Supplementary Materials

A family of robust Dirac cone materials: Two-dimensional hexagonal M_3X_2 (M = Zn/Cd/Hg, X=Si/Ge)

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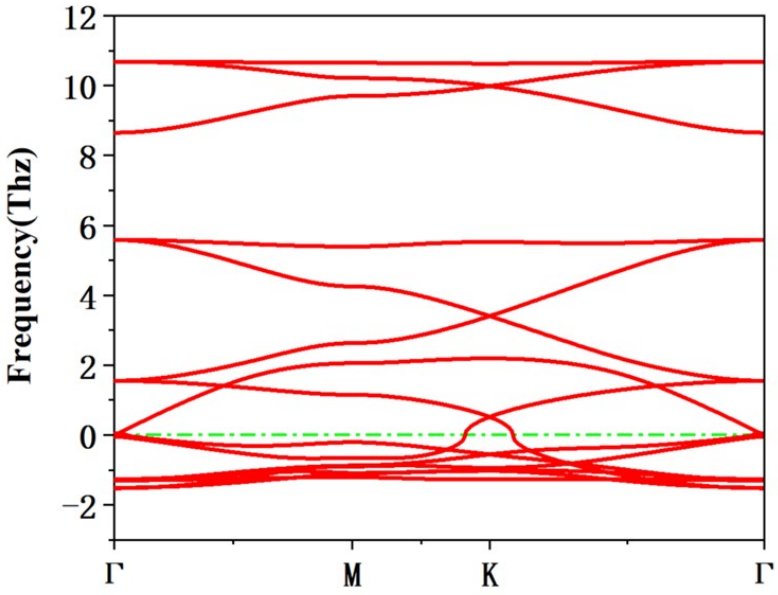

Fig.S1. Phonon spectrum of 3×3 superlattice Hg_3Ge_2

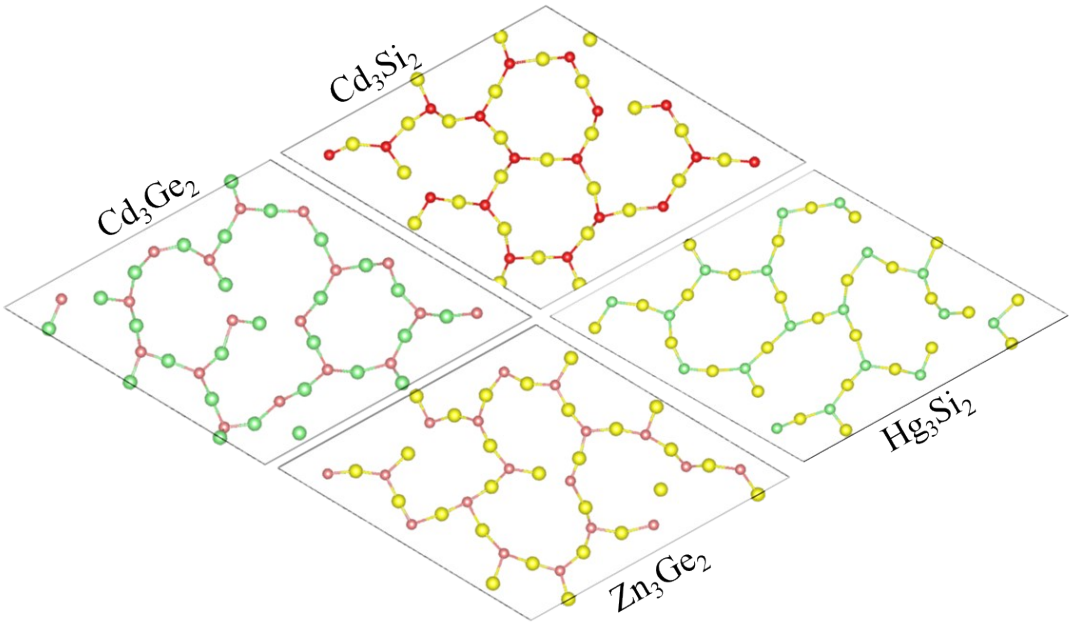

Fig.S2 Snapshots for the equilibrium structures of the M_3X_2 monolayers at 900K temperatures.

