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Prediction of Superhard B_2N_3 with Two-dimensional Metallicity

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Table S1. The optimized structural parameters of *R*3*m*-, *P1*-, and *t*-B_2N_3 at ambient pressure.

Space group	*a*,*b*,*c* (Å,deg)	Volume(Å^3/f.u.)	Atomic position
*R*3*m*	*a*=*b*=5.0263	91.30	B1(3*a*) (0, 0, 0.98)
	c=25.0377		B2(9*b*) (0.5, 0.5, 0.98)
			N1(3*a*) (0.67, 0.33, 0.79)
			N2(3*a*) (0.33, 0.67, 0.17)
			N3(3*a*) (0, 0, 0.65)
			N4(9*b*) (0.33, 0.67, 0.317)
*P*1	*a*=5.0264	85.63	B1(1*a*) (0.88, 0.77, 0.49)
	b=5.0258		B2(1*a*) (0.38, 0.77, 0.49)
	c=7.6927		B3(1*a*) (0.38, 0.27, 0.49)
	α=92.23		B4(1*a*) (0.88, 0.27, 0.49)
	β=79.98		N1(1*a*) (0.16, 0.07, 0.97)
	γ=120.0034		N2(1*a*) (0.03, 0.82, 0.01)
			N3(1*a*) (0.55, 0.6, 0.49)
			N4(1*a*) (0.05, 0.1, 0.49）
			N5(1*a*) (0.55, 0.1, 0.49)
			N6(1*a*) (0.05, 0.6, 0.49)
*P*4$_2$/*mmc*	a=b=2.5706	32.20	B1(4*i*) (0, 0.5, 0.85)
	c=9.7436		N1(4*h*) (0.5, 0.5, 0.93)
			N2(2*e*) (0, 0, 0.25)

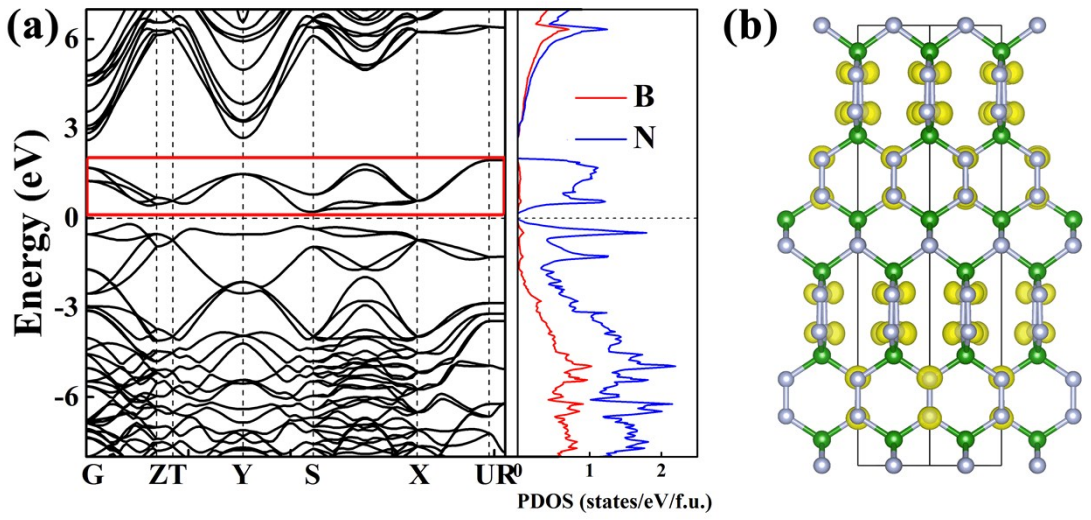

Figure S1. Band structure and PDOS for *C*222$_1$-B_3N_5. The band decomposed charge density of *C*222$_1$-B_3N_5 above Fermi level, respectively (marked by red lines). The Fermi level is set to zero.

