Impact of Defects on Electronic Transmission Properties and Spin Transport in Monolayer Silicene

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Abstract: In this work, we report an ab-initio study on the effect of lattice defects on the spin polarized electronic transmission in Armchair and Zigzag type Silicene Nanoribbons (ASiNR and ZSiNR). We have incorporated various defects such as edge roughness, single vacancy and Stone-Wales defects, and studied the transmission in ASiNR super-cell of dimensions (1x18x20)Å and that in ZSiNR super-cell of dimensions (1x16x19)Å using density functional theory (DFT) - non equilibrium green's function (NEGF) under a small bias. The results show a decrease in the difference (up – down) in spin transmission with increasing surface roughness in both ASiNR and ZSiNR. The total transmission decreases, by approximately 35% in ASiNR and 60% in ZSiNR for single vacancy defect compared to pristine.

Keywords: Density functional theory; spin polarized; transmission spectrum; silicene; defects; projected device density of dtates.

1 INTRODUCTION

Silicene is a dimensionally confined monolayer of Si atoms, analogous to graphene. Extensive research is being carried out in virtue of silicene, in order to integrate it with silicon based devices, as Silicon forms the foundation in all electronic devices [1].

However, it is difficult to always fabricate pristine nanoribbon of silicene. Deformations in nanomaterials (during fabrication) are common phenomena. Laser irradiation and electronic beam cause vacancy defects or point defects [2, 3]. Surface roughness is another pragmatic defect, to be dealt with. These defects condition the material properties. So if we can use the defects to our advantage, the onerous task of engendering perfect nanomaterial can be avoided. In fact, defects may also be purposefully created in nanomaterials in order to tune material properties.

We have attempted to investigate the premise that silicene favours or opposes up-spin or down-spin transmission depending on various factors [4] like the defects or the metrics of the materials. To conduct this research we have used atomistic DFT-NEGF studies in QuantumWise ATK [5].

We have made comparative studies for armchair and zigzag Silicene nanoribbon (ASiNR and ZSiNR) structures of pristine and defective nature.

The modelled defective structures for both ASiNR

and ZSiNR are: (1) with one atom missing on each edge (total two atoms missing), labeled edge2a, (2)

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with two atoms missing on each edge (total four atoms missing), labeled edge4a, (3) Stone-Wales (SW) and (4) Single vacancy defect, labeled single. The first two types mainly account for edge roughness.

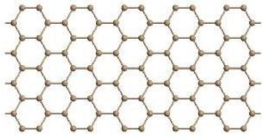
Fig. 1. Pristine ASiNR.

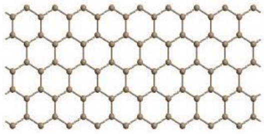
Fig. 2. Pristine ZSiNR.

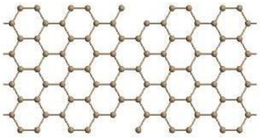
Fig. 3. Edge 2a ASiNR.

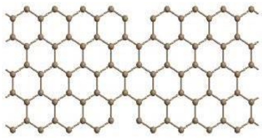
Fig. 4. Edge 2a ZSiNR.

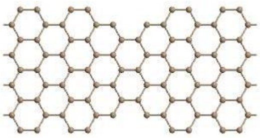
Fig. 5. Edge 4a ASiNR.

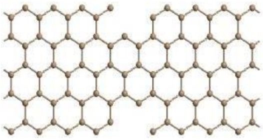
Fig. 6. Edge 4a ZSiNR.

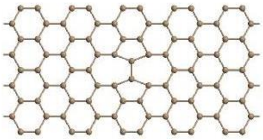
Fig. 7. SW ASiNR.

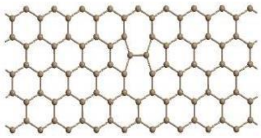
Fig. 8. SW ZSiNR.

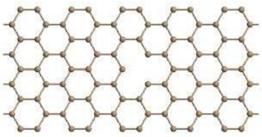
Fig. 9. Single ASiNR.

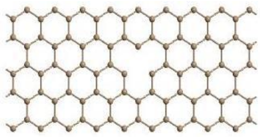
Fig. 10. Single ZSiNR.