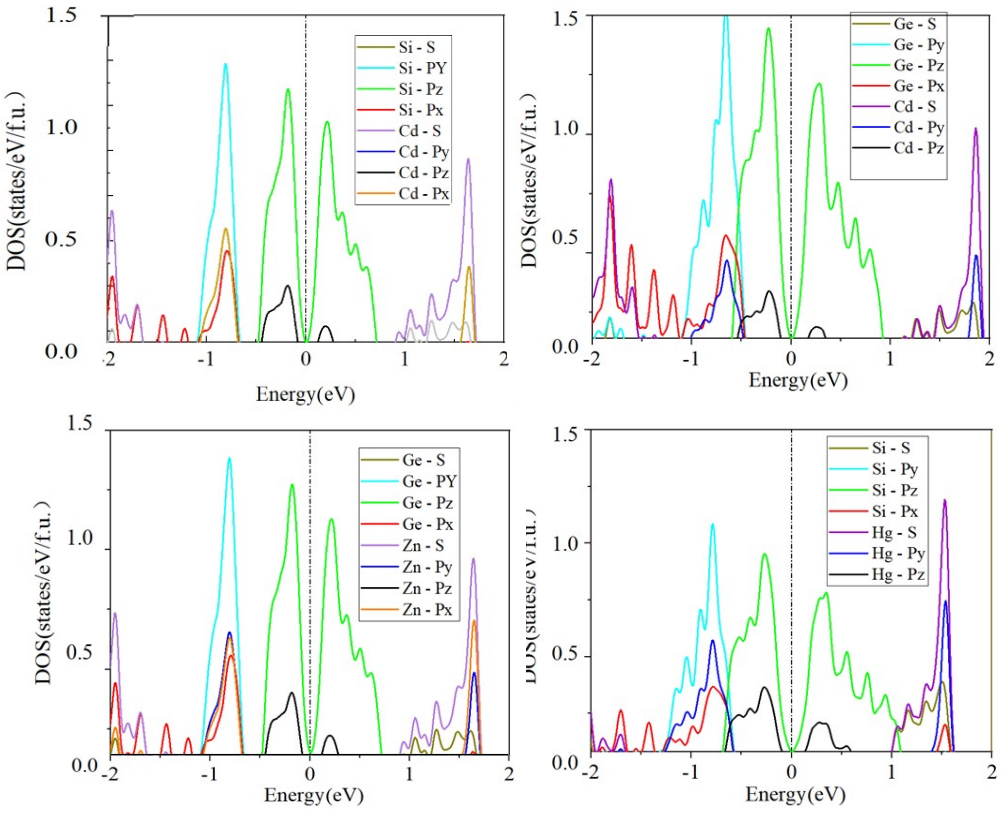

Fig.S3 Partial density of state (PDOS) of M_3X_2.

