Electronic Supplementary Information (ESI)

Silicene-Supported TiO_2 Nanostructures: Theoretical Study of Electronic and Optical Properties

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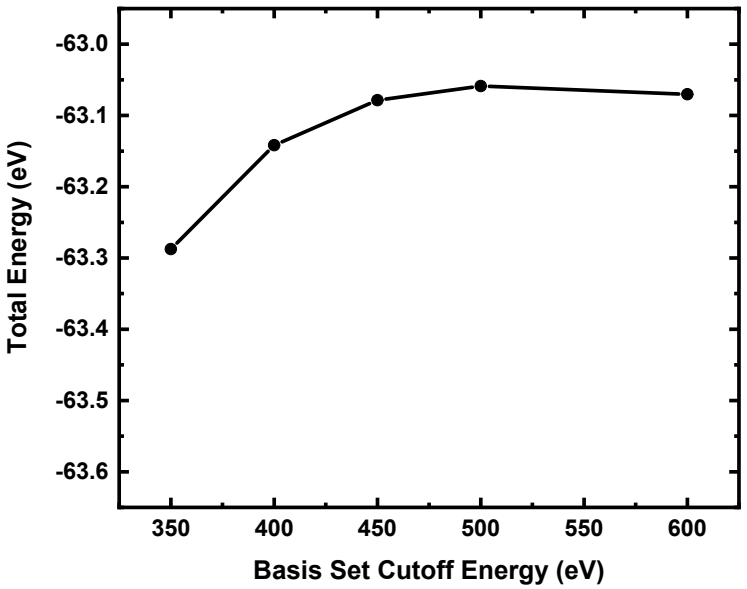
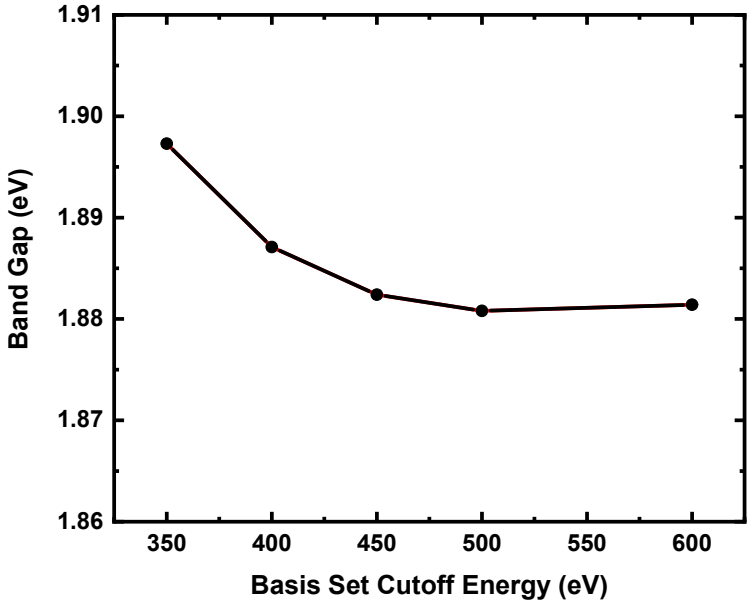
Table S1. Charges and magnetic moments of Ti^{3+} ions in the supported structures based on Bader charge analysis.

Supported structures	Q_1 (e)	μ_1 (μ_B)	Q_2 (e)	μ_2 (μ_B)
$(TiO_2)_3$/Silicene	1.84	0.96	1.93	0.98
$(TiO_2)_8$/Silicene	1.93	0.87	1.90	0.96
$(TiO_2)_{15}$/Silicene	2.07	-0.87	-	-
TiO_2 (101) nanosheet/Silicene	2.02	0.90	2.02	0.90



(a)



(b)

Figure S1. Convergence tests of (a) the total energy and (b) the band gap as a function of the basis set cutoff energy for a $(TiO_2)_3$ cluster.

