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Predicting a Graphene-like WB_4 Nanosheet with Double Dirac Cone, the Ultra-high Fermi Velocity and Significant Gap Opening by Spin-orbit Coupling

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Method

The band gap are calculated in the generalized gradient approximation in the Perdew, Burke, and Ernzerhof form (GGA -PBE) PBE calculations[1] (Figure S1), which underestimate the band gap compared with HSE method. A damped van der Waals correction was incorporated using Grimme's scheme[2] to better describe the nonbonding interaction. Monkhorst−Pack k-points[3] of 15 ×15 × 1 were used for sampling in the first Brillouin zone during geometry optimizations of the WB_4 monolayer. All of the atoms were fully relaxed until the residual force and energy converged to 0.001 eV/Å and 10^{-6}eV, respectively. To make sure of the dynamical stability of the obtained structures, phonon dispersion analysis was performed by the finite displacement method[4] using the Phonopy code[5] interfaced with the density functional perturbation theory[6] as implemented in VASP. In phonon calculations, an increased plane wave energy cutoff of 500 eV was employed, accompanied by more stringent convergence criteria for energy (10^{-8} eV) and force (0.001 eV/Å).

Next, we estimate the elastic limit of the WB_4 monolayer by calculating the strain−stress relation subject to a biaxial tensile tension. The maximum stress is the ultimate strength that a material can withstand while being stretched, and the corresponding strain is called the ideal strain strength, which is determined by the intrinsic bonding strengths. The maximum stress that 2D WB_4 can withstand while being stretched is about 3.5N/m with the corresponding ideal strain of 17% (Figure S2, S3), which is camparable to that of other well-known 2D materials such as MoS_2 (20%)[7] and graphene (24%)[8] suggesting the high mechanical strength and robust of two Dirac cone of the monolayer.WB_4.

Ab initio molecular dynamics (AIMD) simulations with canonical ensemble was performed to evaluate the thermodynamic stability. The structure did not collapse with time change for 10ps at 300 K and 1000K (Figure S4), which confirms our structure is stable at both room temperature and high temperature.

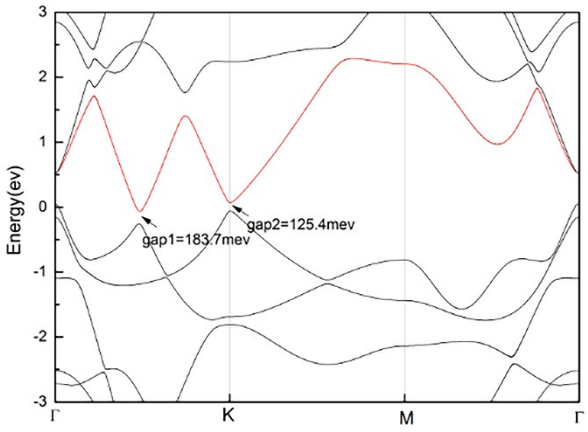

Figure S1. Calculated SOC band structures for 2D P6/mmm WB_4 with PBE method (183.7mev for cone 1and 125.4 mev for cone 2, respectively).

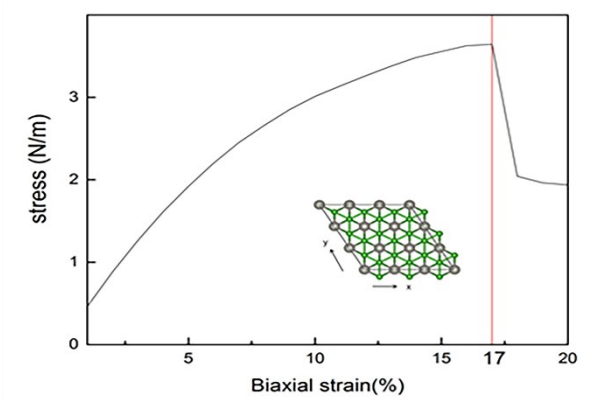

Figure S2. The stress in the WB_4 monolayer subjected to biaxial strain. The structural snapshots under 17% strain. The strain directions are marked by x, y arrows.