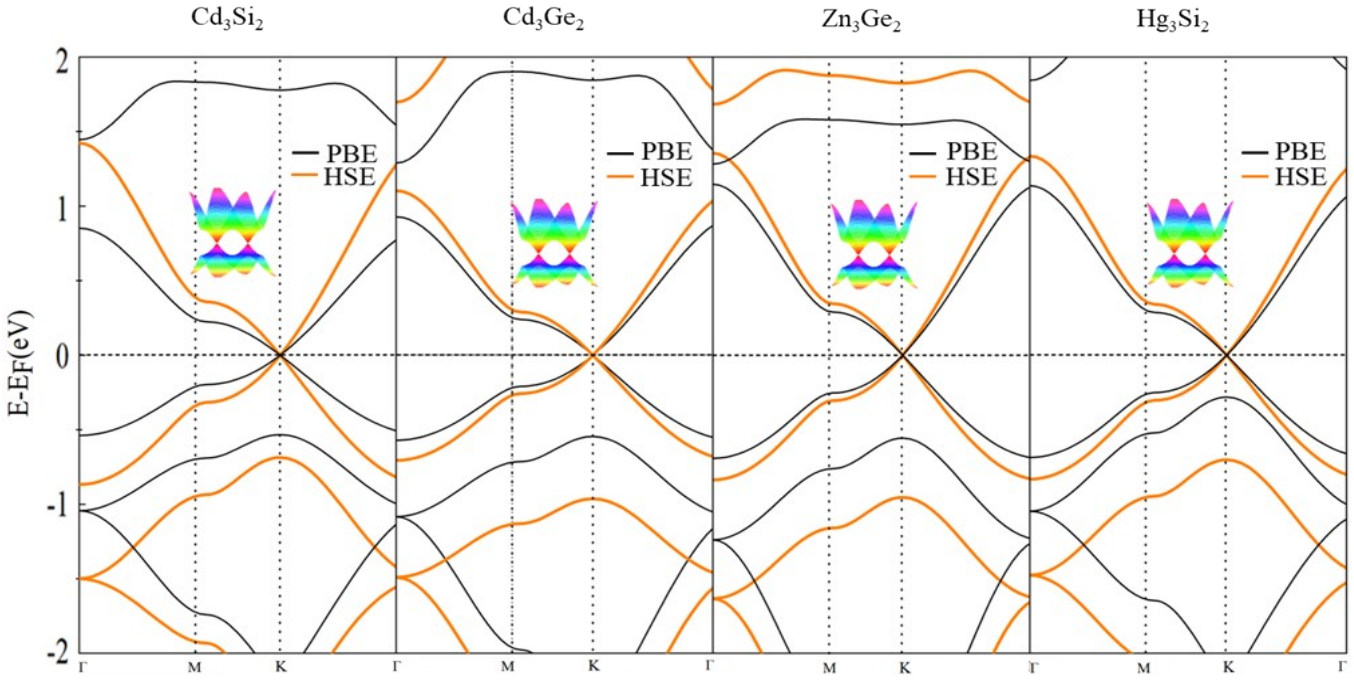

Fig.S4 The calculated band structure (3D band structure) of the M_3X_2 lattice without SOC. Yellow and black solid lines represent the HSE and PBE functional, respectively.