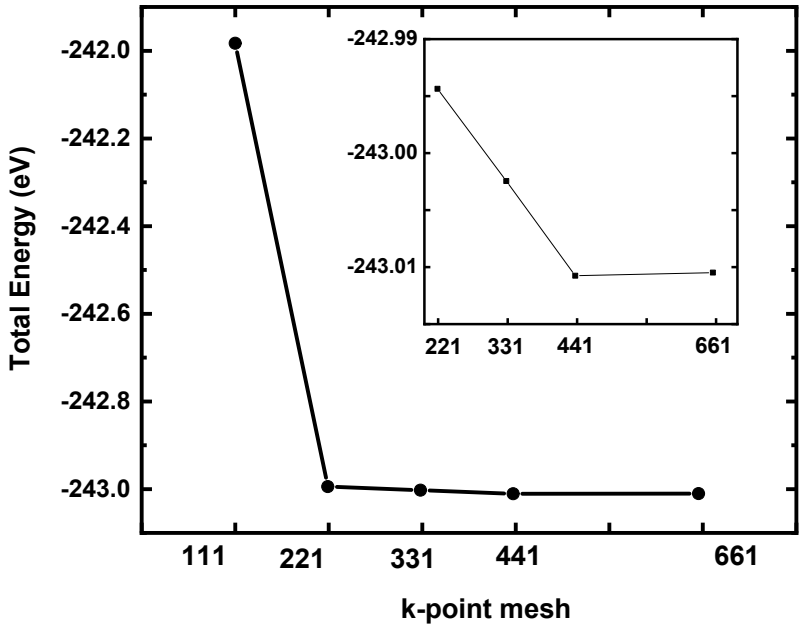


Figure S2. Convergence test of the total energy as a function of the k point mesh for the 5×5 silicene sheet.

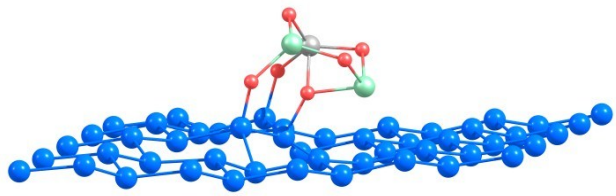
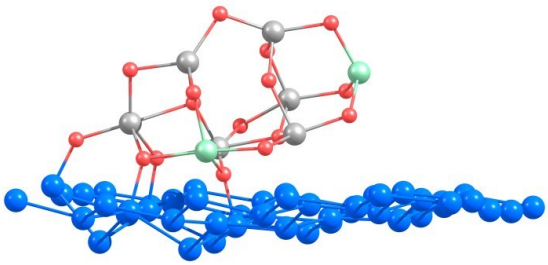
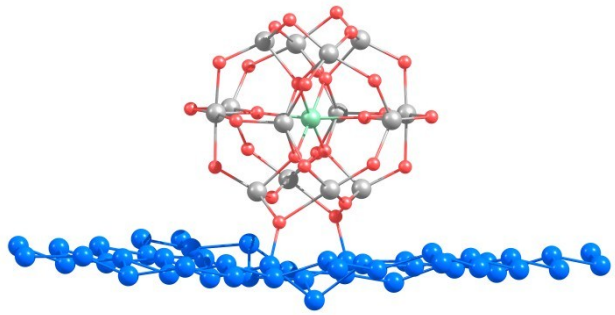
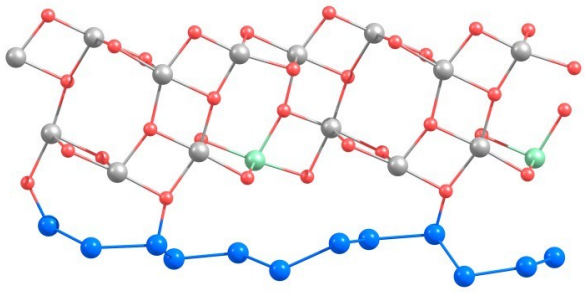
a) Silicene-supported $(TiO_2)_3$ cluster	b) Silicene-supported $(TiO_2)_8$ cluster
	
c) Silicene-supported $(TiO_2)_{15}$ cluster	d) Silicene-supported TiO_2 nanosheet
	

Figure S3. Distribution of Ti^{3+} ions in silicene-supported TiO_2 nanostructures. Color code: Si-navy blue, O-red. Ti^{4+}-gray, Ti^{3+}-green. Note that for clarity, only one supercell is shown for each case.

