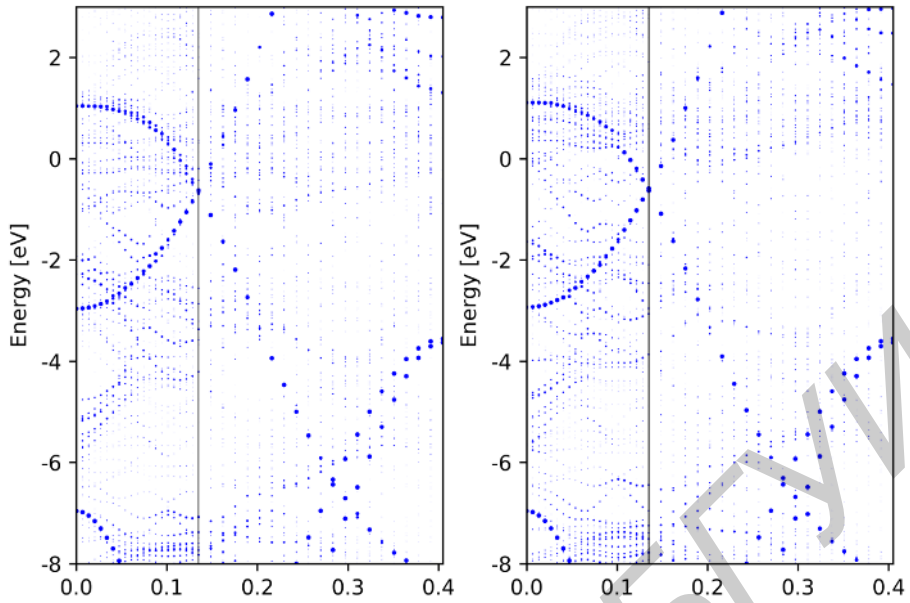


Figure 2 – Band structure of grapheme on the $MoS_2$ substarate (a) and $WSe_2$ substarate (b)

Vertical electric field has little effect on the bandgap $WSe_2$/G and $MoS_2$/G. The heterostructures have a direct band gap under influence Efield of 0.15 V/Å. Analysis of the results showed that a vertical external electric field can regulate charge transfer between monolayers and graphene.

## III. CONCLUSIONS

In summary, bilayered heterostructures of WSe2/G and MoS2/G have been theoretically simulated. Energy dispersion of graphene sheet in heterostructure has similar character to the pristine grapheme. Vertical electric field (0.15 V/Å) weakly affects on the bandgap WSe2/G and MoS2/G and can regulate charge transfer between monolayers and graphene. Utilization of Efield would lead to the realization of electronic properties engineering of the materials.

## ACKNOWLEGMENTS

This work was supported by the grants 2.53 of Belarusian National Scientific Research Program “Physical Materials Science, Novel Materials and Technologies” and 3.02 Belarusian National Scientific Research Program “Convergence 2020”.

## REFERENCES

[1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos and A. A. Firsov, Science, 2007, 306, 666–669
[2] G. Kresse and D. Joubert, Phys. Rev. B: Condens. Matter Mater. Phys., 1999, 59, 1758–1775
[3] G. Kresse and J. Furthmüller, Comput. Mater. Sci., 1996, 6, 15–50
[4] J. P. Perdew, K. Burke and M. Ernzerhof, Phys. Rev. Lett., 1996, 77, 3865
[5] H. J. Monkhorst and J. D. Pack, Phys. Rev. B: Condens. Matter Mater. Phys., 1976, 13, 5188
[6] S. Grimme, J. Antony, S. Ehrlich and H. Krieg, J. Chem. Phys., 2010, 132, 154104–154119
[7] P. E. Blöchl, Phys. Rev. B: Condens. Matter Mater. Phys., 1994, 50, 17953–17979
[8] K. Momma and F. Izumi, J. Mineral. Petrol. Sci., 2010, 39, 136–145