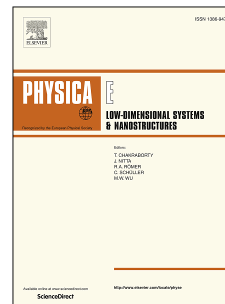
Accepted Manuscript



First principles study of single-layer $SnSe_2$ under biaxial strain and electric field: Modulation of electronic properties

Nguyen D. Hien, Nguyen Q. Cuong, Le M. Bui, Pham C. Dinh, Chuong V. Nguyen, Huynh V. Phuc, Nguyen V. Hieu, Hamad R. Jappor, Le T.T. Phuong, Bui D. Hoi, Le C. Nhan, Nguyen N. Hieu

PII: S1386-9477(19)30132-8

DOI: https://doi.org/10.1016/j.physe.2019.03.025

Reference: PHYSE 13511

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

Received Date: 23 January 2019

Revised Date: 9 March 2019

Accepted Date: 22 March 2019

Please cite this article as: N.D. Hien, N.Q. Cuong, L.M. Bui, P.C. Dinh, C.V. Nguyen, H.V. Phuc, N.V. Hieu, H.R. Jappor, L.T.T. Phuong, B.D. Hoi, L.C. Nhan, N.N. Hieu, First principles study of single-layer $SnSe_2$ under biaxial strain and electric field: Modulation of electronic properties, *Physica E: Low-dimensional Systems and Nanostructures* (2019), doi: https://doi.org/10.1016/j.physe.2019.03.025.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

First principles study of single-layer $SnSe_2$ under biaxial strain and electric field: Modulation of electronic properties

Nguyen D. Hien [a,b], Nguyen Q. Cuong [c], Le M. Bui [d,e,*], Pham C. Dinh [f], Chuong V. Nguyen [g], Huynh V. Phuc [h], Nguyen V. Hieu [i], Hamad R. Jappor [j], Le T.T. Phuong [c], Bui D. Hoi [c], Le C. Nhan [k], Nguyen N. Hieu [ℓ,*]

[a]*Laboratory of Magnetism and Magnetic Materials, Advanced Institute of Materials Science, Ton Duc Thang University, Ho Chi Minh City, Viet Nam*

[b]*Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Viet Nam*

[c]*Department of Physics, University of Education, Hue University, Hue, Viet Nam*

[d]*NTT Hi-Tech Institute, Nguyen Tat Thanh University, Ho Chi Minh City, Viet Nam*

[e]*Center of Excellence for Green Energy and Environmental Nanomaterials (CE@GrEEN), Nguyen Tat Thanh University, Ho Chi Minh City, Viet Nam*

[f]*School of Materials Science and Technology, Hanoi University of Science and Technology, Ha Noi 100000 Viet Nam*

[g]*Department of Materials Science and Engineering, Le Quy Don Technical University, Ha Noi 100000, Viet Nam*

[h]*Division of Theoretical Physics, Dong Thap University, Dong Thap 870000, Viet Nam*

[i]*Physics Department, University of Education, The University of Da Nang, Da Nang 550000, Viet Nam*

ACCEPTED MANUSCRIPT

[j]Department of Physics, College of Education for Pure Sciences, University of Babylon, Hilla, Iraq

[k]Department of Environmental Science, Saigon University, Ho Chi Minh City, Viet Nam

[ℓ]Institute of Research and Development, Duy Tan University, Da Nang 550000, Viet Nam

---

Abstract

In this study, we investigate systematically the effect of strain engineering and electric field on electronic properties of single-layer $SnSe_2$ using density functional theory. Our calculated results indicate that the single-layer SnSe2 is a semiconductor with a small band gap of 0.715 eV at the equilibrium state. The electronic states near the Fermi level are mainly contributed by Sn-d and Se-p orbitals, especially the contribution of the Se-p orbital to the valence band is dominant. Under biaxial strain, the band gap of the single-layer $SnSe_2$ changes abnormally. While compressive biaxial strain reduces band gap rapidly, the band gap of the single-layer $SnSe_2$ only increases slightly when increasing the tensile biaxial strain. In contrast to the strain-dependence case, the influence of the external electric field on the electronic properties of the single-layer $SnSe_2$ is quite small and the energy gap of the single-layer $SnSe_2$ does not depend on the direction of the perpendicular electric field. Our calculated results can provide more information for application possibility of the single-layer $SnSe_2$ in nanoelectronic devices.

