ZINC-DOPED SILICENE NANORIBBONS IN THE ELECTRIC FIELD: A DFT STUDY

Vo Van On[(1)], Nguyen Thanh Tung[(1)], Nguyen Duy Khanh[(1)], Huynh Thi Phuong Thuy[(1)], Trieu Quynh Trang[(2))], Hoang Van Ngoc[(1*)]

[1]*Institute of Applied Technology, Thu Dau Mot University*

[2]*Nam Dinh Teacher Training's College*

Abstract: *Silicene nanoribbons are one-dimensional materials made of silicene with hydrogen-modified edges. This work studies the doping of element Zn into silicene nanoribbons in the presence of an external electric field. There are two configurations studied here, top-configuration, valley-configuration. By using density functional theory (DFT) and VASP software, the energy band structures and state densities of the configurations are plotted, analyzed, and discussed. The top configuration is the most stable and optimal configuration among the studied configurations. The study also shows that there are external electric field intervals that increase the formation energy of the system, there are external electric field intervals that decrease the formation energy of the system, this represents the strength of the bonds in the material under the influence of an external electric field.. Research helps guide practical applications to create new materials and adjust material properties by external electric fields.*

Keywords: *Silicene nanoribbons, doping configurations, zinc doping, external electric field.*

Received 5 January 2022

Revised and accepted for publication 26 January 2022

(*) Email: ngochv@tdmu.edu.vn

1. INTRODUCTION

Low-dimensional materials play an important role in science and technology, the research of new materials creates products with outstanding properties. Preliminary studies have signaled the existence of silicene [1-3]. Silicene together with graphene, and germanene ushered in a new era in the study of low-dimensional materials. Scientists first observed the hexagonal honeycomb structure of silicene while growing it [4,5]. The result is achieved through direct condensation of a stream of silicon atoms onto a single crystal substrate under ultra-high vacuum conditions. A highly ordered silicon structure, arranged in a honeycomb lattice, was synthesized and produced two silicon subunits occupying positions at different

heights (0.02 nm) indicating hybridization potential. sp2-sp3 [5]. The first silicene structure was produced when it was grown on Ag, it's not flat structure, it's atomically flexible [4-6]. The DFT studies also produced similar results [7-9]. The buckling of silicene is due to a mixture of sp3 hybridized orbitals and sp2 planar bonds [10]. Due to the compatibility of silicene with silicon, it opens up many promising applications in microelectronics technology [11]. Early studies on silicene showed that different substances doped in silicene could modulate its band gap, which has many applications in semiconductor technology. A relatively large band gap can be opened at the Dirac point of silicene without degrading the electronic properties of silicene with n-type doping by Cu, Ag and Au adsorption, p-doping by Ir and Au adsorption, and neutral doping by adsorption of Pt [12]. The band gap of silicene is also regulated by an external electric field carrying energy and momentum [13-17]. The band gap in silicene can be opened up at the Fermi level by an external electric field by breaking the inverse symmetry, the band gap varying linearly with the strength of the external electric field [15]. Silicene nanoribbons (SNRs) are one-dimensional structures with edges edited by chemical elements. Studies on SNRs show that this is a one-dimensional material with many outstanding structural properties [18-21]. SiNRs are structurally stable if the edge atoms are hydrogenated, and those with armchair edges often exhibit much better thermoelectric performance than their zigzag counterparts [21]. This work studies SNRs with modified edges by hydrogen, the doped element here is Zn, and the system is placed in an external electric field. With the appearance of Zn and an external electric field, the structural and electrical properties of SNRs are changed.

2. CONTENT

2.1. Research methods

Density functional theory (DFT) is a method of quantum mechanical modeling, it is used in physics, chemistry, materials science to investigate the electronic structure of a many-particle system. DFT theory is based on the postulate that the physical quantities of a system of interacting electrons can be described by a function of the ground-state electron density n0(r). A functional is a mapping from the space of functions into a number field (in the particular case of electronic systems, functions of electron density).

