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Electronic Supplementary Information

Two-dimensional Hexagonal M_3C_2 (M = Zn, Cd, Hg) Monolayer: Novel Quantum Spin Hall Insulators and Dirac Cone Materials

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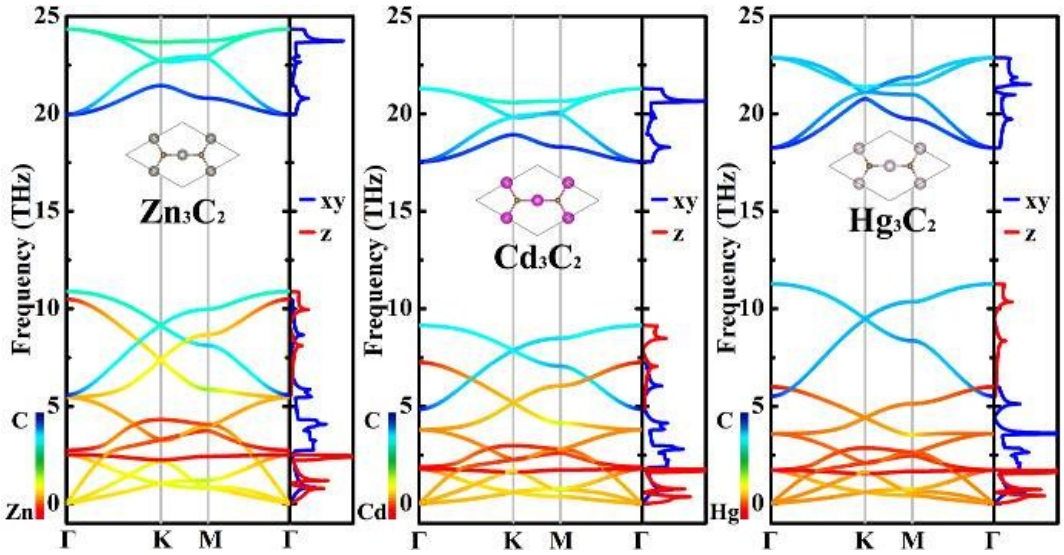

Figure S1. The orbital-resolved phonon spectra and projected phonon density of states for the M_3C_2 monolayers.

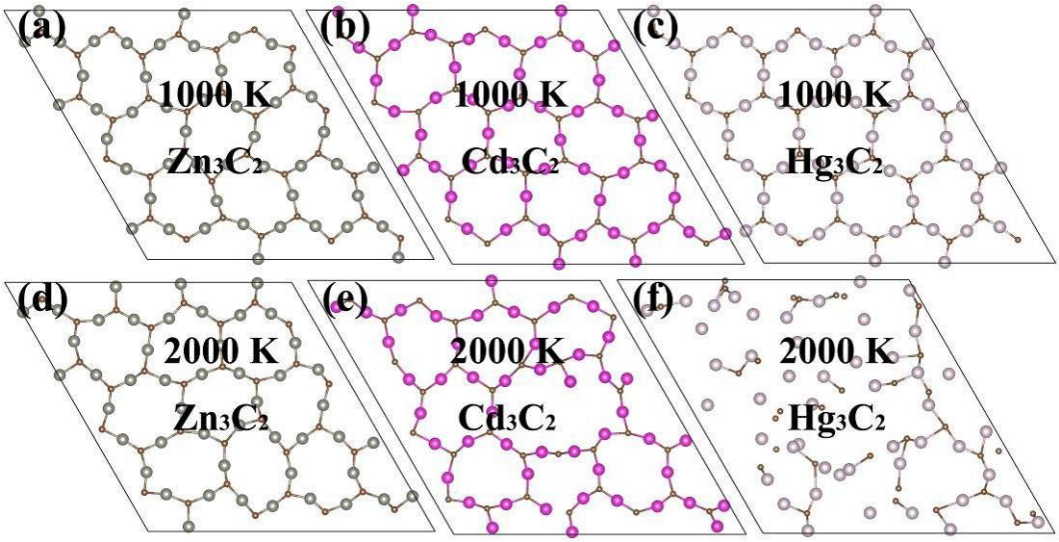

Figure S2. The top views of monolayers after the *ab-initio* molecular dynamics simulation.

