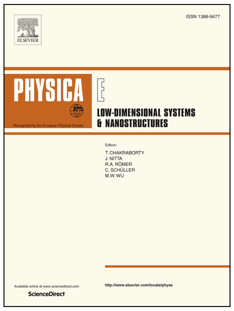

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Stability and electronic properties of edge functionalized silicene quantum dots: A first principles study

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ABSTRACT

The stability and electronic properties of hexagonal and triangular silicene quantum dots are investigated under the effect of edge passivation by different elements and molecular groups. The structures experience a considerable alternation in shape depending on the attached elements or groups. The most noticeable alternations occur in zigzag triangular flakes passivated with sulfur and in all selected flakes when OH groups are attached to the edge atoms. The resulting structure has a spherical shape with a large total dipole moment. All the studied clusters have been proven to be stable by the calculated positive binding energies. Flexible structure transformation from insulator (conductor) to conductor (insulator) is obtained in zigzag hexagonal-H (zigzag triangular-H) and zigzag hexagonal-S (zigzag triangular-OH), respectively. The magnetic properties of triangular zigzag depend on the parity of the total number of Si atoms such that flakes with an even number of Si atoms will have antiferromagnetic properties while flakes with an odd number of Si atoms can have ferromagnetic or antiferromagnetic properties depending on the attached element or group. Thus, a proper choice of the attached functional groups or elements to silicene flakes allows tailoring of their properties to different application. In particular, hydrogenated or fluorinated flakes are highly interactive with the surrounding and can be used for sensor applications while clusters passivated with S or OH are insensitive to edge defects and have tunable electronic properties that make them promising in semiconductor device applications.

1. INTRODUCTION

The recently synthesized silicon version of graphene – a single layer of silicon atoms, arranged in a honeycomb structure called silicene [1-3], has attracted much interest. [4-7] Similar to graphene, in silicene propagating electrons behave like massless Dirac fermions with Fermi velocity ranging from 10^5 to 10^6 ms^{-1} [8]. This innovative material exhibits striking properties and effects similar to those of graphene:

quantum spin Hall effect [9, 10] and half metallicity [11, 12] etc... In addition, silicene is compatible with silicon-based solid state technology.

Unlike graphene, the stable silicene has buckled structure due to the large ionic radius of silicon [3, 14]. Thus, the large spin-orbit coupling of silicene induces a gap equal to 1.55 meV which makes the quantum spin Hall effect or topological insulator state experimentally attainable.[15, 16] This new state of matter, formed due to the combination of spin-orbit coupling and time-reversal symmetry, is expected to have interesting properties [17]. The band structure of silicene can be controlled by applying external electric field where a topological phase transition occurs from a topological insulator to a band insulator by increasing the electric field. [18, 19] Moreover the tunable energy gap induced by an electric field makes it an efficient field effect transistor at room temperature [20].

The chemical functionalization has proved to be a powerful tool to tune the electronic, magnetic, and optical properties in various two dimensional materials such as graphene [21-25], phosphorene [26, 28], and silicene.[29-32] Huang et al. [29] found that chemical modification of silicene lead to a spontaneous structure transition as a result of the sp^3 hybridization of silicon atoms. They also predict that new functional materials, such as Si_8P_4 via substitutional doping, are potential candidates for thin film solar cell absorbers. Functionalization of monolayer silicene with H, CH3, F, and OH enables precise adjustment of the optical band gap by making silicene a semiconductor or metal depending on the type and concentration of the attached groups. [30] Size-controllable energy gap can be achieved by cutting silicene sheet into nanoribbons, Cahangirov et al. [31] show that bar and hydrogenated silicene nanoribbons (SiNRs) have remarkable electronic and magnetic properties depending on the size and edge termination of the nanoribbons. Asymmetric edge functionalization of silicene nanoribbons with H and F can transform zigzag SiNRs from antiferromagnetic semiconductor to ferromagnetic metals and bipolar spin gapless semiconductors. [32]

Additional method to open a controllable energy gap in silicene sheet is to cut it into small flakes or quantum dots where the effects of shape, size and edge morphology must play decisive role. [33-35] In this article, we focus on studying the stability and electronic properties of flake-like silicene quantum dots (SQDs) with different shape (triangular and hexagonal), edge termination (zigzag and armchair), and chemical functionalization. The effect of chemical modification is studied by attaching OH and CN groups and H, F, O, and S elements to the edges of the SQDs. In what follows, we present the computational model in section II, the results and discussion in section III, and the conclusion in section IV.

2. COMPUTATIONAL MODEL

The structure stability and electronic properties of silicene nanodots are investigated using density functional theory (DFT) calculations [36, 37]. The DFT is used as implemented in Gaussian 09 [38] where the basis sets are of the Gaussian type orbital functions. Four types of silicene quantum dots are used; (a) hexagonal with armchair termination (AHEX), (b) triangular with armchair termination (ATRI), (c) hexagonal with zigzag termination (ZHEX), and (d) triangular with zigzag termination (ZTRI). All the selected flakes, under various edge passivation, is then fully optimized at the B3LYB/3-21G level of theory [39–41] without symmetry constraint. To check the adequacy of the 3-21G basis set, we compare its calculated energy gap for AHEX ($Si_{42}H_{18}$) with the energy gap (E_g) calculated using 6-31G(d). We found that E_g =1.76 eV when using the 3-21G basis set and E_g =1. 68 eV for 6-31G(d) where the time taking by the later basis set is almost double the time taken by the former one. Therefore the 3-21G basis can be considered as a sufficient basis set with respect to both results accuracy and computational time.

3. RESULTS AND DISCUSSION

Edge passivation of silicene flakes with different elements may provide tunable electronic properties that are useful for different applications. Here we consider the effect of edge passivation on the stability, electronic energy levels, energy gap, charge distribution and total dipole moment of SQDs.

3.1 STRUTURE STABILITY

Fig. 1 shows the optimized structures of AHEX and ATRI silicene passivated with various elements. Due to the large Si-Si bond length, silicene has a buckled structure with sp^3- like hybridization. As a result of the buckling, the optimized structures of SQDs largely depend on their shapes and passivation elements, as shown in Fig. 1. For SQDs terminated with H and F the alternation is very small with bond lengths (see Table 1) similar the Si-Si bond length calculated for bulk silicene, $d_{Si\text{-}Si}$=2.27 Å, and similar buckled structure.[42] In contrast to this, for passivation with O and S a significant structure alternation occurs. As seen in Fig. 1, the most profound structural modification is observed in AHEX passivated with S where the edge rings are out of the structure plane. Fig. 2 presents the optimized structures of edge functionalized ZHEX and ZTRI dots. Similar to the corresponding armchair flakes, passivation with F or H atoms has negligible effect on the geometrical structure. However, when functionalized with O, zigzag clusters undergo transformation whereby the buckling totally disappears for ZTRI or ZHEX (Fig. 2) and a planar structure is obtained similar to that of graphene.