VASP software is software written based on DFT theory to simulate structural properties and electromagnetic properties of materials. To run a program using VASP, four input files are required: INCAR, KPOINTS, POSCAR, and POTCAR. In this work, we use KPOINTS with 1 1 11 division points to study one-dimensional silicene nanoribbons.

2.2. Configuration of pristine and doping systems

Figure 1 is the structure of the pristine system. This configuration consists of 12 Si atoms and 4 H atoms per unit cell. After optimization, this structure is stable, the largest distance between two adjacent Si atoms is 2.278Å , the smallest distance between two adjacent Si atoms is 2.218Å, its buckling is about 0.538 Å.

The configuration parameters are shown in Table 1, Here d(Si-Si) is the distance between adjacent Si atoms; d(Si-Zn) is the distance between two adjacent atoms Si and Zn.

Compared without doping, it is found that the distance between the atoms has changed and the buckling of the post-doping system has also changed. The closer to the doped atom (Zn), the more flat the configuration of the system tends to be, and the presence of Zn causes the structure of the SNRs to be flatter.

Figures 2 and 3 are the top and valley configurations of the doped system, respectively. These configurations are stable after doping. The formation energy of the doped system is calculated by the formula [22]:

$$E_f = E_t - E_p + E_{Si} - E_{Zn} \quad , \qquad (1)$$

here, E_f is the total energy of doping system, E_p is the total energy of pristine system, E_{Si} and E_{Zn} are the energy of free energy of Si and Zn atoms, respectively.

Table 1. *Configuration parameters of the systems after optimization*

Configurations	d(Si-Si)($\mathring{A}$)		d(Si-Zn) ($\mathring{A}$)		Buckling ($\mathring{A}$)	
	Maximum	Minimum	Maximum	Minimum	Maximum	Minimum
Top	2.296	2.232	2.369	2.347	0.411	0.02
Valley	2.83	2.224	2.354	2.346	0.371	0.023