Key words: Single-layer $SnSe_2$, Electric field, Biaxial strain, Band gap, Density functional theory

---

* Corresponding author.
Email addresses: nguyendinhhien@tdtu.edu.vn (Nguyen D. Hien), blminh@ntt.edu.vn (Le M. Bui), hieunn@duytan.edu.vn (Nguyen N. Hieu).

ACCEPTED MANUSCRIPT

1 Introduction

In recent decades, low-dimensional materials have attracted a lot of interest from the scientific community because they have many outstanding physical properties due to quantum confinement effects. Graphene [1] is considered as one of the materials of particular interest for a long time [2]. Besides graphene, graphene-like layered two-dimensional (2D) nanostructures, such as silicene [3] and transition metal dichalcogenides [4, 5], have extensively been investigated in the past recent years due to their potential applications in electronic and optoelectronic devices [6–8].

Single-layer tin diselenide ($SnSe_2$) is one of the typical examples of group IV-VI metal chalcogenides, which has been noticed recently [9, 10]. Bulk $SnSe_2$ has been studied for a long time [11, 12] and thin film SnSe of about 20 nm has been successfully synthesized by several methods [13–15]. Recently, using density functional theory (DFT) calculations, one showed that the structural properties of few-layer $SnSe_2$ are almost independent of the number of layers of the material [10]. Based on the calculated results of phonon spectrum, Sun's group indicated that the single-layer SnSe2 is dynamically stable [16]. The layers of Sn–Se–Sn in the $SnSe_2$ are held together by weak van der Waals force. Also, we expect that the weak bonding between the $SnSe_2$ layers in the bulk structure allows us to easily isolate single-layer by exfoliation technique as one did in SnS_2 [17]. Shafique and coworkers indicated that the single-layer $SnSe_2$ has a high electron mobility of 462.61 $cm^2V^{-1}s^{-1}$ and very low lattice thermal conductivity of 3.82 $Wm^{-1}K^{-1}$ [18]. These are important features in using $SnSe_2$ to thermoelectric devices. Due to outstanding electronic and thermoelectric properties, the single-layer $SnSe_2$ is expected to potential candidate for electronic [19, 20] and thermoelectric applications [16, 21].

Electronic properties of the single-layer $SnSe_2$ have been theoretically inves-

ACCEPTED MANUSCRIPT

tigated recently [10, 22]. Li and co-workers demonstrated that at equilibrium, the single-layer $SnSe_2$ is an indirect semiconductor [21] and and its band gap ranges from 0.79 eV to 1.07 eV [9, 10, 21]. The electronic properties of single-layer $SnSe_2$ depend strongly on external impacts. For example, semiconductor–metal phase transition can occur in the single-layer $SnSe_2$ at large compressive biaxial strain of 12% [9] or hydrogenation leads to significantly modulation of the electronic properties, especially the band gap, of the single-layer $SnSe_2$ [22]. Besides, the energy gap of the single-layer $SnSe_2$ will also be reduced rapidly when the applied pressure increases [23]. They also pointed out that the energy gap of the single-layer $SnSe_2$ is greater than that of a bulk one [9]. In addition, based on the calculated results of the effect of thickness on the electronic properties of $SnSe_2$ using DFT calculations, Gonzalez and Oleynik indicated that energy gap increases as the number of layers decreases and the energy gap of single-layer $SnSe_2$ is greatest compared to the bulk case [10]. However, many problems of the electronic properties of single-layers $SnSe_2$ are still unclear and need to be studied systematically. In the present study, we investigate the effect of biaxial strain ε_b and electric field $\mathbf{E}$ on the electronic properties of the single-layer $SnSe_2$ by DFT calculations. We focus on investigating the changes in the band structure and especially the energy gap of the single-layer $SnSe_2$ under the biaxial strain and the electric field.