2 METHODOLOGY

We have studied the spin-dependent electronic transport properties of two-probe system, containing left electrode, right electrode and central region. The two electrodes are semi-infinite and pristine in nature and of the same material as the central region. The central region is a 1D channel. Calculations have been performed, based on Atomistic Toolkit (ATK) package, which is based on real-space, nonequilibrium Green's function (NEGF) formalism and DFT. We have adopted the spin polarized generalized gradient approximation and revised Purdew Burke Ernzerhof (SGGA.RPBE) [6]-[8] exchange correlation coupled with double-zeta double polarized basis set, which is a recipe for an accurate calculator.

We have set the parameters as follows: k-point grid has been kept 1 x 1 x 75, electron temperature set at 300 Kelvin. FFT2D poisson solver has been implemented. This is deemed sufficient as the vacuum along the direction A and B is sufficiently large (approximately six Angstrom on each side of the nanoribbon).

The transmission spectra have been calculated for 0.3V finite bias applied to the right electrode for the range -5 to 5 eV using Recursion self-energy Calculator with Monkhorst pack Grid [9] class, 3 x 3 k-point sampling.

The transmission coefficient is used to calculate the current [10-12].

$$I(V_L, V_R, T_L, T_R) = \frac{e}{h}\sum_{\sigma}\int T_\sigma(E)\left[f\left(\frac{E-\mu_R}{k_B T_R}\right) - f\left(\frac{E-\mu_L}{k_B T_L}\right)\right]dE,$$

$$\mu_L = E_F^L - eV_L,$$

$$\mu_R = E_F^L - eV_R$$

Where f is Fermi function,

$T_{L/R}$ is the electron temperature of the left/right electrode,
$T_\sigma(E)$ is the transmission coefficient for the spin component σ,
$\mu_{L/R}$ is chemical potential of left/right electrode,
E_F^L is Fermi level of left electrode,
$(V_L - V_R)$ is the applied bias.

3 RESULTS AND DISCUSSIONS

3.1 Current Transmission

The current in ZSiNR reduces drastically from 23 μA to 8.9 μA (going from Pristine to defective NRs) as shown in Table 1.

The total transmission in ASiNR goes down by 35.46% and that in ZSiNR goes down by 61.52% for single vacancy defect.

Table 1. Total Current in Pristine and Defectivs ASiNR and ZSiNR.

Current (μA)	Pristine	Edge 2a	Edge 4a	Stone-Wales	Single
ASiNR	7.36	6.91	3.87	5.27	4.75
ZSiNR	23.13	17.36	13.89	10.59	8.9

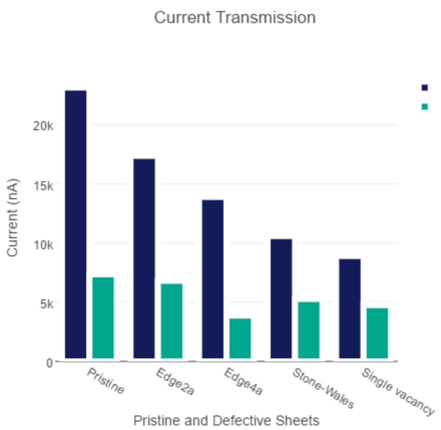

Fig. 11. Comparison of current transmission in ASiNR and ZSiNR.

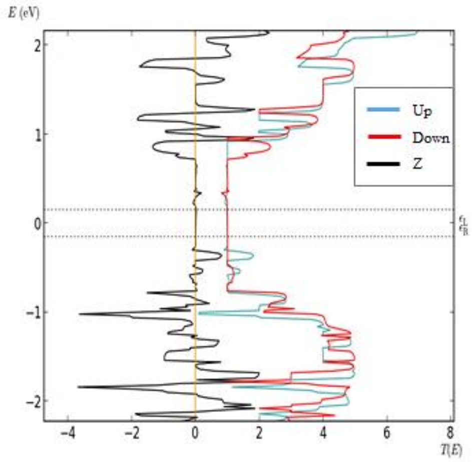

Fig. 13. Transmission spectrum of pristine ZSiNR.

3.2 Transmission Spectrum

The following graphs compare the transmission in pristine ZSiNR and ASiNR. The Up/down curve indicates the up/down spin transmission spectrum and the Z curve represents the difference between up and down spin transmission (Up – Down).

