

## Electronic Supplementary Material (ESI)

### Motif based high-throughput structure prediction of superconducting monolayer titanium boride

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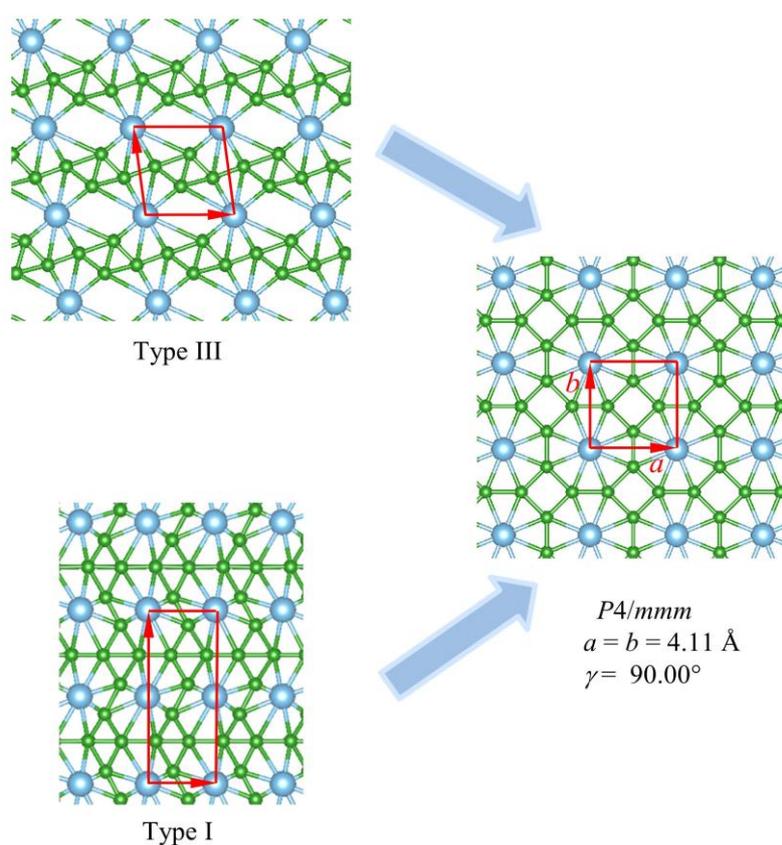


Fig. S1. The top views of two initial configurations and the fully relaxed counterpart of TiB<sub>4</sub>.