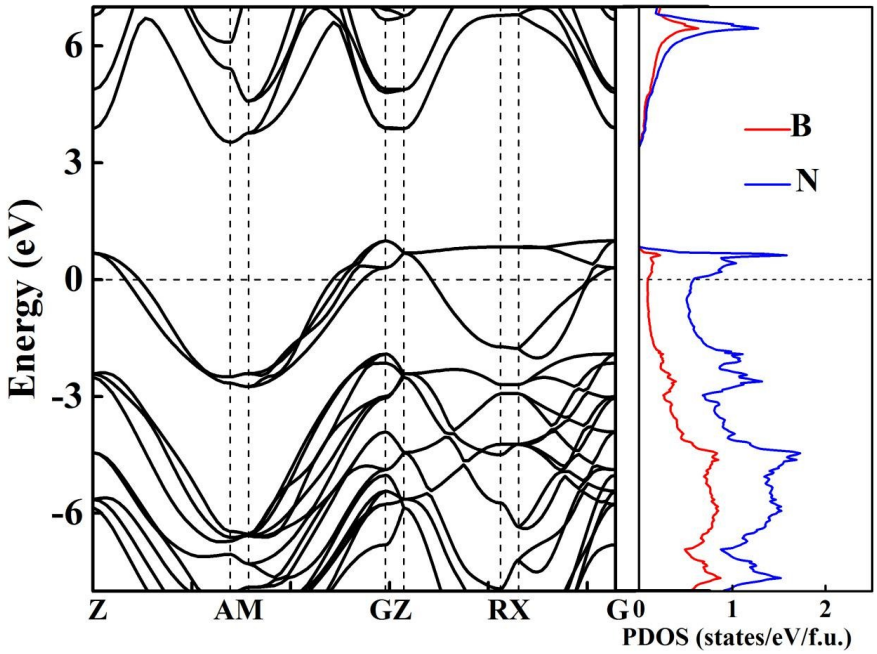

Figure S2. Band structure and PDOS for *t*-B_3N_4. The Fermi level is set to zero.

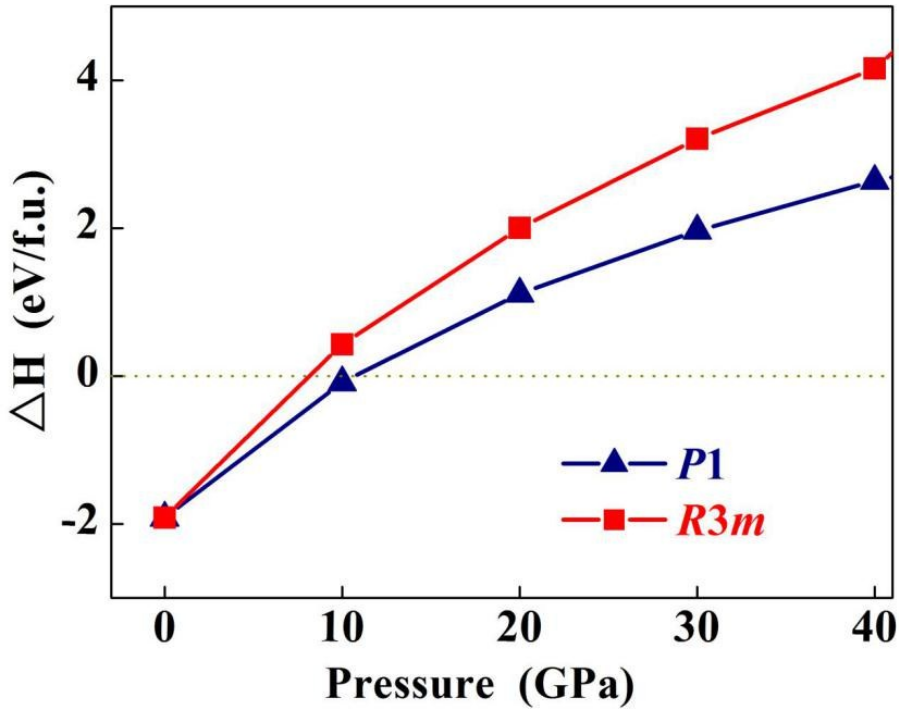

Figure S3. Calculated enthalpy curves of *R*3*m*- and *P1*-B_2N_3 relative to *t*-B_2N_3 as a function of pressure.

