Electronic Supplementary Information

Structural, electronic and mechanical properties of sp^3-hybridized BN phases

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Table SI. Crystalline information of the predicted BN structures in group I.

structure	Space group	Lattice Parameters	Inequivalent sites
bct-BN	$P4_2/mnm$	a=b= 4.86Å,	B1 (0.8259, 0.8259, 0.5)
		c=2.52 Å,	N1 (1.1877, 0.8123, 0.5)
bct_2W_1	$Cmc2_1$	a=2.53 Å,	B1(0.0, 0.3922, -0.1056); B3(0.0, 0.7257, -0.2632);
		b=13.17 Å,	B5(0.0, 0.0558, -0.1073);
		c=4.28 Å,	N1(0.0,0.2734,-0.1301); N2(0.0, 0.3931, -0.7362);
			N5(0.0, 0.0565, -0.7359)
bct_1W_1	$Pbam$	a=8.79 Å,	B1(-0.9117, 0.1716, 0.0); B5(-1.1659, 0.3288, -0.5)
		b=4.24 Å,	N1(-0.9113, 0.7995, 0.0); N5(-1.1661, 0.7001, -0.5)
		c=2.53 Å,	
bct_2W_2	$Pmn2_1$	a=2.53 Å,	B1(0.5, 0.7139, 0.8839); B2(0.5, 0.2083, 0.8822);
		b=8.78 Å,	B3(0.5, 0.5364, 0.2247); B7(0.0, 0.9586, 0.8818)
		c=4.25 Å,	N1(0.5, 0.5358, 0.8567); N3(0.0, 0.9592, 0.2564);
			N4(0.0, 0.2856, 0.7539); N5(0.0, 0.7914, 0.7538)

Table SII. Crystalline information of the predicted BN structures in group II

structure	Space group	Lattice Parameters	Inequivalent sites

M2-BN	*Pnma*	*a*= 4.81Å,	B1（0.8401, 0.25, 0.9079)
		b= 2.56Å,	N1（0.6794, 0.25, 0.6073)
		c=4.25 Å,	
$M2_1W_1$	*Cmc2₁*	*a*=2.56 Å,	B1(0.0, 0.7787, -0.9113); B2(0.0, 0.8850, -0.4084); B5(0.0, 0.5519, -0.2421)
		b=13.13 Å,	N1(0.0, 0.7770, -0.2824); N3(0.0, 0.4474, -0.3744);
		c=4.38 Å,	N5(0.0, 0.1145, -0.2804)
$M2_1bct_1$	*C2/m*	*a*=13.17 Å,	B1(-0.7190, 0.0, 0.1717);B2(-0.6112, 0.0, 0.6678);
		b=2.54 Å,	B5(-0.0582, 0.0, 0.1704);
		c=4.30 Å,	N1(-0.6097, 0.0, 0.3005); N2(-0.2807, 0.0, 0.2080);
		β=90.79°	N5(-0.0594, 0.0, 0.7998)

Table SIII Crystalline information of the predicted BN structures in group III.

structure	Space group	Lattice Parameters	Inequivalent sites
AW-BN	*Pbca*	*a*= 4.39Å,	B1（0.5872, 0.6707, 1.3665)
		b=4.34 Å,	N1（0.4079, 0.6941, 0.6346)
		c=5.05 Å,	
AW_1W_1	$Cmc2_1$	*a*=5.09 Å,	B1(0.2404,-0.3301,0.9820);B5(0.0,-0.4164, 0.4846);
		b=8.74 Å,	B7(0.0, -0.9233, 0.6488);
		c=4.33 Å,	N1(0.2411,-0.6693,0.1131); N5(0.0,-0.0787,0.5118);
			N7(0.0,-0.5832, 0.6122)
AW_1M2_1	$Cmc2_1$	*a*=7.62 Å,	B1(0.3269, 0.3376, 0.4967); B5(0.0, 0.3443,0.6638) N1(0.3271, 0.6578, 0.6311); N5(0.0, 0.3456,0.0213)
		b=4.37 Å,	
		c=4.42 Å,	
AW_1bct_1	*P-3m1*	*a*=*b*=5.09 Å,	B1(0.8279,0.1721,0.8299); B7(0.3333,0.6667,0.6643);
		c=4.39 Å,	N1(0.1720, 0.8280,0.7942);
		γ=120°,	N7(0.3333,0.6667,0.2988);

