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SUPPLEMENTARY MATERIAL

Theoretical study on the controllable preparation of superhard BC_2N under high pressure

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Table S1. Lattice constant and atomic Wyckoff positions of the five BC_2N structure at ambient pressure.

Structure	Symmetry	*a* (Å)	*c* (Å)	Atomic Position
*R*3*m*-BC_2N	*R*3*m*	2.540	25.179	C_1:3a (1, -1, -0.054), C_2:3a (1, -1, -0.116)
				C_3:3a (0.333, -0.333, -0.033), C_4:3a (0.667, -0.667, -0.136)
				B_1:3a (0.333, -0.333, -0.218), B_2:3a (0.667, -0.667, 0.-0.302)
				N_1:3a (0.333, -0.333, -0.279), N_2:3a (0.667, -0.667, -0.196)
*P*2/*m*-BC_2N	*P*2/*m*	8.866	4.277	C_1:2n (-0.091, 0.5, 0.181), C_2:2n (0.086, 0.5, 0.187)
				C_3:2m (0.162, 0, 0.317), C_4:2m (-0.165, 1, 0.317)
				B_1:2n (0.590, 0.5, 0.332), B_2:2m (0.334, 0, 0.177)
				N_1:2n (0.415, 0.5, 0.297), N_2:2m (0.670, 0, 0.201)
*P*2/*m*-BC_2N-2	*P*2/*m*	9.061	4.230	C_1:2n (0.417, -0.5, 0.395), C_2:2m (0.663, 0, 0.141)
				C_3:2m (0.337, 0, 0.488), C_4:2n (0.582, 0.5, -0.021)
				B_1:2m (0.834, 0, 0.09), B_2:2n (1.092, 0.5, 0.380)
				N_1:2m (1.173, 0, 0.290), N_2:2n (0.916, 0.5, 0.252)
R-3*m*-BC_2N	*R*-3*m*	2.547	25.309	C_1:6c (0.333, -0.333, -0.303), C_2:6c (1, -1, -0.282)
				B_1:6c (1, -1, -0.219), N_1:6c (0.667, -0.667, -0.136)
*R*3*m*-BC_2N-2	*R*3*m*	2.540	25.188	C_1:3a (-2, -1, 0.046), C_2:3a (-0.667, -0.333, -0.225)
				C_3:3a (-1.333, -0.667, 0.026), C_4:3a (-1.333, -0.667, -0.205)
				B_1:3a (-2, -1, -0.057), B_2:3a (-1.333, -0.667, -0.140)
				N_1:3a (-2, -1, -0.118), N_2:3a (-1.333, -0.667, -0.035)

Table S2. Calculated elastic constants C_{ij} (GPa) of five BC_2N at ambient pressure.

Properties	*R*3*m*-BC_2N	*P*2/*m*-BC_2N	*P*2/*m*-BC_2N-2	*R*-3*m*-BC_2N	*R*3*m*-BC_2N-2
C_{11}	1007.25	929.93	995.97	1003.41	1002.76
C_{22}	1008.11	1035.37	1030.75	985.4	1006.37
C_{33}	1088.47	954.96	1038.42	981.23	1066.46
C_{44}	400.27	382.53	376.11	395.65	396.27
C_{55}	399.21	327.91	360.52	378.28	396.86
C_{66}	456.01	418.39	429.65	438.57	455.99
C_{12}	106.38	96.60	104.91	84.83	106.73
C_{13}	55.26	77.14	49.76	53.74	61.05
C_{14}	8.29	--	--	4.50	6.64
C_{15}	31.09	25.28	29.75	-27.23	35.09
C_{23}	55.96	40.64	33.80	72.47	59.93
C_{25}	-10.75	3.77	7.90	40.57	-15.60
C_{35}	-22.73	19.66	20.72	-11.76	-21.49
C_{46}	-10.26	12.36	12.22	43.34	-14.68

