

Electronic properties of armchair and zigzag sp^3 -hybridized silicane nanoribbons

Jiseok Kim, Shela Aboud[†], and Massimo V. Fischetti

The University of Texas at Dallas, Richardson, TX 75080, USA

[†]Stanford University, Stanford, CA 94305, USA

e-mail: jiseok.kim@utdallas.edu

Recently, sp^2 - and sp^3 -hybridized silicene, so called silicane, has been shown to exhibit a band gap [2], [3], [4] with the sp^3 -hybridization in low-buckled silicane structure being more stable and favorable [5], [3]. In this study, the electronic properties of arm-chair and zigzag edge sp^3 -hybridized silicane nanoribbons (aSiNRs and zSiNRs, respectively) are calculated using nonlocal empirical pseudopotentials (EP) [1] benchmarked to the results from density function theory (DFT), as implemented in the Vienna *ab-initio* simulation package (VASP) [7] with a plane wave basis expansion and the energy cutoff of 450 eV. The electron-ion core interaction is represented by the projector augmented wave (PAW) method and we have employed the Perdew-Burke-Ernzerhof (PBE) exchange correlation functional in generalized gradient approximation (GGA).

Figure 1 shows the atomic configuration of an aSiNR (a) and of a zSiNR (b); all Si dangling bonds, including those at the top and bottom of the monolayer surfaces, are passivated by hydrogen, thus causing the sp^3 -hybridized bonding. The width of the SiNR is characterized by the number of Si-Si dimer lines or zigzag chains along the ribbon for the aSiNR or zSiNR, respectively, as done for graphene nanoribbons (GNRs) [8]. Note that we have used the unrelaxed atomic configuration when employing EPs while we have allowed relaxation to occur when using DFT. These two atomic configurations are shown in Fig.2. The geometrical relaxation is performed using the conjugate gradient (CG) algorithm in which the force-tolerance is set to 0.02 eV/Å. The calculated band structure for a 4-zSiNR is shown in Fig.3 using (a) EPs and (b) DFT with unrelaxed and relaxed geometry where the relaxed geometry for EPs is obtained from DFT. Both results exhibit a direct band gap at Γ , but the gap obtained using DFT is ~ 1 eV smaller. As it can be seen in Fig. 3, this can be attributed to the

‘band-gap problem’ of DFT, since even using an unrelaxed atomic configuration the DFT band gap remains smaller than the EPs-gap.

The dependence of the band gap on the ribbon width are investigated using EPs. As shown in Fig. 4 the band gap of both aSiNRs and zSiNRs decreases nonlinearly with increasing width due to confinement effects. However, the well-known dependence of the band gap of aGNRs [8] and of edge-only hybridized aSiNR [10] on their chirality is not observed in the case of both aSiNRs and zSiNRs. This is the result of the sp^3 bonding which ensures 4-fold coordination for all Si atoms and therefore is not affected by the Clar resonances which control the edge structure in the sp^2 bonding of aGNRs, as shown in inset from Ref. [9]. Also note that both aSiNRs and zSiNRs exhibit a wide band-gap with the band gap of aSiNRs being larger than that of zSiNRs of similar width. In addition, for all widths we have considered aSiNRs exhibit an indirect gap, while the gap of zSiNRs is direct. The 1D ballistic conductance and the density of states (DOS) calculated using EPs – shown in Fig. 5 – indicates that zSiNRs enjoy better electron transport properties, although their DOS is smaller than that of aSiNRs.

In conclusion, we have studied the electronic properties of sp^3 -hybridized aSiNRs and zSiNRs using EPs benchmarked to DFT calculations. Both types of ribbons exhibit band-gaps sufficiently large for nanoelectronics application. In addition, the smooth dependence of the band-gap with width, unlike aGNRs, renders them less sensitive to line-edge roughness in such applications.

REFERENCES

- [1] J. Kim and M. V. Fischetti, *Empirical pseudopotential calculations of the band structure and ballistic conductance of strained [001], [110], and [111] silicon nanowires*, J. Appl. Phys. **110**, 033716 (2011)

- [2] L. C. Lew Yan Voon, E. Sandberg, R. S. Aga, and A. A. Farajian, *Hydrogen compounds of group-IV nanosheets*, Appl. Phys. Lett., **97**, 163114 (2010)
- [3] M. Houssa, A. Scalise, K. Sankaran, G. Pourtois, V. V. Afanas'ev, and A. Stesmans, *Electronic properties of hydrogenated silicene and germanene*, Appl. Phys. Lett., **98**, 223107 (2011)
- [4] P. De Padova, C. Quaresima, B. Olibveri, P. Perfetti, and G. Le Lay, *sp^2 -like hybridization of silicon valence orbitals in silicene nanoribbons*, Appl. Phys. Lett., **98**, 8 (2011)
- [5] T. Osborn, A. A. Farajian, O. Pupyshcheva, R. A. Aga, and L. C. Lew Yan Voon, *Ab initio simulation of silicene hydrogenation*, Chem. Phys. Lett., **511**, 101 (2011)
- [6] G. Guzmán-Verri and L. C. Lew Yan Voon, *Electronic structure of silicon-based nanostructures*, Phys. Rev. B, **76**, 075131 (2007)
- [7] G. Kresse and J. Hafner, *Ab initio molecular dynamics for liquid metals*, Phys. Rev. B, **47**, 558 (1993)
- [8] Y. Son, M. L. Cohen, and S. G. Louie, *Energy gaps in graphene nanoribbons*, Phys. Rev. Lett., **97**, 216803 (2006)
- [9] L. Yang, C.-H. Park, Y.-W. Son, M. L. Cohen, and S. G. Louie, *Quasiparticle energies and band gaps in graphene nanoribbons*, Phys. Rev. Lett., **99**, 186801 (2007)
- [10] Y. Ding, and J. Ni *Electronic structures of silicon nanoribbons*, Appl. Phys. Lett., **95**, 083115 (2009)

