Supplementary information

Novel superhard semiconducting structures of $C_8B_2N_2$ predicted using the first-principles approach

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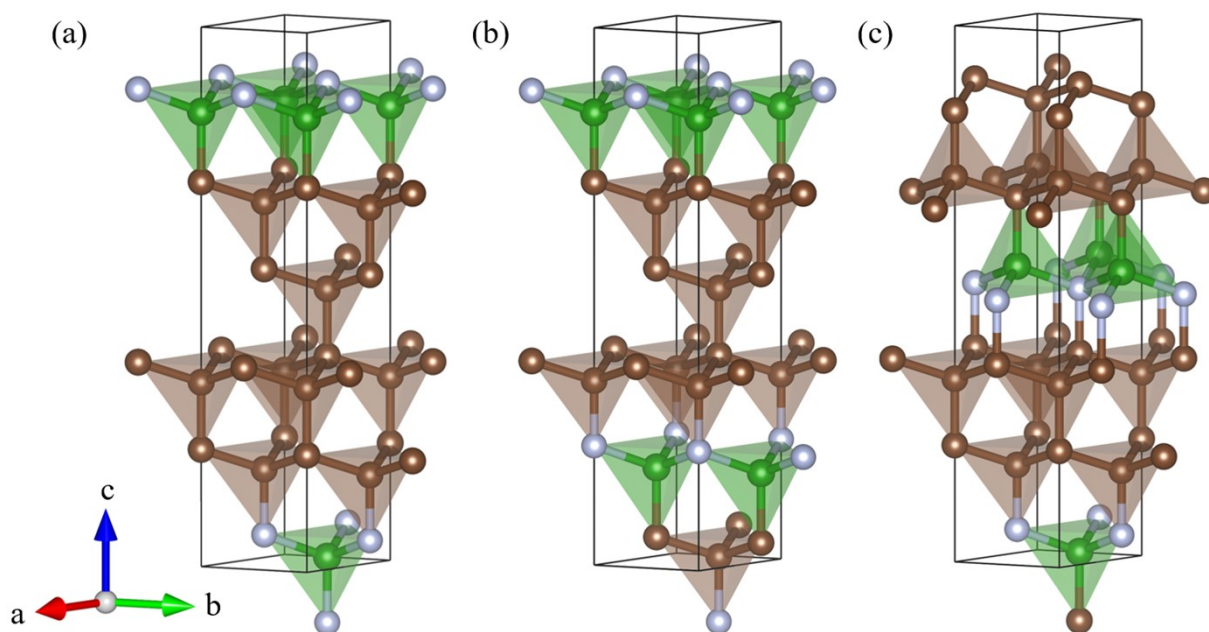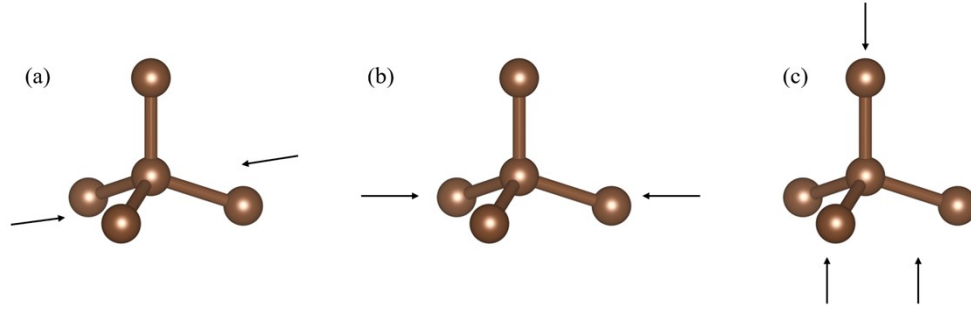
Fig. S1 Polyhedral view of the (a) a-$C_8B_2N_2$, (b) b-$C_8B_2N_2$ and (c) c-$C_8B_2N_2$

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Fig. S2 Schematic diagram of a C5 tetrahedra under compression along the (a) *a*-, (b) *b*- and (c) *c*-axes, respectively

Table S1 The optimized lattice constants (Å) and atomic coordinates of the BCN and *x*-$C_8B_2N_2$ (*x* = *a*, *b*, *c*)

	Space group	Lattice constants		Atomic coordinates
		a	*c*	
BCN	*P*3*m*1	2.546	6.293	C1 1*b* (0.333, 0.667, 0.015)
		2.550	6.301	C2 1*c* (0.667, 0.333, 0.093)
				B1 1*c* (0.667, 0.333, 0.353)
				B2 1*a* (0, 0, 0.685)
				N1 1*b* (0.333, 0.667, 0.770)
				N2 1*a* (0, 0, 0.440)
a-$C_8B_2N_2$	*P*3*m*1	2.536	12.456	C1 1*c* (0.667, 0.333, 0.176)
				C2 1*c* (0.667, 0.333, 0.672)
				C3 1*c* (0.667, 0.333, 0.548)
				C4 1*a* (0, 0, 0.342)
				C5 1*a* (0, 0, 0.217)
				C6 1*a* (0, 0, 0.713)
				C7 1*b* (0.333, 0.667, 0.507)
				C8 1*b* (0.333, 0.667, 0.383)
				B1 1*a* (0, 0, 0.843)
				B2 1*b* (0.333, 0.667, 0.010)
				N1 1*c* (0.667, 0.333, 0.055)
				N2 1*b* (0.333, 0.667, 0.889)
b-$C_8B_2N_2$	*P*3*m*1	2.534	12.511	C1 1*c* (0.667, 0.333, 0.048)
				C2 1*c* (0.667, 0.333, 0.672)
				C3 1*c* (0.667, 0.333, 0.549)
				C4 1*a* (0, 0, 0.343)
				C5 1*a* (0, 0, 0.713)
				C6 1*b* (0.333, 0.667, 0.008)
				C7 1*b* (0.333, 0.667, 0.384)
				C8 1*b* (0.333, 0.667, 0.508)
				B1 1*c* (0.667, 0.333, 0.178)
				B2 1*a* (0, 0, 0.843)
				N1 1*a* (0, 0, 0.222)
				N2 1*b* (0.333, 0.667, 0.887)

c-C$_8$B$_2$N$_2$	$P3m1$	2.537	12.496	C1 1c (0.667, 0.333, 0.177)
				C2 1c (0.667, 0.333, 0.677)
				C3 1a (0, 0, 0.341)
				C4 1a (0, 0, 0.218)
				C5 1a (0, 0, 0.841)
				C6 1a (0, 0, 0.718)
				C7 1b (0.333, 0.667, 0.383)
				C8 1b (0.333, 0.667, 0.883)
				B1 1c (0.667, 0.333, 0.548)
				B2 1b (0.333, 0.667, 0.011)
				N1 1c (0.667, 0.333, 0.057)
				N2 1b (0.333, 0.667, 0.502)