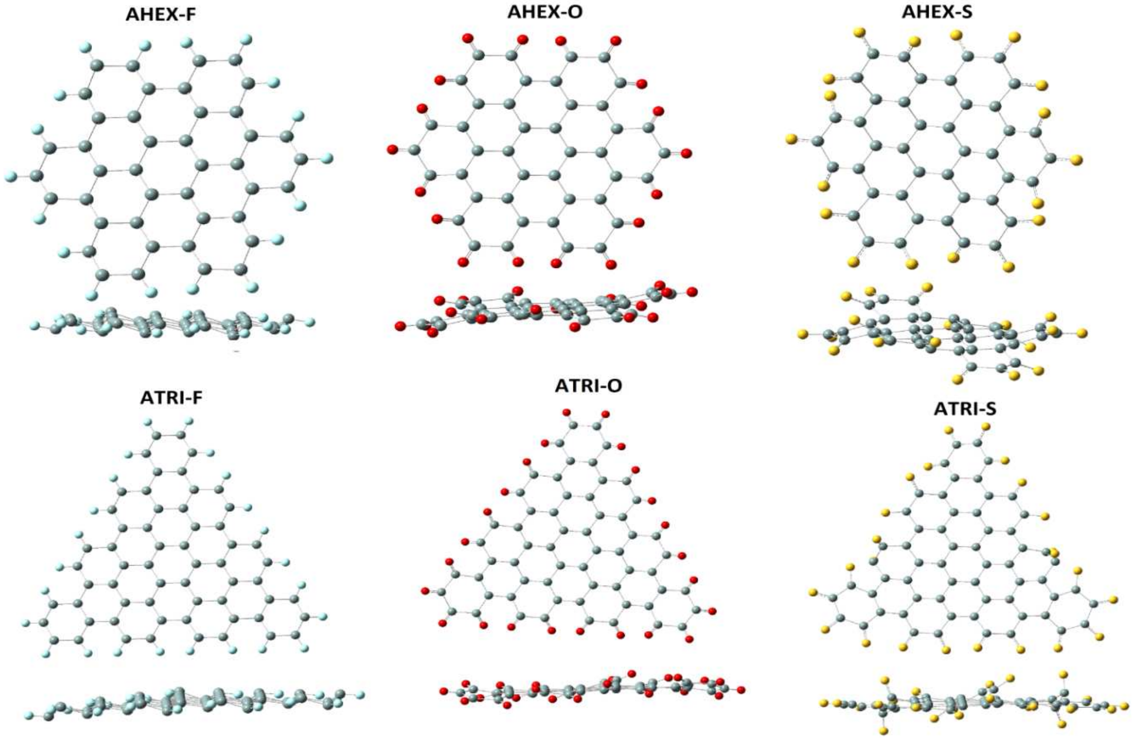

Fig. 1. The optimized structure of AHEX and ATRI silicene quantum dots passivated with F, O, and S.

Moreover for ZTRI with S atoms at the edges, the structure bends taking a hemispherical shape. The observed structure transformation in flakes passivated with S or O is due to the change in the bond length between Si atoms at the edges. It is seen in Table 1, that $d_{Si\text{-}Si}$ equal 2.4 to 2.43 Å at the edges represents the highest increase in the bond length with respect to its value in bulk sheet ($d_{Si\text{-}Si}$=2.27 Å). The distance between the attached element (d_{XSi}) and the edge atom is nearly the same regardless of the shape or edge type of the SQDs with the highest d_{XSi}~2.1 Å observed for passivation with S atoms.