Pristine ZSiNR shows conduction in the bias region (with a transmission coefficient of 1.5) In the bias region, pristine ZSiNR is not showing support to any particular spin. The Z curve is approximately a flat line. Whereas, pristine ASiNR shows support to the up spin transmission of holes (transmission coefficient is 2). Substantial difference between the up and down spin transmissions is observed in ASiNR as compared to ZSiNR as the intermittent peaks in ASiNR are greater in number. In pristine ASiNR, the average up spin transmission coefficient is 2.2 and the average down spin transmission coefficient is 1.97, and those in pristine ZSiNR are 3.76 and 3.75 respectively.

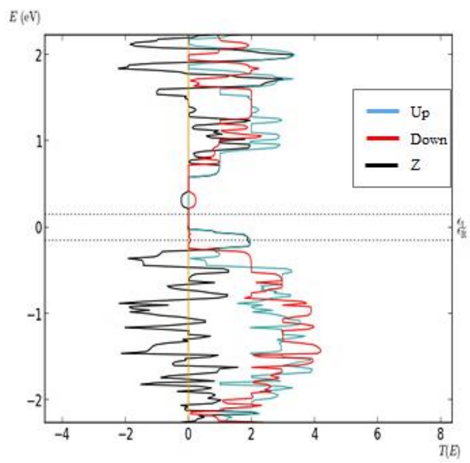

Fig. 12. Transmission spectrum of pristine ASiNR.

However, in ASiNR, we find that the difference between the up and down spin electron transmissions (represented by Z curve) reduces in the nanoribbons with SW and single vacancy defect and goes further down for edge4a defect but in the case of holes the reduction is not significant.

Pristine ASiNR shows a tendency to support up spin transmission, that support decreases in the nanoribbon with edge4a defect but, in edge2a defect that propensity is boosted.

On the other hand, pristine ZSiNR shows support to down spin holes, that tendency reduces in nanoribbons with edge4a, SW and single vacancy defects and again is boosted in case of edge2a defect.

Average up spin support is 0.91 for Stone-Wales defect and 0.84 for single vacancy in ASiNR.

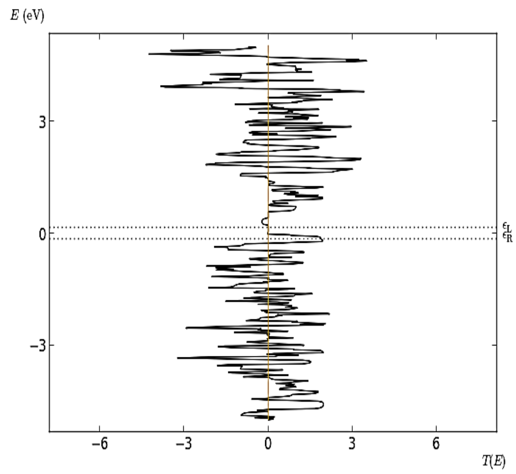

Fig. 14. Difference between up and down spin transmission in pristine ASiNR.

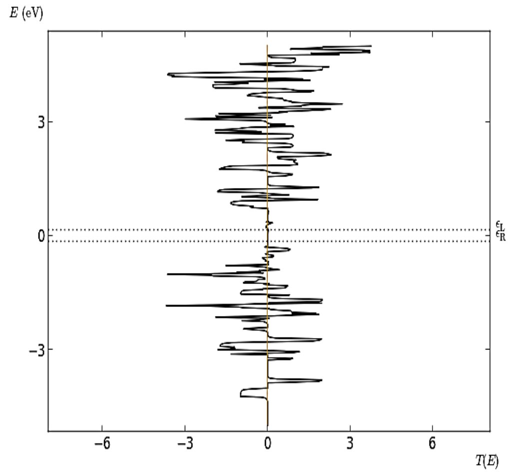

Fig. 15. Difference between up and down spin transmission in pristine ZSiNR.

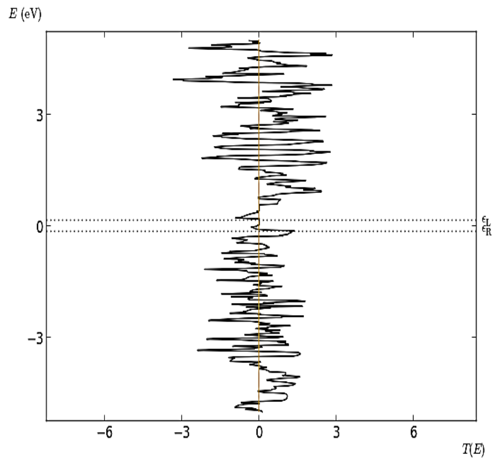

Fig. 16. Difference between up and down spin transmission in ASiNR with single vacancy defect.

