

**Supplemental Material for**  
**“The Dirac Cone in Two-Dimensional Tetragonal Silicon Carbide:**  
**Ring Coupling Mechanism”**

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	a (Å)	b (Å)	c (Å)	$\theta$ (°)	Bond length (Å)			$E_c$ (eV)
					C-C	Si-Si	C-Si	
graphene	2.468	2.468	PL	120	1.425			9.141
	2.461 <sup>a</sup>	2.461 <sup>a</sup>	PL	120 <sup>a</sup>	1.421 <sup>a</sup>			9.259 <sup>a</sup>
T graphene (planar)	3.447	3.447	PL	90	$b_1$ :1.374	$b_2$ :1.466		8.626
	3.41 <sup>b</sup>	3.41 <sup>b</sup>	PL	90 <sup>b</sup>				
silicene	3.867	3.867	0.453	120	2.278			4.698
	3.865 <sup>a</sup>	3.865 <sup>a</sup>		120 <sup>a</sup>	2.276 <sup>a</sup>			4.784 <sup>a</sup>
h-SiC	3.097	3.097	PL	120	1.787			6.941
	3.084 <sup>a</sup>	3.084 <sup>a</sup>	PL	120 <sup>a</sup>	1.780 <sup>a</sup>			7.076 <sup>a</sup>
T1 SiC	6.094	6.094	PL	90	$b_1$ :1.813	$b_2$ :1.747		6.676
T2 SiC	6.246	6.246	PL	90	1.465	2.264	1.781	6.378
T3 SiC	4.032	4.758	0.536	90	1.374	2.292	1.854	6.459

a Reference 1.

b Reference 2.

Table.S1 The lattice information and cohesive energy( $E_c$ ) of T-SiC are calculated. In order to evaluate the structural characteristics and stability of T-SiC, the corresponding parameters of graphene, T graphene, silicene, and h-SiC are calculated, and the corresponding values in the literature are also given. It can be seen that the two are quite consistent.

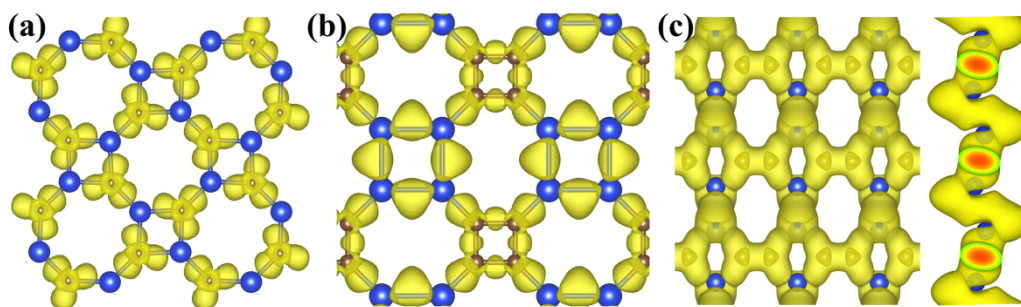


Fig.S1 Electron localization function(ELF) of (a)T<sub>1</sub>-SiC (b)T<sub>2</sub>-SiC and (c)T<sub>3</sub>-SiC.

Charge distribution (Bader analysis)				
	h-SiC	T1-SiC	T2-SiC	T3-SiC
C	6.51	6.48	4.62-5.03	5.23-5.47
Si	1.49	1.51	3.03-3.31	2.62-2.68

Table.S2 The number of electrons around an atom calculated using Bader charge analysis.

