ELECTRONIC SUPPLEMENTARY INFORMATION

Novel three-dimensional boron nitride allotropes from compressed nanotube bundles

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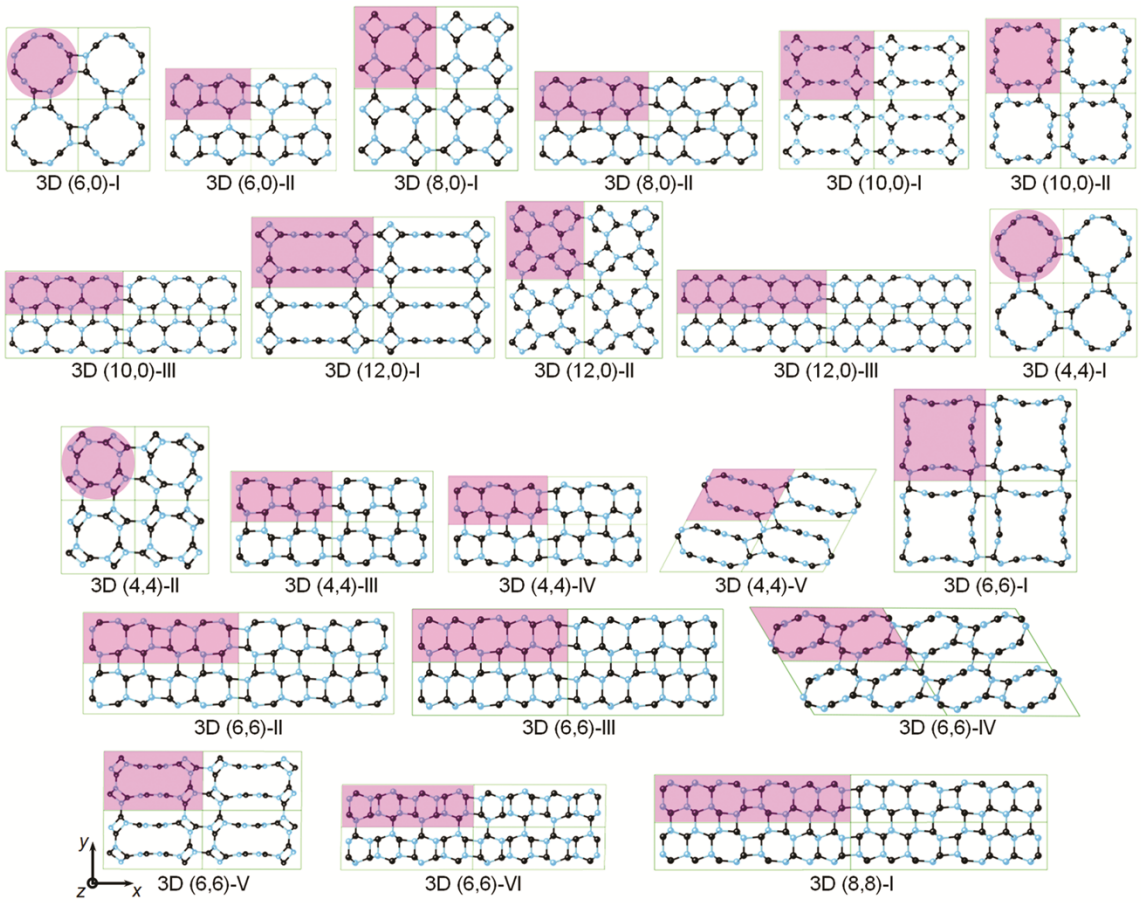

Fig. S1 3D BN allotropes viewed along the axial direction of original BNNTs.

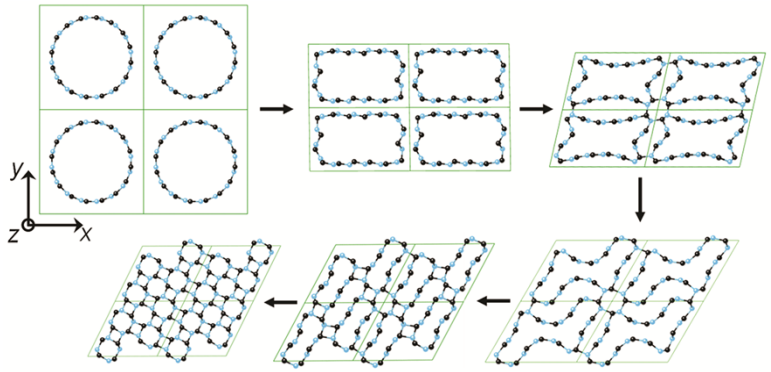

Fig. S2 Structural evolutions of (8,8) BNNT bundles under non-hydrostatic pressure of 45/50/50 GPa.

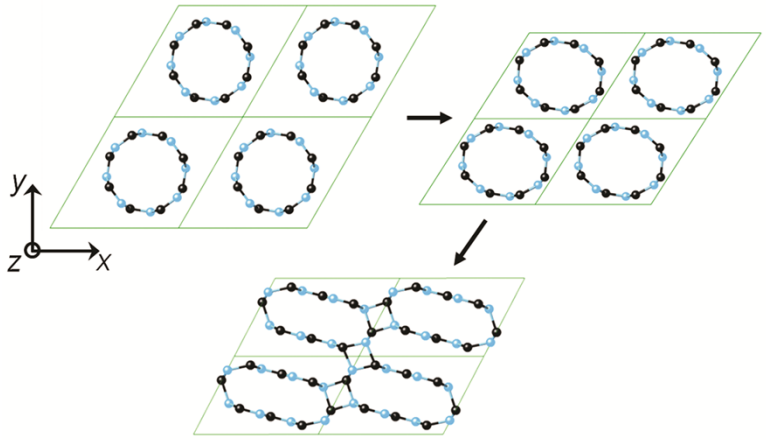

Fig. S3 Structural evolutions of hexagonal arranged (4,4) BNNT bundles under hydrostatic pressure of 30 GPa.