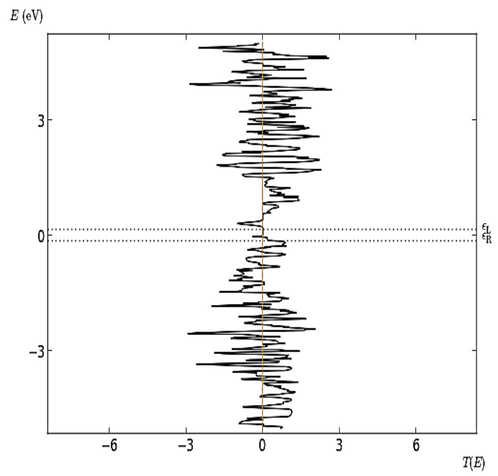

Fig. 17. Difference between up and down spin transmission in ASiNR with edge4a defect.

3.3 Density of States

Figs. 18-20 show the projected device density of states (PDDOS). The Up Spin curve shows the density of available up spin states and the Down Spin curve shows the density of available down spin states. The DOS in ZSiNR shows stronger peaks in certain energies near the Fermi level in comparison to that in ASiNR.in pristine as well as defective ones. We observe that the density of states (DOS) shoots up intermittently in both the defective ASiNR and ZSiNR as compared to the pristine one. The DOS seemingly increase with defects, which can be of utility. The intermittent peaks reduce in the nanoribbons with stone-wales and single vacancy defects. In Fig. 18 we can see that DOS in ASiNR shoots up for down spin showing support to down spin holes. DOS in pristine ZSiNR shows support to down spin electrons and up spin holes. The support for down spin electrons (in ZSiNR) is maintained in edge2a nanoribbon but reduces significantly in other defects. Whereas, in ASiNR the down spin electrons receive substantial support in the edge4a, Stone-Wales and single vacancy defective nanoribbons in comparison to that in pristine ASiNR and edge2a defect.

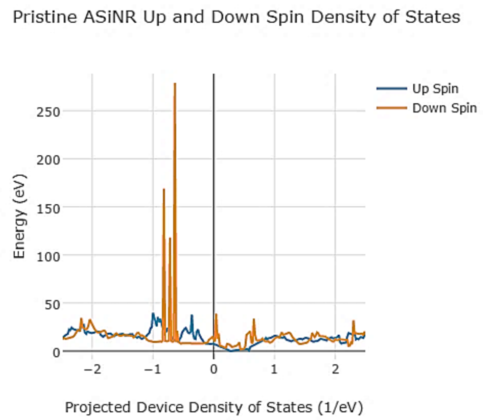

Fig. 18. Up and down spin PDDOS of pristine ASiNR.

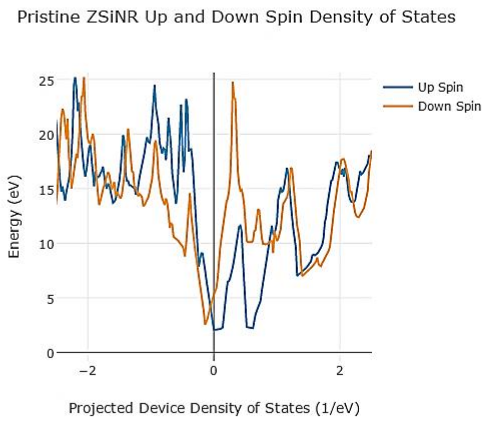

Fig. 19. Up and down spin PDDOS of Pristine ZSiNR.

