Supplemental Material for Modulating the electronic properties of silicene allotropes through the synergistic effect of different geometric configurations and edge hydrogenation

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Here, we provide all the geometric structures (S1 and S2), band structures and density of states (S3 and S4) of TO-SiNRs in the calculation process. S1 is the structure diagram of intrinsic TO-SiNRs before and after relaxation. S2 is the structure diagram of TO-SiNRs before and after relaxation under edge hydrogenation. S3 is the band structure and density of states diagram of intrinsic TO-SiNRs; s4 is the band structure and density of states of TO-SiNRs after edge hydrogenation.

Fig. S1.

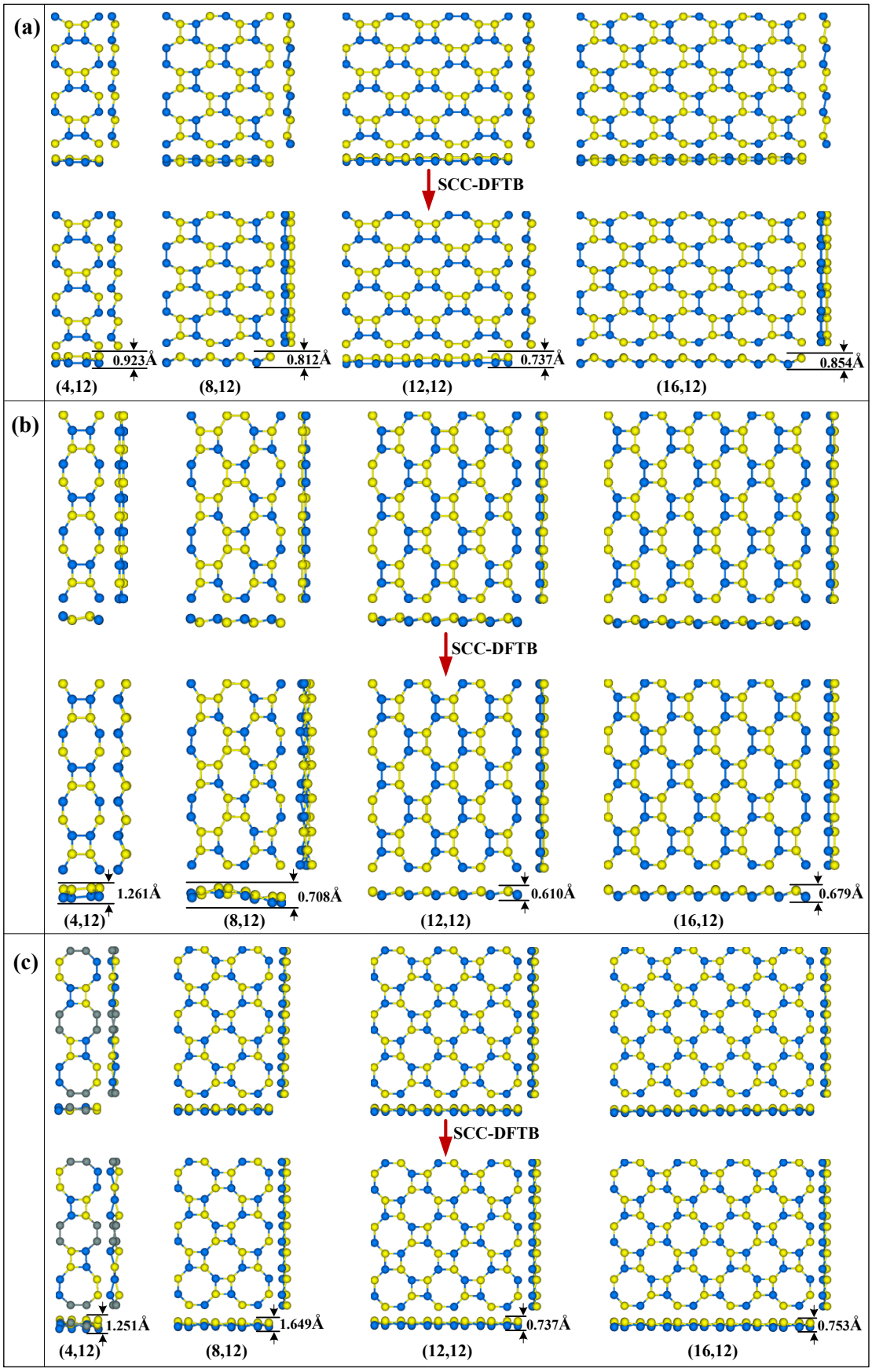

(a)
SCC-DFTB
0.923Å
0.812Å
0.737Å
0.854Å
(4,12)
(8,12)
(12,12)
(16,12)
(b)
SCC-DFTB
1.261Å
0.708Å
0.610Å
0.679Å
(4,12)
(8,12)
(12,12)
(16,12)
(c)
SCC-DFTB
1.251Å
1.649Å
0.737Å
0.753Å
(4,12)
(8,12)
(12,12)
(16,12)