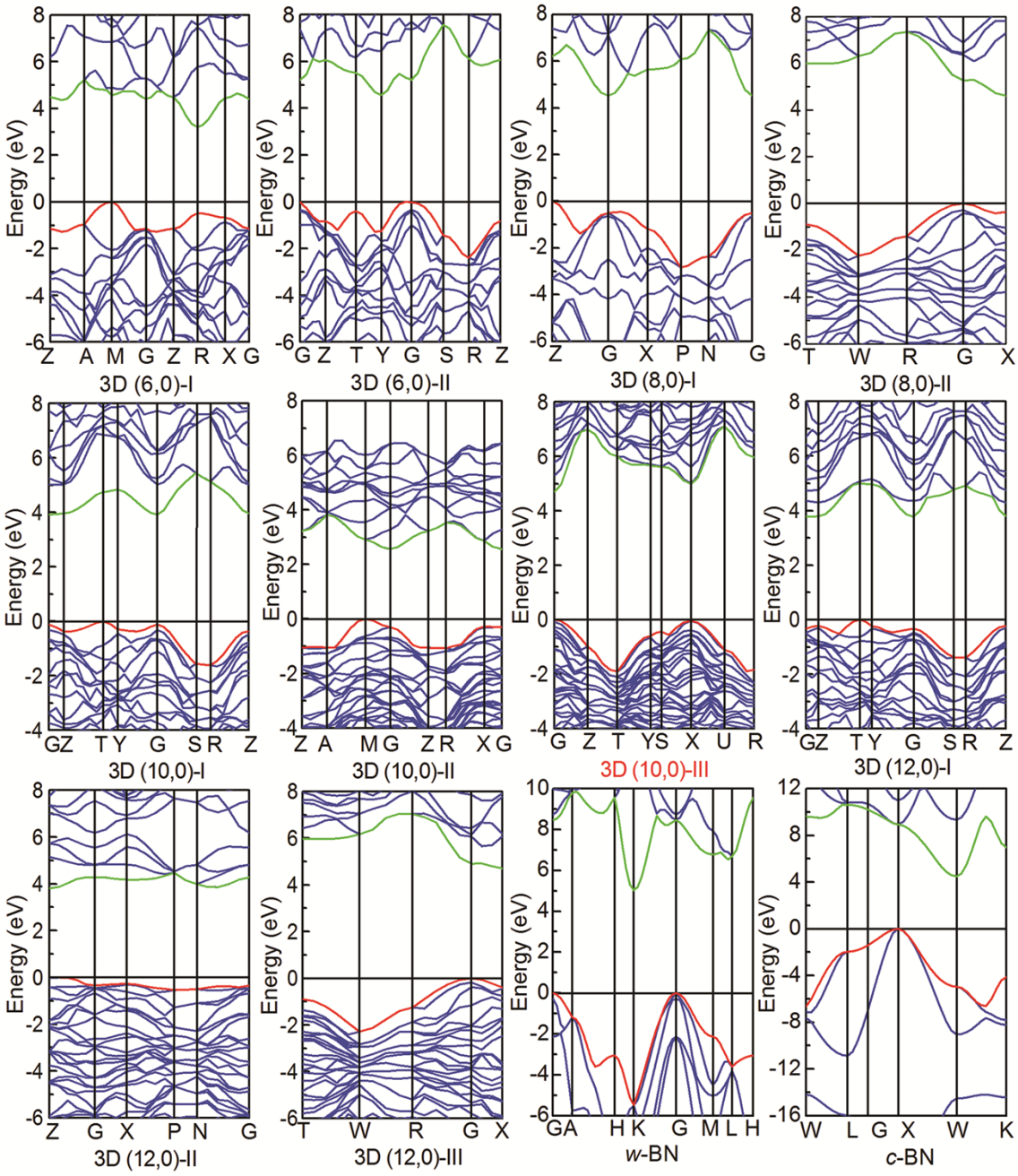

Fig. S4 Band structures of 3D BN allotropes from (n,0) BNNT bundles. The top valence band and bottom conducting band are marked in red and green, respectively. Band structures of wBN and cBN are also shown for comparison. 3D (10,0)-III with a direct bandgap are emphasized with red.