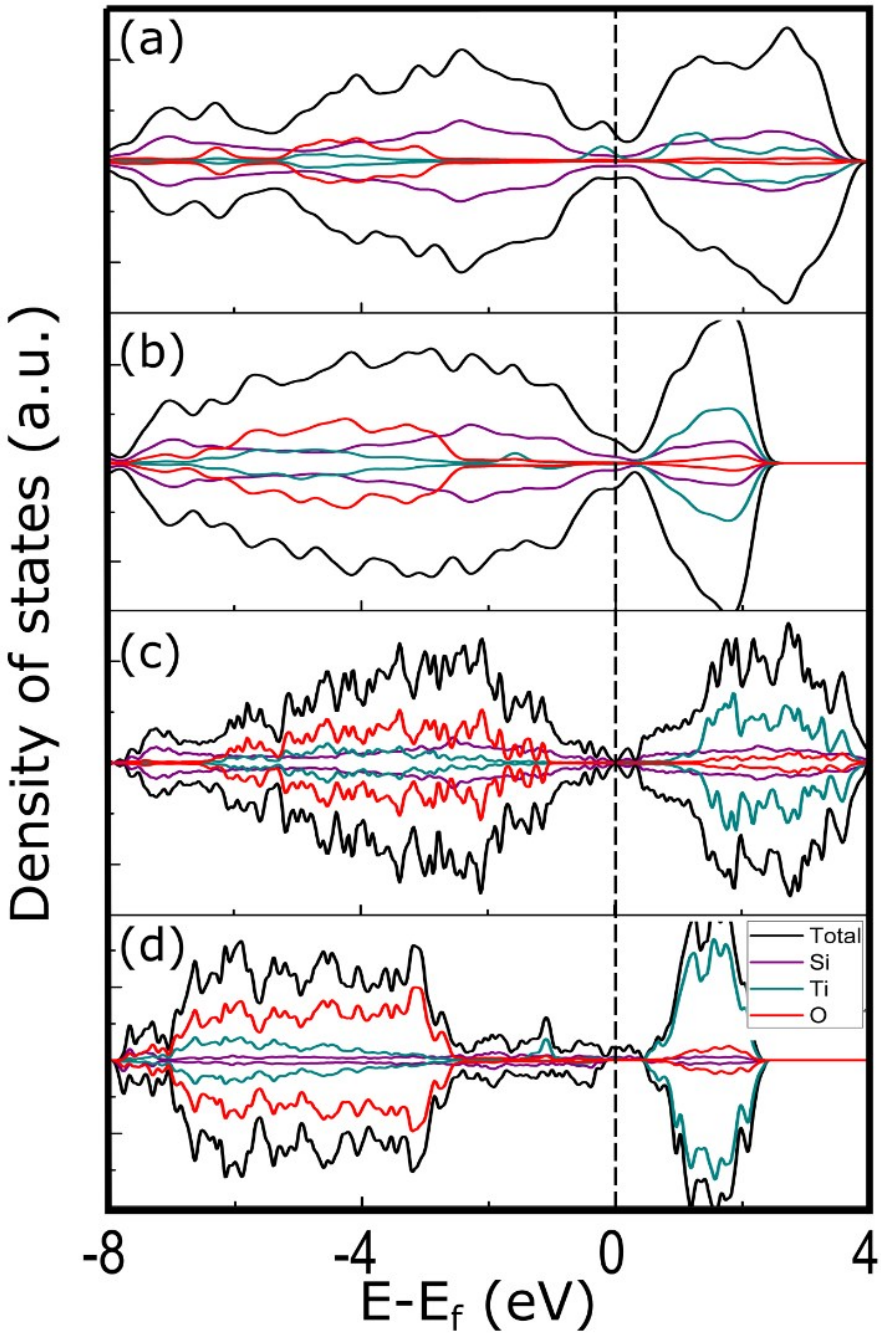
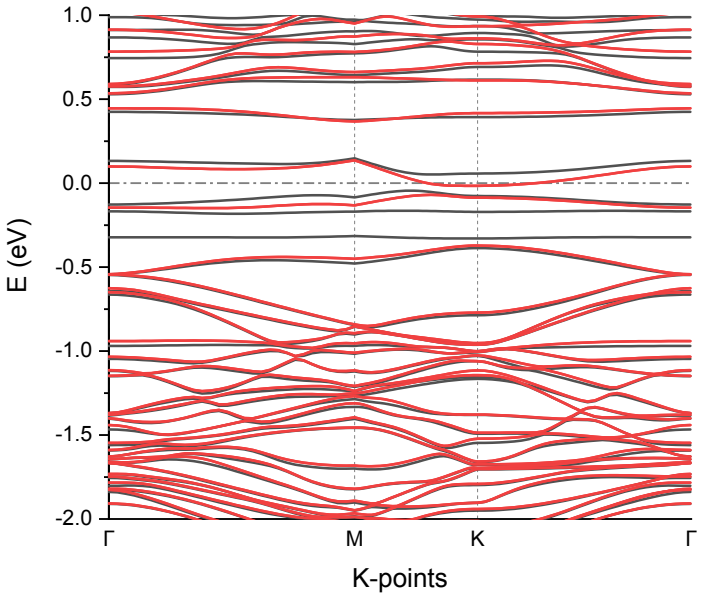