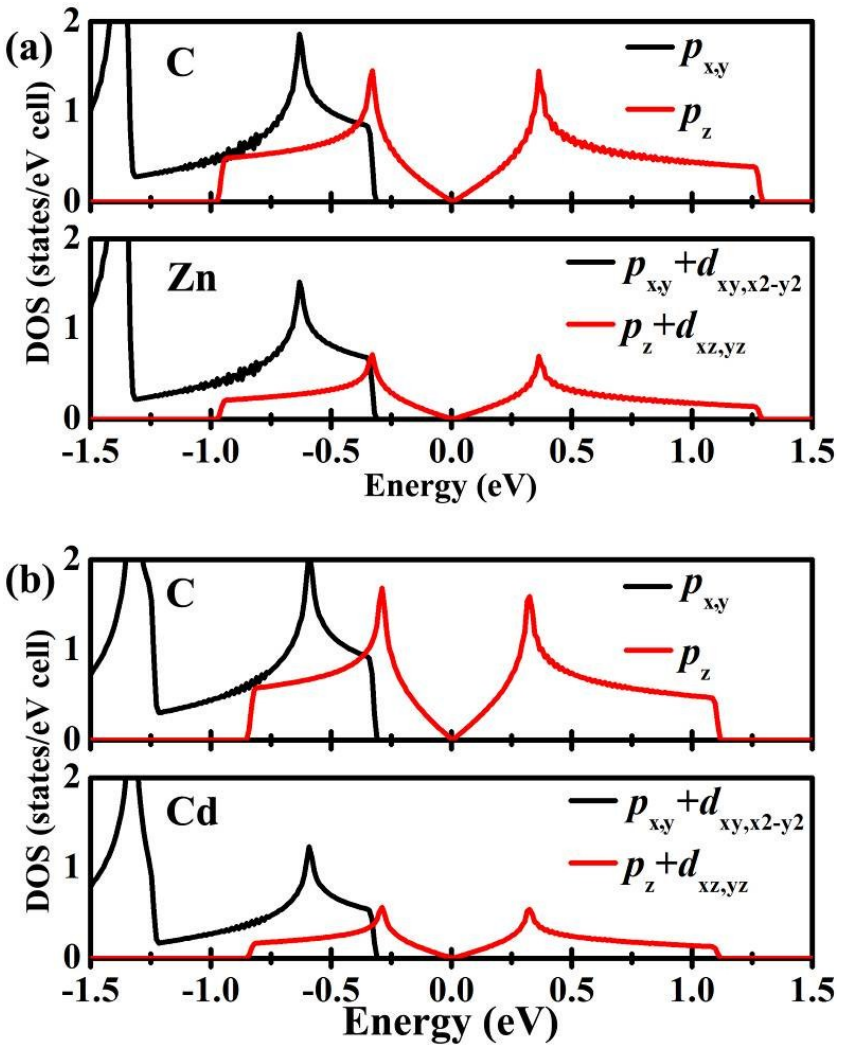

Figure S3. The density of states for the Zn_3C_2 and Cd_3C_2 monolayers.

Comp.	Parities of occupied spin-degenerate bands	Product
Zn_3C_2	+ - + + + + + + + + + + + + + + + - - -	Γ (+)
	- + - - - + + - - + - - + - - + - - + - + +	M (-)
Cd_3C_2	+ + - + + + + + + + + + + + + + + + - - -	Γ (+)
	- + - - + - + - - - + - + - - + - - + - + +	M (-)
Hg_3C_2	+ - + + + + + + + + + + + + + + + + - - -	Γ (+)
	- + - - + + - - - - + + - - + - - + - - + +	M (-)

Figure S4. The parities of occupied bands at Γ (red color) and M (black color) points for the M_3C_2 monolayers. The product of Γ and M points are + 1 and – 1 for M_3C_2 monolayers.

