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Tunable band gap of silicene nanoribbons- a review

Gurleen Kaur Walia[1], Deep Kamal Kaur Randhawa[2] and Kanwalpreet Singh[3]

[1]*Department of Electronics and Electrical Engineering, Lovely Professional University (LPU), Phagwara, Punjab, India*
[2]*Department of Electronics and Communication Engineering, Guru Nanak Dev University, Regional Campus, Jalandhar, Punjab, India*
[3]*Department of Computer Science and Engineering, UIET, Panjab University, Swami Sarvanand Giri Regional Centre, Hoshiarpur, Punjab, India*

Abstract –

A band gap is the foremost feature required for any material to be useful in the electronic industry. So a device must be flexible enough that its band gap can be tuned in numerous ways, if initially it has a zero band gap. So an extensive review has been carried out in analyzing a nanomaterial, silicene for its band gap tuning. The results reveal that the pristine silicene, which is actually a semimetal, exhibits varied levels of band gap tuning on introducing vacancy defect and gas molecule adsorption.

Keywords*: band gap, defect, adsorption, ASiNR*

1. INTRODUCTION

Today's world is the world of nanotechnology. So there is always a need of such a nanomaterial which finds applications in day-to-day life. Silicene is considered as a wonder material, after graphene, which exhibits outstanding properties and is found to have applications in numerous fields these days. A material needs to have an electronic band gap for it to be useful in electronics. Silicene has an advantage over graphene in having this feature. Pristine silicene is a semimetal having no band gap, which can be tuned using different methods [1-4].

2. COMPUTATIONAL DETAILS

Non-equilibrium Green's theorem along with density functional theory (DFT) is used to find the electronic calculations using Virtual Nano Lab Atomistix Tool Kit (VNL-ATK) software by Quantumwise [5]. Armchair silicene nanoribbon of width of 9 atoms is considered with a buckling of 0.44 Å. The exchange correlation functional of local density approximation is used along with 75 Ha density mesh cut-off. Silicene is a silicon counterpart of graphene.

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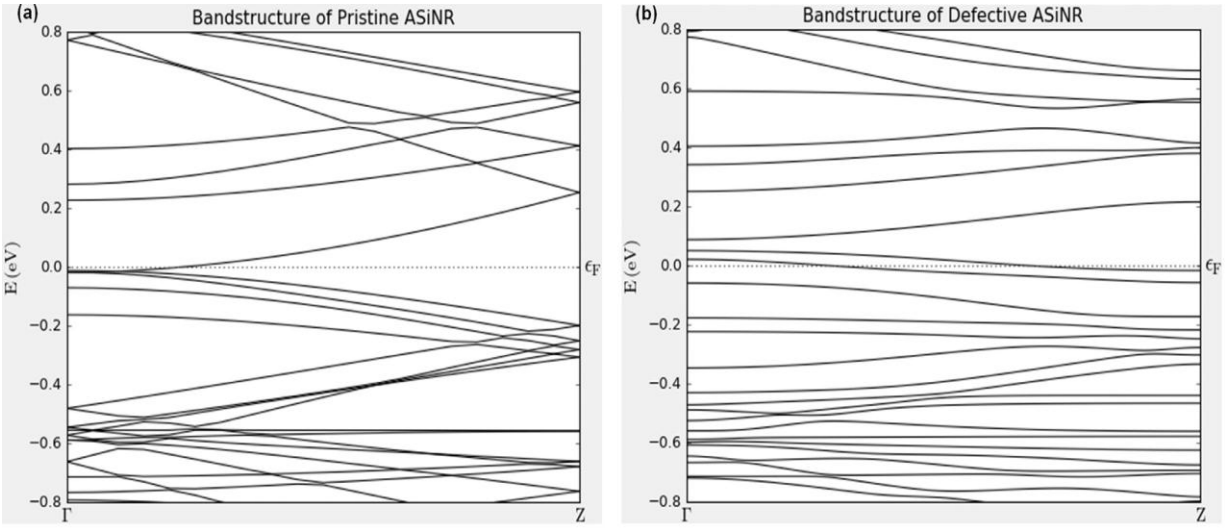


Figure 1. Bandstructure diagrams of (a) pristine ASiNR and (b) defective ASiNR [6]