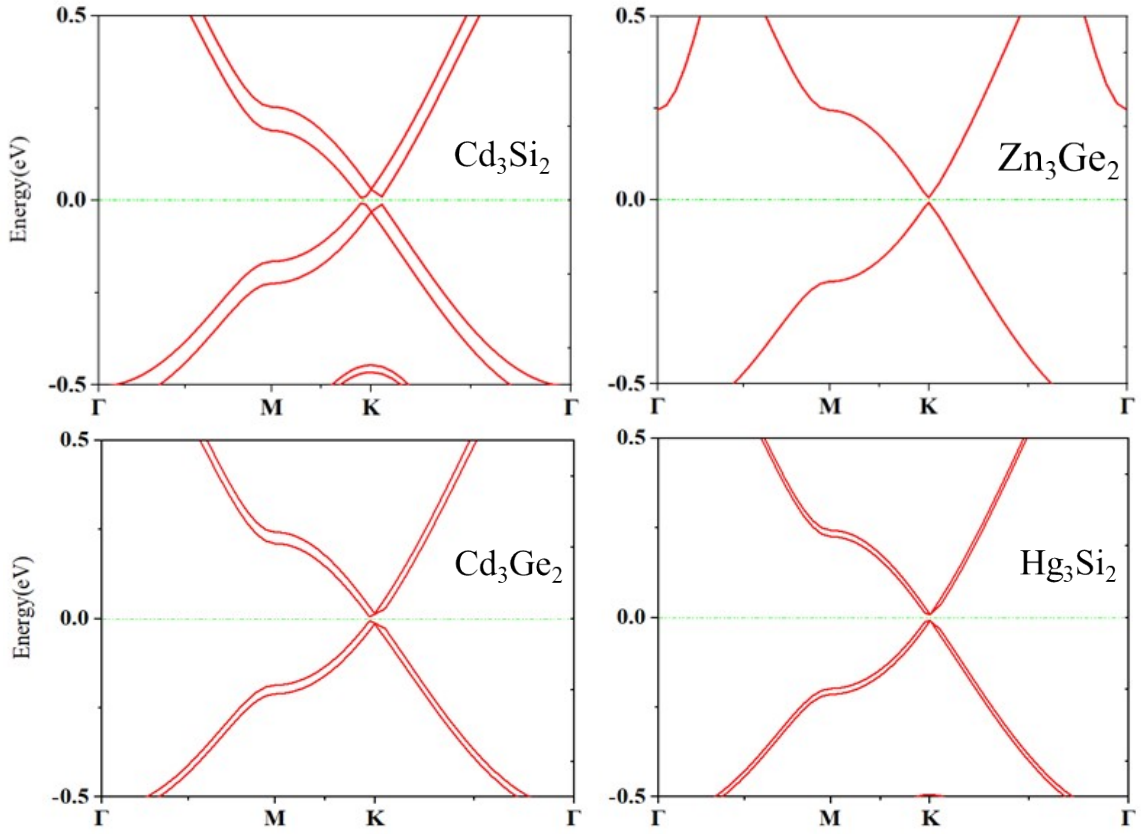

Fig.S5 Band structures of M_3X_2 with SOC around K point.

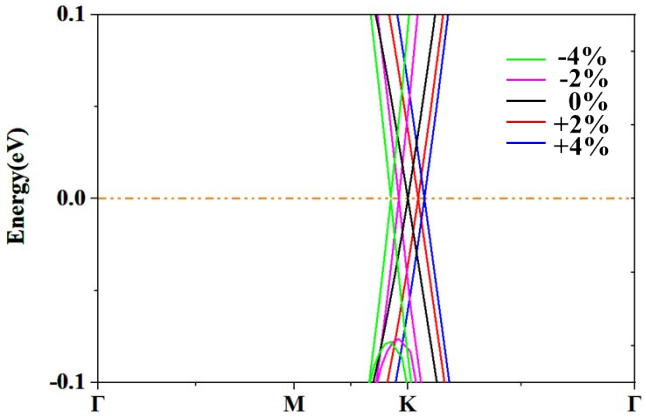

Fig.S6 Variations of electronic band structure against different in-plane biaxial strains (-4%~+4%).

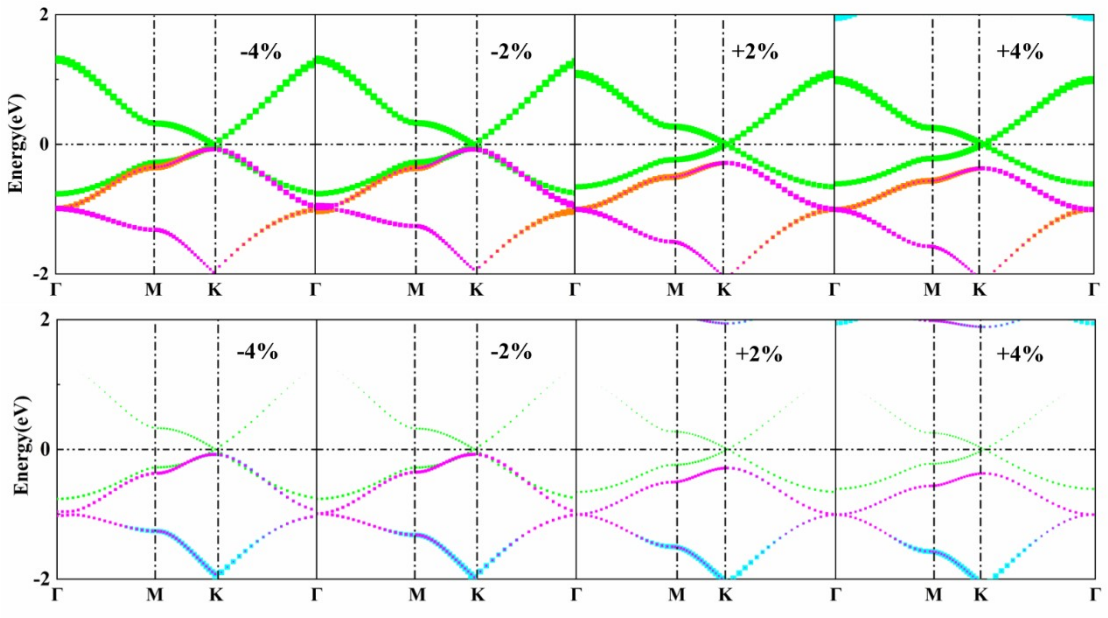

Fig. S7 Orbital-resolved band structures of Cd_3Si_2 monolayer under mild tensile or compressional strains (-4% ~ 4%), under which the Dirac cone persist evidently. The green, yellow, blue and purple dots represent the contributions from the p_z, p_x, p_y and s atomic orbitals, respectively.