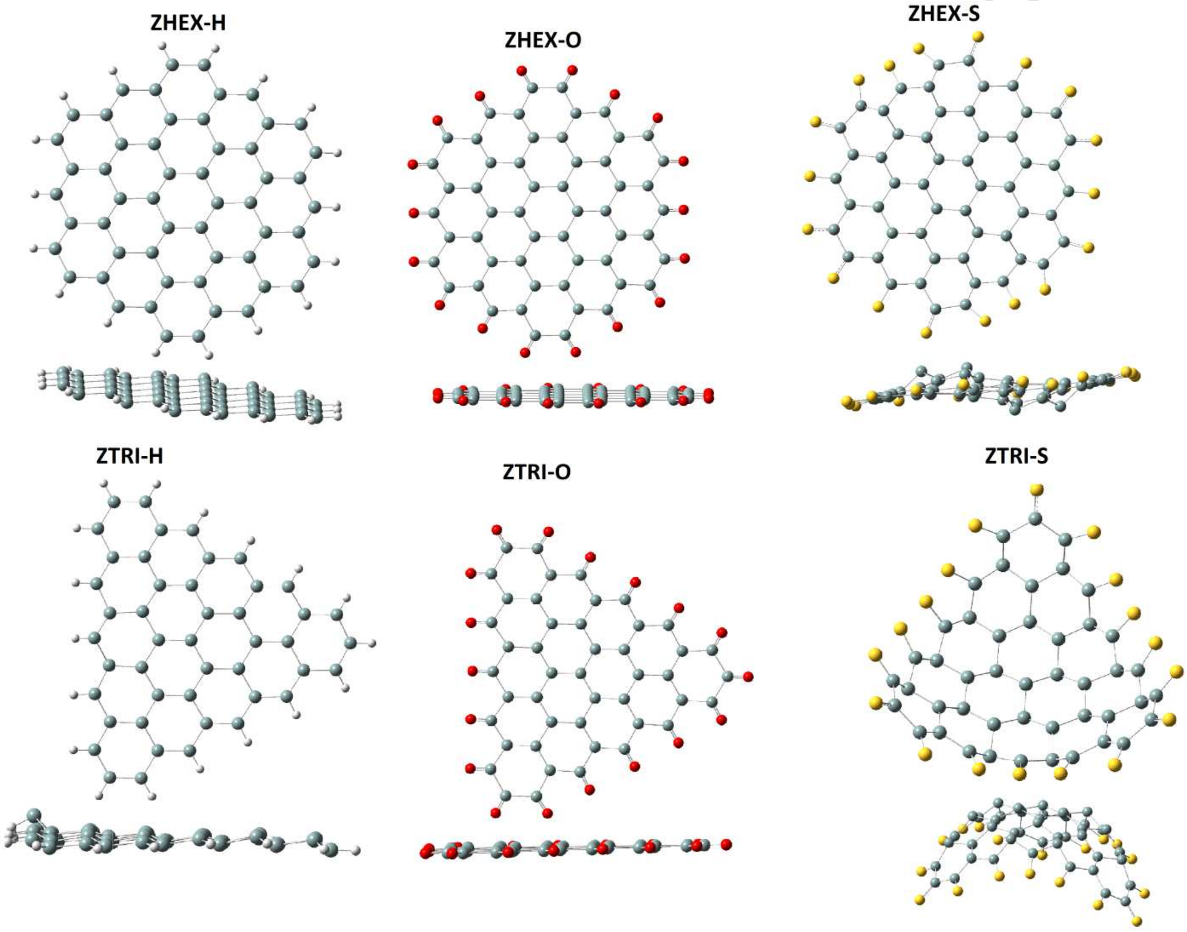

Fig. 2. The optimized structure of ZHEX (a-c) and ZTRI (d-f) terminated with different elements.

All the investigated SQDs are stable; this is confirmed by the calculated positive binding energies (**E_B**), presented in Table 1. We use the following formula to calculate E_B per unit atom:
E_B= (N_XE_X+$N_{Si}E_{Si}$-E_C)/N.With N_X, N_{Si}, and N are the number of X atoms, X=H, F, O, S, and OH, the number of silicon atoms, and the total number of atoms, respectively. E_X, E_{Si}, and E_C are the corresponding total energies of the terminating atoms, silicon atoms, and the resultant compound, respectively. The maximum binding energies are achieved when SQDs are terminated with O atoms making the optimized structures almost planar.

Table I. The optimal bond lengths between the attached element or group (***d_{XSi}***) and the Si edge atoms, between Si-Si atoms (***$d_{Si\text{-}Si}$***), and the corresponding binding energy.

Structure		***d_{XSi}*****(A^0)**	***$d_{Si\text{-}Si}$*** **(A^0)**	**E_B (eV)**
AHEX ($Si_{42}X_{18}$)	H	1.5	2.25-2.32	3.75
	F	1.7	2.29-2.32	4.27
	O	1.6	2.22-2.42	5.06
	S	2.1	2.26-2.39	4.23
	OH	1.68-1.76	2.29-2.37	4.09
ATRI ($Si_{60}X_{24}$)	H	1.5	2.24-2.31	3.78
	F	1.7	2.28 -2.35	4.28
	O	1.6	2.23 -2.43	5.03
	S	2	2.24-2.42	4.26
	OH	1.66-1.76	2.28-2.37	4.12
ZHEX ($Si_{54}X_{18}$)	H	1.5	2.22 -2.3	4.34
	F	1.7	2.26-2.33	4.84
	O	1.6	2.21-2.39	5.56
	S	2.1	2.25-2.39	4.79
	OH	1.76	2.25-2.45	4.134
ZTRI ($Si_{46}X_{18}$)	H	1.5	2.24-2.31	3.76
	F	1.7	2.25-2.32	4.26
	O	1.6	2.24-2.40	4.98
	S	2.1	2.30-2.40	4.25
	OH	1.68-1.76	2.24-2.254	4.08

3.2 DENSITY OF STATES AND ENERGY GAP

The electronic density of states (DOS) is shown in Fig. 3 for AHEX, ATRI, ZHEX, and ZTRI silicene quantum dots passivated with different elements. The energy levels are represented by Gaussian function $\frac{1}{\sqrt{2\pi\alpha}}\exp\left[\frac{-(\varepsilon-\varepsilon_i)^2}{2\alpha^2}\right]$ with broadening $\alpha = 0.1\ eV$. The Fermi level is fixed, $E_F = (E_{HOMO}+E_{LUMO})/2$, where E_{HOMO} is the highest occupied molecular orbital (HOMO) energy and E_{LUMO} is the lowest unoccupied molecular orbital (LUMO) energy. It is clear from Fig. 3 that the energy gap strongly depends on the shape and edge termination of the silicene flakes and chemical modification. AHEX dot is characterized by large energy gap (E_g =1.74 eV) while ZTRI dot has a tiny gap (E_g = 0.27 eV). The small energy gap in hydrogenated ZTRI can be doubled (see Table 2) when passivated with S instead of H. On the other hand, the effect of chemical modification on the energy gap of AHEX is not pronounced where the lowest energy gap in AHEX-S, E_g=1.4 eV, can be considered as a wide energy gap with respect to the lowest values in other flakes. Similar to hydrogenated AHEX, the ATRI and ZHEX have a high energy gap however it can be considerably decreased by edge passivation.