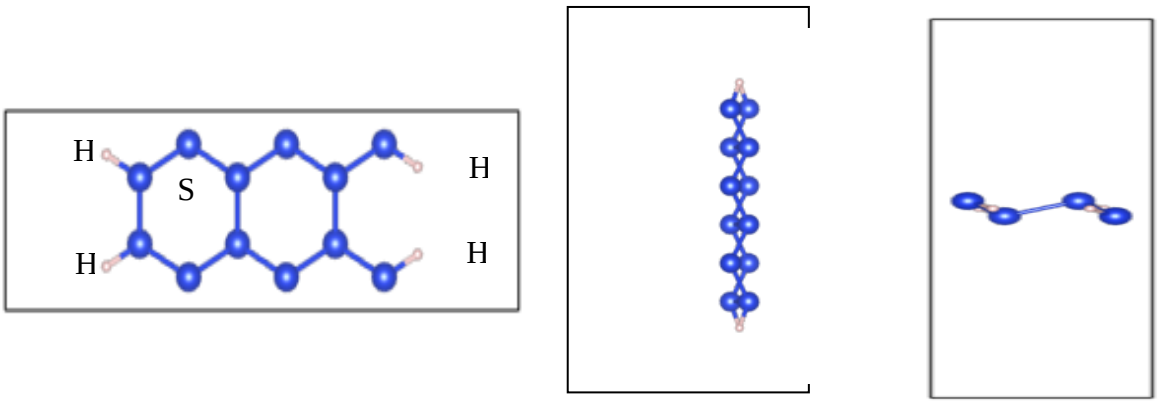

Fig. 1. *The pristine configuration*

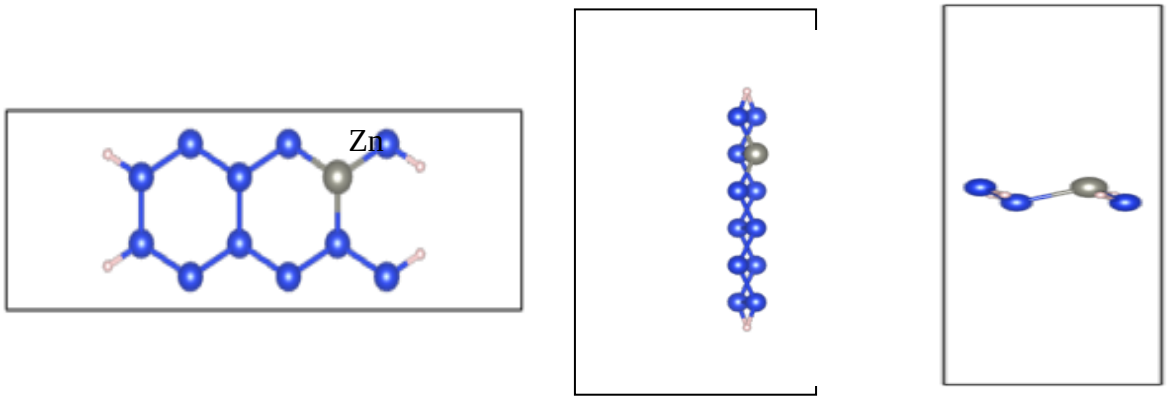

Fig. 2. *The top-configuration*

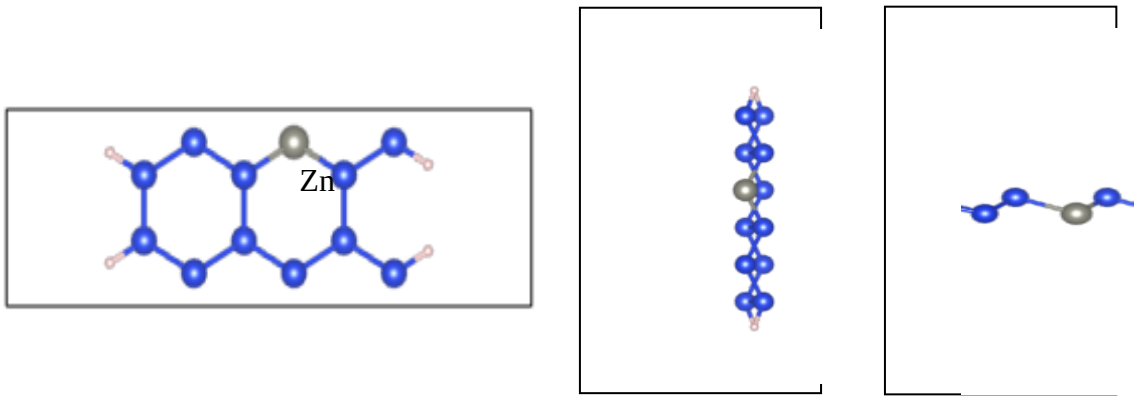

Fig. 3. *The valley-configuration*

Table 2. *The formation energy of the systems in the presence of the external electric field*

Doping systems	E_t(eV)	E_p(eV)	E_{Si} (eV)	E_{Zn}(eV)	E_f(eV)
Top	-65.701958	-64.408218	-0.13534420	-0.013485993	-1.415598207
Valley	-65.616263	-64.408218	-0.13534420	-0.013485993	-1.329903207

Table 2 shows the formation energy of the system. With the top configuration for the smallest formation energy, this is the more optimal of the two configurations. Since the top configuration is the more optimal configuration, we will focus on studying this configuration.