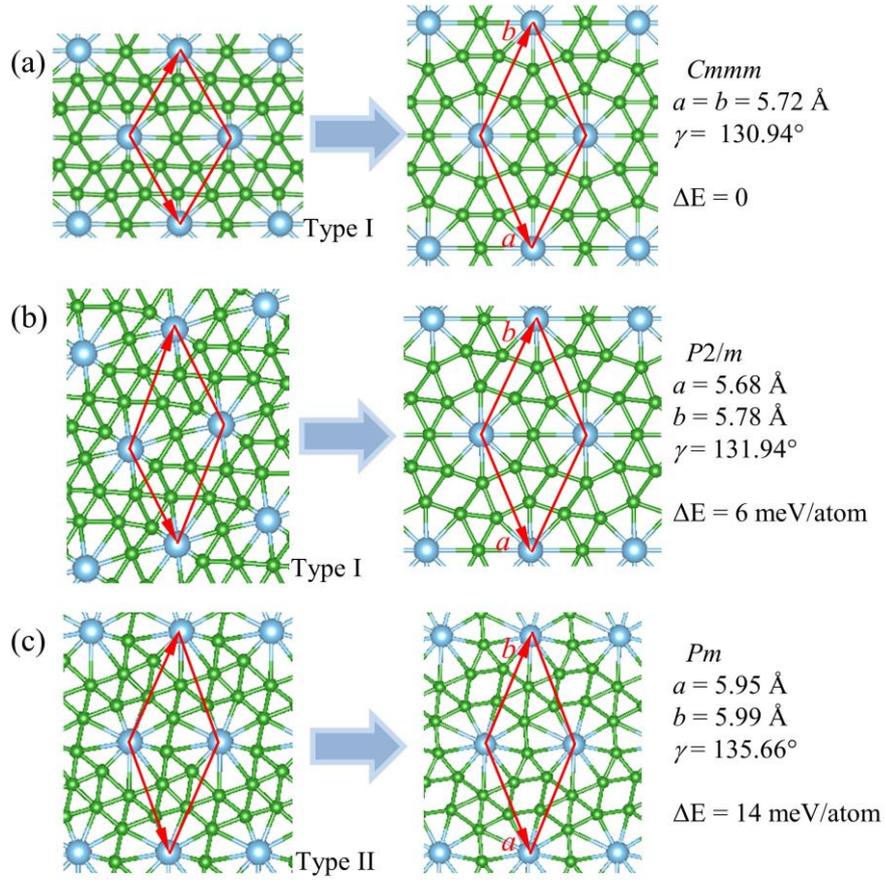


Fig. S2. The top views of the initial configurations and the fully relaxed counterparts of  $\text{TiB}_7$  with (a) the lowest, (b) the second-lowest and (c) the third-lowest formation energy.

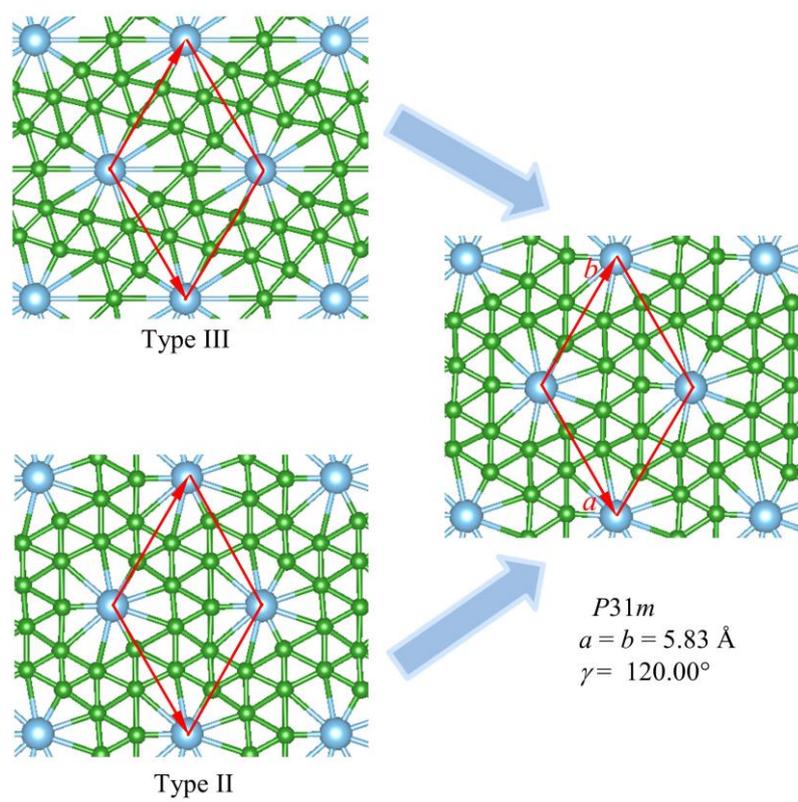


Fig. S3. The top views of two initial configurations and the fully relaxed counterpart of TiB<sub>9</sub>.