Fig. S2.

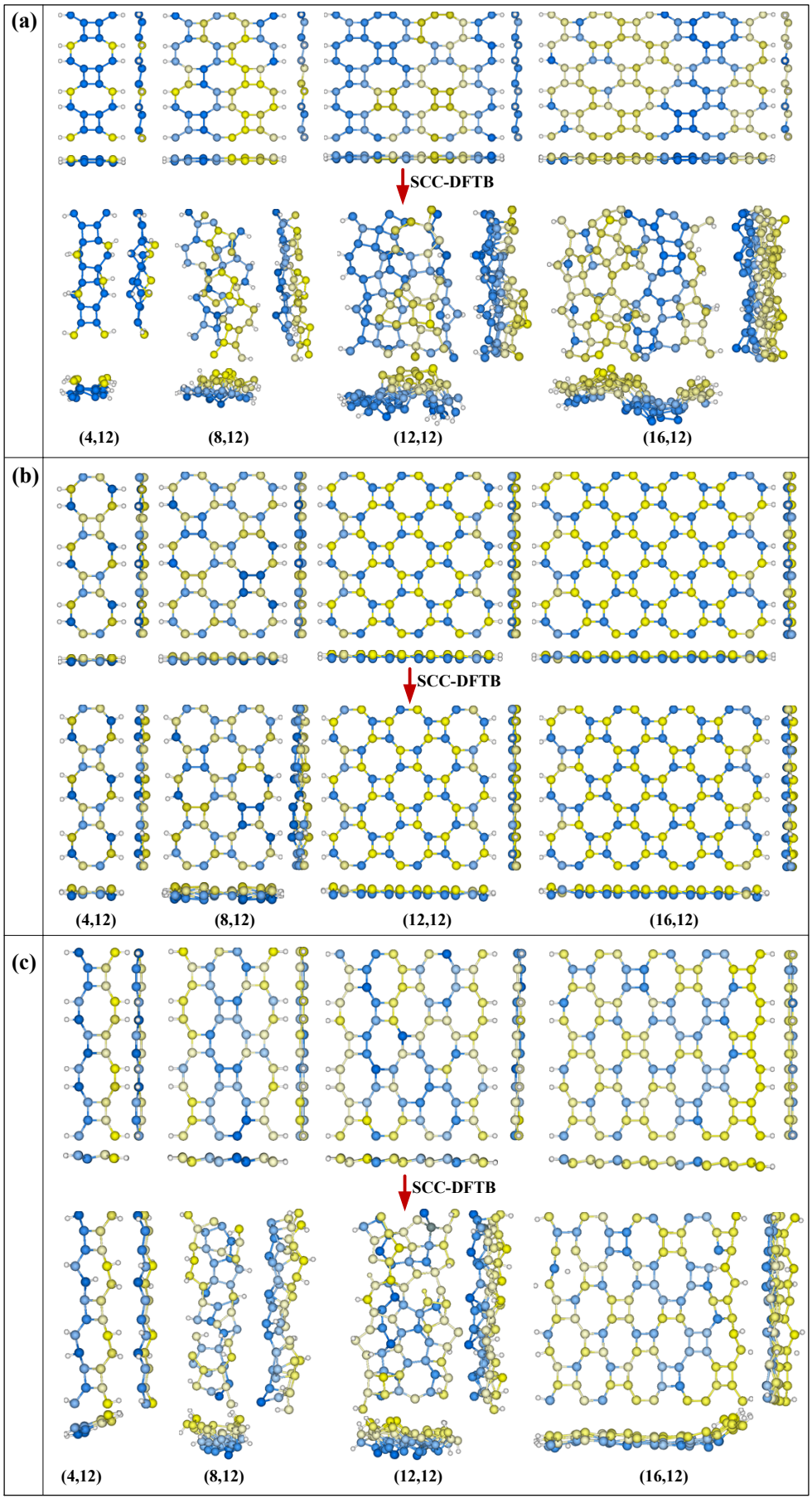

(a)
SCC-DFTB
(4,12)
(8,12)
(12,12)
(16,12)
(b)
SCC-DFTB
(4,12)
(8,12)
(12,12)
(16,12)
(c)
SCC-DFTB
(4,12)
(8,12)
(12,12)
(16,12)

Fig. S3.