2.3. Structural properties of the doped system

2.3.1. Band structure, density of states (DOS)

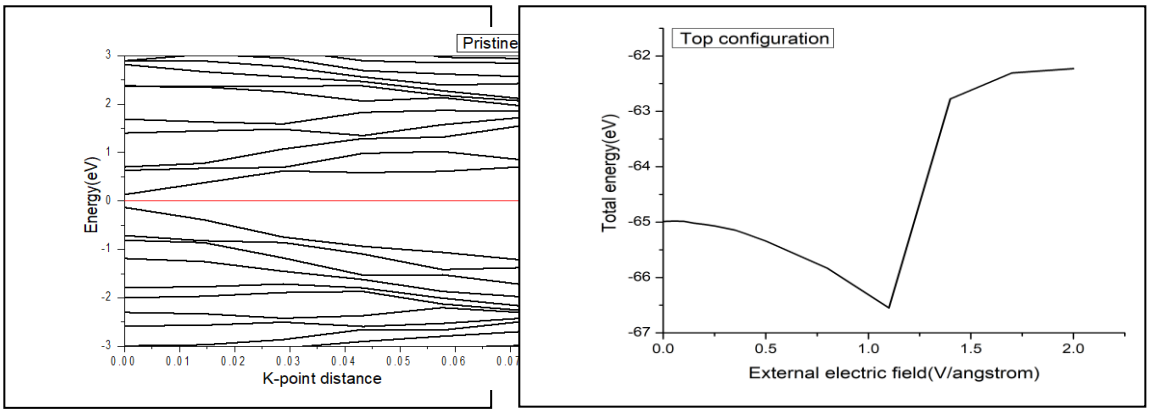

Fig. 4. *Band structure of pristine system (a), the dependent of E_t on electric field (b)*

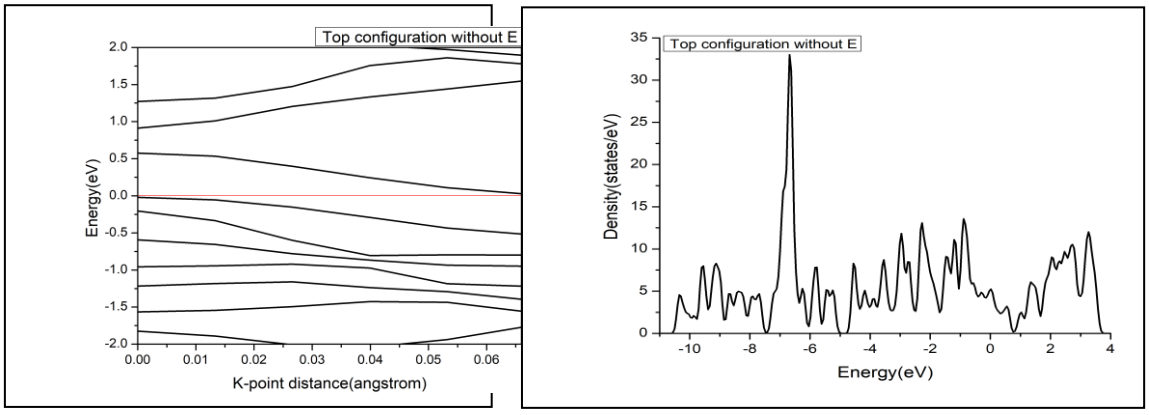

Fig. 5. *Band structure (a) and DOS (b) of top-configuration without electric field*

The energy band and DOS structure of the undoped system is a semiconductor with a direct band gap of 0.325eV (Figure 4a). Figure 4b examines the variation of the energy of the top configuration with the magnitude of the external electric field. When the external electric field is in the range of 0 < E < 1.1V/angstrom, the energy of this configuration decreases over time, when E > 1.1V/angstrom, the energy starts to increase. This problem can be explained as follows: When the electric field is small, its effect is not enough to change the party, including the mobility of electrons. When the electric field is large, the electric field pulls the bonds between the atoms apart, which reduces the energy of formation.

The energy band structure and state density of the top configuration in the absence of electric field are seen in Figure 5. This is a semiconductor with a very narrow mute band, the band gap is 0.063eV, with such a narrow band gap, the system will always conduct electricity under all conditions without any significant stimulus.