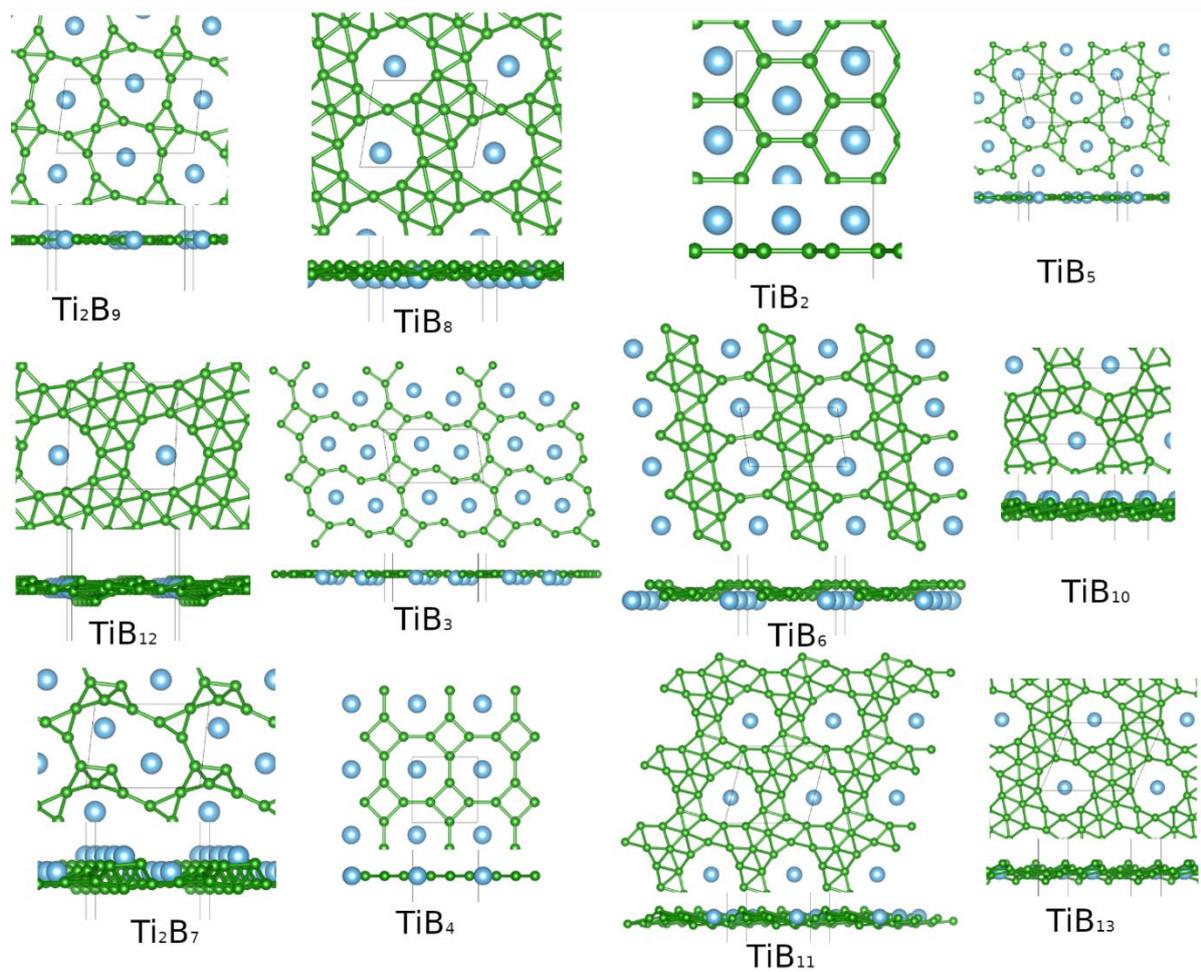


Fig. S4. The top and side views of the atomic structure of titanium boride monolayers as a function of concentration of titanium.

