Supplemental Material

Structural, strength, and fracture mechanisms of superconducting transition metal nitrides TM_3N_5 (TM = W and Mo)

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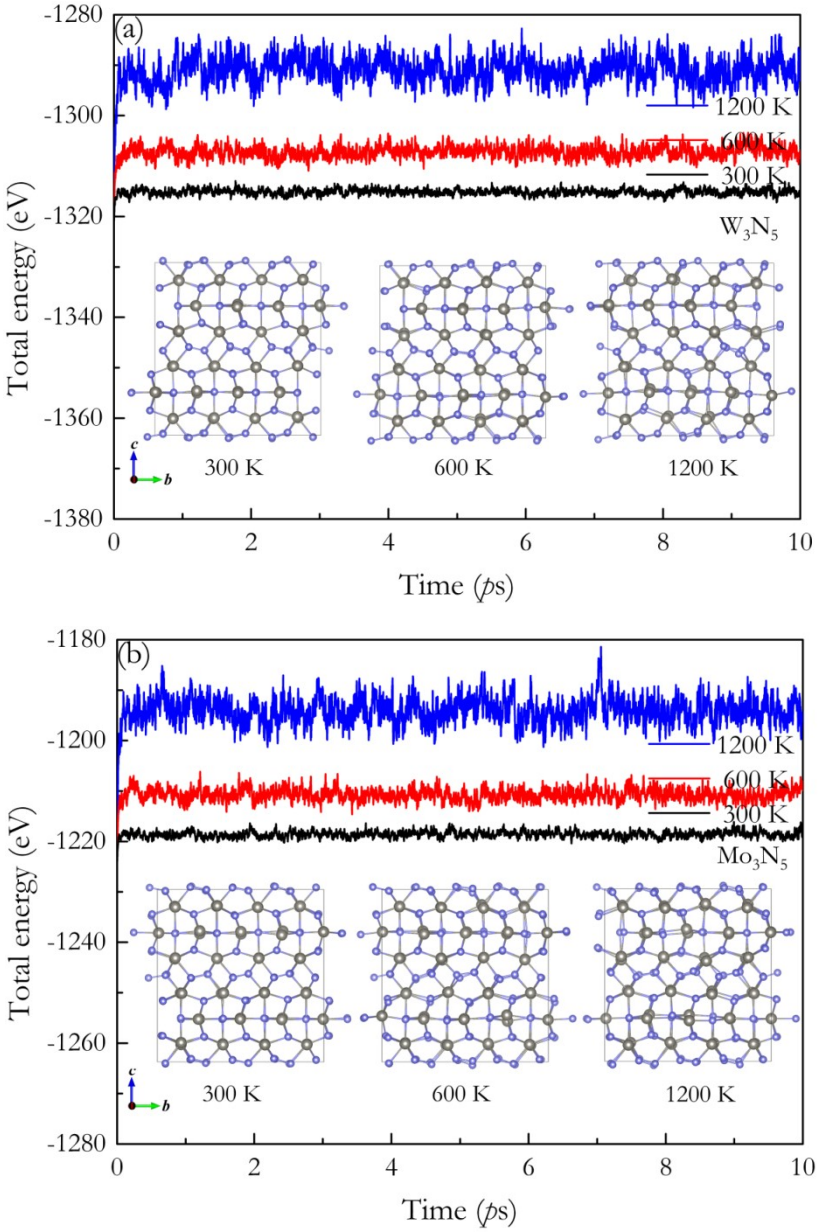

Fig. S1 AIMD simulations at 300, 600, and 1200 K for W_3N_5 (a) and Mo_3N_5 (b) at ambient conditions. Insets are the equilibrium structures after 10 *p*s.