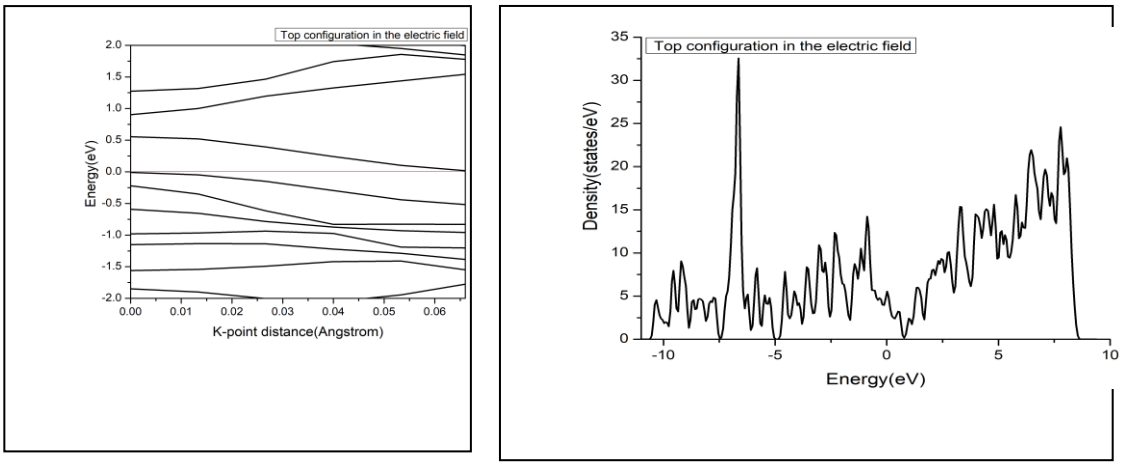

Fig. 6. *Band structure (a) and DOS (b) of top-configuration in electric field*

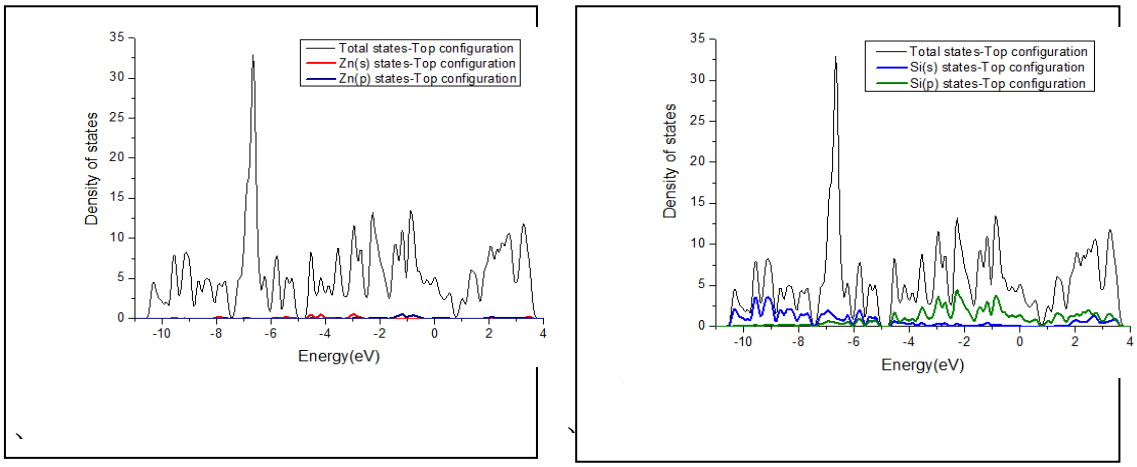

Fig. 7. *The contribution of s, p states of Si (a) and Zn (b) in the top configuration*

When placed in the top configuration an electric field, its energy band structure, and state density are seen in figure 6, the magnitude of the electric field is 0.6V/angstrom. Looking at the energy band structure (Figure 6a), we see that the band gap of the system is almost unchanged compared to when there is no electric field (Figure 5a), the change here is just a redistribution of states. (Figure 6b). Compared with the absence of an electric field, the states in the presence of an electric field extend more towards the top of the conduction band. Figures 7 shows the contributions of the partial states Si(s), Si(p), Zn(s), Zn(p) in the top configuration. We see that the contribution of the Si(s), Si(p) states is large, while the contributions of the Zn(s), Zn(p) states are small. This is because the density of doped Zn particles per unit cell is small. The s-states mainly contribute to the formation of the valence band bottom and the conduction band top, while the p-states mainly contribute to the formation around the Fermi level. The contribution of Zn is limited also because zinc belongs to group 2 while Si belongs to group 4, after bonding, Zn no longer has mobile electrons, the system conducts electricity mainly through holes.