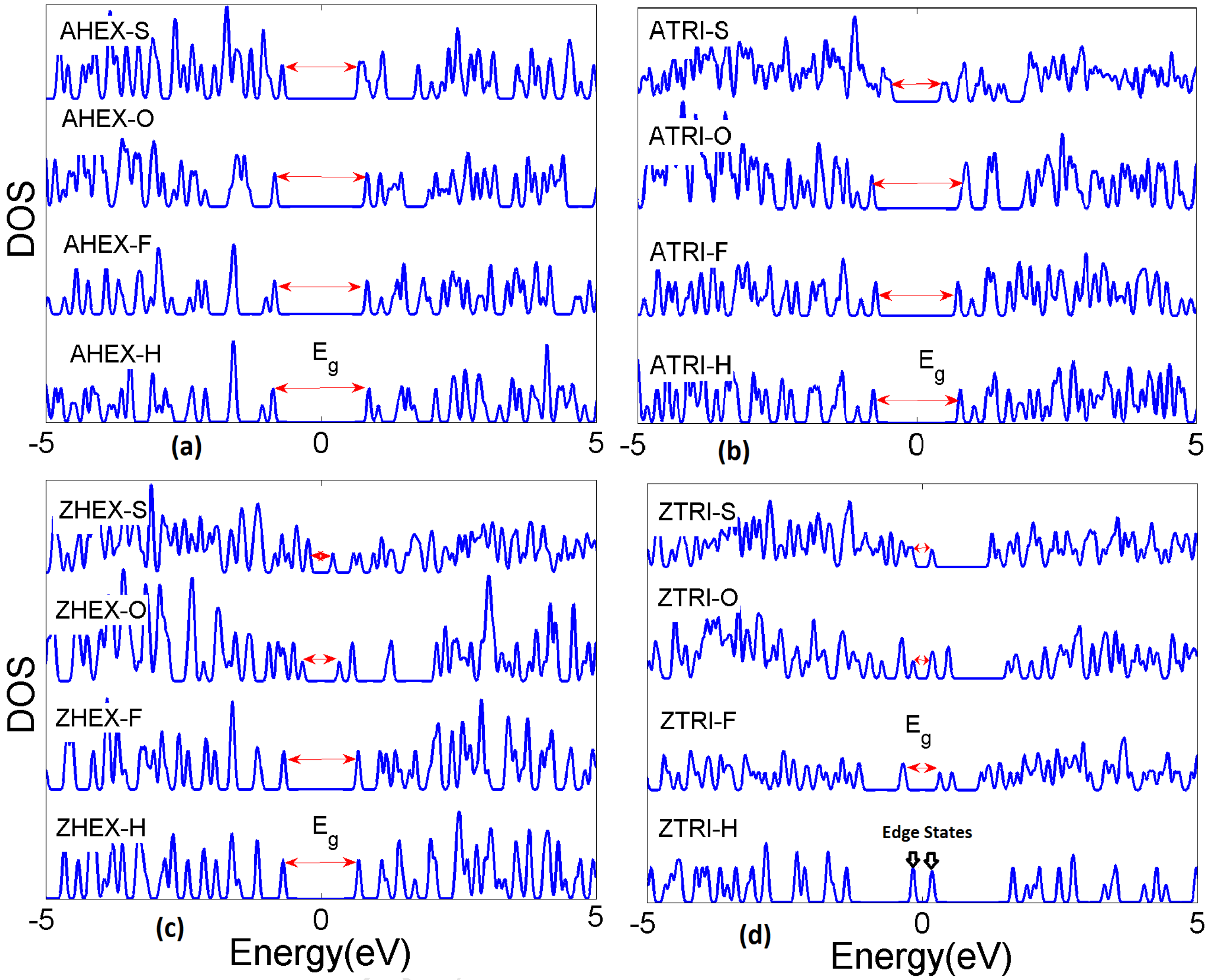

Fig. 3. Density of states of AHEX (a), ATRI (b), ZHEX (c), and ZTRI (d) clusters relaxed by various elements.

For instance, the gap in ZHEX decreases from 1.38 to 0.43 eV for H and S terminations, respectively. The reason behind this considerable decrease of the energy gap in SQD passivated with O or S is the lone pairs of electrons, situated in the energy gap, provided by these large atoms. Moreover, the small energy gap in ZTRI-H can be significantly increased by replacing H with OH group, namely E_g=1.1 eV . As a result of the geometrical shape of the ZTRI, it will have certain number of edge states due to electrons from edge atoms (it will be discussed briefly in the following section) that are detached from other states. These states appear in the energy gap as seen in Fig. 3 (d). In case of ZTRI-H, these edge electrons will interact with each other to form the high energy antibonding pi-orbitals. While in ZTRI-OH, they will interact with the near O atoms instead of the far Si atoms (see numbered atoms in Fig. 4 (k)) to form strong pi-bonds and therefore get shifted to lower energy.

In order to study the effect of size and generalize our results, we investigate the effect of different passivation on larger SQDs. The AHEX (114 atom) and ZTRI (118 atom) are chosen as a representative examples of the large flakes. Increasing the flake size leads to decrease of the energy gap, where for AHEX-H ($Si_{114}H_{30}$) the energy gap decrease to 1.16 eV from 1.74 eV for AHEX-H ($Si_{42}H_{18}$). In case of ZTRI-H, E_g =0.15 eV which also means that increasing size decrease the energy gap. The effect of chemical passivation in large flakes is similar to its effect in small flakes, the energy gap of AHEX ($Si_{114}H_{30}$) decreases from 1.16 eV to 0.82 eV when passivated with S instead of H. This small decrease in energy gap is similar to the decrease in energy gap in small AHEX ($Si_{42}H_{18}$) flakes. The effect of chemical functionalization in large ZTRI is similar to small ones, where a considerable energy gap can be opened when passivation with OH group Eg=0.81 eV with respect to the small E_g=0.15 eV in ZTRI ($Si_{118}H_{30}$). Therefore the present results are valid for the small as well as the large silicene quantum dots having triangular or hexagonal shapes with zigzag or armchair termination subjected to different edge passivation.

TABLE II. The energy gap (E_g) and the total dipole moment (TDM) of SQDs passivated with OH group and various elements.

Structure		E_g (eV)	TDM (D)	Structure		E_g (eV)	TDM (D)
AHEX	H	1.74	0.00	ATRI	H	1.56	0.002
	F	1.68	0.00		F	1.47	0.08
	O	1.67	0.00		O	1.61	0.01
	S	1.4	0.00		S	0.94	7.38
	OH	1.6	8.94		OH	1.42	15.4
					pristine	1.33	0.014
ZHEX	H	1.38	0.00	ZTRI	H	0.27	3.32
	F	1.36	0.00		F	0.65	2.1
	O	0.67	0.00		O	0.33	3.3
	S	0.43	0.00		S	0.36	16.89
	OH	1.1	24.03		OH	1.06	6.05
					pristine	0.62	4.93

3.3 EDGE STATES AND HOMO/LUMO

Fig. 4 shows the distribution of the HOMO and LUMO states in the four selected SQDs with different passivation. It is observed that for hydrogenated armchair flakes, the HOMO and LUMO distribute over the surface and the edges of the flakes. Hydrogen atoms passivate one of the two free electrons in silicon leaving one free electron on each edge atom which in addition to the electrons from bulk atoms lead to the distribution over the edge and the surface of the flake. In this type of passivation the edge and the surface of the SQDs are highly interactive with the surrounding which can be used in many applications such as sensors. As a result of sp3 hybridization in sulfur, the two unpaired electrons from sulfur in S-armchair flakes totally neutralize the edge atoms therefore the HOMO (as seen in Fig. 4 (e)) has negligible