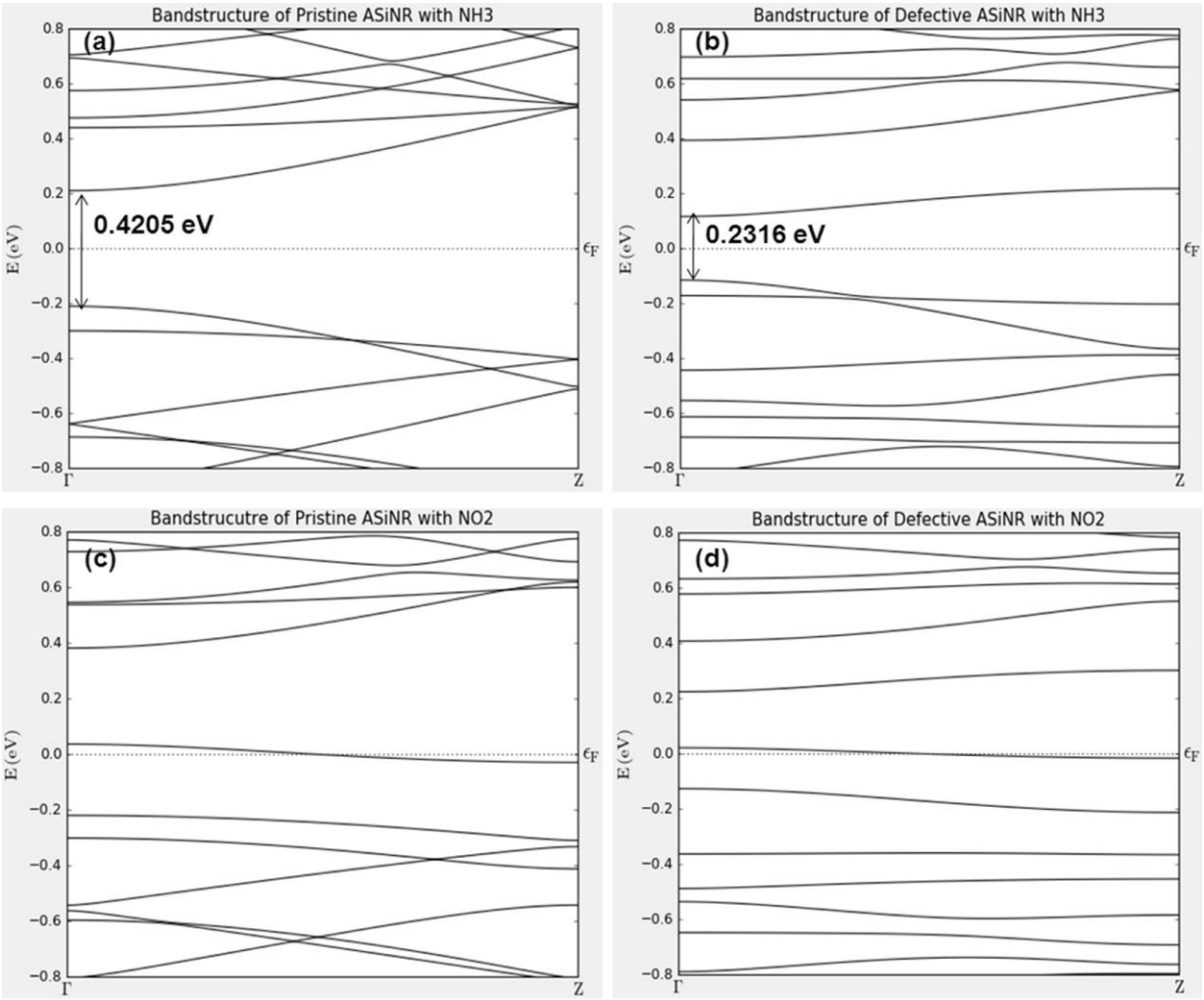


Figure 2. Bandstructure diagrams of pristine and defective ASiNRs on adsorption of N-based gases [7]