2 Model and computational details

In this study, we calculate the electronic properties of the single-layer $SnSe_2$ by first-principles calculations using Quantum Espresso simulation package [24] with the generalized gradient approximations (GGA). The Perdew-Burke-Ernzerhof (PBE) exchange–correlation energy functional [25, 26] and a semi-empirical DFT-D2 method by Grimme [27] have been used in the present work. A $(15 \times 15 \times 1)$

ACCEPTED MANUSCRIPT

k-mesh Monkhorst-Pack grid has been used to sample the Brillouin zone. To optimize the atomic structure, the convergence threshold for a force of 10^{-6} eV/Å was used and the cut-off energy of 500 eV was employed in the present numerical simulations. We used a vacuum space of 20 Å to eliminate interactions between the considered single-layer and the nearest neighbors layers. It is well-known that, in DFT calculations, the results of the energy gap problem of 2D materials depend strongly on the functional. The difference between the results obtained by DFT calculations using different functionals, such as local-density approximations (LDA), GGA, Heyd-Scuseria-Ernzerhof (HSE06)..., is obvious. However, despite the difference in energy gap values, the physical properties of the material almost do not depend on the calculated approach, i.e., fucntionals were used in DFT calculations. It is well-known that DFT method has proven to be a reliable method to predict various physical and chemical phenomena on the atomic scale. However, the conventional DFT method typically underestimates the band gaps of semiconductors because of the self-interaction errors. This problem can be resolved by using the hybrid HSE06 functional or quasi particle self-consistent GW methods. However, in the present work, we mainly focus on the general trends, which are expected in the electronic properties of $SnSe_2$ as well as the effect of strain and electric field, rather than emphasizing quantitatively the exact values of the band gaps. We believe that GGA functional can also perfectly describe the general trends in electronic properties of 2D materials.

To demonstrate the biaxial strain effect on the electronic properties, the biaxial strain ε_b has been defined through the lattice constants as $\varepsilon_b = (\Delta - \Delta_0)/\Delta_0$, where Δ and Δ_0 are respectively the lattice constants of the single-layer $SnSe_2$ with and without biaxial strain. In this work, we only consider the single-layer $SnSe_2$ under small biaxial strain ε_b ranging from -5% to 5%. The minus sign of the elongation ε_b refers to the compressive strain. To evaluate the effect of an external electric

ACCEPTED MANUSCRIPT

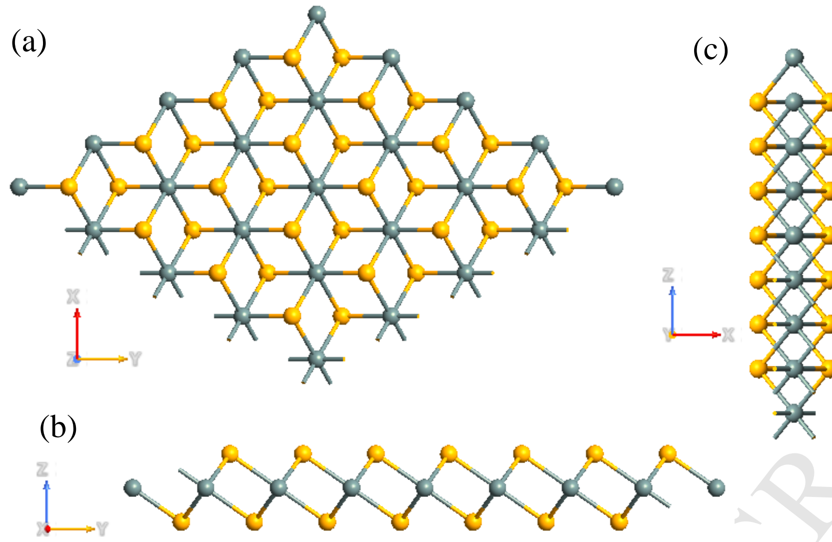


Fig. 1. Top view (a), side view (b), and front view (c) of atomic structures of single-layer $SnSe_2$. Turquoise and yellow and balls stand respectively for the Sn and Se atoms.

field on the electronic properties of the materials, an electric field **E** is applied perpendicular to the two-dimensional plane of the material, i.e., along the z-axis as illustrated in Fig. 1. The negative value of the electric field E is implied that the applied electric field direction is opposite to the positive direction of the z-axis.