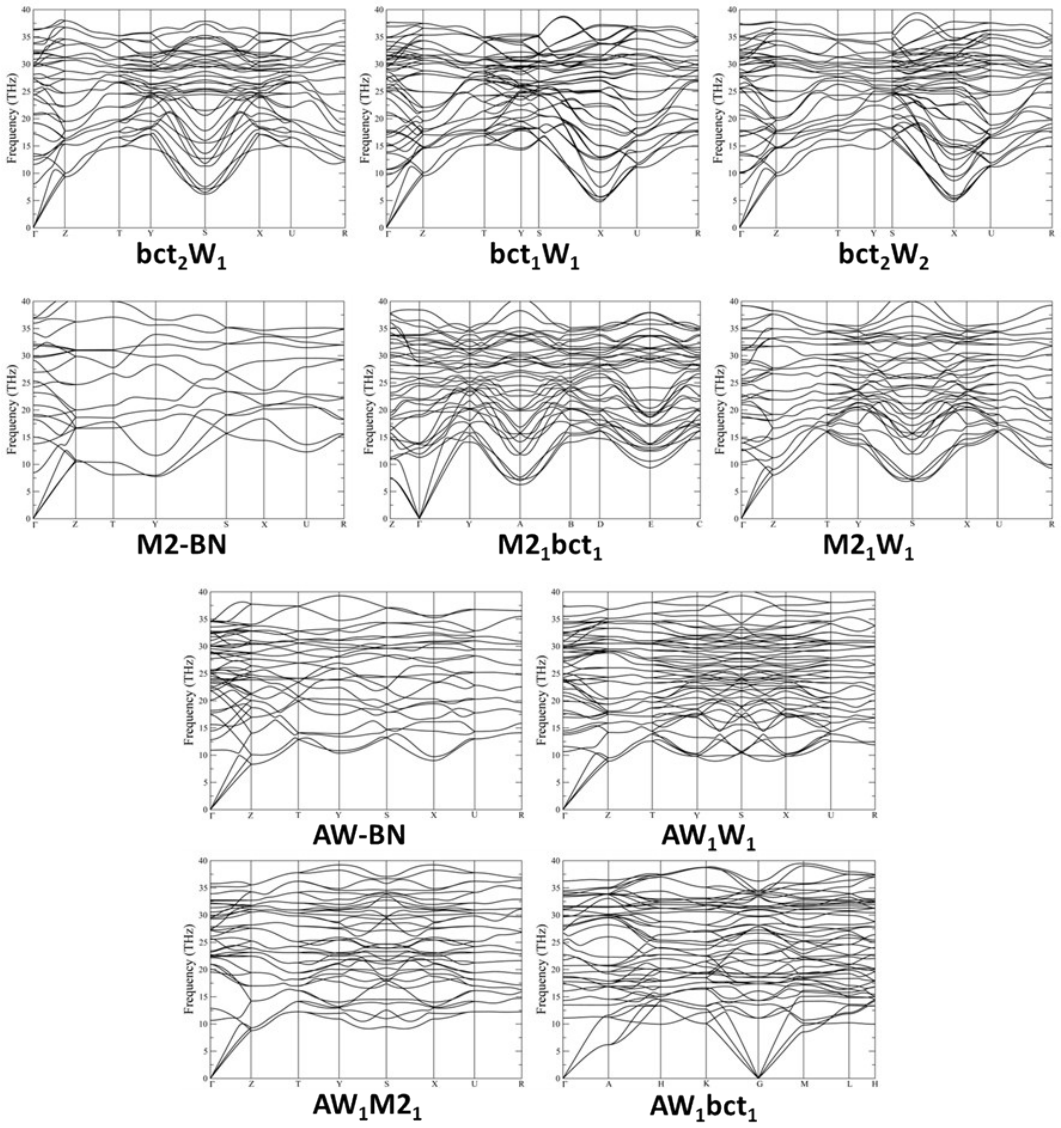

Figure S1 Phonon spectra of the ten new phases of BN under 0 GPa.

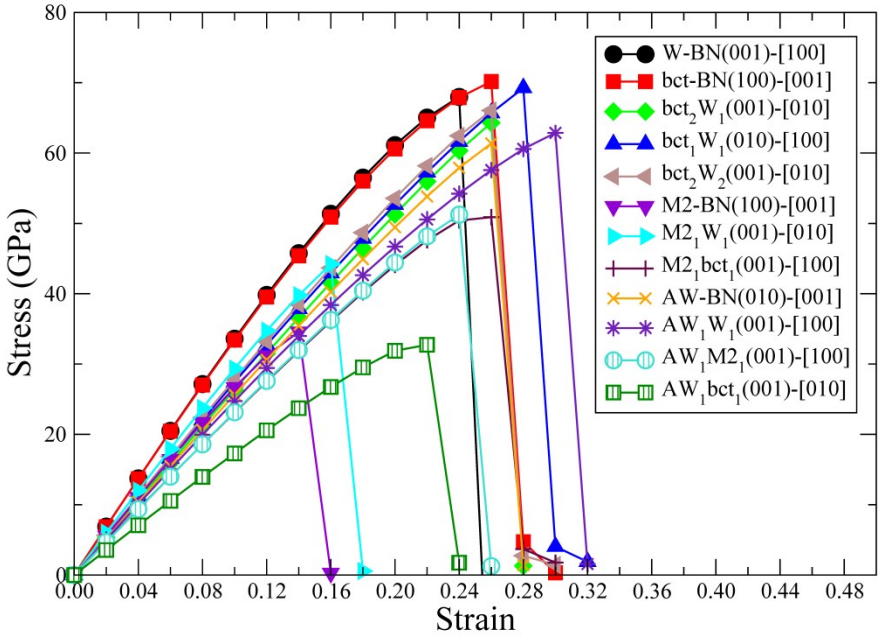

Figure S2 Stress-strain relationships of various BN structures under shear load in the weakest slip planes.