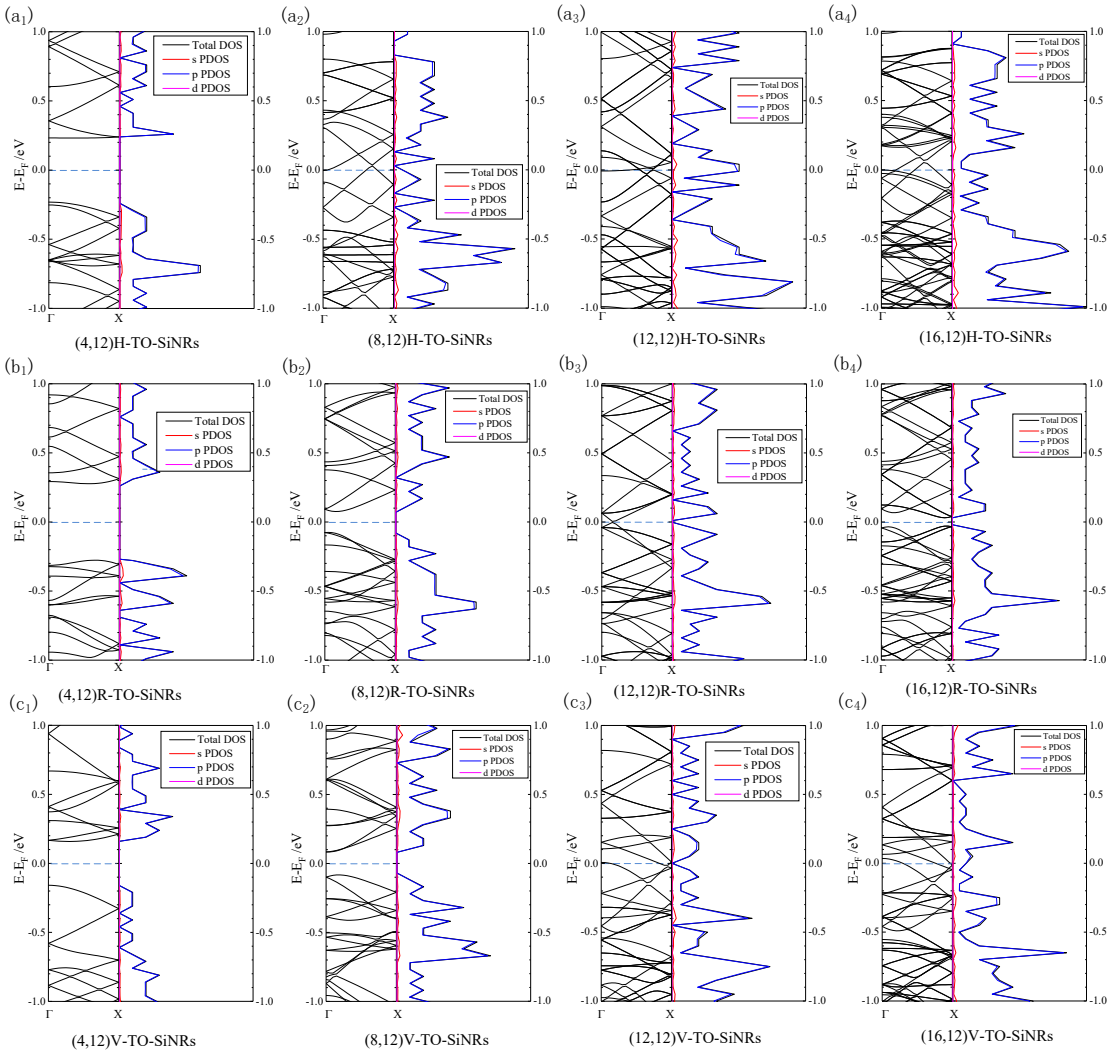
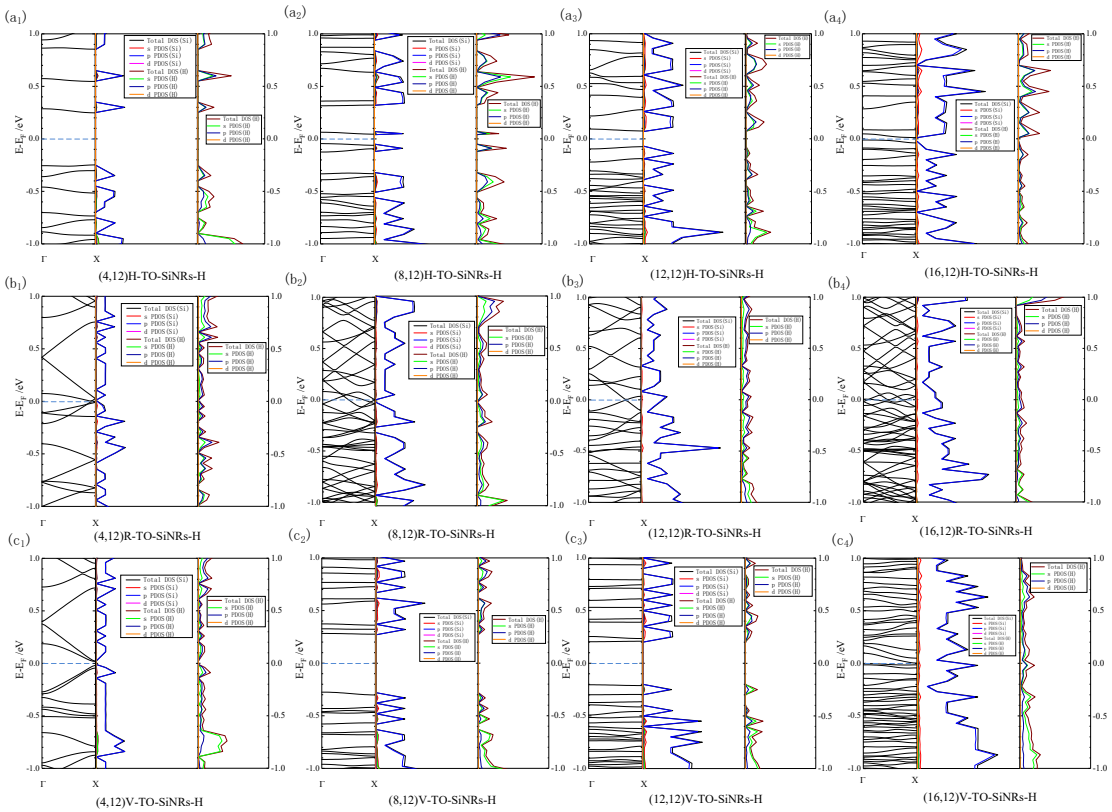