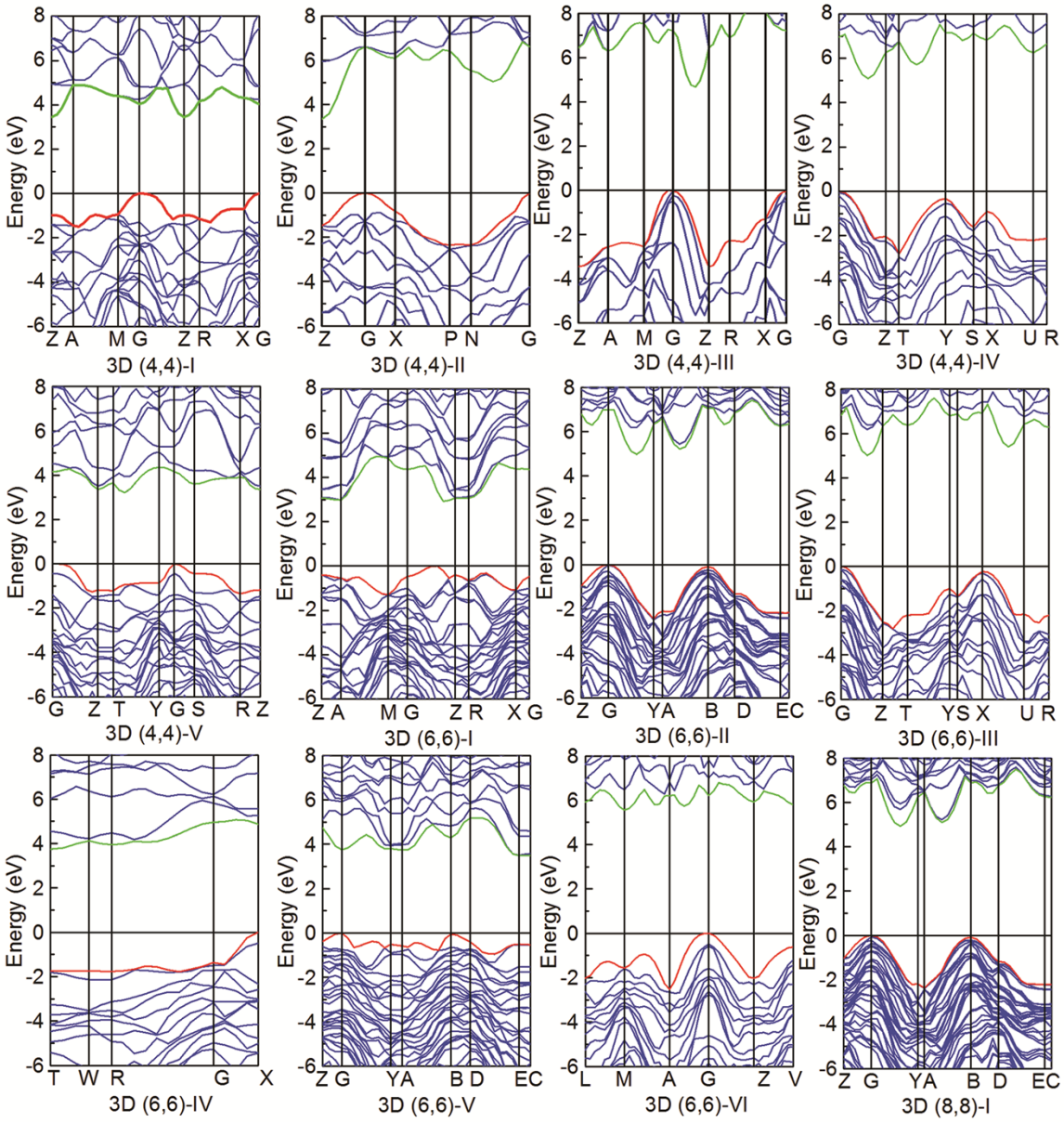

Fig S5 Band structures of 3D BN allotropes from (n,n) BNNT bundles. The top valence band and bottom conducting band are marked in red and green, respectively.

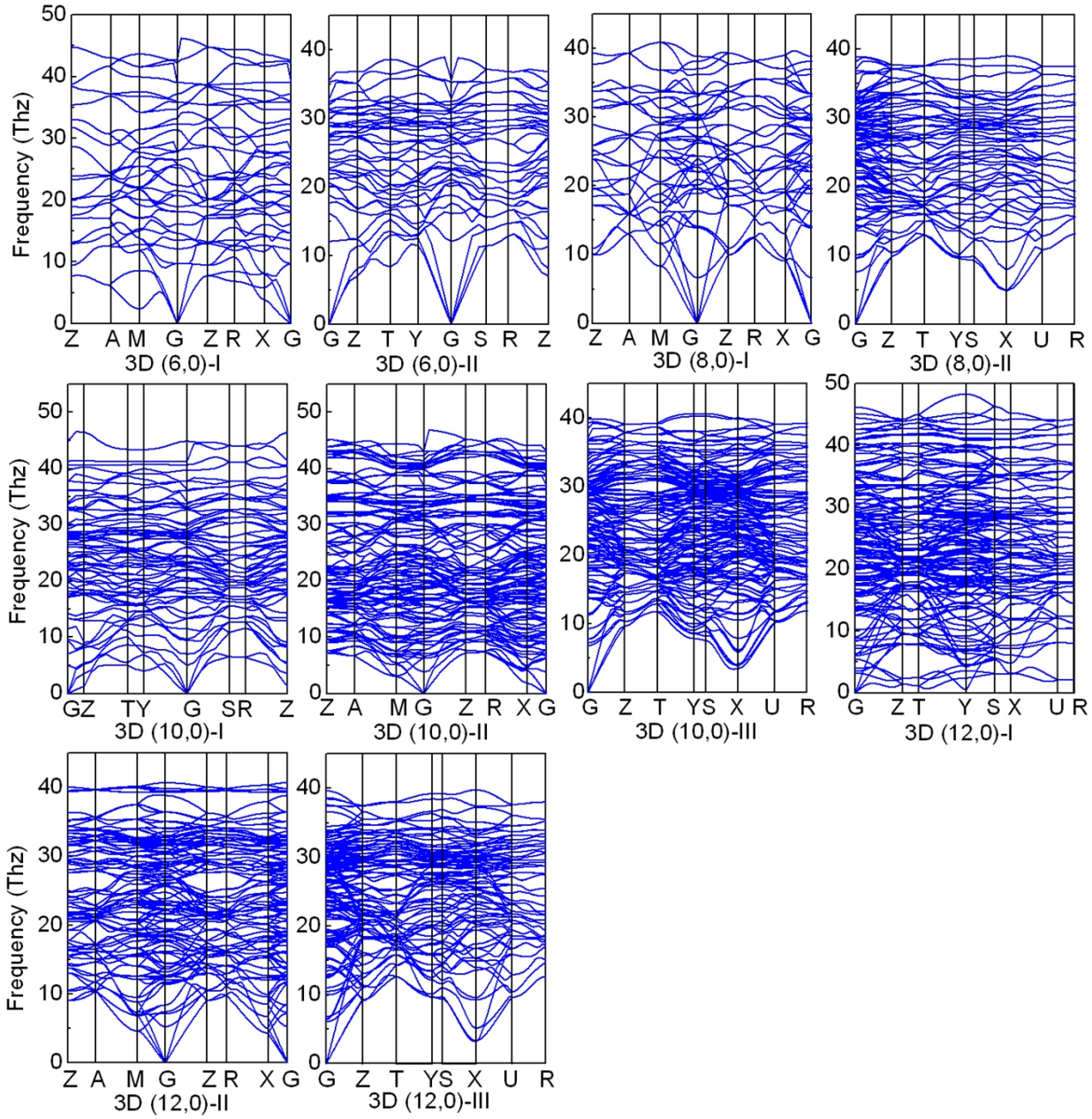

Fig S6 Phonon dispersion curves of 3D BN allotropes from (n,0) BNNT bundles.