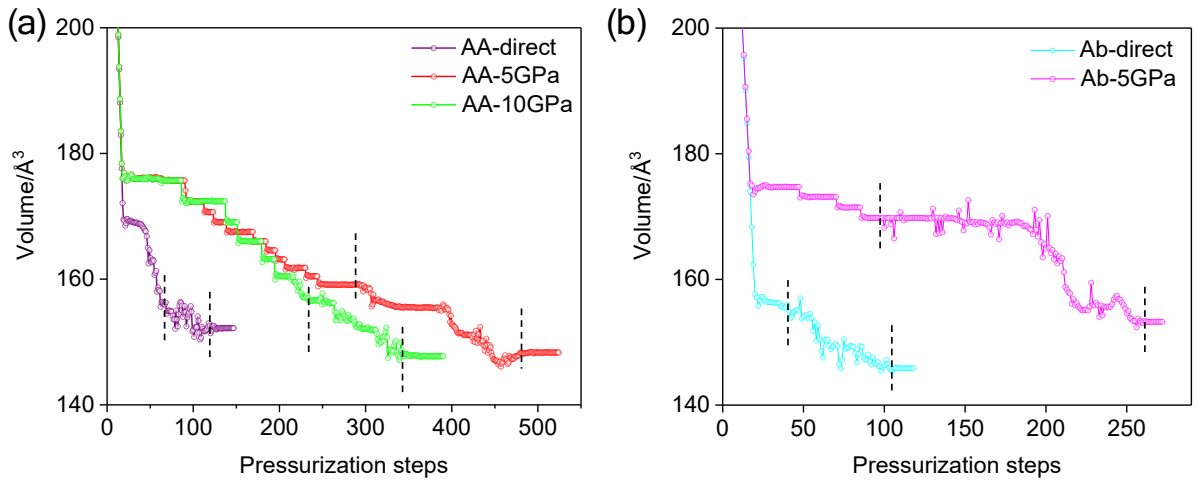

Figure S1. (a) is the volume change curve of AA superlattice under different pressurization methods. (b) is the volume change curve of Ab superlattice under different pressurization methods.

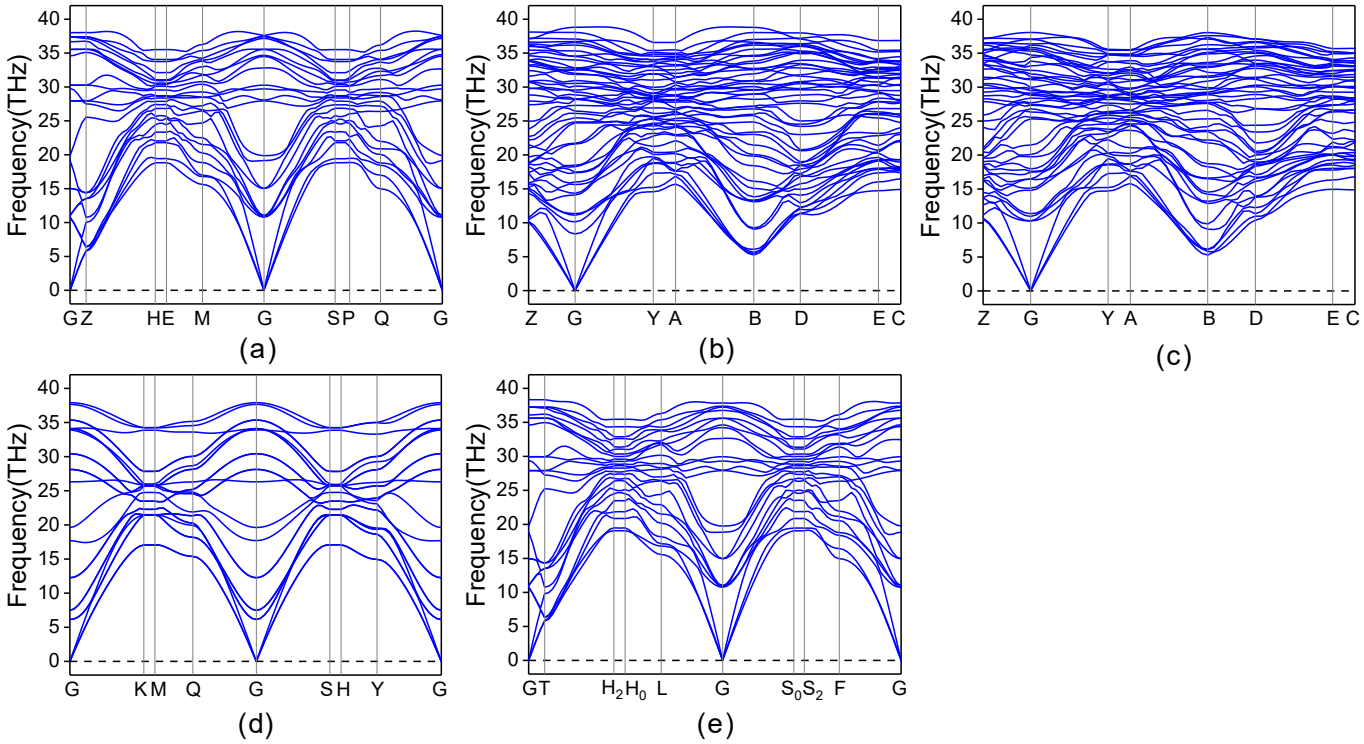

Figure S2. Phonon spectra of five BC_2N at ambient pressure (a) *R*3*m*-BC_2N (b) *P*2/*m*-BC_2N (c) *P*2/*m*-BC_2N-2 (d) *R*-3*m*-BC_2N (e) *R*3*m*-BC_2N-2.