3 Results and discussion

In Fig. 1, we show the atomic structure of single-layer $SnSe_2$ at equilibrium. Structure of the single-layer $SnSe_2$ has a sandwich type of the Se–S–Se atom three-layer and its geometry belongs to the P$\bar{3}m1$ group space [10]. At the equilibrium state, the lattice constant of the single-layer $SnSe_2$ is $a = b = 3.81$ Å and the thickness of the single-layer (Se–Se distance) is 2.74 Å. This DFT results are in good agreement with available data [22].

To check the stability of the single-layer $SnSe_2$, we calculate its phonon dispersion relations at the equilibrium state. Our calculated results for phonon dispersion curves of the single-layer $SnSe_2$ is shown in Fig. 2. We can see that, as

ACCEPTED MANUSCRIPT

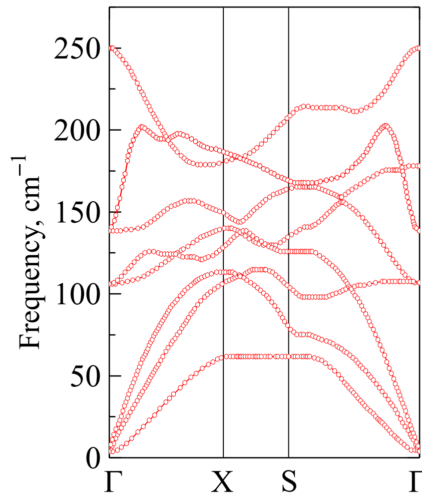


Fig. 2. Phonon dispersion curves of the single-layer $SnSe_2$ at the equilibrium state.

shown in Fig. 2, there are no soft phonon modes in the phonon dispersion curves of the single-layer $SnSe_2$. It means that at the equilibrium state, the single-layer $SnSe_2$ is stable. Band structure of the single-layer $SnSe_2$ is shown in Fig. 3(a). Our calculated results indicate that, the single-layer $SnSe_2$ at equilibrium is an indirect semiconductor. As shown in Fig. 3(a), we can clearly see that, an indirect band gap of 0.715 eV is formed near the Fermi level with the conduction band maximum (CBM) located at the X-point and the valence band maximum (VBM) located in the ΓX-path. Our calculated result for the band gap is in good agreement with previous DFT calculations [9, 21]. This value of the energy is smaller than that of single crystal $SnSe_2$ which is around 1.0 eV as shown in the available data [11, 28, 29]. The total energy of the single-layer $SnSe_2$ is -820.70 eV at the equilibrium. We see that, in terms of energy, the distance between the VBM (located in the ΓX-path) and the maximum of the valence band at the Γ-point is very small at the equilibrium state and we can believe that the position of VBM can be changed by external factors. However, the difference between VBM and maximum energy at the X-point is quite large, therefore indirect–direct gap transition is difficult to occur. Focusing on contribution of the atom orbitals to the energy structure, the partial

ACCEPTED MANUSCRIPT

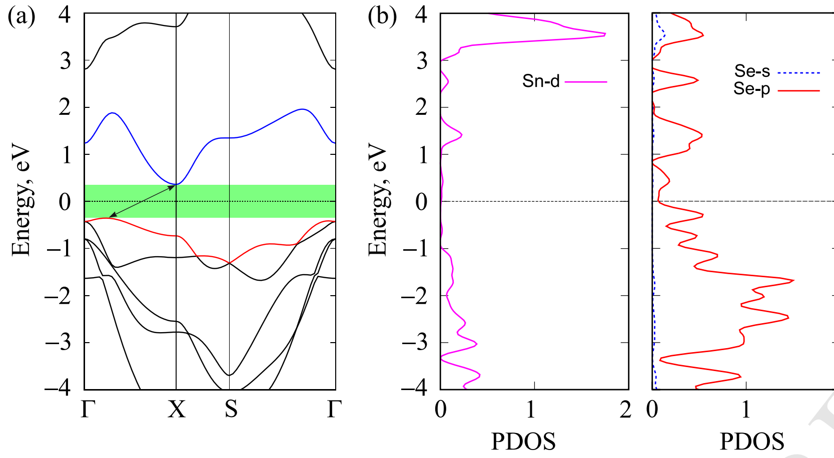


Fig. 3. (a) Band structure and (b) PDOS of single-layer $SnSe_2$ at the equilibrium state.