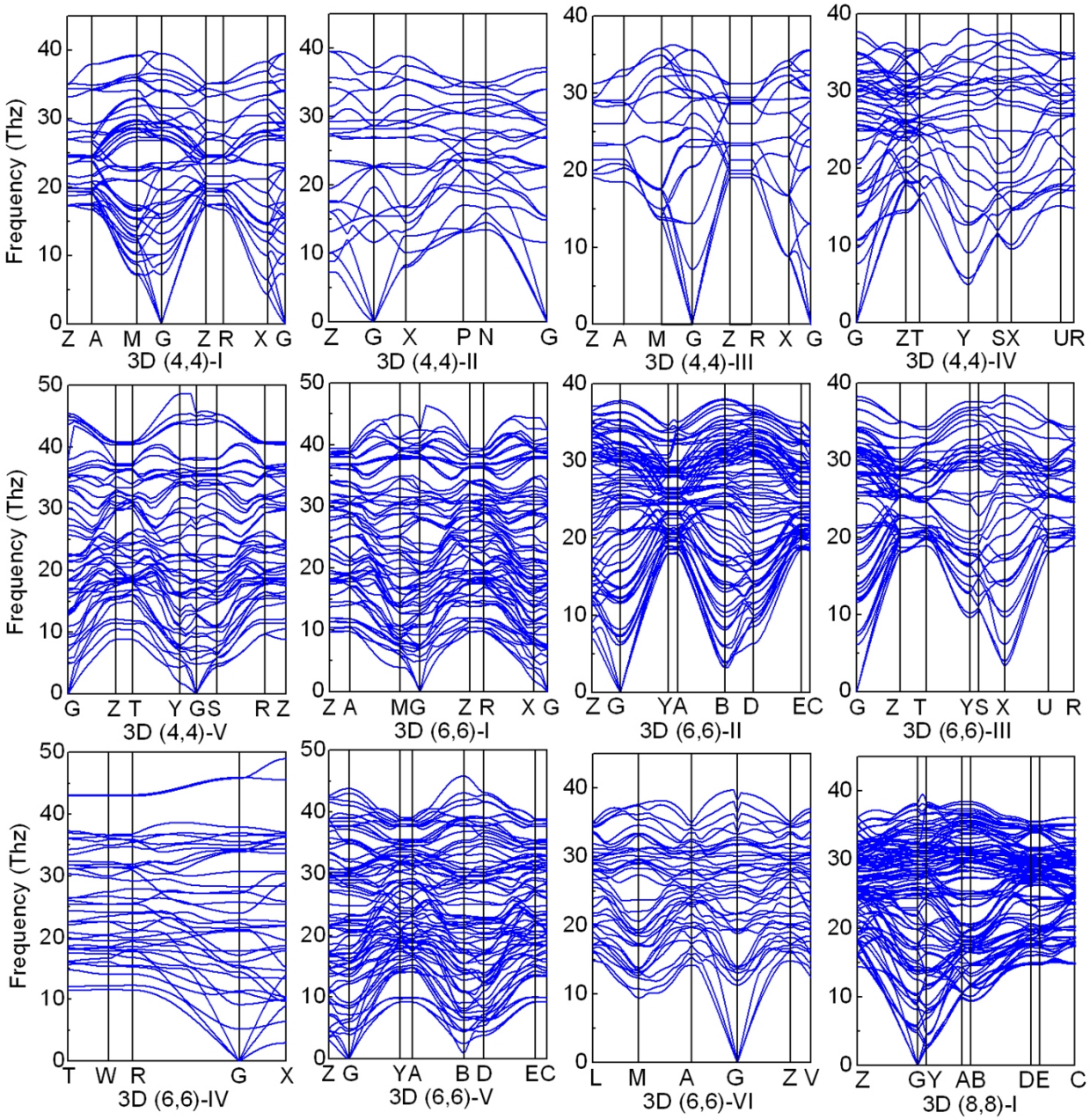

Fig S7 Phonon dispersion curves of 3D BN allotropes from (n,n) BNNT bundles.

Table S1 Space group (S.G.), lattice parameters (Å), and atomic Wyckoff positions of 3D BN allotropes at ambient pressure.

Structure	S.G.	*a*	*b*	*c*	*β*	Atomic positions
3D (6,0)-I	*P42mc* (105)	4.788		4.221		B 4*d* (0, 0.221, 0.697); B 4c (0, 1/2, 0.175); N 4d (0, 0.231, 0.333); N 4*c* (0, 1/2, 0.845);
3D (6,0)-II	*Abm2* (39)	4.592	7.708	4.185		B 8*d* (0.344, 0.0939, 0.697); B 4c (0.847, 1/4, 0.696); N 8d (0.323, 0.095, 0.326); N 4c (5/6, 1/4, 0.326)
3D (8,0)-I	*I4cm* (108)	4.970		4.192		B 8*c* (0.354, 0.854, 0.689) ; N 8*c* (0.343, 0.843, 0.321)
3D (8,0)-II	*Iba2* (45)	4.528	10.257	4.185		B 8*c* (0.342, 0.072, 0.704); B 8*c* (0.158, 0.188, 0.203); N 8*c* (0.324, 0.071, 0.333); N 8*c* (0.167, 0.188, 0.831)
3D (10,0)-I	*Abm2* (39)	9.564	7.013	4.223		B 8*d* (0.817, 0.104, 0.666); B 4*c* (0.923, 1/4, 1/6); B 4*c* (0.438, 1/4, 0.147); B 4*c* (0.294, 1/4, 2/3); N 8*d* (0.817, 0.093, 0.299); N 4*c* (0.931, 1/4, 0.799); N 4*c* (0.434, 1/4, 0.814); N 4*c* (0.301, 1/4, 0.301);
3D (10,0)-II	*P42cm* (101)	9.155		4.235		B 8e (0.864, 0.566, 0.648); B 8e (0.910, 0.709, 0.168); B 4d (0.827, 0.827, 0.642); N 8e (0.856, 0.568, 0.315); N 8e (0.909, 0.708, 0.803); N 4d (0.839, 0.839, 0.315)
3D (10,0)-III	*Pcc2* (27)	4.700	12.791	4.187		B 4*e* (0.844, 0.556, 0.668); B 4*e* (0.654, 0.650, 0.167); B 4e (0.353, 0.943, 0.167); B 4e (0.149, 0.857, 0.668); B 4e (0.846, 0.743, 0.667); N 4*e* (0.825, 0.557, 0.297); N 4*e* (0.664, 0.650, 0.796) N 4*e* (0.333, 0.941, 0.799) N 4*e* (0.168, 0.859, 0.299) N 4*e* (0.828, 0.742, 0.297)
3D (12,0)-I	*Abm2* (39)	12.051	7.003	4.234		B 8*d* (-0.355, 0.396, 0.512); B 4*c* (-0.0528, 3/4, 0.494); B 4*c* (-0.267, 3/4, 0.513); B 4*c* (-0.154, 3/4, 0.991); B 4*c* (-0.439, 1/4, 1.013); N 8*d* (-0.354, 0.407, 0.145); N 4*c* (-0.0512, 3/4, 0.159); N 4*c* (-0.156,3 /4, 0.659); N 4*c* (-0.262, 3/4, 0.146); N 4*c* (-0.446, 1/4, 0.644)