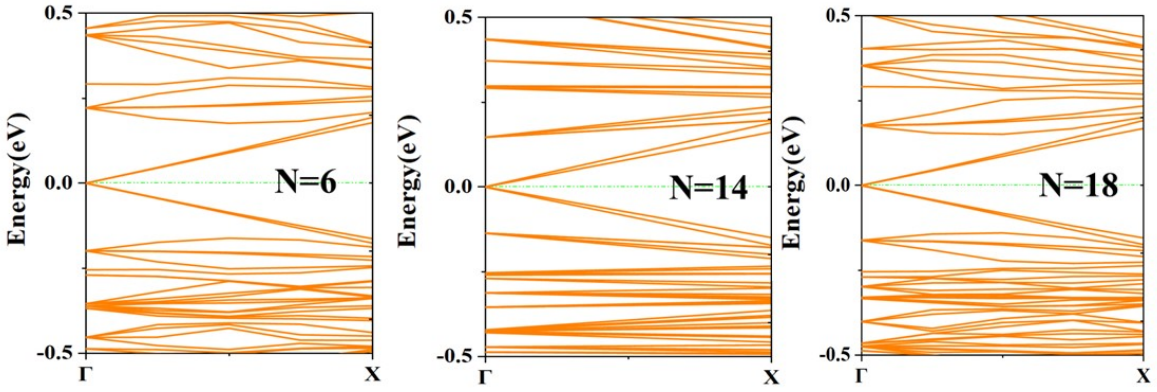

Fig.S8 electronic band structure of 1D zigzag nanoribbons of Cd_3Si_2 cut from the width(N=6~18).