density of states (PDOS) of the single-layer $SnSe_2$ at the equilibrium state are also calculated as shown in Fig. 3(b). We can see that the contribution of the Sn-d and Se-p orbitals to the energy bands near the Fermi level is dominant. Especially, the contribution from the Se-p orbital to the valence band is huge compared to the rest. Overal, Meanwhile, the contribution of other atom orbitals to the energy bands is quite small in comparison with the Sn-d and Se-p orbitals. Overall, the contribution to the energy bands of the orbitals of the Se atom is greater than that of the S atom. However, it is mainly from the Se-p orbital because the contribution of Se-s is quite small as shown in Fig. 3(b).

To exam the influence of the strain engineering on electronic properties, we apply a biaxial strain ε_b from -5% to 5% to the single-layer $SnSe_2$. In Fig. 4 we show the band structure of the single-layer $SnSe_2$ under different levels of ε_b. In the limit of small biaxial strain ε_b, our DFT calculations demonstrate that there is no indirect–direct band gap transition in the single-layer $SnSe_2$. However, the band gap of the single-layer $SnSe_2$ depends strongly on the applied biaxial strain ε_b, especially in the case of the compressive biaxial strain ($\varepsilon_b < 0$). Dependence of the energy gap of the single-layer $SnSe_2$ on the applied biaxial strain ε_b is shown in Fig. 5. As shown in Fig. 5 we can see that, the band gap of the single-layer $SnSe_2$

ACCEPTED MANUSCRIPT

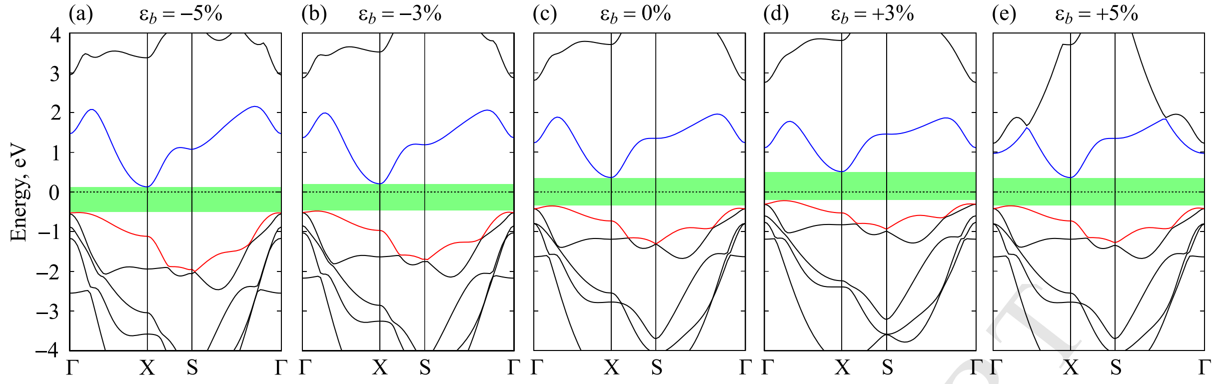


Fig. 4. Band structure of single-layer $SnSe_2$ under biaxial strain ε_b: (a) $\varepsilon_b = -5\%$, (b) $\varepsilon_b = -3\%$, (c) $\varepsilon_b = 0\%$ (at equilibrium), (d) $\varepsilon_b = 3\%$, and (e) $\varepsilon_b = 5\%$.

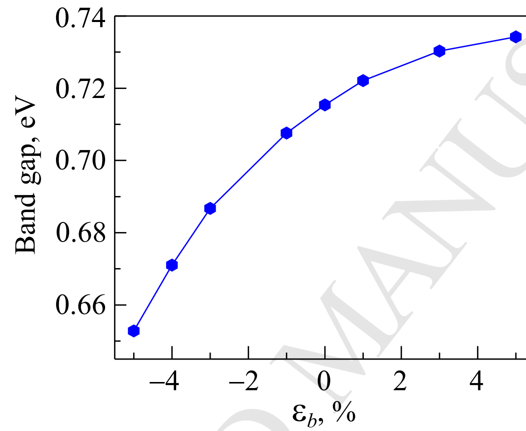


Fig. 5. Dependence of band gap of single-layer $SnSe_2$ on biaxial strain ε_b.