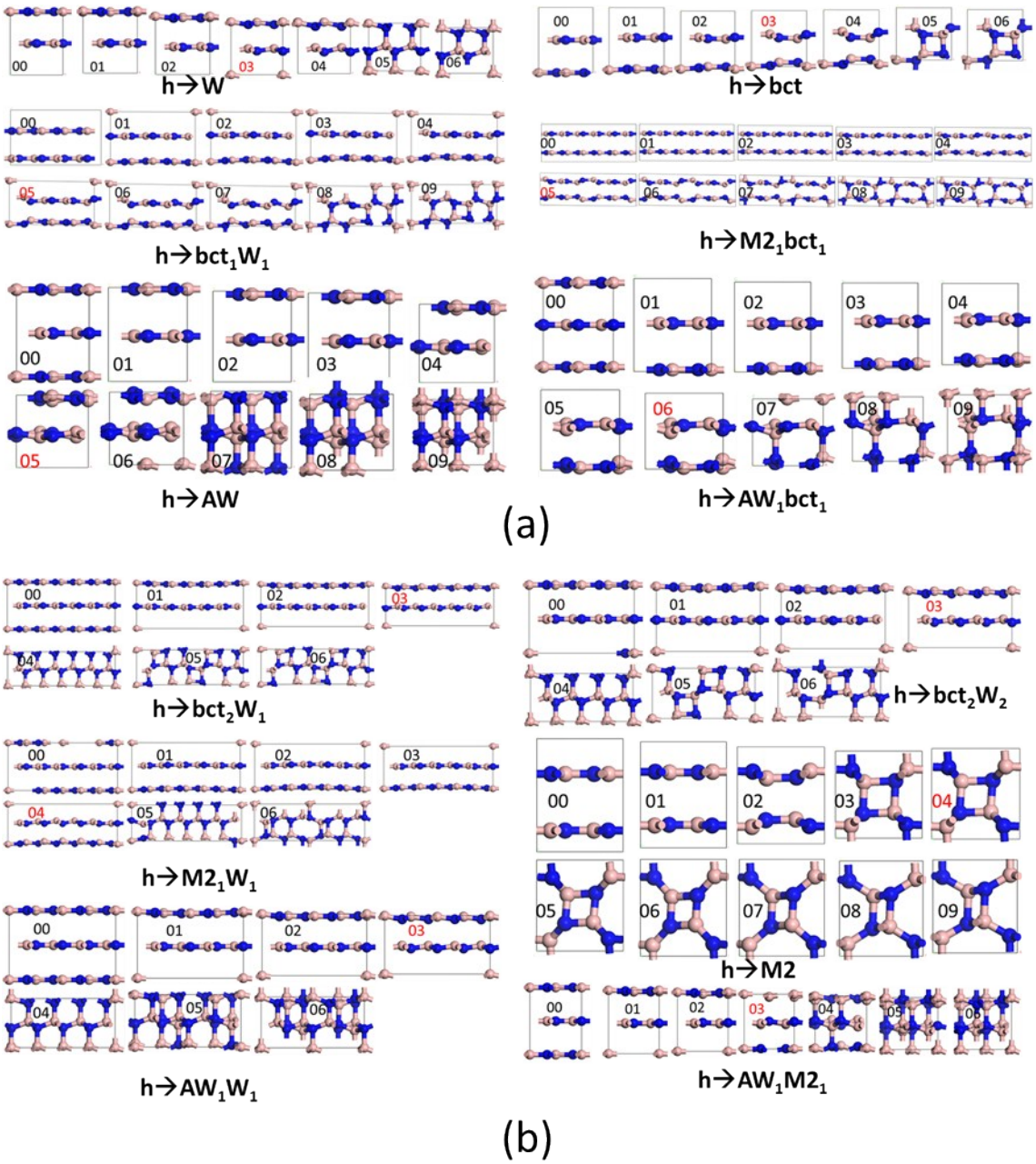

Figure S3 The structures of each image in the transition path from h-BN to different BN structures. The image marked in red color is the transition state of each path. (a) transition without intermediate phases (b) transition with an intermediate phase.