3D (12,0)-II	*I4cm* (108*)*	8.790		4.177		B 16*d* (0.709, 0.582, 0.418); B 8*c* (0.84, 0.66, 0.892); N 16*d*(0.702, 0.583, 0.045); N 8*c* (0.854, 0.646, 0.56)
3D (12,0)-III	*Iba2* (45)	4.469	15.338	4.185		B 8*c* (0.341, 0.547, 0.304); B 8*c* (0.336, 0.709, 0.305); B 8c (0.159, 0.627, 0.804); N 8c (0.323, 0.548, 0.933); N 8*c* (0.167, 0.626, 0.432); N 8*c* (0.332, 0.709, 0.930)
3D (4,4)-I	*P4/mbm* (127)	7.443		2.513		B 4*h* (0.688, 0.188, 1/2); B 4*g* (0.606, 0.894, 0); N 4*h* (0.68, 0.82, 1/2); N 4*g* (0.614, 0.114, 0)
3D (4,4)-II	*I4/m* (87)	6.528		2.553		B 8h (0.292, 0.874, 1/2); N 8h (0.717, 0.895, 1/2)
3D (4,4)-III	*P42/mnm* (136)	4.382		2.527		B 4g (0.826, 1.174, 0); N 4f (0.188, 1.188, 0)
3D (4,4)-IV	*Pbam* (55)	8.811	4.253	2.532		B 4h (0.666, 0.671, 1/2); B 4g (0.412, 0.828, 0); N 4h (0.334, 0.7, 1/2); N4g (0.589, 0.799, 0)
3D (4,4)-V	*Cmmm* (65)	14.910	6.177	2.508		B 4*h* (0.633, 1/2, 1/2); B 4*i* (1/2, 0.678, 0); B 4*h* (0.576, 0, 1/2); B 4*g* (0.723, 0, 0); N 4*g* (0.581, 1/2, 0); N 4*j* (1/2, 0.81, 1/2); N 4*h* (0.773, 0, 1/2); N 4*g* (0.629, 0, 0)
3D (6,6)-I	*P42/m* (84)	8.703		2.497		B 4*j* (0.866, 0.334, 0); B 4*j* (0.421, 0.85, 0); B 4*j* (0.093, 0.169, 0); N 4*j* (0.862, 0.66, 0); N 4*j* (0.0921, 0.836, 0); N 4*j* (0.412, 0.155, 0)
3D (6,6)-II	*P12/m1* (10)	13.205	2.53	4.288	90.02	B 2*m* (0.559, 0, 0.673); B 2*m* (0.892, 0, 0.828); B 2*m* (0.774, 0, 0.171); B 2*n* (0.941, 1/2, 0.33); B 2*n* (0.611, 1/2, 0.173); B 2*n* (0.722, 1/2, 0.673); N 2*m* (0.774, 0, 0.802); N 2*m* (0.893, 0, 0.196); N 2*m* (0.559, 0, 0.301); N 2*n* (0.723, 1/2, 0.302); N 2*n* (0.61, 1/2, 0.801); N 2*n* (0.94, 1/2, 0.695)
3D (6,6)-III	*Pnnm* (58)	4.229	13.196	2.532		B 4*g* (0.829, 0.559, 1/2); B 4*g* (0.829, 0.889, 1/2); B 4*g* (0.829, 0.723, 1.0); N 4*g* (0.703, 0.777, 1/2); N 4*g* (0.701, 0.611, 0); N 4*g* (0.702, 0.941, 0)

3D (6,6)-IV	*Immm* (71)	10.532	2.501	6.046		B 4*i* (1.0, 0, 0.324); B 4*e* (0.688, 0, 0); B 4*f* (0.894, 1/2, 0); N 4*e* (0.819, 0, 0); N 4*j* (1.0, 1/2, 0.19); N 4*f* (0.614, 1/2, 0)
3D (6,6)-V	*P12/m1* (10)	10.853	2.525	6.478	90.33	B 2*m* (0.924, 0, 0.709); B 2*m* (0.819, 0, 0.121); B 2*m* (0.428, 0, 0.258); B 2*n* (0.626, 1/2, 0.249); B 2*n* (0.229, 1/2, 0.216); B 2*n* (0.878, 1/2, 0.37); N 2*m* (0.936, 0, 0.274); N 2*m* (0.562, 0, 0.259); N 2*m* (0.175, 0, 0.11); N 2*n* (0.364, 1/2, 0.253); N 2*n* (0.873, 1/2, 0.601); N 2*n* (0.759, 1/2, 0.215)
3D (6,6)-VI	*C12/m1* (12)	13.216	2.551	4.311	89.17	B 4*i* (0.558, 1/2, 0.167); B 4*i* (0.781, 1/2, 0.826); B 4*i* (0.611, 0, 0.662); N 4*i* (0.78, 1/2, 0.214); N 4*i* (0.559, 1/2, 0.795); N 4*i* (0.609, 0, 0.295)
3D (8,8)-I	*P12/m1* (10)	17.601	2.532	4.261	89.99	B 2*n* (0.67, 1/2, 0.669); B 2*n* (0.917, 1/2, 0.672); B 2*n* (5/6, 1/2, 0.172); B 2*n* (0.581, 1/2, 0.328); B 2*m* (0.545, 0, 0.83); B 2*m* (0.792, 0, 0.672); B 2*m* (0.956, 0, 0.172); B 2m (0.708, 0, 0.171); N 2*n* (0.58, 1/2, 0.696); N 2*n* (5/6, 1/2, 0.797); N 2*n* (0.917, 1/2, 0.3); N 2*n* (0.67, 1/2, 0.3); N 2*m* (0.708, 0, 0.799); N 2*m* (0.956, 0, 0.799); N 2*m* (0.792, 0, 0.297); N 2*m* (0.545, 0, 0.196)

Tabel S2 Elastic constants C_{ij} (GPa) of 3D BN allotropes.