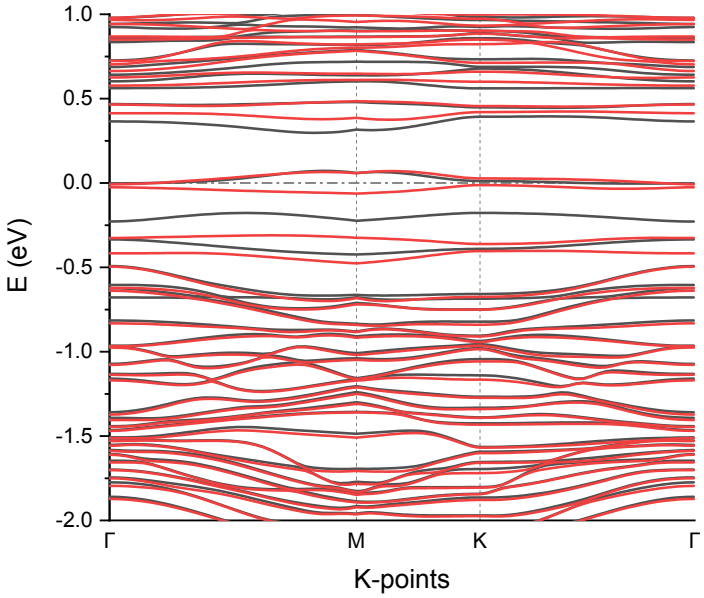