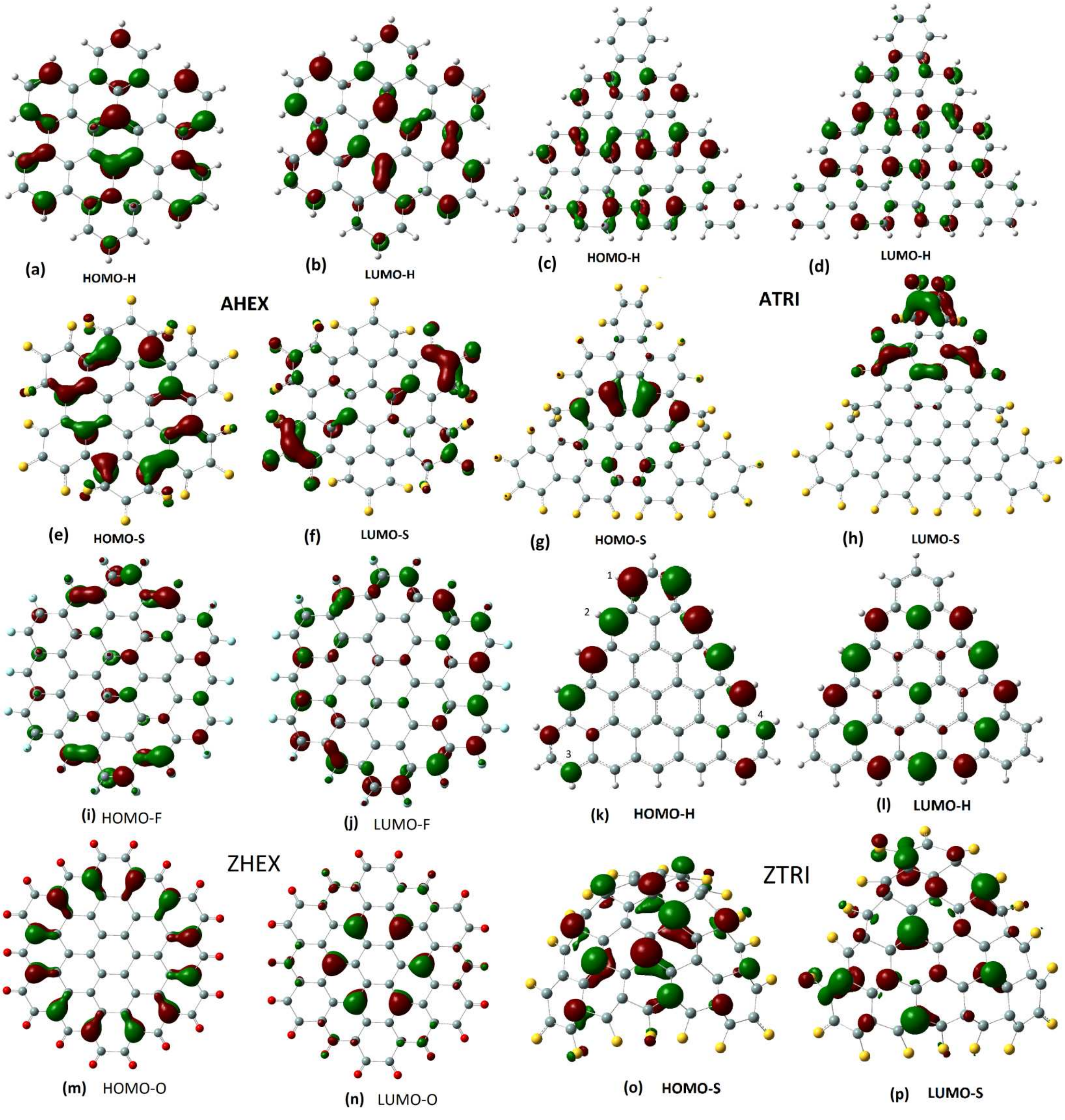

Fig. 4. Distribution of the HOMO/LUMO orbitals in hexagonal and triangular silicene flakes under passivation with various elements with the dark purple and green (online only) denote the positive and negative sign of the molecular orbital wave function.

distribution over the edge atoms. The electronic states of the edge atoms experience decrease in energy and move to lower energy in valance band or conduction band this can be noticed in the distribution of LUMO in Fig. 4 (f). Therefore, edge modified SQDs by S are insensitive to edge defects that is frequantly occur during the experimental fabrication. The distribution of the HOMO and LUMO in F- and O-passivated AHEX and ATRI is qualitatively similar to that in H- and S-passivated flakes, respectively, therefore we do not present their results here.

The distribution in silicene flakes with zigzag edges is significantly different, especially for ZTRI clusters. It can be observed from Fig. 3 (d) for ZTRI-H that there are two peaks inside the gap between conduction band and valance band states. These two peaks are due to the edge states from electrons in the four edge atoms shown in Fig. 4 (k). Two electronic energy levels (HOMO and HOMO-1) will be formed from the four electrons provided by these four atoms that are totally detached from the bulk states and distribute only on the edge atoms. The HOMO in ZTRI-H is shown in Fig.4 (k), it is localized on single atoms at the edges forming antibonding orbitals. In this type of bonding the electrons are weakly bounded to the silicene system. This interesting effect has been observed also in triangular graphene with zigzag edges [25]. The number of edge states in GQDs with the same number of atoms from tight binding model is four states.[43] This number is exactly the same as in SQDs however in graphene these states are only P electrons while in silicene, due to the sp3 hybridization they can be s or p electrons. It was shown that the low-energy electronic band structure of silicene is dominated by pi-electrons.[31] Thus the number and type of edge states in silicene is similar to those in graphene. The edge effect in zigzag cluster is still observed in ZHEX. However, due to the small separation between the edge states in ZHEX and the bulk states as in Fig. 4 (i) and (j) the HOMO has a finite distribution at the bulk atoms. When SQDs with zigzag termination are passivated with O, the two unpaired electrons from the sp3 hybridized orbitals of oxygen interact with two electrons from edge silicon atom forming strong Si=O double bond which forces the ZHEX or ZTRI quantum dot to transformation to planar structure. In armchair flakes such planar structure is observed only in their interior because the distance between Si atoms at the edge is large in comparison with that in zigzag flakes which leads to a small deformation at the edges.