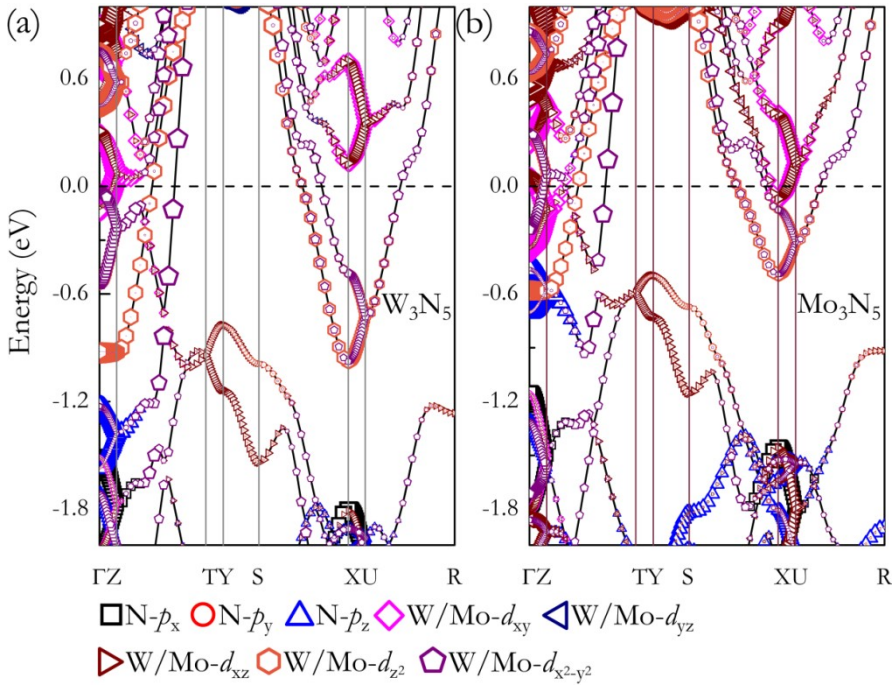

Fig. S2 Projected weights of atomic orbitals in the band structures of W_3N_5 (a) and Mo_3N_5 at ambient pressure. The E_F is indicated by horizontal dashed lines.

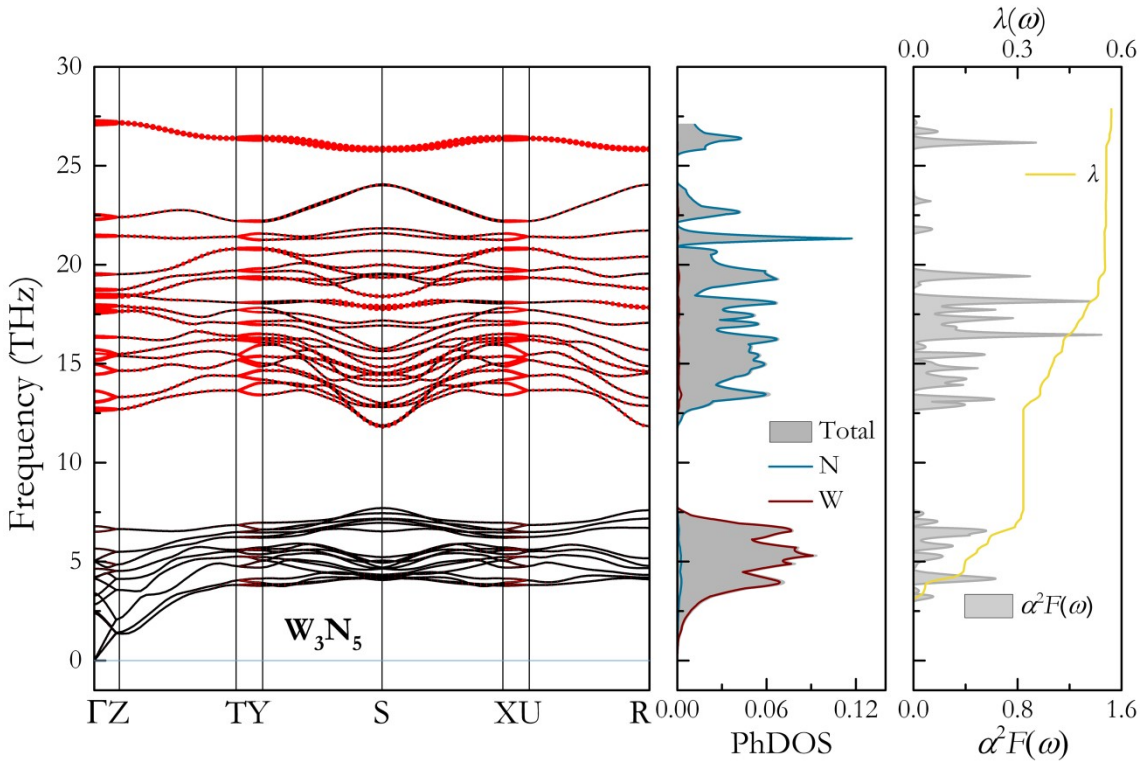

Fig. S3 Phonon dispersion curves, projected phonon density of states, Eliashberg spectral function $\alpha^2F(\omega)$, and the EPC parameter λ for W_3N_5 at ambient pressure.