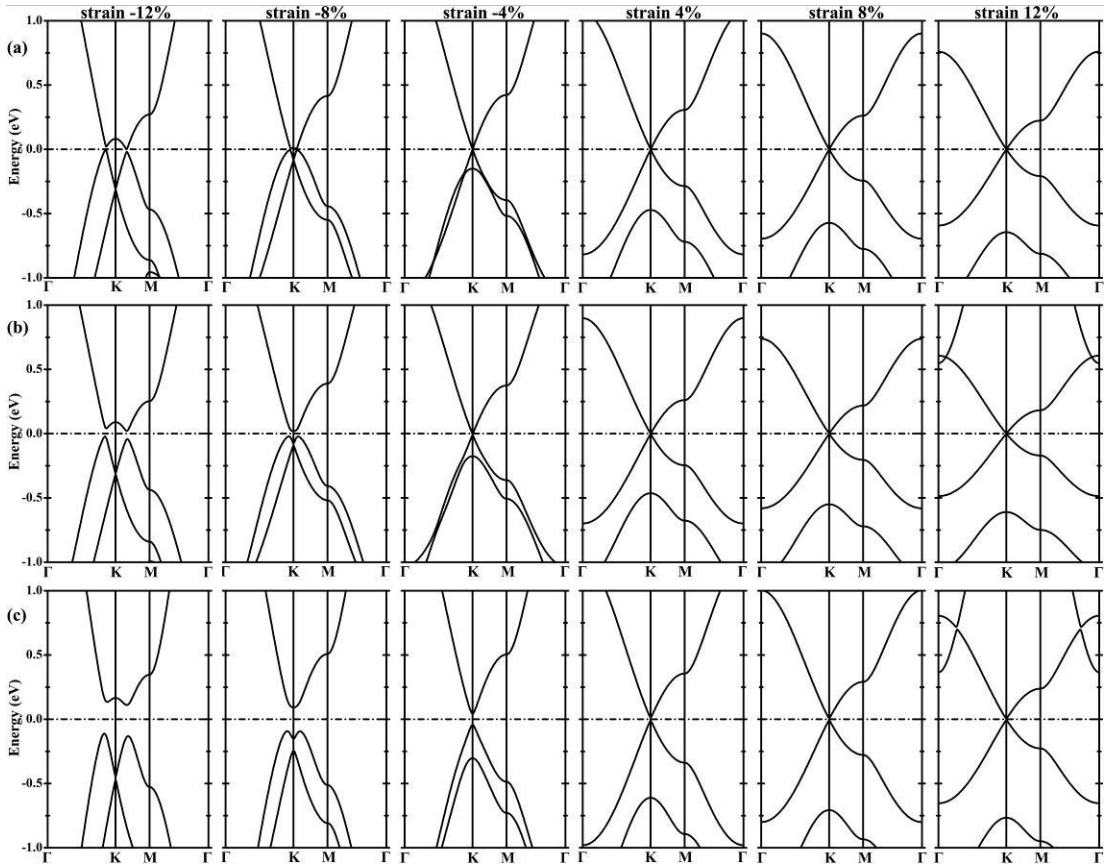

Figure S5. The calculated band structures of (a) Zn_3C_2 (b) Cd_3C_2 and (c) Hg_3C_2 monolayers with SOC under external strain from −12% to 12%. The Fermi level is set to zero.

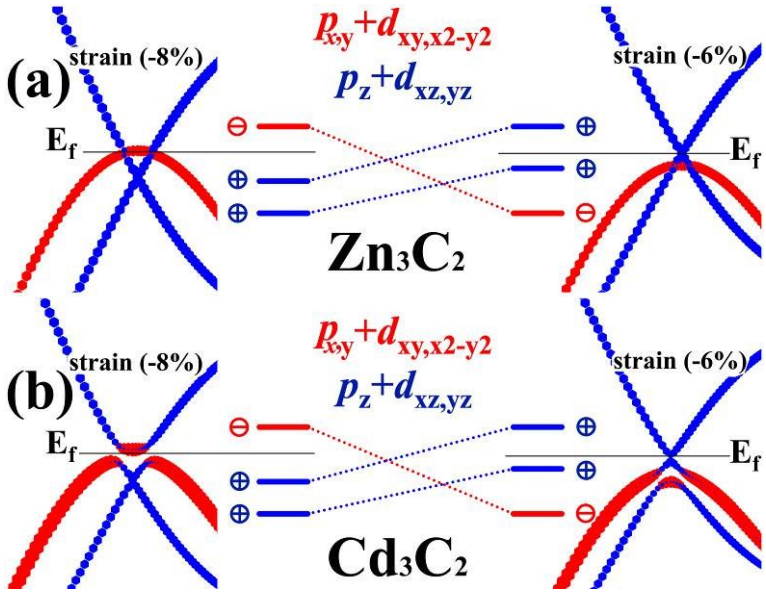

Figure S6. Schematic illustration of the band evolution around the Fermi level at K point for the (a) Zn_3C_2 and (b) Cd_3C_2 monolayers.