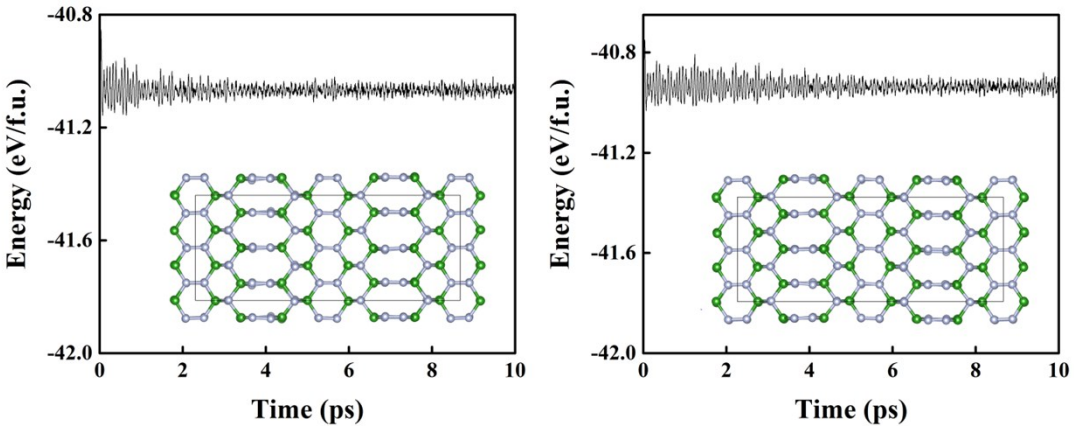

Figure S4. Snapshots of the final frame of t-B_2N_3 at temperatures of 300 K at the end of 10 ps AIMD simulations at (a) 0 GPa and (b) 20 GPa.

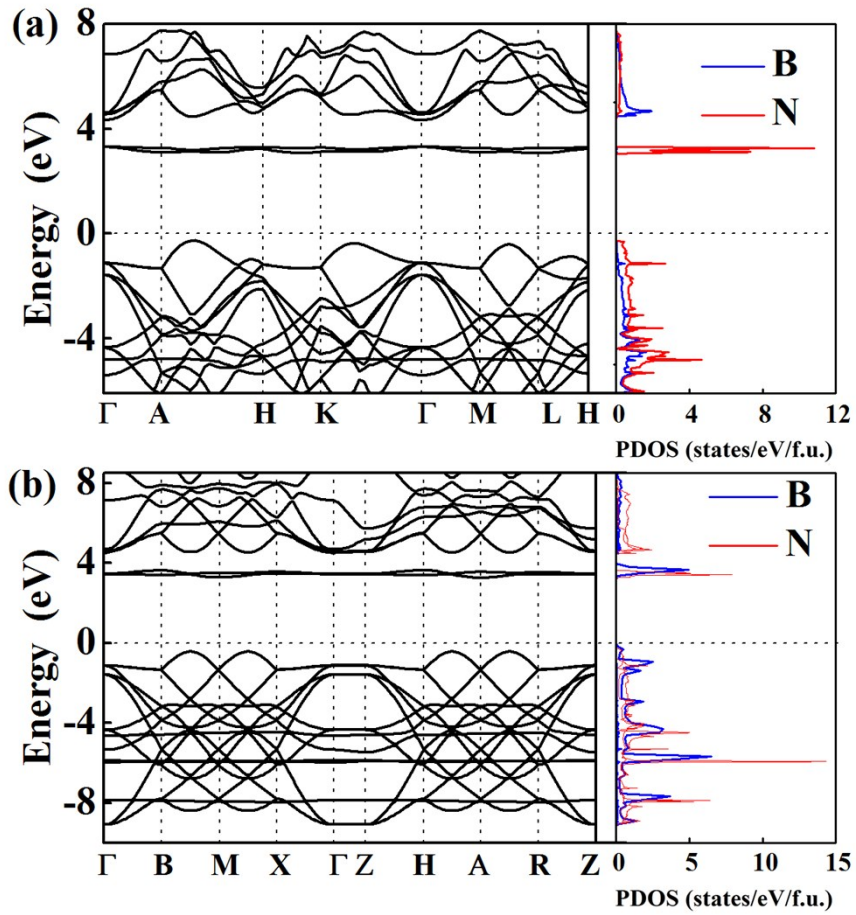

Figure S5. The calculated band structures and PDOS of $R3m$-B_2N_3 (a) and $P1$-B_2N_3 (b) at ambient pressure.