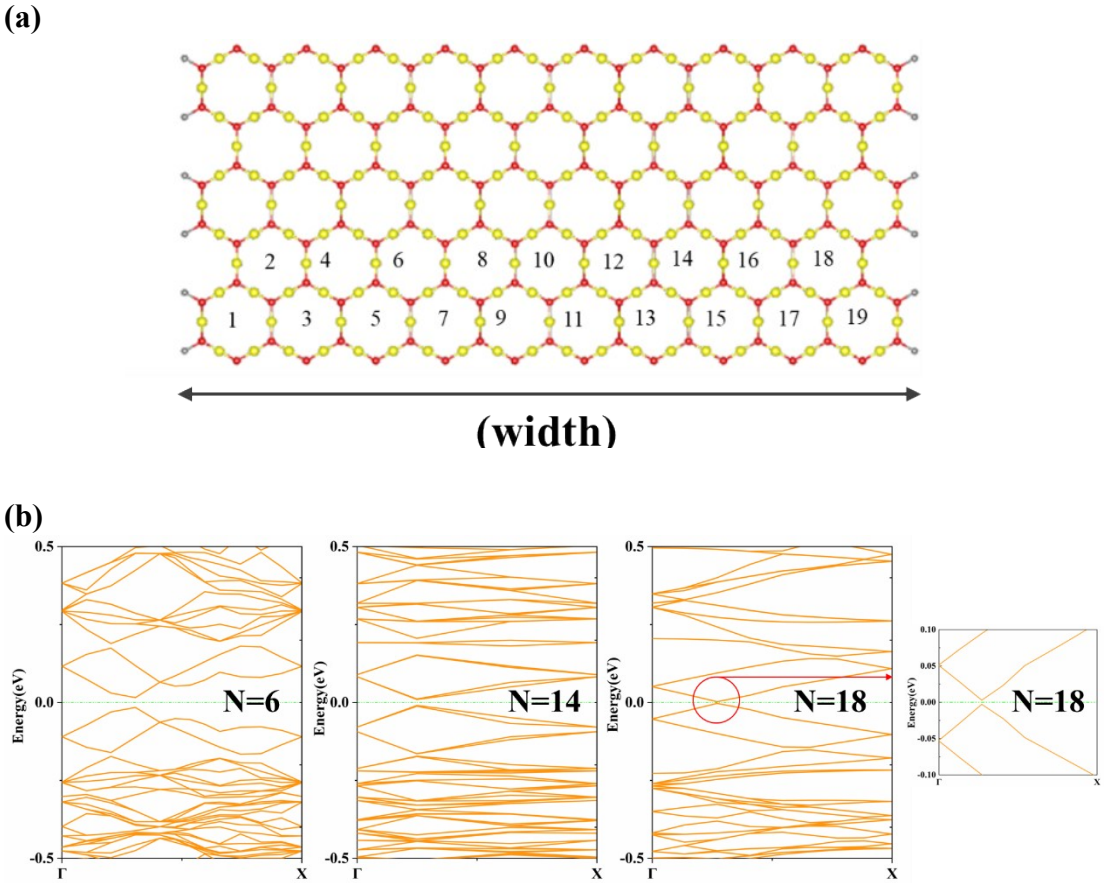

Fig.S9 (a) Structural model of armchair nanoribbon of Cd_3Si_2. (b) Band structures of the 1D armchair nanoribbons from the Cd_3Si_2.

Table.S1 The band gaps of Cd_3Si_2 nanoribbons with various widths.

Width(N)/Band gap(eV)	6	14	18
zigzag	sm[a]	sm[a]	sm[a]
armchair	0.0616	0.0313	0.0056

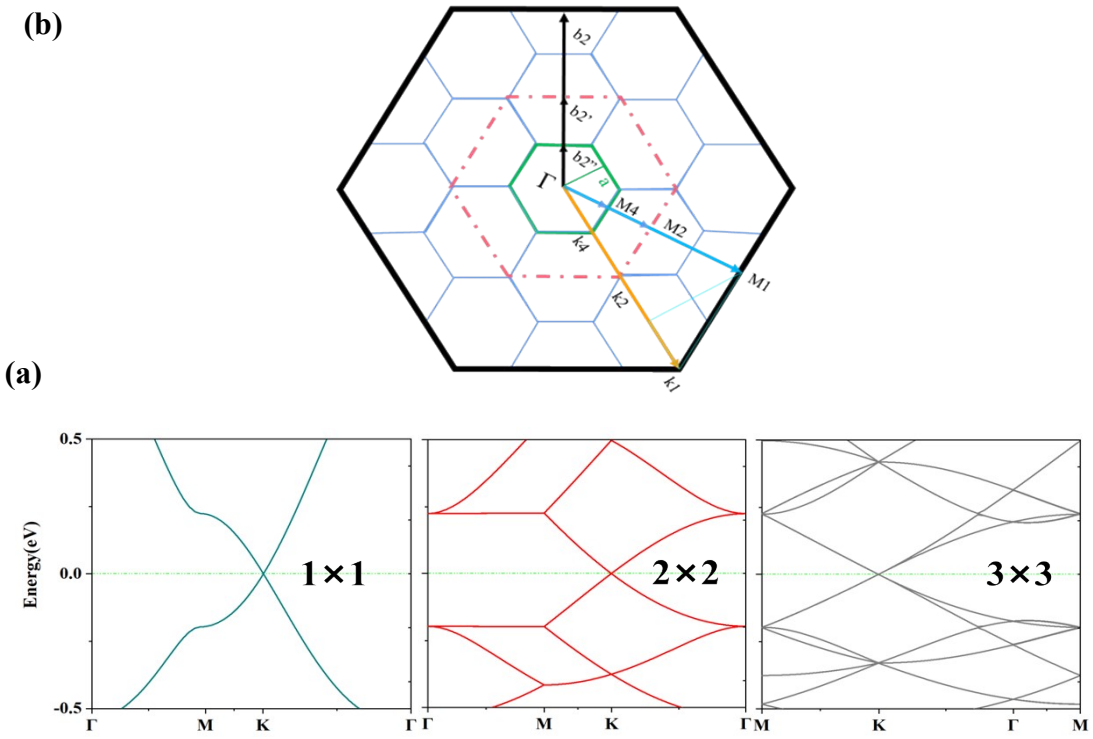

Fig.S10 (Color online) The first Brillouin zones of the primitive (green line), 2 ×2 supercell (red dash line), 3 × 3 supercell (black line) of Cd_3Si_2 and their corresponding band structure.