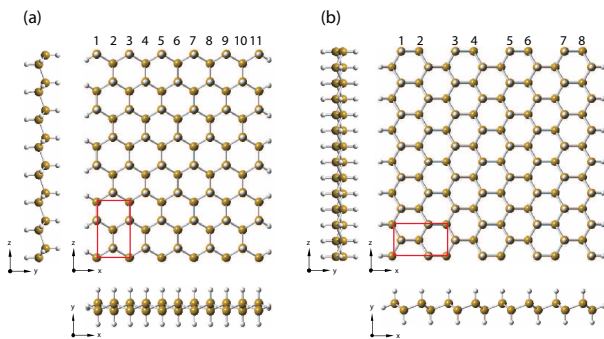


Fig. 1. Atomic configurations of (a) an 11-aSiNR and (b) an 8-zSiNR. All the Si (gold balls) dangling bonds are passivated by H (white balls). Note the H atoms passivate the dangling bonds in alternating pairs at the top and bottom sides of the monolayer.

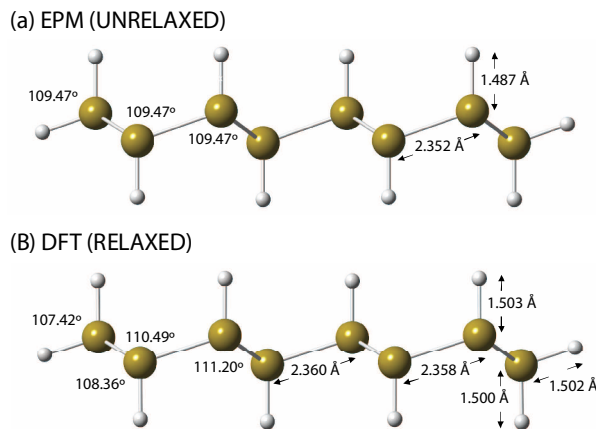


Fig. 2. Atomic configuration of an unrelaxed (a) and relaxed (b) 4-zSiNR for EPs and DFT calculations, respectively.

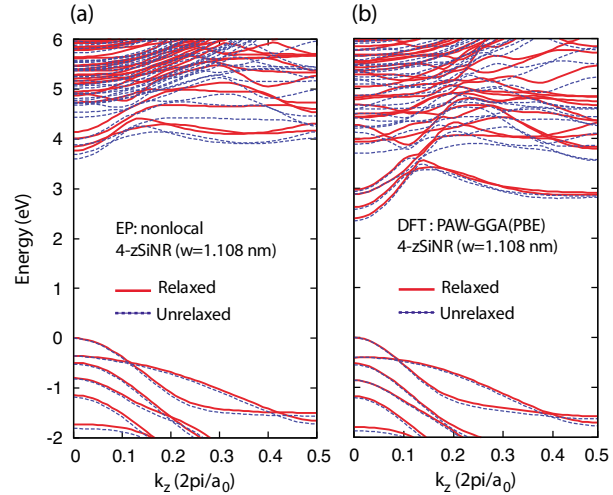


Fig. 3. Electronic band-structure of a 4-zSiNR using (a) EPs and (b) DFT with an unrelaxed and fully relaxed geometry.

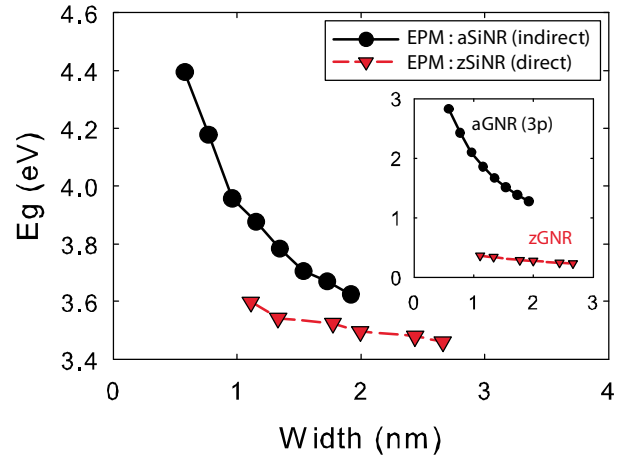


Fig. 4. Energy band gap of an aSiNR (black solid circles) and a zSiNR (red solid circles) as a function of ribbon width calculated using EPs with an unrelaxed geometry. The inset shows the band gap variation with width of aGNR (3p) and zGNR from Ref. [9] using GW self-energy correction.

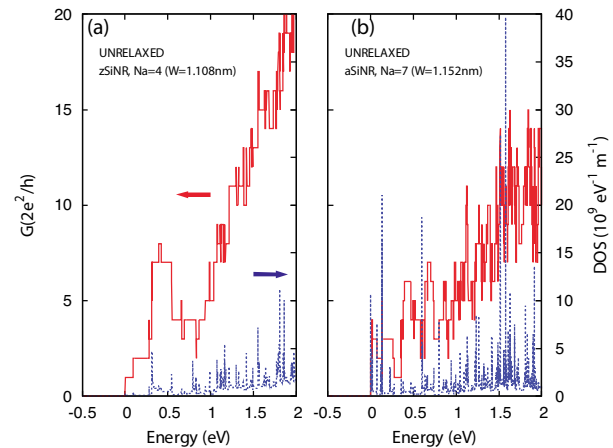


Fig. 5. 1D ballistic conductance (red solid lines) and density of states (blue dotted lines) of (a) a 4-zSiNR and (b) a 7-aSiNR calculated using EPs with an unrelaxed geometry.