Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Material for Structure searches and superconductor discovery in XB_2 (X= Sc, Ti, V, Cr, and Tc)

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Compound	Formation enthalpy (eV/atom)	Lattice parameter (Å) a	c	λ
ScB_2	-0.85	3.14	3.52	0.28
TiB_2	-1.08	3.04	3.22	0.1
VB_2	-0.73	3.0	3.0	0.3

TABLE SI. Formation enthalpy and lattice parameter, the calculated electron-phonon coupling strength (λ) for compounds of ScB_2, TiB_2, and VB_2 at ambient pressure.

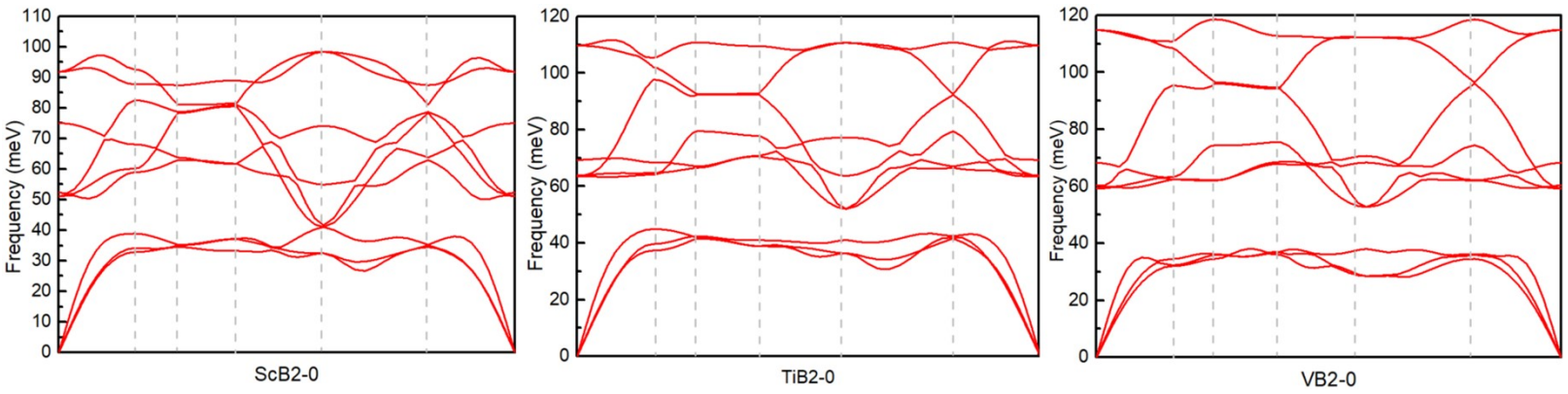

Fig. S1. phonon-dispersion curves of ScB_2, TiB_2, and VB_2 at ambient pressure.