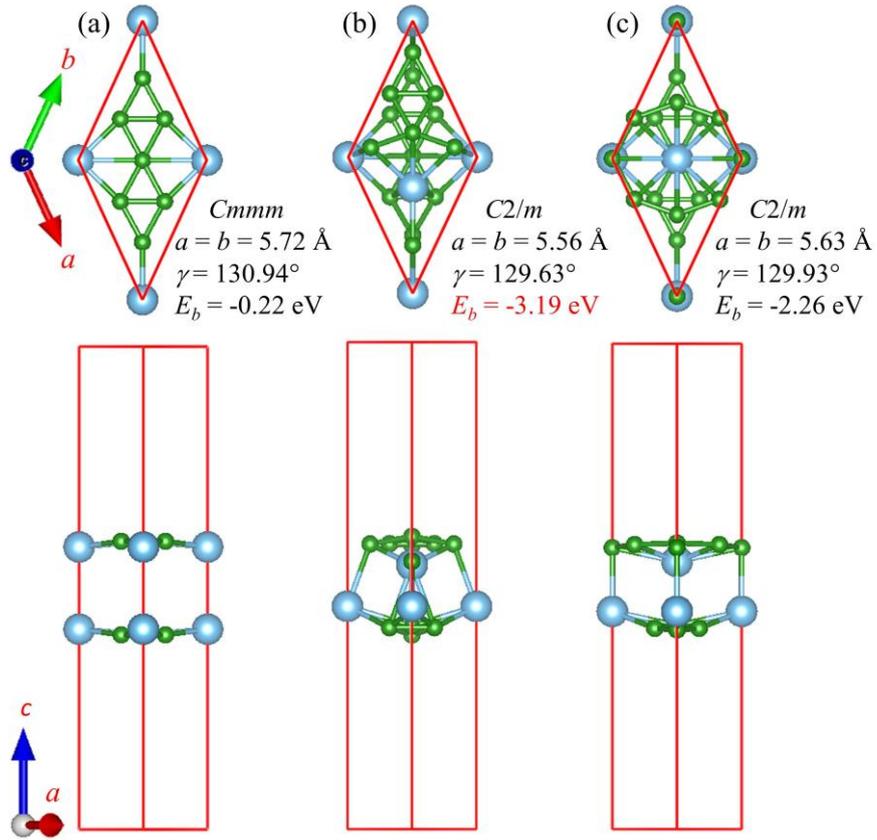


Fig. S5. The top and side views of the atomic structure of bilayer  $TiB_7$  with stacking order of (a)AA , (b) AB (B: the center of an acute triangle) and (c)AC (C: the rhombic center).