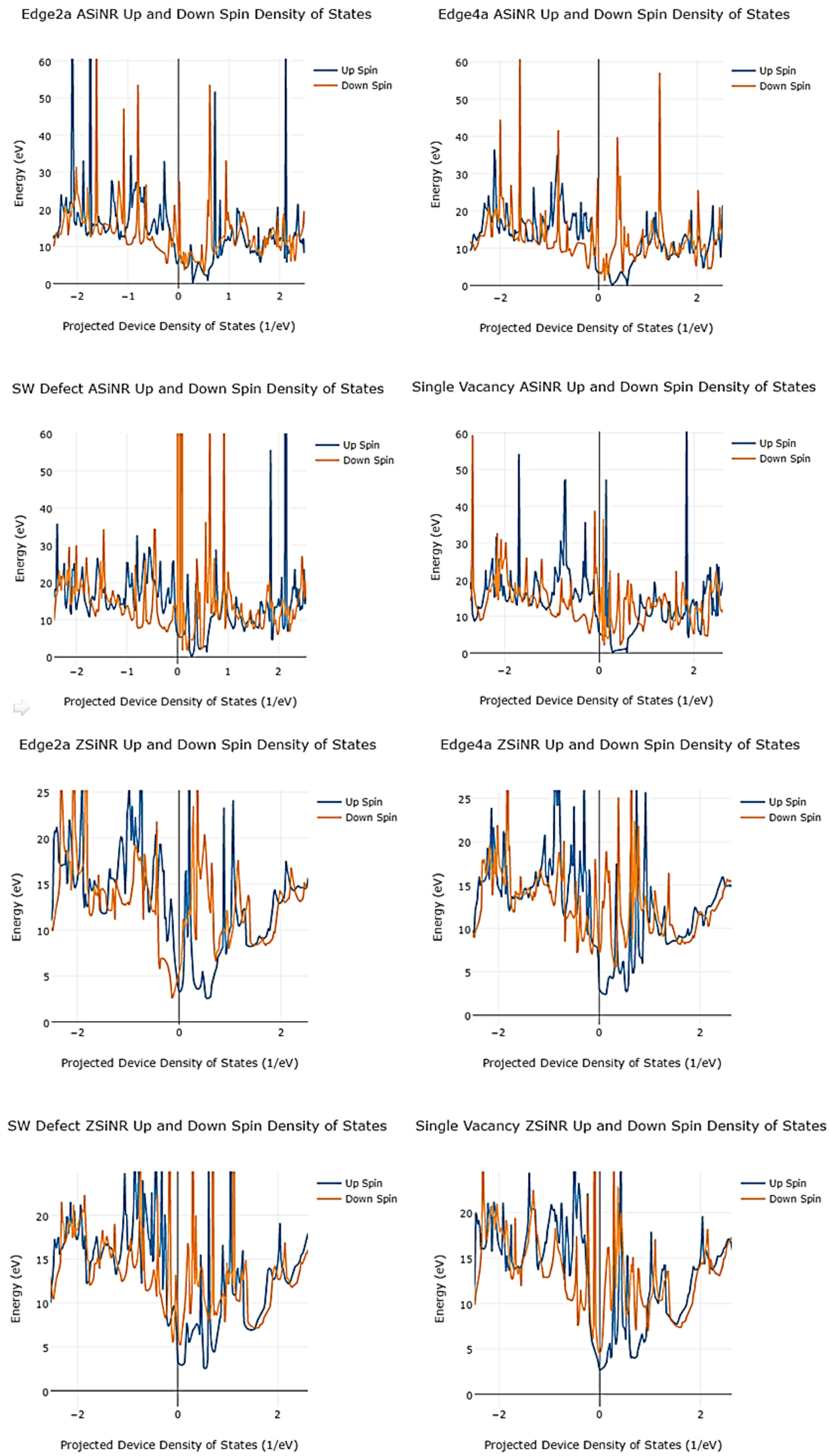

Fig. 20. Projected device density of dtates of ASiNR and ZSiNR pristine and defective nanoribbons.

3.4 Bandstructure

In Figs. 21 and 22 we have zoomed the conduction and valence bands near the fermi energy as those bands mainly contribute for the electronic transport properties. As we are performing ab-initio calculations on a supercell containing large number of atoms, multiple bands overlap and the effect that we see is attributable to Brilloune zone folding. The bandstructure has been calculated atomistically, which is more accurate, rather than using a classical or semi-classical E-k relation.