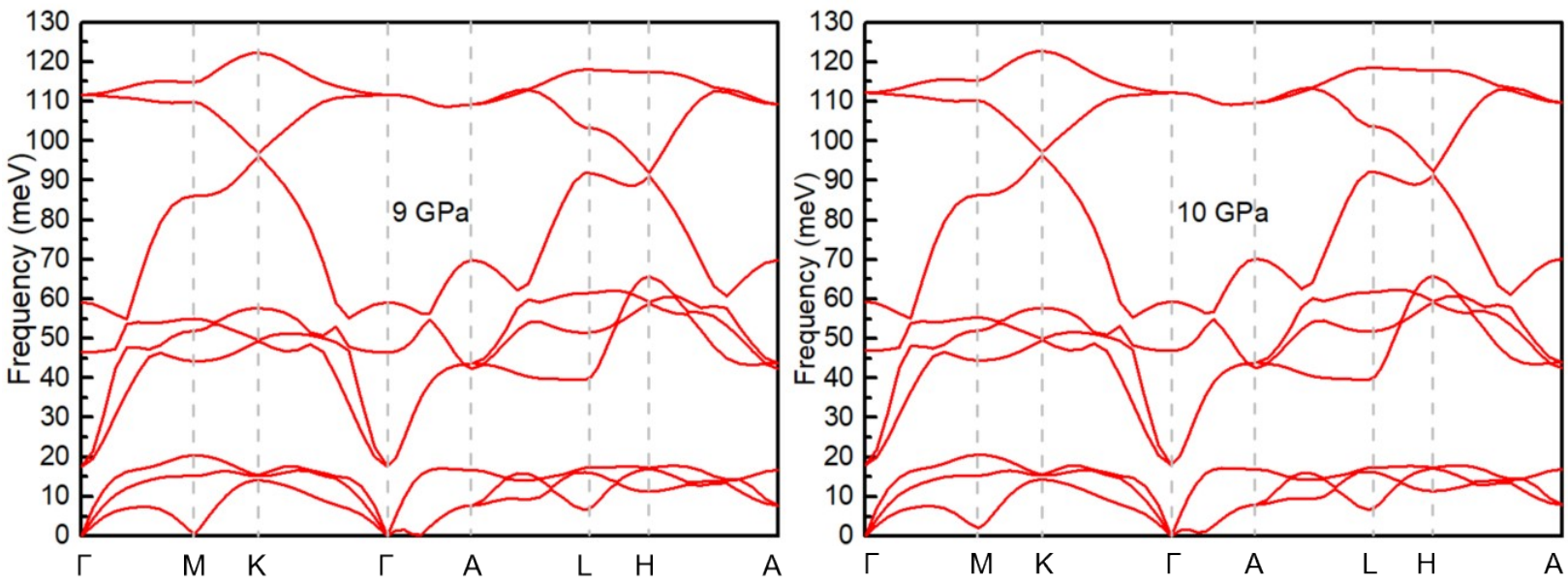

Fig. S2. Phonon-dispersion curves of TcB_2 at 9 GPa and 10 GPa.

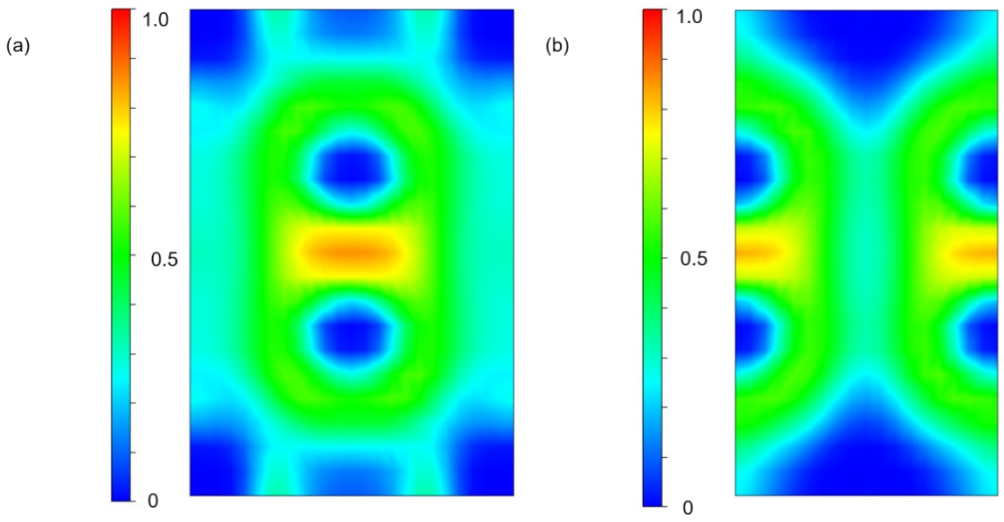

Fig. S3. The calculated ELF of (a) TcB_2 at 20 GPa and (b) CrB_2 at 108 GPa on the (1 1 0) plane.