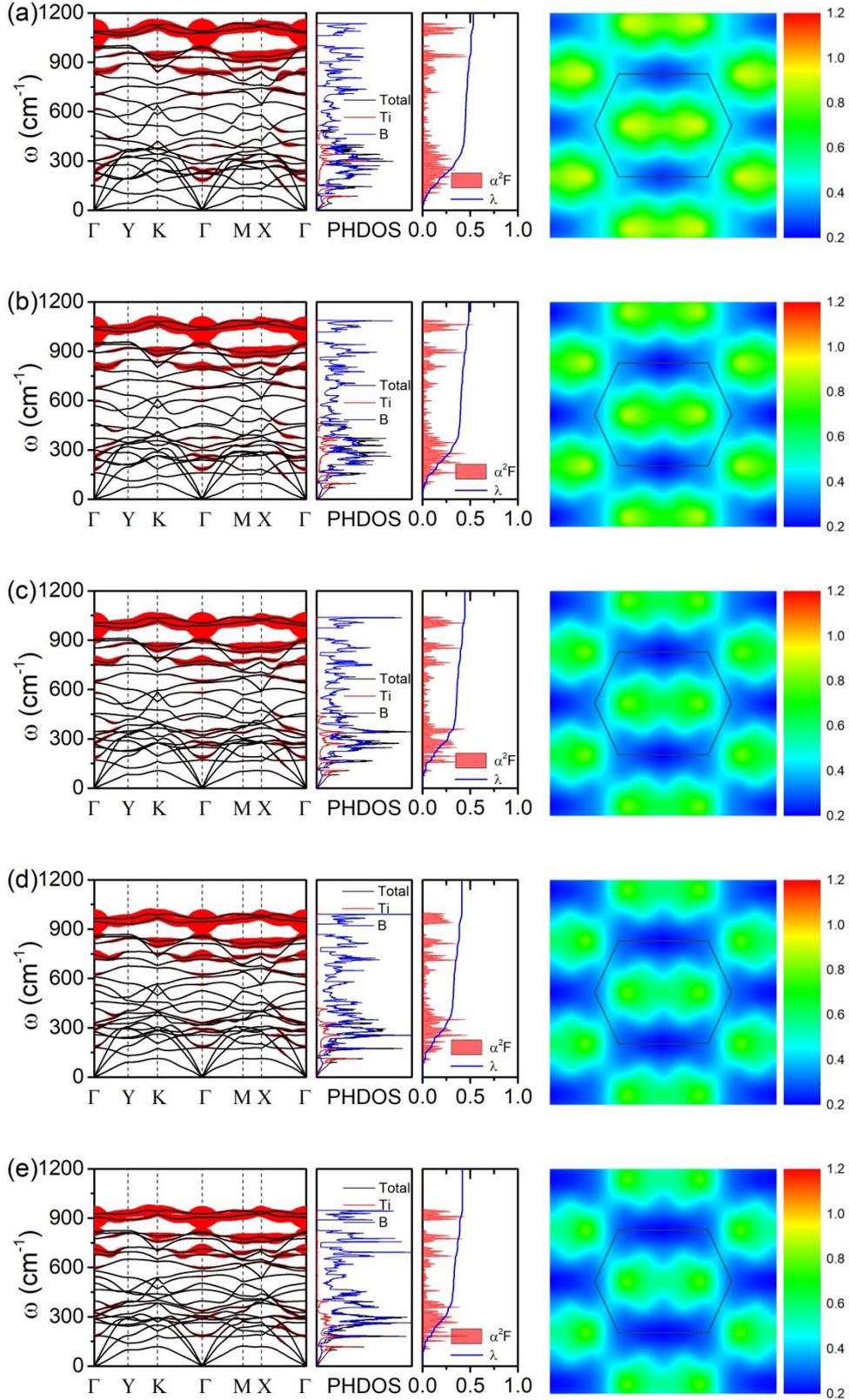


Fig. S6. Phonon dispersions with phonon linewidth  $\gamma_{q\nu}$  in red bubble, phonon density of states, Eliashberg function  $\alpha^2F(\omega)$  with  $\lambda(\omega)$  and EPC distribution of monolayer  $\text{TiB}_7$  under the equibiaxial tensile strain of (a) 1%, (b) 2%, (c) 3%, (d) 4%, and (e) 5%.

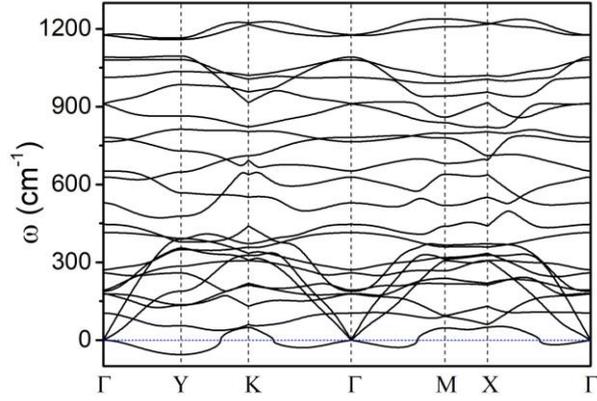


Fig. S7. Phonon dispersion of monolayer  $\text{TiB}_7$  under the equibiaxial compressive strain of 1%.