Structure	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{15}	C_{23}	C_{25}
3D(6,0)-I	597.79		812.26	215.79		28.46	29.77	72.85			
3D(6,0)-II	647.63	830.67	1011.04	338.41	264.63	280.89	203.94	38.62		65.30	
3D(8,0)-I	815.04		980.40	293.63		133.52	89.21	55.77			
3D(8,0)-II	701.42	855.63	1024.69	337.94	288.47	363.60	191.99	40.15		62.86	
3D(10,0)-I	817.382	587.37	918.19	207.49	305.92	64.85	65.37	98.22		41.29	
3D(10,0)-II	183.90		708.10	165.32		46.56	94.22	17.28			
3D(10,0)-III	571.49	761.67	997.01	326.95	267.08	316.14	243.74	40.46		65.15	
3D(12,0)-I	825.37	468.22	894.98	162.18	311.34	41.72	49.43	113.53		33.81	
3D(12,0)-II	437.06		887.56	247.42		173.73	194.00	31.08			
3D(12,0)-III	781.65	890.30	1035.98	341.28	302.01	372.22	173.66	42.71		60.39	
3D(4,4)-I	278.18		779.80	186.48		172.50	248.68	85.06			
3D(4,4)-II	630.44		761.55	241.60		93.82	191.66	72.82			
3D(4,4)-III	746.60		986.41	339.97		246.25	171.61	104.15			
3D(4,4)-IV	880.77	895.35	972.65	341.23	383.06	277.98	85.34	129.31		69.42	
3D(4,4)-V	818.92	291.71	947.11	120.27	351.06	32.38	96.78	161.53		39.87	
3D(6,6)-I	476.33		889.40	200.49		46.11	51.89	68.84			
3D(6,6)-II	838.72	977.16	831.34	340.91	266.78	371.55	126.03	110.94		81.04	
3D(6,6)-III	946.15	902.69	968.08	391.47	339.84	295.45	75.73	61.47		130.23	
3D(6,6)-IV	780.48	951.71	402.19	172.88	66.41	345.66	145.56	134.04		58.93	
3D(6,6)-V	717.43	834.48	363.62	150.10	51.72	274.62	110.99	112.85		52.58	
3D(6,6)-VI	888.03	911.96	731.59	258.48	241.94	377.59	132.13	98.56	18.45	72.47	15.42
3D(8,8)-I	883.43	871.52	973.72	384.94	341.28	280.27	97.41	72.61		127.06	

Table S3 Calculated tensile strength, σ_a, of 3D BN polymorphs in the axial direction of the parent BNNTs. Bond length d_{AB}, EBVE number $n_{AB,}$ and the density of broken bonds across (*hkl*) plane S_{hkl}.

Structure	d_{AB} (Å)	n_A	n_B	n_{AB}	S_{hkl} ($\times 10^{20}$ m^{-2})	σ_a (GPa)	σ_{total} (GPa)
3D(6,0)-I	1.392	1	1	0.707	0.044	25.46	60.7
	1.537	0.75	1.25	0.643	0.087	35.26	
3D(6,0)-II	1.555	0.75	1.25	0.643	0.170	67.54	67.5
3D(8,0)-I	1.546	0.75	1.25	0.643	0.162	64.93	64.9
3D(8,0)-II	1.556	0.75	1.25	0.643	0.172	68.46	68.5
3D(10,0)-I	1.556	0.75	1.25	0.643	0.030	11.86	64.9
	1.548	0.75	1.25	0.643	0.089	35.82	
	1.405	1	1	0.707	0.030	17.19	
3D(10,0)-II	1.546	0.75	1.25	0.643	0.048	19.14	60.5
	1.393	1	1	0.707	0.024	13.92	
	1.408	1	1	0.707	0.048	27.44	
3D(10,0)-III	1.555	0.75	1.25	0.643	0.100	39.72	66.4
	1.545	0.75	1.25	0.643	0.067	26.71	
3D(12,0)-I	1.554	0.75	1.25	0.643	0.071	28.32	64.8
	1.562	0.75	1.25	0.643	0.024	9.38	
	1.406	1	1	0.707	0.024	13.65	
	1.421	1	1	0.707	0.024	13.46	
3D(12,0)-II	1.558	0.75	1.25	0.643	0.104	41.10	71.2
	1.397	1	1	0.707	0.052	30.07	
3D(12,0)-III	1.557	0.75	1.25	0.643	0.117	46.37	69.3
	1.568	0.75	1.25	0.643	0.058	22.97	
3D(4,4)-I	1.480	0.75	1	0.600	0.072	26.15	77.3
	1.478	1	1.25	0.781	0.072	51.16	
3D(4,4)-II	1.559	0.75	1.25	0.643	0.188	74.46	74.5
3D(4,4)-III	1.525	0.75	1.25	0.643	0.208	85.07	85.1
3D(4,4)-IV	1.537	0.75	1.25	0.643	0.214	86.31	86.3
3D(4,4)-V	1.477	1	1.25	0.781	0.043	30.80	88.5
	1.460	1	1	0.707	0.043	23.80	
	1.484	0.75	1	0.600	0.043	15.67	
	1.495	0.75	1.25	0.643	0.043	18.20	
3D(6,6)-I	1.545	0.75	1.25	0.643	0.053	21.20	80.4
	1.435	1	1	0.707	0.106	59.22	
3D(6,6)-II	1.522	0.75	1.25	0.643	0.071	28.92	86.0
	1.538	0.75	1.25	0.643	0.141	57.04	

3D(6,6)-III	1.537	0.75	1.25	0.643	0.143	57.96	86.6
	1.551	0.75	1.25	0.643	0.072	28.63	
3D(6,6)-IV	1.488	1	1.25	0.781	0.063	44.11	92.7
	1.492	0.75	1	0.600	0.063	22.51	
	1.505	0.75	1.25	0.643	0.063	26.10	
3D(6,6)-V	1.545	0.75	1.25	0.643	0.114	45.67	77.3
	1.444	1	1	0.707	0.057	31.67	
3D(6,6)-VI	1.552	0.75	1.25	0.643	0.140	55.98	84.8
	1.518	0.75	1.25	0.643	0.070	28.82	
3D(8,8)-I	1.552	0.75	1.25	0.643	0.053	21.30	86.3
	1.538	0.75	1.25	0.643	0.107	43.12	
	1.522	0.75	1.25	0.643	0.053	21.86	

Table S4 Calculated tensile strength, σ_r, of 3D BN polymorphs in the radial direction of the parent BNNTs. Bond length d_{AB}, EBVE number $n_{AB,}$ and the density of broken bonds across (*hkl*) plane S_{hkl}.