It is worth noting that the magnetic state of ZTRI silicene depends on the number of Si atoms such that flakes with an even number of Si atoms will have nonmagnetic properties while flakes with an odd number of Si atoms will have ferromagnetic/nonmagnetic properties depending on the attached element. To investigate the ferromagnetic properties of ZTRI with odd number of Si atoms, we plot Fig. 5 that shows the electronic density of states and HOMO-1, HOMO, and LUMO of ZTRI (Si_{33}) saturated with H, OH, F, and O. In order to determine the number of edge atoms from which these edge states arise we plot Fig. 5 (b) where we first determine the shape that does not have edge states (any shape that have even number of sides such as hexagonal or square) as seen by yellow in Fig. 5 (b). The other atoms are then allowed to share their electrons with the nearest atoms (shown in red) the remaining atoms (three atoms) are the edge atoms. The total number of edge states is then equals three states detached from other states and located in the energy gap as seen in Fig. 5 (a). The distribution of HOMO-1, HOMO, and LUMO confirm that these states are distributed over the edges and form week antibonding pi orbitals, as in Fig. 5 (c)-(f). The energy gap in ZTRI-H ($Si_{33}H_{15}$) equals 0.91 eV which is very high comparing to the small gap, E_g=0.27 eV, in ZTRI-H ($Si_{46}H_{18}$). The reason of the high energy gap in hydrogenated flakes could be due to the unpaired edge electrons in that repulse each other in the alpha MOs or in beta MOs.

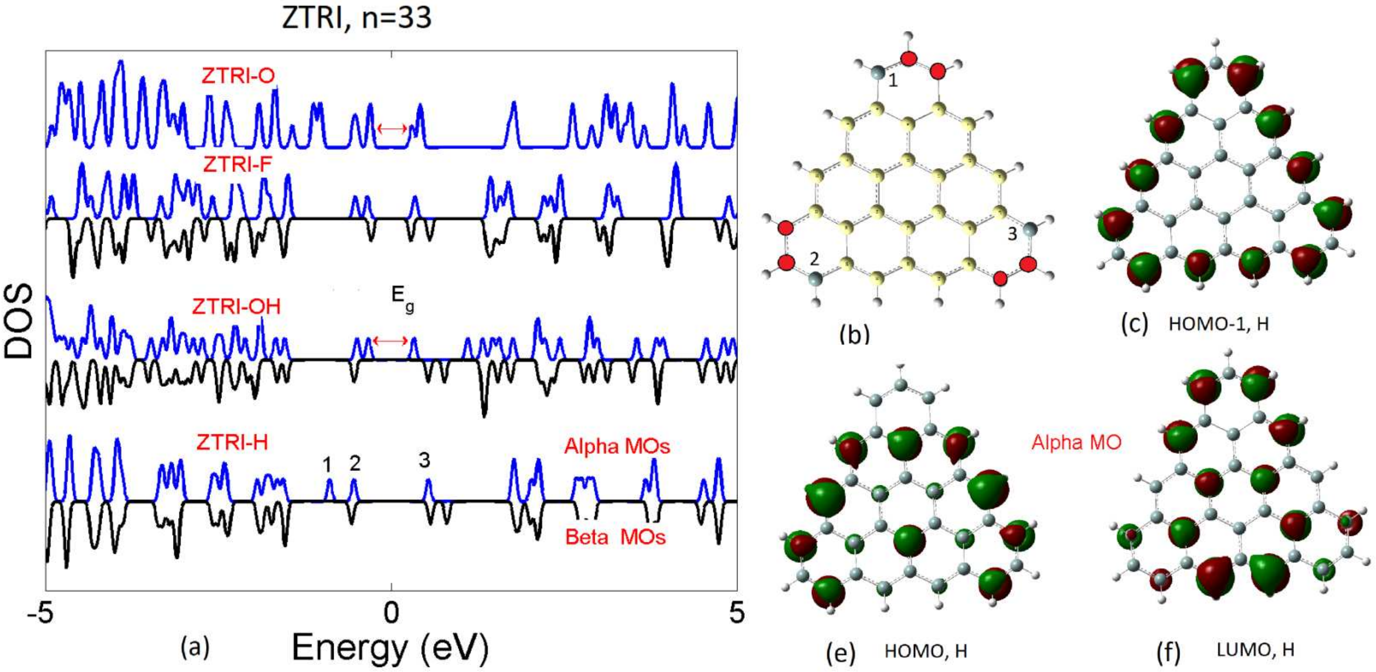

Fig. 5. (a) Density of states of ZTRI with non-zero total spin and (b) edge atoms corresponding to the edge states of ZTRI are illustrated. The alpha MOs distribution of the three edge states are shown for ZTRI-H, namely HOMO-1, HOMO, and LUMO.

Attaching larger atoms such as F or OH to the ZTRI edges will decrease the repulsion between alpha or beta edge states and lead to the decrease of the energy gap. The magnetic state observed in zigzag triangular can be transformed to nonmagnetic state by edge termination with O or S. One of the two unpaired electrons from the sp3 hybridized O or S will neutralize one of the three edge electrons which convert the system from doublet state to singlet with zero total spin.

3.4 CHARGE DISTRIBUTION AND TOTAL DIPOLE MOMENT

Shape modification due to edge relaxation using large atoms has a considerable effect on the total dipole moment (TDM) of the SQDs. Fig. 6 presents the charge distribution and TDM of selected SQDs with high and low deformation. The TDM of AHEX and ZHEX with attached H, F, O, and S equal to zero (D) due to the symmetric distribution of attached edge atoms on the six sides of the flakes which ensures the local dipoles cancel each other. Even in the case of passivation with large atoms as shown in Fig 6 (a), the resultant deformation in hexagonal quantum dots is symmetric around the edges which eventually leads to a zero TDM. The situation, however, is different in triangular dots where due to the existence of three sides there must be a finite value of TDM in the direction of the base regardless of the attached element. The value of TDM in triangular strongly depends on the attached element, for instance ATRI-F has TDM= 2.1 D while ZTRI-S has TDM= 16.9 D, as given in Table 2. The non-zero TMD induces an intrinsic electric field which affects the electronic structure of the SQDs. A carefully engineered edge functionalization of triangular SQDs thus can be used to build-in electric fields and in this way tailor their band gaps for various device applications. This approach offers an alternative to the external field tunability having been studied not only in silicene but also in graphene and phosphorene quantum dots [44-46] and nanoribbons. [47-50]

Passivation with chemical groups can also control the TDM of SQDs. For example passivation with OH (as shown in Fig. 6 (c)) shows that a giant dipole, with respect to the original zero value, can be achieved in ZHEX (TDM=24 D) when passivated with OH. The increase in the TDM occurs due to the considerable structural modification; the local dipoles between O and H in the OH group are responsible for the giant increase in the total dipole moment. As can be seen from Fig.6 c almost all the O-H bonds are in the positive x-y plane, therefore they sum together to increase the TDM.