decreases quite rapidly when increasing compressive biaxial strain ε_b. Besides, the maximum valence band tends to shift to the Γ-point when increasing compressive biaxial strain and it located at the Γ-point at $\varepsilon_b = -5\%$. Meanwhile, the band gap increases slowly with the increase of the tensile biaxial strain ε_b. The band gap at $\varepsilon_b = 5\%$ is 0.734 eV compared with 0.715 eV at equilibrium. The slow increase in energy gap due to the increase of tensile biaxial strain ε_b in our calculations is consistent with the trend of changing energy gap that Huang and co-workers presented in the previous calculations [9].

We next investigate the influence of the external electric field **E** on electronic properties of the single-layer $SnSe_2$. The electric field **E** is applied perpendicular to

ACCEPTED MANUSCRIPT

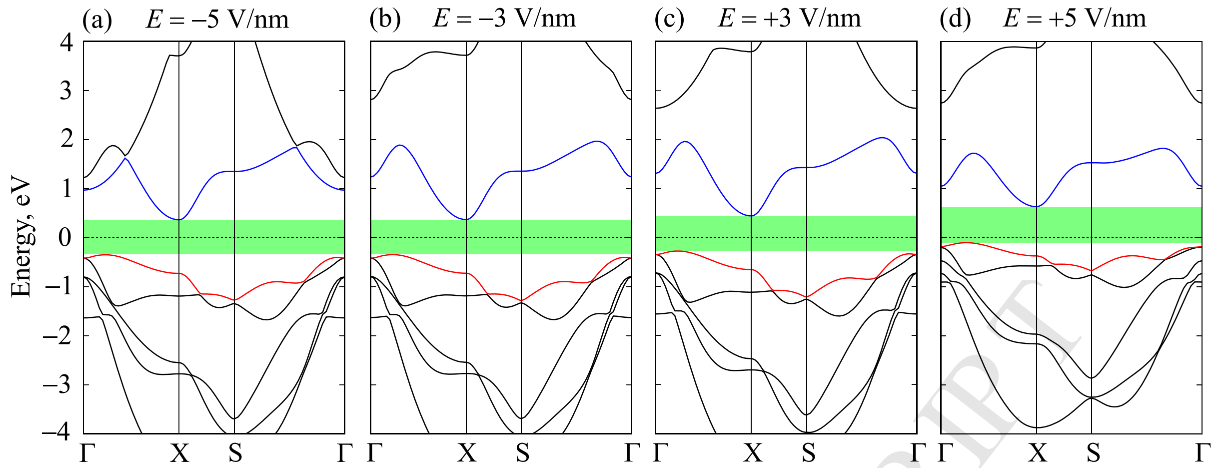


Fig. 6. Band structure of single-layer $SnSe_2$ under an external electric field E: $E = -5$ V/nm (a), $E = -3$ V/nm (b), $E = 3$ V/nm (c), and $E = 5$ V/nm (d).

the 2D plane of the single-layer $SnSe_2$ and its direction along the positive direction of the z-axis. In this case, the negative value of the electric field implies that the electric field direction is opposite to the z-axis positive direction. Band structure of the single-layer $SnSe_2$ under an applied electric field $\mathbf{E}$ is shown in Fig. 6. As shown in Fig. 6, we see clearly that the single-layer $SnSe_2$ is still an indirect semiconductor under electric field ranging from 0 to 5 V/nm. It can be anticipated that the electronic properties of monolayer $SnSe_2$ respond differently to the direction of the external electric field due to the spontaneous polarization. That is the reason why the band structure of single-layer $SnSe_2$ depends on the direction of the electric field in the case of a strong electric field. This behavior was also observed in other 2D materials under electric field, such as silicene [30] or GaN [31].