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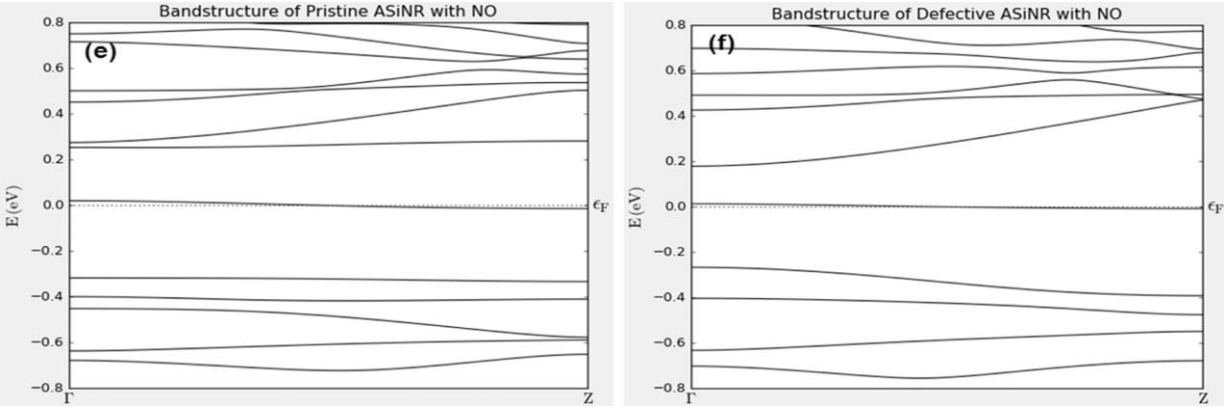
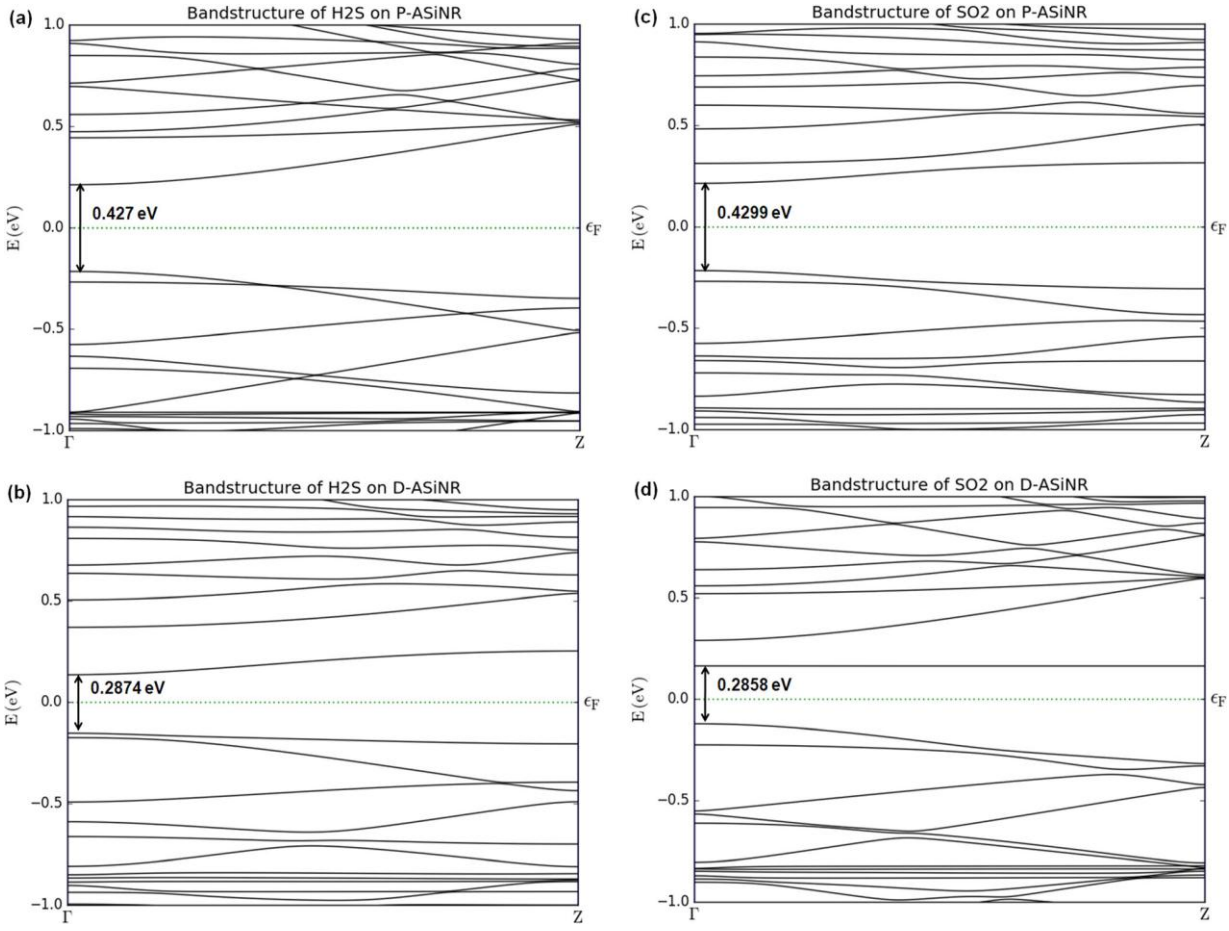