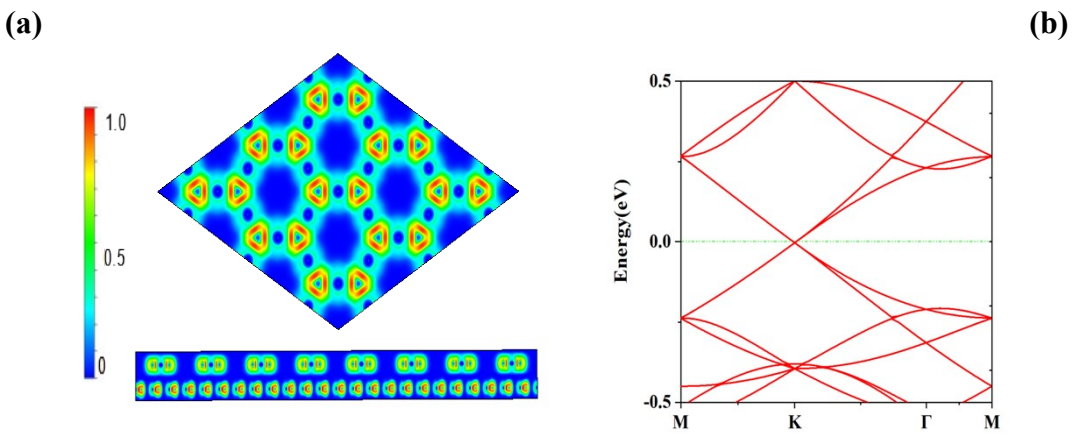

Fig.S11 (a)The ELF of Cd_3Si_2/h-BN heterostructure (b) the band structures of Cd_3Si_2 on h-BN substrate.

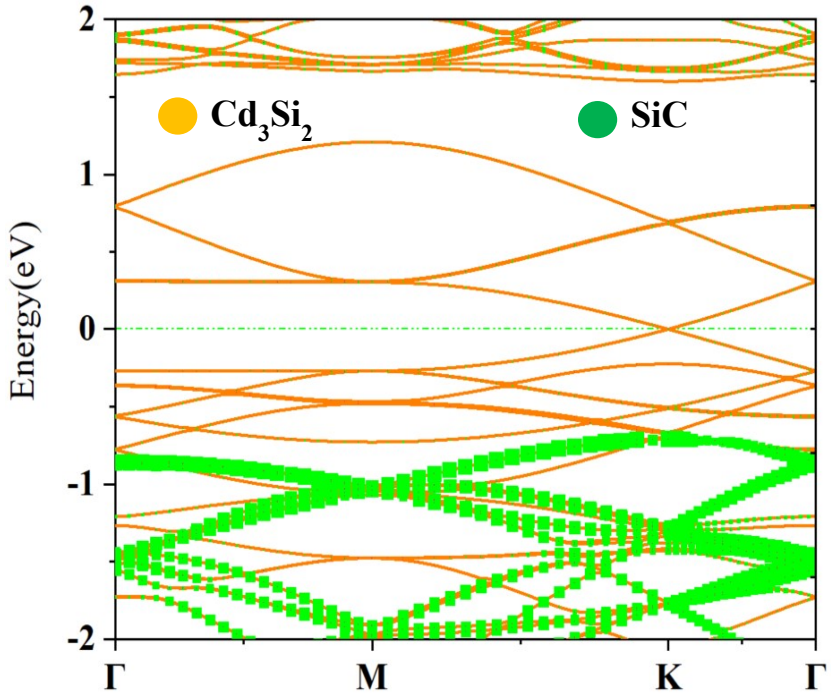

Fig.S12 Calculated band structure of the Cd_3Si_2 / SiC heterostructure.