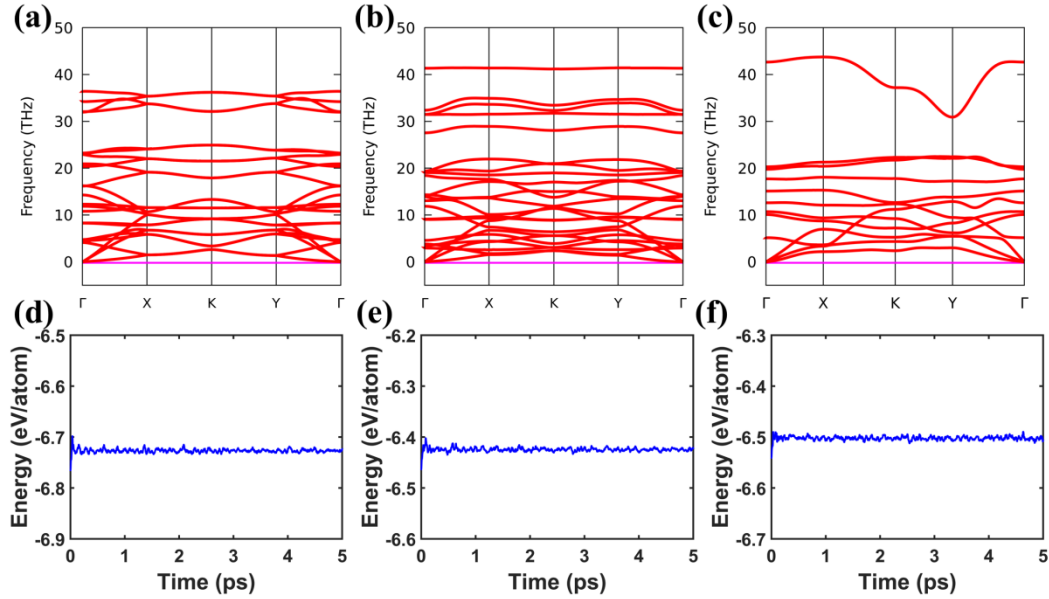


Fig.S2 Phonon spectra of (a) $T_1$ -SiC (b) $T_2$ -SiC and (c) $T_3$ -SiC, all branches have positive frequencies. And finite temperature(300k) molecular dynamics (MD) simulations of (d) $T_1$ -SiC (e) $T_2$ -SiC and (f) $T_3$ -SiC, The energy oscillates only slightly over time.

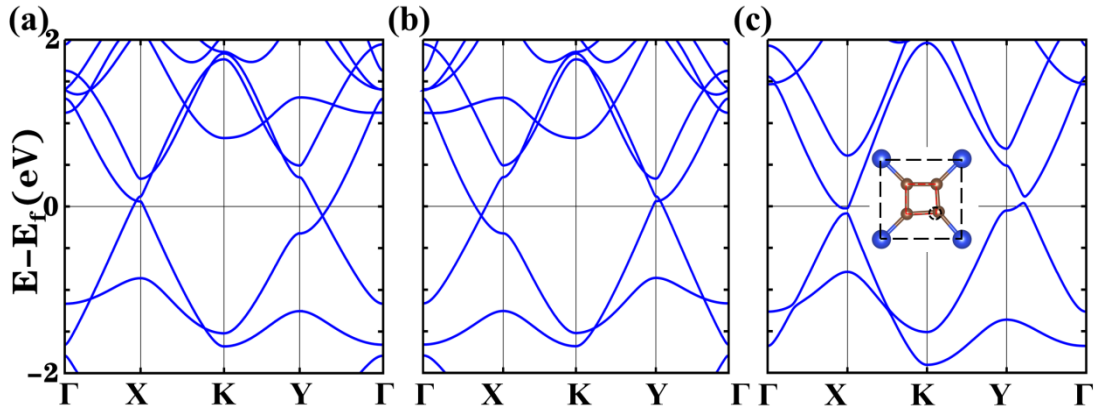


Fig.S3 Band structure of  $T_2$ -SiC with 8% strain applied along the (a)X-axis and (b)Y-axis, respectively. (c)The Dirac cone is opened when the structural symmetry is broken.

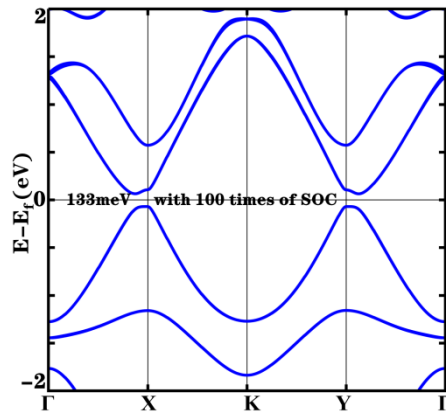


Fig.S4 Band structures with 100 times SOC of T<sub>2</sub>-SiC.