Structure	d_{AB} (Å)	n_A	n_B	n_{AB}	S_{hkl} ($\times 10^{20}$ m^{-2})	σ_r (GPa)
3D(6,0)-I	1.637	0.75	1.25	0.643	0.140	52.0
3D(6,0)-II	1.562	0.75	1.25	0.643	0.124	49.1
3D(8,0)-I	1.496	0.75	1.25	0.643	0.136	56.8
3D(8,0)-II	1.585	0.75	1.25	0.643	0.186	72.3
3D(10,0)-I	1.492	0.75	1.25	0.643	0.099	41.6
3D(10,0)-II	1.761	0.75	1.25	0.643	0.103	34.8
3D(10,0)-III	1.583	0.75	1.25	0.643	0.149	58.1
3D(12,0)-I	1.492	0.75	1.25	0.643	0.078	32.9
3D(12,0)-II	1.551	0.75	1.25	0.643	0.109	43.5
3D(12,0)-III	1.575	0.75	1.25	0.643	0.187	73.1
3D(4,4)-I	1.637	0.75	1.25	0.643	0.107	39.8
3D(4,4)-II	1.508	0.75	1.25	0.643	0.120	49.7
3D(4,4)-III	1.587	0.75	1.25	0.643	0.181	70.0
3D(4,4)-IV	1.581	0.75	1.25	0.643	0.179	69.9
3D(4,4)-V	1.633	0.75	1.25	0.643	0.107	39.9
3D(6,6)-I	1.614	0.75	1.25	0.643	0.092	34.9
3D(6,6)-II	1.584	0.75	1.25	0.643	0.180	69.7
3D(6,6)-III	1.577	0.75	1.25	0.643	0.180	70.2
3D(6,6)-IV	1.497	0.75	1.25	0.643	0.073	57.3
3D(6,6)-V	1.618	0.75	1.25	0.643	0.150	30.5
3D(6,6)-VI	1.585	0.75	1.25	0.643	0.119	46.0
3D(8,8)-I	1.580	0.75	1.25	0.643	0.180	70.0

Tabel S5 Calculation parameters for Vickers hardness of 3D BN allotropes. V, d, n, N_e, and f_i are the unit cell volume, bond length, bond multiplicity in unit cell, valence electron density, and bond ionicity, respectively. $H_{V,\ calc}$ is Vickers hardness from specific bond. H_V is averaged Vickers hardness. Data for partially sp^3-hybridized structures are marked with red color.

Structure	d (Å)	n	V (Å^3)	N_e (Å^{-3})	f_i	$H_{V,\ calc}$ (GPa)	H_V (GPa)
3D (6,0)-I	1.393	2	96.79	0.814	0.256	98.23	56.1
	1.450	4		0.609		73.22	
	1.474	4		0.623		71.33	
	1.538	4		0.454		51.93	
3D (6,0)-II	1.555	12	148.12	0.657	0.256	64.65	63.4
	1.564	36		0.645		62.99	
3D (8,0)- I	1.546	8	103.43	0.621	0.256	63.17	60.6
	1.565	24		0.598		59.79	
3D (8,0)-II	1.561	48	194.38	0.657	0.256	64.07	64.3
	1.557	16		0.662		64.81	
3D (10,0)-I	1.410	8	282.35	0.790	0.256	93.42	58.8
	1.463	4		0.707		79.13	
	1.473	4		0.744		80.48	
	1.551	16		0.528		56.24	
	1.578	44		0.501		52.04	
3D (10,0)-II	1.393	4	354.91	0.662	0.256	85.61	55.1
	1.412	16		0.636		80.54	
	1.500	16		0.448		54.79	
	1.504	16		0.477		56.78	
	1.545	8		0.364		44.34	
	1.761	8		0.246		24.61	
3D (10,0)-III	1.551	16	251.76	0.651	0.256	64.71	62.4
	1.566	44		0.633		61.96	
	1.573	20		0.624		60.73	
3D (12,0)-I	1.422	20	357.35	0.799	0.256	92.11	58.1
	1.461	4		0.621		72.82	
	1.477	4		0.646		72.72	
	1.556	16		0.457		50.70	
	1.578	44		0.438		47.60	
3D (12,0)-II	1.397	8	322.80	0.976	0.256	110.03	62.2
	1.514	16		0.695		71.75	
	1.527	16		0.630		65.83	
	1.558	16		0.528		55.60	
	1.584	32		0.502		51.61	
3D (12,0)-III	1.559	72	286.86	0.670	0.256	65.10	65.0
	1.561	24		0.667		64.72	
3D (4,4)-I	1.387	4	139.20	0.700	0.256	89.80	55.3
	1.478	8		0.488		60.24	
	1.480	8		0.522		62.80	
	1.637	8		0.319		35.17	
3D (4,4)-II	1.552	16	108.80	0.592	0.256	60.64	60.0
	1.559	16		0.584		59.42	

3D (4,4)-III	1.525 1.587	8 8	48.48	0.702 0.623	0.256	70.96 59.31	64.9
3D (4,4)-IV	1.537 1.576	16 16	94.76	0.702 0.651	0.256	69.57 62.15	65.8
3D (4,4)-V	1.396 1.460 1.477 1.484 1.495 1.633	8 8 8 8 8 16	231.00	0.880 0.804 0.588 0.622 0.504 0.386	0.256	98.57 80.56 68.28 70.11 59.78 40.18	62.4
3D (6,6)-I	1.436 1.451 1.526 1.536 1.545 1.614	16 4 4 4 8 4	189.13	0.667 0.528 0.454 0.478 0.388 0.341	0.256	69.61 66.43 52.95 53.93 46.30 38.04	57.0
3D (6,6)-II	1.533 1.580	24 24	143.25	0.703 0.642	0.256	70.13 61.21	65.5
3D (6,6)-III	1.542 1.571	24 24	141.13	0.709 0.670	0.256	69.47 63.88	66.6
3D (6,6)-IV	1.377 1.488 1.492 1.505 1.618	4 8 8 8 16	164.07	0.992 0.659 0.702 0.566 0.456	0.256	115.37 72.37 74.99 63.57 45.90	62.9
3D (6,6)-V	1.444 1.454 1.463 1.482 1.545 1.568	8 2 2 2 16 14	177.53	0.780 0.763 0.633 0.654 0.477 0.457	0.256	87.34 84.46 73.46 72.69 53.13 49.71	59.9
3D (6,6)-VI	1.541 1.583	24 24	145.53	0.683 0.630	0.256	67.86 60.12	63.9
3D (8,8)-I	1.537 1.576	32 32	189.58	0.707 0.656	0.256	69.91 62.45	66.1
c-BN	1.551	16	45.91	0.697	0.256	67.75	67.8
w-BN	1.556	8	23.2	0.689	0.256	66.66	66.7

Table S6 Coordinates of the high symmetry points in reciprocal space for calculated band structures of 3D BNNTs polymorphs.