2.3.2. Charge density difference and partial charge density

Figure 8 is the charge density difference of the top (a) and valley (b) configurations. Blue is where the negative charge is concentrated (electrons move towards the blue), yellow is where the positive charge is concentrated (negative charge is lost). Looking at the figure, we see that the negative charges move towards the Zn-doped atom, causing clouds of negative charge around Zn to appear. This charge concentration is due to Zn being an electron acceptor and to the presence of an external electric field. Figure 10 shows the partial charge density of the top (a) and valley (b) configurations. Yellow is represented as the charge clouds around the atoms in the unit cell. Clouds have a difference between top and valley configurations, where thicker clouds indicate greater charge density.

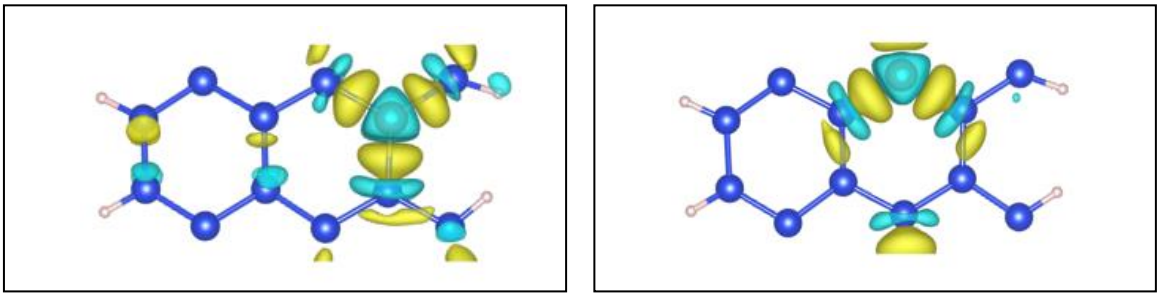

Fig. 8. *Charge density difference of the top (a) and the valley (b) configurations*

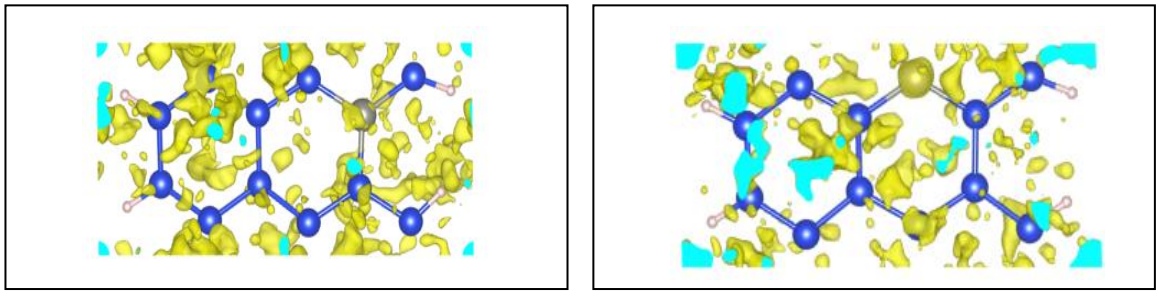

Fig. 9. *Partial charge density of the top (a) and the valley (b) configurations*

3. CONCLUSION

The work of doping Zn into SNRs with the appearance of an external electric field. There are two configurations studied here, the top configuration and the valley configuration. Both configurations are stable after doping. Using DFT theory we calculated the formation energies of the two systems and found that the top configuration gives smaller formation energy, so this is the more stable configuration. The appearance of electric field and Zn doping changed the energy band structure of the system, from a semiconductor with a narrow band gap has become a semimetal (with valley configuration) and a semiconductor with a near-zero width (top configuration). The contributions of the partial states of Si are significant because the density of Si particles is large. The charge density difference and partial charge density of the two configurations are also plotted and investigated, with Zn receiving a relatively large amount of charge from neighboring atoms.