(a1)
(a2)
(a3)
(a4)
(4,12)H-TO-SiNRs
(8,12)H-TO-SiNRs
(12,12)H-TO-SiNRs
(16,12)H-TO-SiNRs
(b1)
(b2)
(b3)
(b4)
(4,12)R-TO-SiNRs
(8,12)R-TO-SiNRs
(12,12)R-TO-SiNRs
(16,12)R-TO-SiNRs
(c1)
(c2)
(c3)
(c4)
(4,12)V-TO-SiNRs
(8,12)V-TO-SiNRs
(12,12)V-TO-SiNRs
(16,12)V-TO-SiNRs
Total DOS
s PDOS
p PDOS
d PDOS
E-E_F /eV
Γ
X

Fig. S4.


(a1)
(a2)
(a3)
(a4)
(4,12)H-TO-SiNRs-H
(8,12)H-TO-SiNRs-H
(12,12)H-TO-SiNRs-H
(16,12)H-TO-SiNRs-H
(b1)
(b2)
(b3)
(b4)
(4,12)R-TO-SiNRs-H
(8,12)R-TO-SiNRs-H
(12,12)R-TO-SiNRs-H
(16,12)R-TO-SiNRs-H
(c1)
(c2)
(c3)
(c4)
(4,12)V-TO-SiNRs-H
(8,12)V-TO-SiNRs-H
(12,12)V-TO-SiNRs-H
(16,12)V-TO-SiNRs-H
E-E_f /eV
Γ
X