Structure	Coordinates
3D (6,0)-I	Z (0, 0, 0.5); A (0.5, 0.5, 0.5);M (0.5, 0.5, 0); G (0, 0, 0); Z (0, 0, 0.5); R (0, 0.5, 0.5); X (0, 0.5, 0); G (0, 0, 0)
3D (6,0)-II	G (0, 0, 0); Z (0, 0, 0.5); T (-0.5, 0.5, 0.5); Y (-0.5, 0.5, 0); G (0, 0, 0); S (0, 0.5, 0); R (0, 0.5, 0.5); Z (0, 0, 0.5)
3D (8,0)-I	Z (-0.5, 0.5, 0.5); G (0, 0, 0); X (0, 0, 0.5); P (0.25, 0.25, 0.25); N (0, 0.5, 0); G (0, 0, 0)
3D (8,0)-II	T (0.5, -0.5, 0); W (0.75, -0.25, -0.25); R (0.5, 0, 0); G (0, 0, 0); X (0.5, -0.5, 0.5)
3D (10,0)-I	G (0, 0, 0); Z (0, 0, 0.5); T (-0.5, 0.5, 0.5); Y (-0.5, 0.5, 0);G (0, 0, 0); S (0, 0.5, 0); R (0, 0.5, 0.5); Z (0, 0, 0.5)
3D (10,0)-II	Z (0, 0, 0.5); A (0.5, 0.5, 0.5); M (0.5, 0.5, 0); G (0, 0, 0);Z (0, 0, 0.5); R (0, 0.5, 0.5); X (0, 0.5, 0); G (0, 0, 0)
3D (10,0)-III	G (0, 0, 0);Z (0, 0, 0.5);T (-0.5, 0, 0.5); Y (-0.5, 0, 0); S (-0.5, 0.5, 0); X (0, 0.5, 0); U (0, 0.5, 0.5); R (-0.5, 0.5, 0.5)
3D (12,0)-I	G (0, 0, 0.); Z (0, 0, 0.5); T (-0.5, 0.5, 0.5); Y (-0.5, 0.5, 0); G (0, 0, 0); S (0, 0.5, 0); R (0, 0.5, 0.5); Z (0, 0, 0.5)
3D (12,0)-II	Z (-0.5, 0.5, 0.5); G (0, 0, 0); X (0, 0, 0.5); P (0.25, 0.25, 0.25);N (0, 0.5, 0); G (0, 0, 0)
3D (12,0)-III	T (0.5, -0.5, 0.0); W (0.75, -0.25, -0.25); R (0.5, 0.0, 0.0); G (0.0, 0.0, 0.0); X (0.5, -0.5, 0.5)
3D (4,4)-I	Z (0, 0, 0.5); A (0.5, 0.5, 0.5); M (0.5, 0.5, 0); G (0, 0, 0);Z (0, 0, 0.5); R (0, 0.5, 0.5); X (0, 0.5, 0); G (0, 0, 0)
3D (4,4)-II	Z (-0.5, 0.5, 0.5); G (0, 0, 0); X (0, 0, 0.5); P (0.25, 0.25, 0.25);N (0, 0.5, 0); G (0, 0, 0)
3D (4,4)-III	Z (0, 0, 0.5); A (0.5, 0.5, 0.5); M (0.5, 0.5, 0); G (0, 0, 0); Z (0, 0, 0.5); R (0, 0.5, 0.5); X (0, 0.5, 0); G (0, 0, 0)
3D (4,4)-IV	G (0, 0, 0); Z (0, 0, 0.5); T (-0.5, 0, 0.5); Y (-0.5, 0, 0); S (-0.5, 0.5, 0); X (0, 0.5, 0); U (0, 0.5, 0.5); R (-0.5, 0.5, 0.5)
3D (4,4)-V	G (0, 0, 0); Z (0, 0, 0.5); T (-0.5, 0.5, 0.5); Y (-0.5, 0.5, 0); G (0, 0, 0); S (0, 0.5, 0); R (0, 0.5, 0.5); Z (0, 0, 0.5)
3D (6,6)-I	Z (0, 0, 0.5); A (0.5, 0.5, 0.5); M (0.5, 0.5, 0); G (0, 0, 0); Z (0, 0, 0.5); R (0, 0.5, 0.5); X (0, 0.5, 0); G (0, 0, 0)
3D (6,6)-II	Z (0, 0, 0.5); G (0, 0, 0); Y (0, 0.5, 0); A (-0.5, 0.5, 0); B (-0.5, 0, 0); D (-0.5, 0, 0.5); E (-0.5, 0.5, 0.5); C (0, 0.5, 0.5)
3D (6,6)-III	G (0, 0, 0); Z (0, 0, 0.5); T (-0.5, 0, 0.5); Y (-0.5, 0, 0); S (-0.5, 0.5, 0); X (0, 0.5, 0); U (0, 0.5, 0.5); R (-0.5, 0.5, 0.5)

3D (6,6)-IV	T (0.5, -0.5, 0); W (0.75, -0.25, -0.25); R (0.5, 0, 0); G (0, 0, 0); X (0.5, -0.5, -0.5)
3D (6,6)-V	Z (0, 0, 0.5); G (0, 0, 0); Y (0, 0.5, 0); A (-0.5, 0.5, 0); B (-0.5, 0, 0); D (-0.5, 0, 0.5); E (-0.5, 0.5, 0.5); C (0, 0.5, 0.5)
3D (6,6)-VI	L (-0.5, 0, -0.5); M (-0.5, -0.5, -0.5); A (-0.5, 0, 0); G (0, 0, 0); Z (0, -0.5, -0.5); V (0, 0, -0.5)
3D (8,8)-I	Z (0, 0, 0.5); G (0, 0, 0); Y (0, 0.5, 0); A (0.5, 0.5, 0); B (0.5, 0, 0); D (0.5, 0, 0.5); E (0.5, 0.5, 0.5); C (0, 0.5, 0.5)