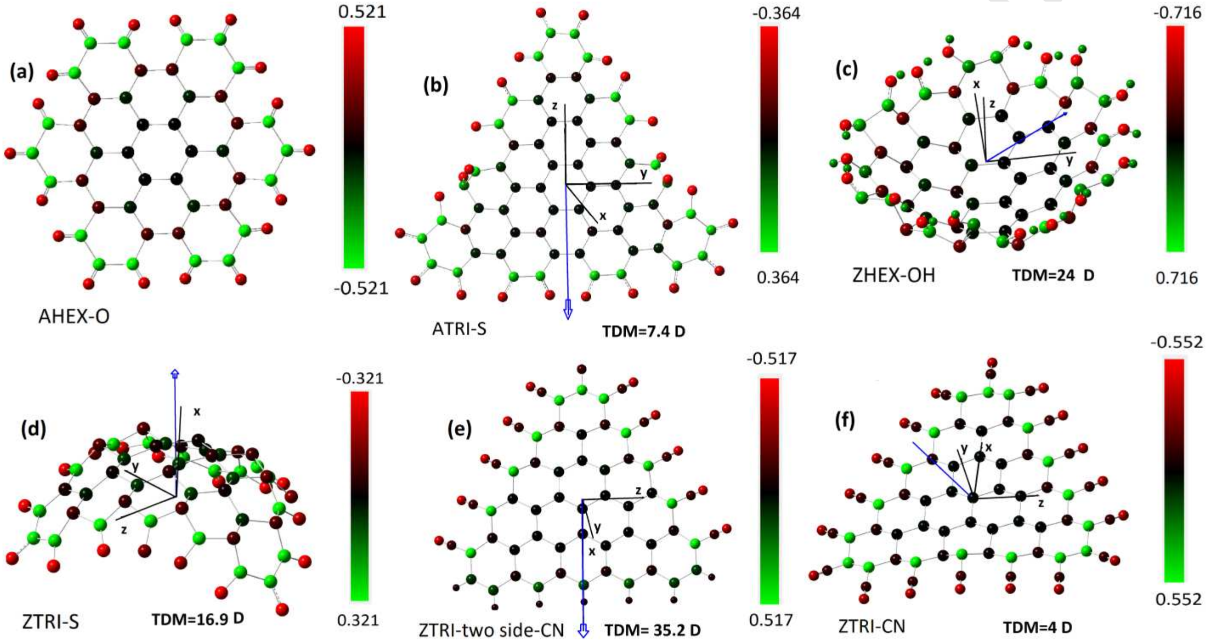

Fig. 6. The charge distribution and total dipole moment of selected silicene flakes subjected to edge passivation using various elements and groups.

The local dipoles from the O-Si bonds sum up to increase the value of total dipole in x direction and negligible increase in y-direction because these bonds are distributed in y-x plane around the positive x-direction. The final case for ZTRI terminated with CN group shows the highest value of TDM=35.2 D, in x-directions as seen in fig. 6 (e). In this case the local dipoles have two components in x-z plane and a very small component in y-direction due to buckling, the dipole moment components in z-direction cancel each other while that in x-direction sum up. Any further addition of CN group to the triangular base leads to a decrease of the TDM, see Fig. 6 (f), because local dipoles from the corresponding Si-CN bonds will be in the opposite x-direction with respect to the local dipoles from the two sides of the triangle.

4. CONCLUSION

The structure stability and electronic properties of the hexagonal and triangular SQDs with armchair and zigzag termination have been investigated under the effect of edge passivation by different elements and chemical groups. Our study shows significant structural modifications with a hemispherical shape being observed in ZTRI-S and in all structure when passivated with OH group. Such structural modifications cause considerable change in the TDM. For instance, in ZHEX quantum dots the TDM increases from zero D when passivated with H, or F, or O, or S to 24 D when passivated with OH group. The largest values of TDM are observed in SQDs with hemispherical shapes. The calculated positive binding energy shows that all the selected clusters are stable under edge relaxation. The highest stability with respect to shape and edge termination is observed for ZHEX silicene quantum dots, especially if it is passivated with oxygen. The O atoms form a very strong double bond with Si atoms stabilizing and flattening buckled silicene structure.

The SQDs show remarkable electronic properties depending on the shape, edge termination, and attached elements or groups. The AHEX has a large energy gap that is approximately unaffected by the attached elements or groups. In contrast, ATRI and ZHEX quantum dots exhibit energy gaps controllable by edge functionalization with flexible transformation from insulator (ZHEX-H) to conductor (ZHEX-S). The lone pair electrons provided by S or O are the reason for the decrease of the energy gap. On the other hand, the H or F atoms provide only one electron to passivate the edge atoms which make the sp3 hybridized system highly interactive with the surrounding due to the free electrons in Si atoms. The ZTRI quantum dot shows peculiar low-energy states localized at the edges, these states make it a conductor. Nevertheless, ZTRI can be converted to a semiconductor material by attaching OH groups to the edge atoms with energy gap ≈ 1 eV. Moreover, ZTRI with odd total number of Si atoms can have tunable ferromagnetic or antiferromagnetic properties depending on the attached element. Therefore by proper choice of the attached chemical groups or elements, the electronic properties can be oriented toward important sensor and transistor applications.

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REFERENCES

[1] B. Lalmi, H. Oughaddou, H. Enriquez, A. Kara, S. Vizzini, B.Ealet, and B. Aufray, Appl. Phys. Lett. 97, 23109 (2010).
[2] P. E. Padova, C. Quaresima, C. Ottaviani, P.M. Sheverdyaeva, P.Moras, C. Carbone, D. Topwal, B. Olivieri, A. Kara, H. Oughaddou,B. Aufray, and G.L. Lay, Appl. Phys. Lett. 96, 261905 (2010).
[3] P. Vogt, P. De Padova, C. Quaresima, J. Avila, E. Frantzeskakis,M. C. Asensio, A. Resta, B. Ealet and G. Le Lay, Phys. Rev. Lett. 108, 155501 (2012).
[4] G. G. Guzmán-Verri and L. C. Lew Yan Voon, Phys. Rev. B 76, 075131 (2007).
[5] C.-C. Liu, W. Feng, and Y. Yao, Phys. Rev. Lett. 107, 076802 (2011).
[6] W.-F. Tsai, C.-Y. Huang, T.-R. Chang, H. Lin, H.-T. Jeng, and A. Bansil, Nat. Commun. 4, 1500 (2013).
[7] Z. Ni, H. Zhong, X. Jiang et al. Nanoscale, 6, 7609 (2014).
[8] C.-C. Liu, W. Feng, and Y. Yao, Phys. Rev. Lett. 107, 076802 (2011).
[9] C.-C. Liu, W. Feng, and Y. Yao, Phys. Rev. Lett. 107 (2011).
[10] M. Ezawa, Phys. Rev. Lett. 109, 055502 (2012).