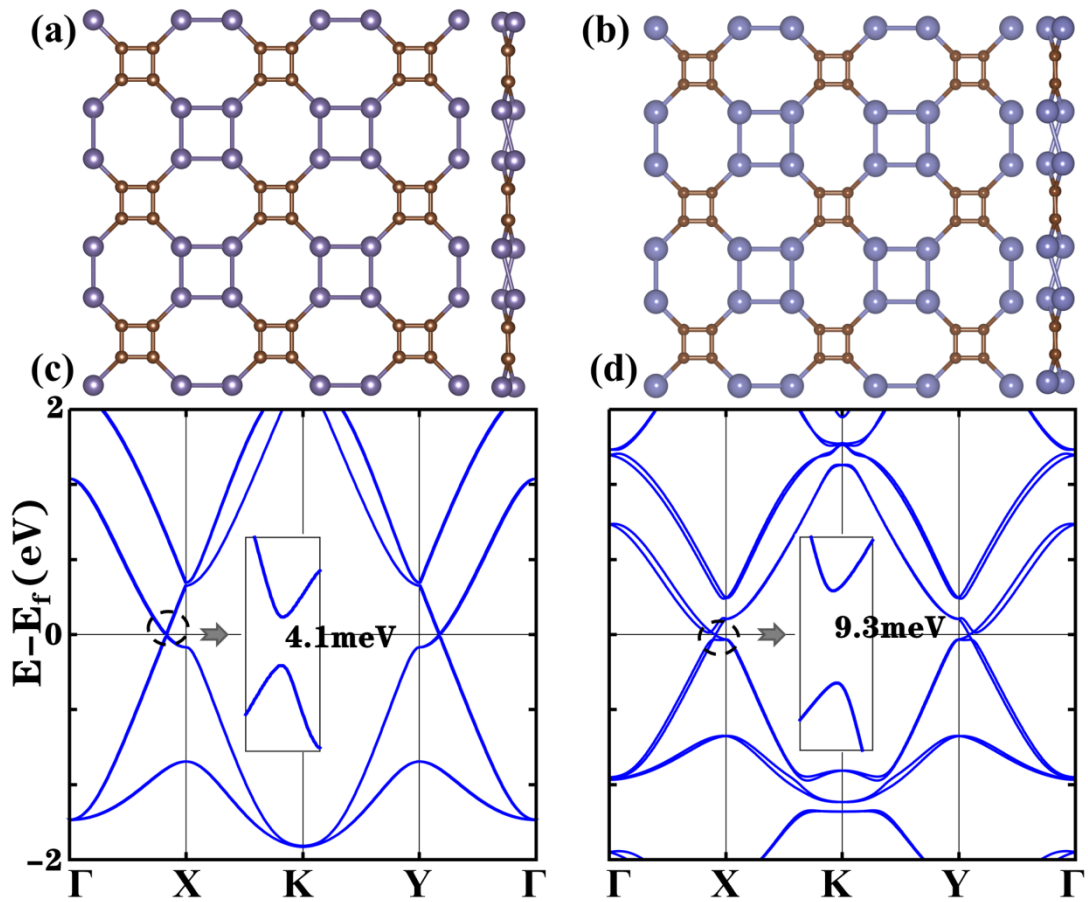


Fig.S5 The structure of (a)T<sub>2</sub>-GeC (b)T<sub>2</sub>-SnC. Band structures with SOC of (c)T<sub>2</sub>-GeC (d)T<sub>2</sub>-SnC.

### References

1. X. Qin, Y. Liu, X. Li, J. Xu, B. Chi, D. Zhai and X. Zhao, *J. Phys. Chem. Lett.*, 2015, **6**, 1333-1339.
2. Y. Liu, G. Wang, Q. Huang, L. Guo and X. Chen, *Phys. Rev. Lett.*, 2012, **108**, 225505.