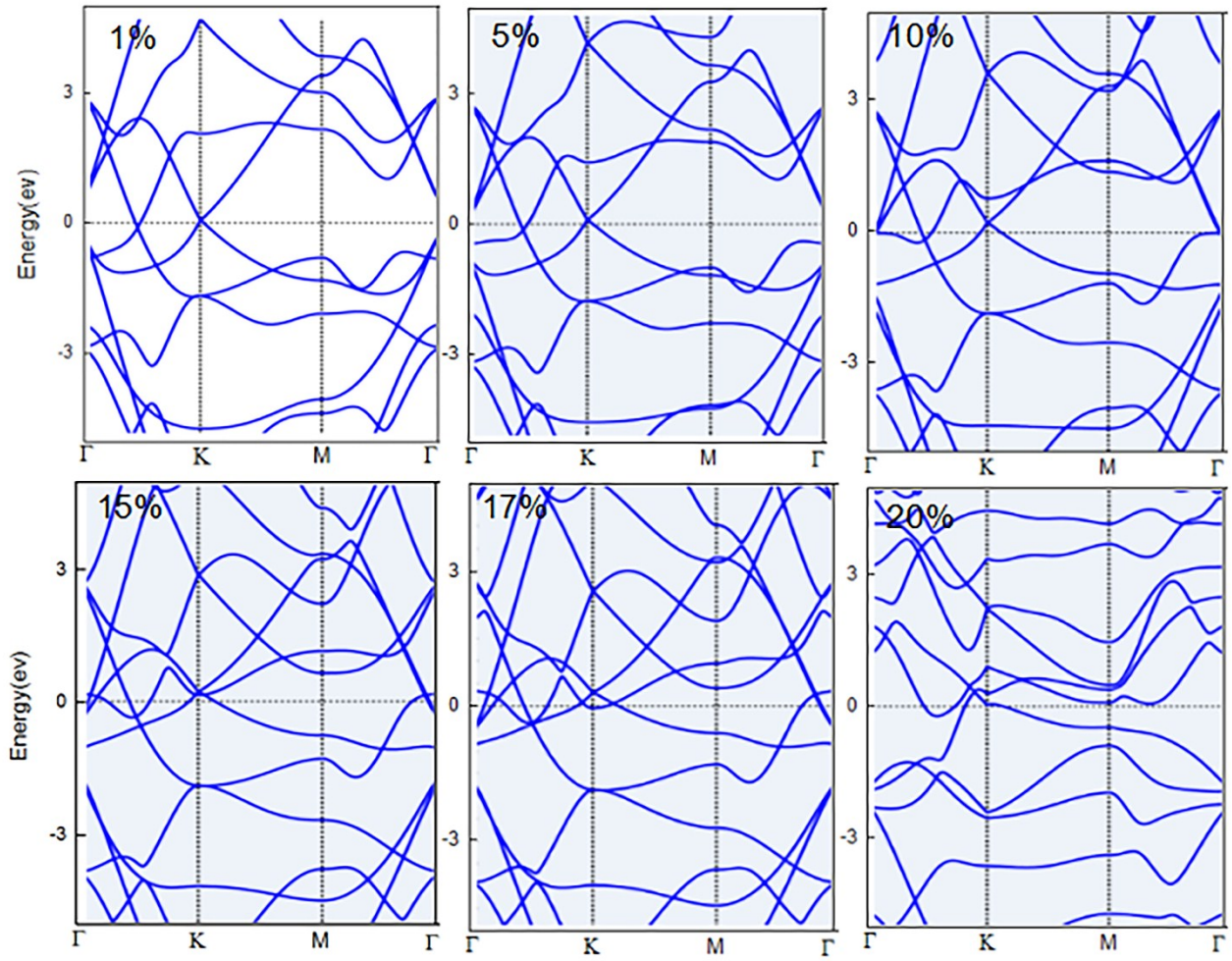

Figure S3, The band structure changes when 1%, 5%, 10%, 15%, 17%, 20% biaxial strain is applied on the monolayer WB_4. Biaxial strain is observed to shift the Dirac points without affecting the metallicity while preserving the Dirac points until 17%, which gives a clear description of the robust of Dirac cone.

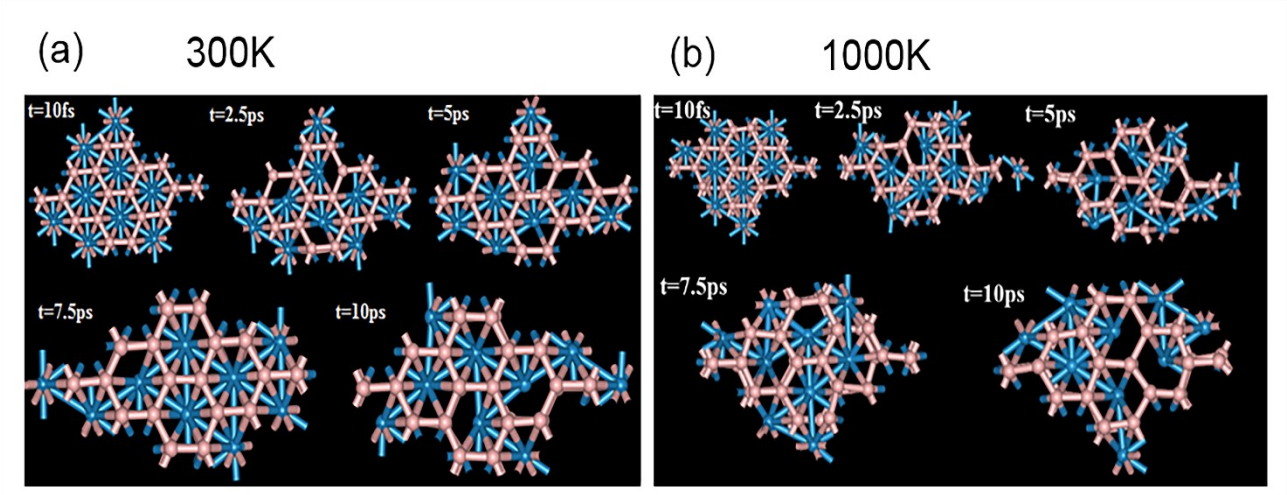

Figure S4. The thermodynamic stability at (a) 300K (b) 1000K of monolayer WB_4 are evaluated through Ab initio molecular dynamics (AIMD) simulations. The figures present configurations from 10fs to 10ps.

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