The energy gap of single-layer $SnSe_2$ will decrease when the external electric field increases as shown in Fig. 7. At the same time, the graph shows the dependence of energy on the positive electric field and the negative is almost symmetrical with each other through the vertical line passing through the point at $E = 0$. This proves that the energy gap of single-layer $SnSe_2$ depends only on the strength of the electric field and it does not depend on the electric field direction in the case of

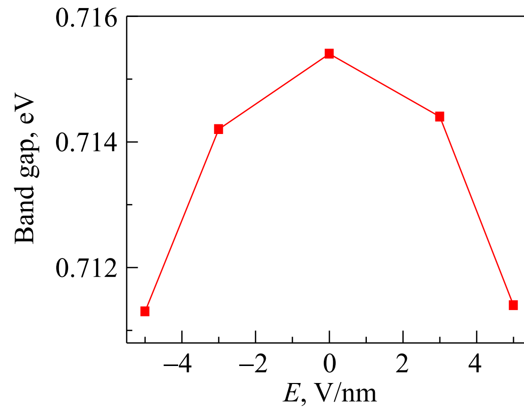


Fig. 7. Dependence of band gap of single-layer $SnSe_2$ on applied electric field E.

the electric field perpendicular to the 2D plane of the material. However, overall, the influence of the applied electric field on the band gap of the single-layer $SnSe_2$ is not very large. The energy gap decreases from 0.715 eV to 0.711 eV when the external electric field increases from 0 to 5 V/nm. This increase in energy is quite small. The electric field affects mainly on the charge transfer between atom layers in the materials. Thus, it leads to the change in the position of the Fermi level of the single-layer $SnSe_2$. In addition, due to the spontaneous electric polarization, the positive and negative electric field affects differently the electronic properties of material. When a negative electric field is applied to the single-layer $SnSe_2$, its CBM shifted downwards to the Fermi level, while its VBM shifted downwards far away from the Fermi level. It indicates that the band gap of the $SnSe_2$ is changed insignificantly when a negative electric field is applied. This phenomenon is also observed in the case of positive electric field.

4 Conclusion

In conclusion, we studied the influence of the strain engineering and electric field on the electronic properties of the single-layer SnS_2 using first-principles calculations based on density functional theory. Our DFT calculations showed that

ACCEPTED MANUSCRIPT

the energy gap of single-layer SnS_2 changes negligibly when the applied electric field varies from 0 to 5 V/nm. However, the electronic properties of the single-layer $SnSe_2$ depend strongly on the biaxial strain ε_b. The energy gap of the single-layer $SnSe_2$ that changes drastically in the presence of the biaxial strain, especially compressive case, can be useful in applying single-layer $SnSe_2$ in nanoelectromechanical systems.

5 Acknowledgments

This research is funded by the Vietnam National Foundation for Science and Technology Development (NAFOSTED) under Grant Number 103.01-2017.309.

References

[1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, A. A. Firsov, Science 306 (2004) 666.

[2] E. P. Randviir, D. A. Brownson, C. E. Banks, Mater. Today 17 (2014) 426.

[3] A. Acun, B. Poelsema, H. J. W. Zandvliet, R. van Gastel, Appl. Phys. Lett. 103 (2013) 263119.

[4] J. N. Coleman, M. Lotya, A. O'Neill, S. D. Bergin, P. J. King, U. Khan, K. Young, A. Gaucher, S. De, R. J. Smith, I. V. Shvets, S. K. Arora, G. Stanton, H.-Y. Kim, K. Lee, G. T. Kim, G. S. Duesberg, T. Hallam, J. J. Boland, J. J. Wang, J. F. Donegan, J. C. Grunlan, G. Moriarty, A. Shmeliov, R. J. Nicholls, J. M. Perkins, E. M. Grieveson, K. Theuwissen, D. W. McComb, P. D. Nellist, V. Nicolosi, Science 331 (2011) 568.

[5] M. Chhowalla, H. S. Shin, G. Eda, L.-J. Li, K. P. Loh, H. Zhang, Nat. Chem. 5 (2013) 263.

ACCEPTED MANUSCRIPT

ACCEPTED MANUSCRIPT

[6] Q. H. Wang, K. Kalantar-Zadeh, A. Kis, J. N. Coleman, M. S. Strano, Nat. Nanotechnol. 7 (2012) 699.

[7] G. Fiori, F. Bonaccorso, G. Iannaccone, T. Palacios, D. Neumaier, A. Seabaugh, S. K. Banerjee, L. Colombo, Nat. Nanotechnol. 9 (2014) 768.