Figure S4. Calculated total and projected DOS of silicene-supported TiO_2 nanostructures. (a) silicene-supported $(TiO_2)_3$ cluster, (b) silicene-supported $(TiO_2)_8$ cluster, (c) silicene-supported $(TiO_2)_{15}$ cluster, and (d) silicene-supported TiO_2 nanosheet. Zero is taken to be Fermi energy of the system. A larger energy range is shown compared to Figure 4.

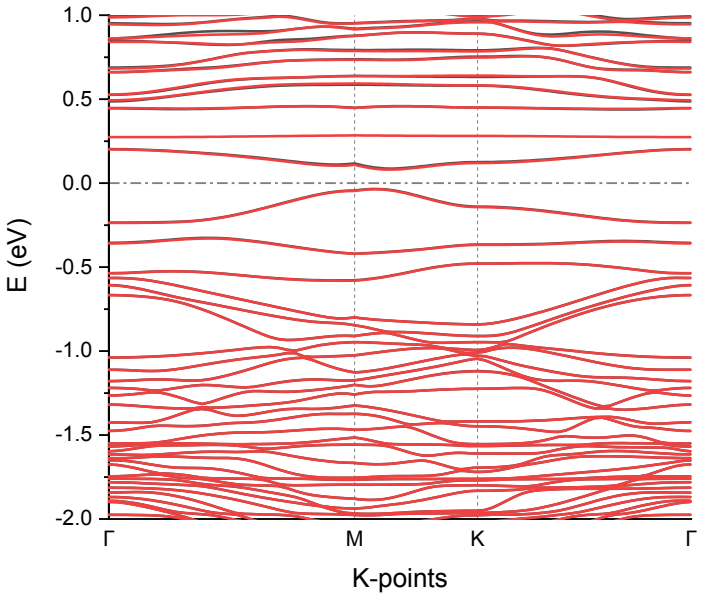
a)


1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
E (eV)
Γ
M
K
Γ
K-points

b)


1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
E (eV)
Γ
M
K
Γ
K-points

c)



d)

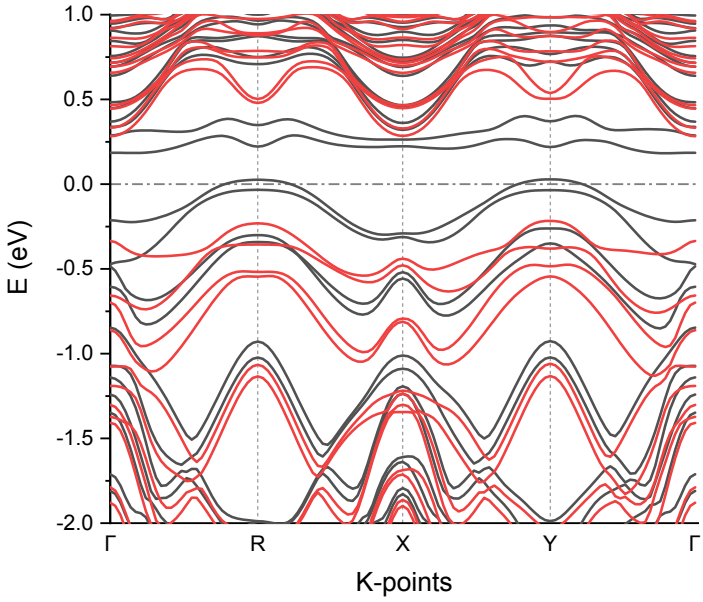


Figure S5. Calculated band structures of silicene-supported TiO_2 nanostructures at the PBE+U level. (a) silicene-supported $(TiO_2)_3$ cluster, (b) silicene-supported $(TiO_2)_8$ cluster, (c) silicene-supported $(TiO_2)_{15}$ cluster, and (d) silicene-supported TiO_2 (101) nanosheet. For figures (a)-(c), Γ=(0 0 0), M=$(0\ \frac{1}{2}\ 0)$, and K=$(\frac{1}{3}\ \frac{1}{3}\ 0)$. For figure (d), Γ=(0 0 0), R=$(\frac{1}{2}\ \frac{1}{2}\ 0)$, X=$(\frac{1}{2}\ 0\ 0)$, Y=$(0\ \frac{1}{2}\ 0)$. Black lines are for spin-up electrons, while red lines for spin-down electrons.