Figure 2. Continued

3. FIRST-PRINCIPLES STUDY ON SILICENE NANORIBBONS

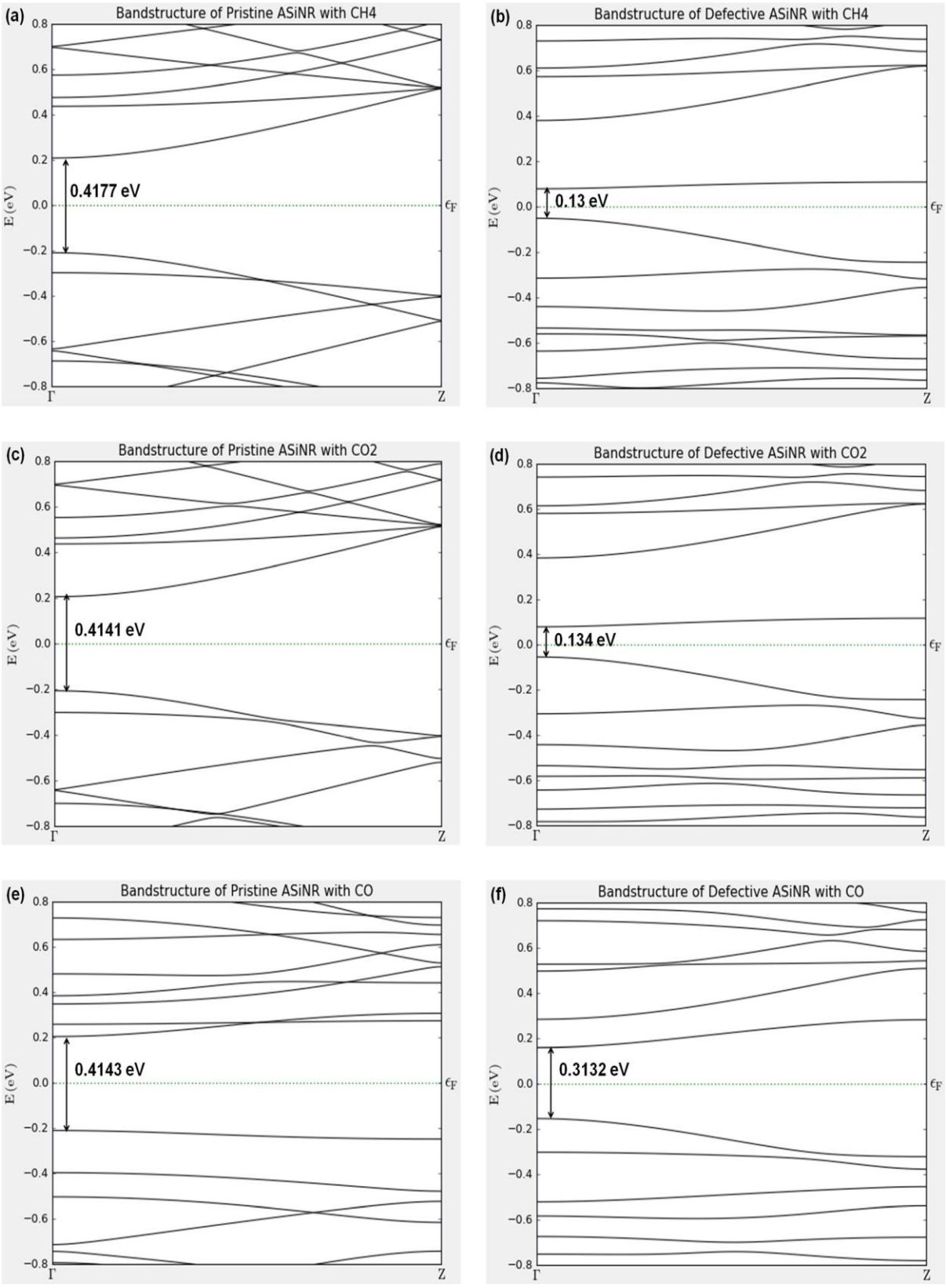
The calculated electronic properties show that pristine silicene nanoribbon is a material with no band gap as shown in Figure 1 (a). When a vacancy defect is created by the removal of a Si atom, there is a variation in the bandstructure of SiNR as shown in Figure 1 (b) [6].