[8] H.-Y. Chang, M. N. Yogeesh, R. Ghosh, A. Rai, A. Sanne, S. Yang, N. Lu, S. K. Banerjee, D. Akinwande, Adv. Mater. 28 (2016) 1818.

[9] Y. Huang, C. Ling, H. Liu, S. Wang, B. Geng, J. Phys. Chem. C 118 (2014) 9251.

[10] J. M. Gonzalez, I. I. Oleynik, Phys. Rev. B 94 (2016) 125443.

[11] G. Domingo, R. S. Itoga, C. R. Kannewurf, Phys. Rev. 143 (1966) 536.

[12] A. J. Smith, P. E. Meek, W. Y. Liang, J. Phys. C Solid State Phys. 10 (1977) 1321.

[13] Y. W. Park, S.-K. Jerng, J. H. Jeon, S. B. Roy, K. Akbar, J. Kim, Y. Sim, M.-J. Seong, J. H. Kim, Z. Lee, M. Kim, Y. Yi, J. Kim, D. Y. Noh, S.-H. Chun, 2D Mater. 4 (2017) 014006.

[14] Y. Huang, K. Xu, Z. Wang, T. A. Shifa, Q. Wang, F. Wang, C. Jiang, J. He, Nanoscale 7 (2015) 17375.

[15] S. Anwar, B. Mishra, S. Anwar, Mater. Chem. Phys. 175 (2016) 118.

[16] B.-Z. Sun, Z. Ma, C. He, K. Wu, Phys. Chem. Chem. Phys. 17 (2015) 29844.

[17] Y. Huang, E. Sutter, J. T. Sadowski, M. Cotlet, O. L. Monti, D. A. Racke, M. R. Neupane, D. Wickramaratne, R. K. Lake, B. A. Parkinson, P. Sutter, ACS Nano 8 (2014) 10743.

[18] A. Shafique, A. Samad, Y.-H. Shin, Phys. Chem. Chem. Phys. 19 (2017) 20677.

[19] M. Sun, Y. Hu, B. Shen, J. Zhai, S. Song, Z. Song, Integ. Ferroelectr. 140 (2012) 1.

[20] T. Pei, L. Bao, G. Wang, R. Ma, H. Yang, J. Li, C. Gu, S. Pantelides, S. Du, H.-j. Gao, Appl. Phys. Lett. 108 (2016) 053506.

ACCEPTED MANUSCRIPT

[21] G. Li, G. Ding, G. Gao, J. Phys. Conden. Matter 29 (2017) 015001.

[22] S. Wen, H. Pan, Y. Zheng, J. Mater. Chem. C 3) (2015) 3714.

[23] Z. Daifeng, Y. Chuanbin, L. Yuhao, O. Yun, G. Yongyi, R. Soc. Open Sci. 5 (2018) 171827.

[24] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. D. Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, R. M. Wentzcovitch, J. Phys. Condens. Matter 21 (2009) 395502.

[25] J. P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 77 (1996) 3865.

[26] J. P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett. 78 (1997) 1396.

[27] S. Grimme, J. Comput. Chem. 27 (2006) 1787.

[28] B. L. Evans, R. A. Hazelwood, J. Phys. D: Appl. Phys. 2 (1969) 1507.

[29] A. K. Garg, O. P. Agnihotri, A. K. Jain, R. C. Tyagi, J. Appl. Phys. 47 (1976) 997.

[30] N. D. Drummond, V. Zólyomi, V. I. Fal'ko, Phys. Rev. B 85 (2012) 075423.

[31] D. Xu, H. He, R. Pandey, S. P. Karna, J. Phys. Condens. Matter 25 (2013) 345302.

ACCEPTED MANUSCRIPT

Highlights

- Single-layer $SnSe_2$ is an indirect semiconductor with band gap of 0.715 eV at equilibrium
- Band gap of single-layer $SnSe_2$ depends strongly on the biaxial strain
- Effect of electric field on band gap of single-layer $SnSe_2$ is quite small
- Control of single-layer $SnSe_2$ band gap by strain is useful in nanoelectronic applications

ACCEPTED MANUSCRIPT