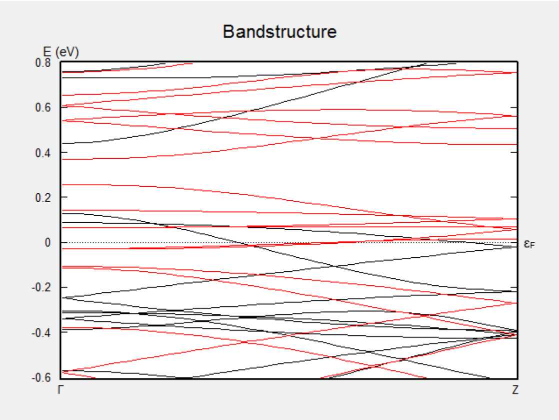

Fig. 21. Banstructure of pristine ASiNR.

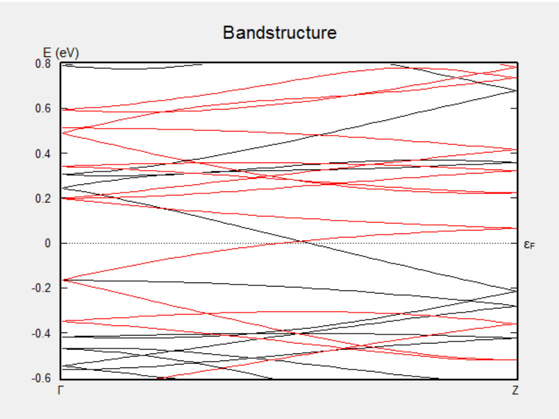

Fig. 22. Banstructure of Pristine ASiNR.

4 CONCLUSION

Our studies show that the difference between the spin transmission deteriorates in presence of edge roughness. Total transmission in ZSiNR is higher than that in ASiNR by 68.2% however, the spin transmission is affected more in ASiNR compared to ZSiNR. For edge roughness in ASiNR the drop in transmission varies from 6.1% (in edge 2a) to 47.42% (edge 4a) and for ZSiNR drop in transmission is 25% (edge 2a) and 40% (edge 4a) compared to pristine. Support to individual spin transmission deteriorates in presence of edge roughness (of edge4a type) but is boosted in edge2a type defective ASiNR and ZSiNR.

In pristine ZSiNR down spin electrons and up spin holes have more states available. This tendency is maintained in edge2a but not in other ZSiNR. In ASiNR, edge4a, Stone-Wales and single vacancy defective nanoribbons show greater availability of states for the down spin electrons in comparison to the number of states existing in pristine ASiNR and edge2a defect.

REFERENCES

[1] H. Li, L. Wang, Q. Liu, J. Zheng, W. Mei, Z. Gao, J. Shi, and J. Lu, 2012. High performance silicene nanoribbon field effect transistors with current saturation, Eur. Phys. J. B, vol. 85, pp. 274.

[2] G. Brumfiel, Sticky problem snares wonder material, Nature, vol. 495, pp. 152-153.

[3] F. Banhart, J. Kotakoski, A. V. Krasheninnikov, Structural defects in graphene, ACS Nano, vol. 5, pp. 26-41.

[4] W. Tsai, C. Huang, T. Chang, H.n Lin, H. Jeng, and A. Bansil. Gated silicene as tunable source of nearly 100% spin-polarized electrons, Nature Communications, vol. 4, ref. no. 1500.

[5] Atomistix ToolKit version 2014. 3, QuantumWise A/S.

[6] J. P. Perdew, K. Burke, and M. Ernzerhof, 1996. Generalized gradient approximation made simple, Phys. Rev. Lett., vol. 77, ref. no. 65.

[7] J. Perdew, K. Burke, and M. Ernzerhof, 1997. Generalized gradient approximation made simple, Phys. Rev. Lett., 78, 1396(E).

[8] Y. Zhang and W. Yang, 1998. Phys. Rev. Lett, vol. 80, pp. 890.

[9] H. J. Monkhorst and J. D. Pack, 1976. Special points for Brillouin-zone integrations, Phys. Rev. B, vol. 13, no. 5188-5192.

[10] ATK Toolkit Reference Manual – Transmission Spectrum http://www.quantumwise.com/documents/manuals/latest/ReferenceManual/index.html/ref.transmissionspectrum.html

[11] ATK Toolkit Reference Manual – Recursion Self Energy http://www.quantumwise.com/documents/manuals/latest/ReferenceManual/index.html/ref.recursionselfenergy.html

[12] M. P. Lopez Sancho, J. M. Lopez Sancho, and J. Rubio, 1985. Highly convergent schemes for the calculation of bulk and surface Green functions, J. Phys. F., vol. 15, pp. 851.