[11]F.-B. Zheng and C.-W. Zhang, “The electronic and magnetic properties of functionalized silicene: a first-principles study,” Nanoscale Research Letters, vol. 7, article 422, 2012.
[12]F. Pan, R. Quhe, Q. Ge, J. Zheng, Z. Ni, Y. Wang, Z. Gao, L. Wang, J. Lu, "Gate-induced half-metallicity in semi hydrogenatedsilicene,"Physica E 56, 43 (2014).
[13]L. Chen, C.-C. Liu, B. Feng et al. Phys. Rev. Lett. 109, 056804 (2012).
[14]C.-C. Liu, H. Jiang, and Y. Yao, Phys. Rev. B, 84, 195430 (2011).
[15]C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 226801 (2005).
[16]M.Z Hasan and C. Kane, Rev. Mod. Phys. 82, 3045 (2010).
[17]X.-L. Qi, and S.-C. Zhang, Phys Today 63, 33 (2010).
[18]M. Ezawa, New J. Phys. 14 (2012).
[19]N. D. Drummond, V. Zólyomi, and V. I. Fal'ko Phys. Rev. B 85, 075423 (2012).
[20]Z. Ni, Q. Liu, K. Tang, J. Zheng, J. Zhou, R. Qin, Z. Gao, D. Yu, and J. Lu, Nano Lett., 12, 113 (2012).
[21]B. Mandal, S. Sarkar, and P. Sarkar, J. Phys. Chem. C 119, 3400 (2015).
[22]C.Spinato, C. Ménard-Moyon, and A. Bianco, in Functionalization Of Graphene, edited by V.Georgakilas (Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany), Chap. 4.
[23]H. Zheng and W. Duley, Phys. Rev B 78, 045421 (2008).
[24]H. Abdelsalam, H. Elhaes, M. A. Ibrahim, Physica B, 537, 77 (2018).
[25]H. Abdelsalam, H. Elhaes, M. A. Ibrahim, Chem. Phys. Lett.,695, 138 (2018).
[26]X. Peng, A. Copple, and Q. Wei, J. Appl. Phys. 116, 144301 (2014).
[27]W. Hu, L. Lin, C. Yang, J. Dai, and J. Yang, Nano Lett. 3, 1675 (2016).
[28]N. Saikia, M. J. Seel, and R. Pandey, J. Phys. Chem. C 120, 20323 (2016).
[29]B. Huang, H. J. Xiang, and S.-H. Wei, Phys. Rev. Lett. 111, 145502 (2013).
[30]P. A. Denis, Phys. Chem. Chem. Phys., 17, 5393 (2015).
[31]S. Cahangirov, M. Topsakal , E. Akturk, H. Sahin, S. Ciraci, Phys. Rev. Lett. 102, 236804 (2009).
[32]S. M. Aghaei, M. M. Monshi, I. Torres, and I. Calizo, RSC Advances, 6, 17046 (2016).
[33]H. Abdelsalam, T. Espinosa-Ortega, I. Lukyanchuk, Superlattices Microstruct. 87, 137 (2015).
[34]H. Abdelsalam, M. H. Talaat, I. Lukyanchuk, M. E. Portnoi, V. A. Saroka, J. Appl. Phys. 120, 014304 (2016).
[35]P. Hu, L. Chen, J.-E. Lu, H.-W. Lee, and S. Chen, *Langmuir* 34, 2834 (2018).
[36]P. Hohenberg and W. Kohn, Phys. Rev. 136, 864 (1964).
[37]W. Kohn and L. J. Sham, Phys. Rev. 140, A1130 (1965).
[38]M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, et al., Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford, CT, 2010.
[39]A.D. Becke, J. Chem. Phys. 98, 5648 (1993).
[40]E. Rudberg, P. Salek, Y. Luo, Nano Lett. 7, 2211 (2007).
[41]K.D. Dobbs, W.J. Hehre, J. Comput. Chem. 8, 880 (1987).
[42]S. Lebègue, O. Eriksson, Phys Rev. B 79, 115409 (2009).
[43]J. Fernández-Rossier and J. J. Palacios, Phys. Rev. Lett. 99, 177204 (2007).
[44]L. L. Li, D. Moldovan, W. Xu, and F. M. Peeters, Nanotechnology 28, 85702 (2017).
[45]V. A. Saroka, I. Lukyanchuk, M. E. Portnoi, and H. Abdelsalam, Phys. Rev. B 96, 85436 (2017).
[46]L. L. Li, D. Moldovan, W. Xu, and F. M. Peeters, Phys. Rev. B 96, 155425 (2017).
[47]C. P. Chang, Y. C. Huang, C. L. Lu, J. H. Ho, T. S. Li, and M. F. Lin, Carbon N. Y. 44, 508 (2006).
[48]M. Ezawa, New J. Phys. 16, 115004 (2014).
[49]V. A. Saroka, K. G. Batrakov, V. A. Demin, and L. A. Chernozatonskii, J. Phys. Condens. Matter 27, 145305 (2015).
[50]M. M. Grujić, M. Ezawa, M. Ž. Tadić, and F. M. Peeters, Phys. Rev. B 93, 245413 (2016).

Highlights

- The stability and electronic properties of edge functionalized silicene quantum dots are investigated using density functional theory.

- The electronic properties of silicene flakes strongly depend on the shape, edge termination, and attached element or chemical groups.

- The zigzag flakes have highly interactive edge states that are localized on the edges.

- Triangular flakes with zigzag termination have tunable magnetic properties depending on the number of atoms and the attached element.

- Careful choice of the attached functional groups or elements to silicene flakes allows tailoring of their properties to different application such as sensors or semiconductor devices.