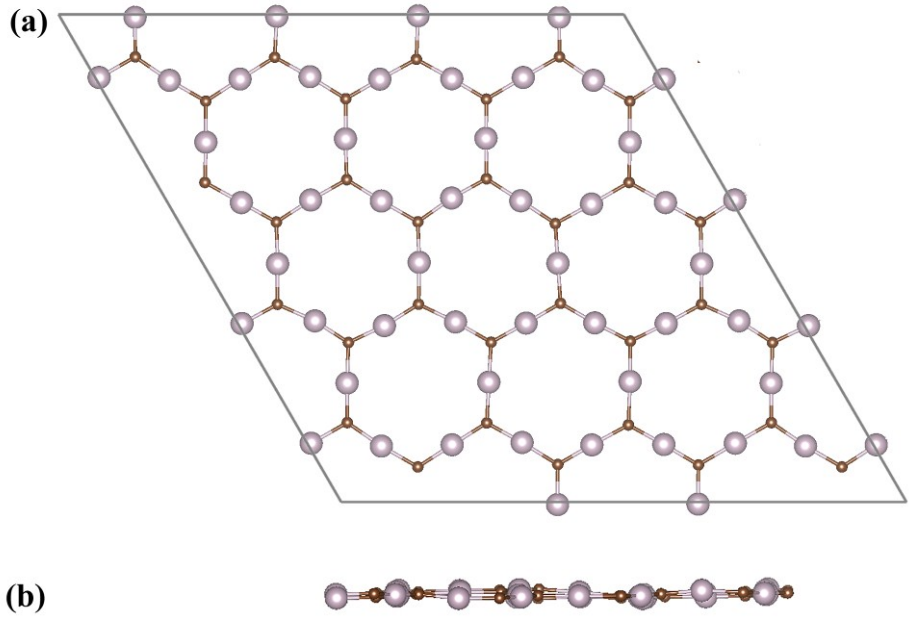

Figure S7. (a) Top and (b) side view of a snapshot of the Hg_3C_2 sheet under 6 % in-plane biaxial tensile strain at 5 ps of *ab-initio* molecular dynamics simulation in the NVT ensemble. The controlled temperature of the system was set to 300K.

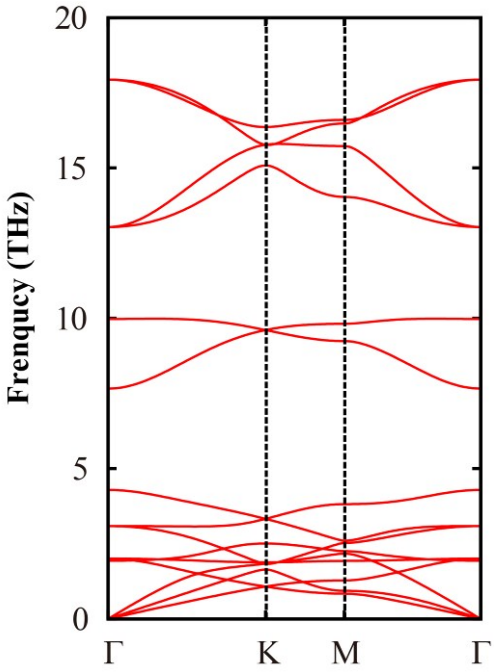

Figure S8. The phonon spectrum of Hg_3C_2 monolayer under 6% in-plane biaxial tensile strain.

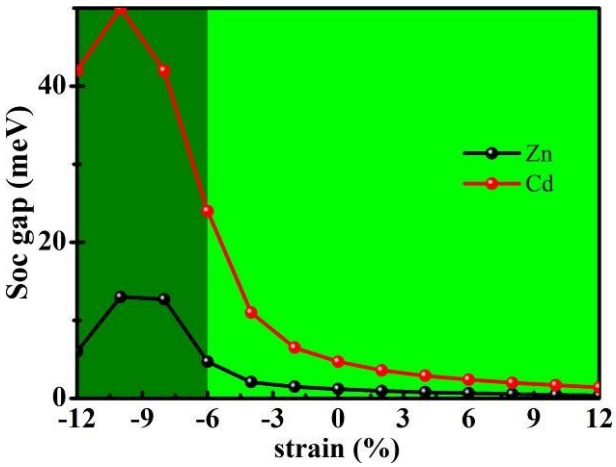

Figure S9. The nontrivial topological gap of the Zn_3C_2 and Cd_3C_2 monolayers as a function of applied external biaxial strain obtained with PBE+SOC technique. Olive region: node-line semimetal phase; green region: single Dirac-point phase.