Acknowledgment: This research is funded by Thu Dau Mot University under grant number DA.21.1-004. This research used resources of the high-performance computer cluster (HPCC) at Thu Dau Mot University (TDMU), Binh Duong Province, Vietnam

REFERENCES

1. Takeda, K.; Shiraishi, K. (1994), "Theoretical possibility of stage corrugation in Si and Ge analogs of graphite", *Physical Review B.,* Vol. 50, No. 20, pp. 14916–14922.
2. Guzmán-Verri, G.; Lew Yan Voon, L. (2007), "Electronic structure of silicon-based nanostructures", *Physical Review B,* Vol. 76, No, 7, p. 075131.
3. Cahangirov, S.; Topsakal, M.; Aktürk, E.; Şahin, H.; Ciraci, S. (2009), "Two- and One-Dimensional Honeycomb Structures of Silicon and Germanium", *Physical Review Letters,* Vol. 102, No. 23, p. 236804.
4. Aufray, B.; Kara, A.; Vizzini, S. B.; Oughaddou, H.; LéAndri, C.; Ealet, B.; Le Lay, G. (2010), "Graphene-like silicon nanoribbons on Ag(110): A possible formation of silicene", *Applied Physics Letters., Vol.* 96, No. 18, p. 183102.
5. Lalmi, B.; Oughaddou, H.; Enriquez, H.; Kara, A.; Vizzini, S. B.; Ealet, B. N.; Aufray, B. (2010), "Epitaxial growth of a silicene sheet", *Applied Physics Letters*., Vol. 97, No. 22, p. 223109.
6. Sone, Junki; Yamagami, Tsuyoshi; Nakatsuji, Kan; Hirayama, Hiroyuki (2014), "Epitaxial growth of silicene on ultra-thin Ag(111) films", *New J. Phys.,* Vol. 16, No. 9, p. 095004.
7. Lay, G. Le; Padova, P. De; Resta, A.; Bruhn, T.; Vogt, P. (2012), "Epitaxial silicene: can it be strongly strained", *Journal of Physics D: Applied Physics*., Vol. 45, No. 39, p. 392001.
8. Bernard, R.; Leoni, T.; Wilson, A.; Lelaidier, T.; Sahaf, H.; Moyen, E.; Assaud, L. C.; Santinacci, L.; Leroy, F. D. R.; Cheynis, F.; Ranguis, A.; Jamgotchian, H.; Becker, C.; Borensztein, Y.; Hanbücken, M.; Prévot, G.; Masson, L. (2013), "Growth of Si ultrathin films on silver surfaces: Evidence of an Ag(110) reconstruction induced by Si", *Physical Review B.,* Vol. 88, No. 12, p. 121411.
9. Colonna, S.; Serrano, G.; Gori, P.; Cricenti, A.; Ronci, F. (2013), "Systematic STM and LEED investigation of the Si/Ag(110) surface", *Journal of Physics: Condensed Matter.,* Vol. 25, No. 3, p. 315301.