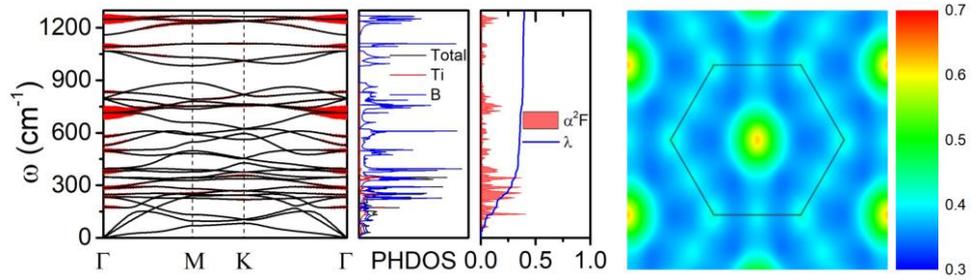


Fig. S8. Phonon dispersion with phonon linewidth  $\gamma_{\text{qv}}$ , phonon density of states, Eliashberg function  $\alpha^2 F(\omega)$  with  $\lambda(\omega)$  and EPC distribution of unstrained monolayer  $\text{TiB}_9$ .

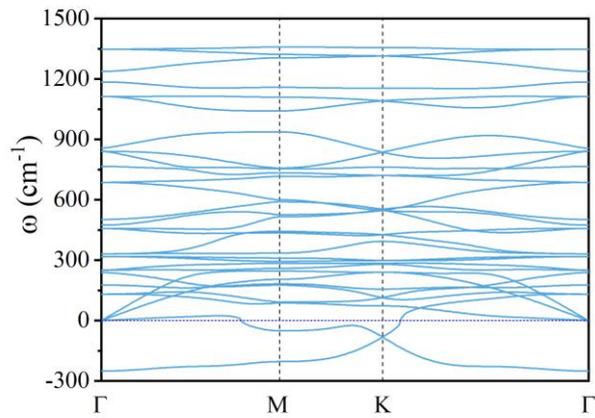


Fig. S9. Phonon dispersion of the planar monolayer  $\text{TiB}_9$ .

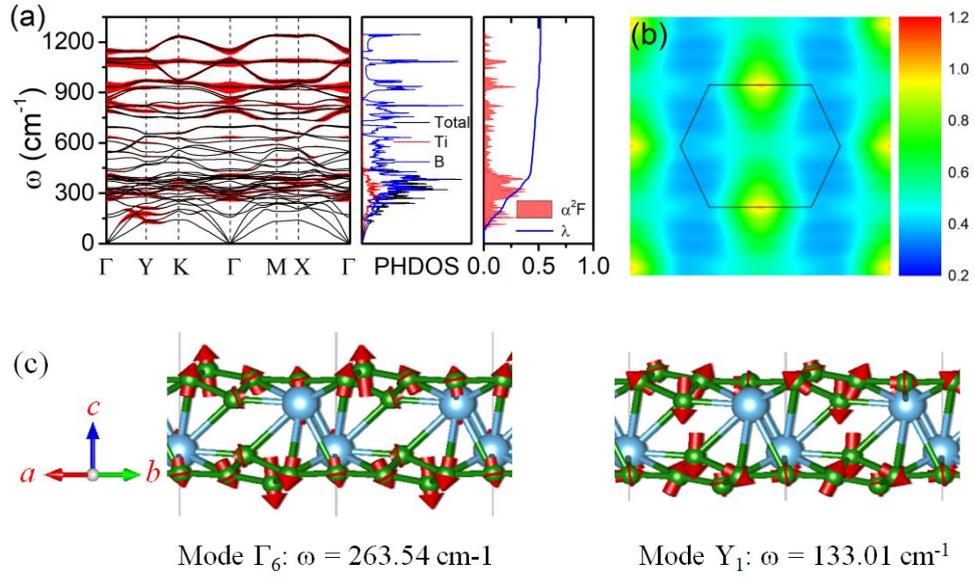


Fig. S10. (a) Phonon dispersion with phonon linewidth  $\gamma_{qv}$ , phonon density of states, Eliashberg function  $\alpha^2F(\omega)$  with  $\lambda(\omega)$  and (b) EPC distribution of AB-stacking bilayer TiB<sub>7</sub>. (c) Some phonon modes. The red arrows and their lengths represent the directions and amplitudes of the corresponding vibrational modes.