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Figure 3. Bandstructure diagrams of pristine ASiNRs and defective ASiNRs on adsorption of H_2S and SO_2 [8]



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Figure 4. Bandstructure diagrams of pristine ASiNRs and defective ASiNRs on adsorption of CH_4, CO_2 and CO [9]

The adsorption of gases plays a major role in altering the bandstructure behaviour of SiNRs. Figure 2 shows the variations in band gap openings on adsorption of nitrogen-based gases, such as NH_3, NO_2 and NO. However, on adsorption of NO_2 and NO, there is formation of flat bands resulting in the metallic behaviour [7]. Sulfur-based gases, viz., H_2S and SO_2, are also analysed for band gap variation of SiNRs. Figure 3 shows the formation of band gaps in SiNRs [8]. Figure 4 shows the bandstructure diagrams on adsorption of carbon-based gases, namely, CH_4, CO_2 and CO on SiNRs. The nanoribbons having methane exhibit the minimum band gap [9]. Highly toxic gas, hydrogen cyanide, is also analysed for band gap tuning of the nanoribbons. Figure 5 shows the same [10].

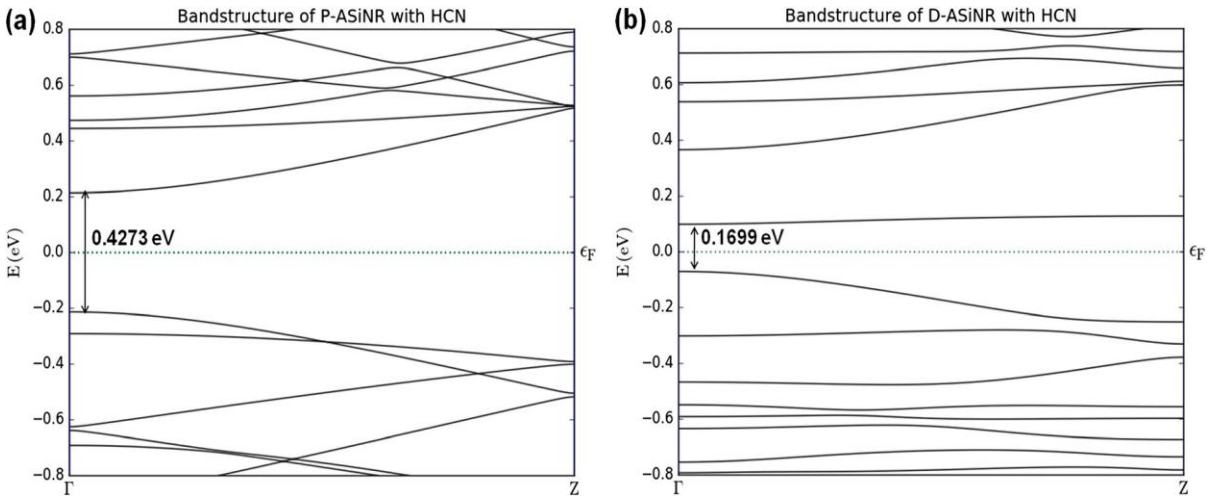


Figure 5. Bandstructure diagrams of pristine ASiNRs and defective ASiNRs on adsorption of HCN [10]

CONCLUSIONS

The electronic property calculation of bandstructure is carried out using VNL-ATK along with DFT study to analyze the effect of adsorption of different gas molecules on the band gap of the silicene nanoribbons. The results reveal that the metallic behaviour of pristine SiNRs is highly tuned by introducing a vacancy defect and adsorption of gases. On the whole, it is analyzed that the defective SiNRs undergo a small variation of band gap in contrast to the pristine counterparts; hence its conductivity is more.

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