10. S. Cahangirov, M. Topsakal, E. Aktürk, H. Şahin, and S. Ciraci (2009), "Two- and One-Dimensional Honeycomb Structures of Silicon and Germanium", *Phys. Rev. Lett.* Vol. 102, p. 236804.
11. Tao, L.; Cinquanta, E.; Chiappe, D.; Grazianetti, C.; Fanciulli, M.; Dubey, M.; Molle, A.; Akinwande, D. (2015), "Silicene field-effect transistors operating at room temperature", *Nature Nanotechnology*. Vol. 10, No. 3, pp. 227–234.
12. Jump up to:a b c d Ni, Z.; Zhong, H.; Jiang, X.; Quhe, R.; Luo, G.; Wang, Y.; Ye, M.; Yang, J.; Shi, J.; Lu, J. (2014), "Tunable band gap and doping type in silicene by surface adsorption: Towards tunneling transistors", *Nanoscale.*, Vol. 6, No. 13, pp. 7609–7616.
13. Motohiko Ezawa (2012), "A topological insulator and helical zero mode in silicene under an inhomogeneous electric field", *New J. Phys.*, Vol. 14, p. 033003.
14. Jhao-Ying Wu, Szu-Chao Chen, Godfrey Gumbs, and Ming-Fa Lin (2016), "Feature-rich electronic excitations of silicene in external fields" *Phys. Rev. B*, Vol. 94, p. 205427.
15. C. Kamal (2012), "Controlling Band Gap in Silicene Monolayer Using External Electric Field", *Mesoscale and Nanoscale Physics*, Vol. 13, pp. 1-10.
16. J.Villarreal, F.Escudero, J.S.Ardenghi, P.Jasen (2021), "Effect of an external electric field on local magnetic moments in silicene", *Journal of Magnetism and Magnetic Materials*, Vol. 524, No. 15, p. 167598.
17. Li Geng, Zhao Yin-Chang, Zheng Rui, Ni Jun, Wu Yan-Ning (2015), "Modulation of electronic properties with external fields in silicene-based nanostructures", *Chinese Physics B*, Vo. 24, No. 8, pp. 087302.
18. Xu C, Luo G, Liu Q, Zheng J, Zhang Z, Nagase S, Gao Z, Lu J. (2012), "Giant magneto resistance in silicene nanoribbons", *Nanoscale*, No. 4, pp. 3111–3117.
19. Kang J, Wu F, Li J. (2012), "Symmetry-dependent transport properties and magneto resistance in zigzag silicene nanoribbons", *Appl Phys Lett*, Vol. 100, No. 23, pp. 233122.
20. Yin Yao, Anping Liu, Jianhui Bai, Xuanmei Zhang & Rui Wang (2016), "Electronic Structures of Silicene Nanoribbons: Two-Edge-Chemistry Modification and First-Principles Study", *Nanoscale Research Letters,* Vol. 11, No. 371, pp. 1-9.
21. Pan L, Liu H, Tan X, Lv H, Shi J, Tang X, Zheng G. (2012), "Thermoelectric properties of armchair and zigzag silicene nanoribbons", *Phys Chem Chem Phys.*, Vol. 14, No. 39, pp. 13588–13593.
22. Qing Pang, Yan Zhang, Jian-Min Zhang, Vincent Jib and Ke-Wei Xuc (2011), "Electronic and magnetic properties of pristine and chemically functionalized germanene nanoribbons", *Nanoscale,* Vol. 3, pp.4330-4338.

PHA TẠP KẼM TRONG CÁC DẢI SILICENE MỘT CHIỀU VỚI SỰ CÓ MẶT CỦA ĐIỆN TRƯỜNG NGOÀI: MỘT NGHIÊN CỨU DFT

Tóm tắt: *Các băng silicene một chiều được tạo ra từ vật liệu silicene với các cạnh được sửa đổi bởi hidro. Công trình này nghiên cứu pha tạp các nguyên tử kẽm vào các băng silicene một chiều, hệ chịu tác động của một trường ngoài. Có hai cấu hình được nghiên cứu, cấu hình top và cấu hình valley. Cấu trúc vùng năng lượng, mật độ trạng thái của các hệ pha tạp sẽ được vẽ và khảo sát bằng lý thuyết phiếm hàm mật độ (DFT) và phần mềm VASP. Cấu hình top là cấu hình tối ưu và ổn định nhất trong các cấu hình được nghiên cứu. Nghiên cứu cũng chỉ ra rằng có những khoảng giá trị điện trường ngoài làm tăng năng lượng hình thành của hệ, có những khoảng giá trị làm giảm năng lượng hình thành của hệ, điều này nói lên khả năng bền vững của vật liệu dưới tác dụng của điện trường ngoài. Nghiên cứu tạo ra định hướng cho việc tạo ra những vật liệu mới và điều khiển các tính chất của vật liệu nhờ sử dụng điện trường ngoài.*

Từ khóa: *Silicene một chiều, cấu trúc pha tạp, pha tạp kẽm, điện trường ngoài.*