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## Supporting Information: Thermodynamic stability of Li-B-C compounds from first principles.

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Figure S1. Quasi-harmonic approximation (QHA) results for LiBC. In these simulations, we (i) generated a uniform grid of volumes around equilibrium by rescaling the lattice constants; (ii) optimized the unit cell shape and atomic positions at each fixed volume with VASP; (iii) used Phonopy and VASP to perform phonon calculations in the harmonic approximation at each volume; (iv) fitted the resulting free energy points at each temperature with a third-order polynomial; and (v) showed the free energy values for every 200 K (black circles), the polynomial fits (black solid lines), the minimum free energy values at the corresponding volumes for every 10 K (red solid line), and the starting volume (red dashed line). At 1800 K, the free energy difference between the standard harmonic formalism and the QHA values was found to be 21.53 meV/atom.



Figure S2. QHA results for Li<sub>0.5</sub>BC. The simulation and analysis procedure is described in Figure S3. At 1800 K, the free energy difference between the standard harmonic formalism and the QHA values was found to be 23.16 meV/atom. These LiBC and Li<sub>0.5</sub>BC results were used to assess the significance of the anharmonic effect on the Gibbs free energy difference defining the phase boundary between Li<sub>2</sub>B<sub>2</sub>C<sub>2</sub> and 1/2Li<sub>2</sub>+LiB<sub>2</sub>C<sub>2</sub> in Fig. 4(a). The volume expansion in the solid phases change the Gibbs free energy difference by  $6 \times (-21.53 \text{ meV/atom}) - 5 \times (-23.16 \text{ meV/atom}) \approx -13.4 \text{ meV/Li}.$ 



(a) Displacement map in  $g-BC_3$ 



Figure S3. Stability analysis of g-BC<sub>3</sub> and its derivatives. (a) A grid of examined displacements in g-BC<sub>3</sub>. The location of each point on the grid corresponds to a rigid shift of one layer in the AB-stacked g-BC<sub>3</sub>. Arbitrary shifts reduce the symmetry to mP16 (P2<sub>1</sub>/m), shifts along the dotted lines result in oS32 (Cmcm), while shift to special points generate higher-symmetry orthorhombic or hexagonal unit cells. The size of each dot shows excess energy calculated without atomic or lattice constant optimizations. After optimization, the oS32 (Fmmm) configuration has the lowest energy, 15 meV/atom below that of g-BC<sub>3</sub>. (b,c) Structures of g- and e-BC<sub>3</sub>. (d,e) Phonon dispersions calculated in the harmonic approximation for g- and e-BC<sub>3</sub>.



Figure S4. Calculated equations of state for graphite, hypothetical BC, and reported h-BC<sub>3</sub> as a function of the in-plane lattice constants. The formation energies are referenced to the energies of graphite and BC at equilibrium. The dotted red line corresponds to the average energy of graphite and BC constrained to the same lattice constant value. The plot illustrates that the dominant part of the h-BC<sub>3</sub> positive formation energy results from the penalty associated with the C-C bond expansion and B-C bond compression.



Figure S5. Comparison of powder XRD patterns adopted from experimental studies on precursor-based synthesis of g-BC<sub>3</sub> by King *et al.* [1], ball-milling preparation of turbostratic carbon by Li et al. [2], and direct synthesis of h-BC<sub>3</sub> by Milashius et al. [3]. The gray data sets correspond to the reported powder XRD patterns of graphite.

$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	Phase	Space	Pearson	$\Delta E_{\rm c}$ hull	$\Delta E_{\rm c}$ hull	$\Delta F_{\rm c}$ hull		Lattic	e parame	eters (Å	or °)		Ref.	Fig.
fec-Li     FmÅm     eF4     0     0     0.0004     4.318	name	group	symbol	w/o ZPE	w/ ZPE	at 600 K	a	b	с С	α	β	$\gamma$		0
bcc-Li         Im\overline         th2         0.002         0.001         0         3.431	fcc-Li	${\rm Fm}\overline{3}{\rm m}$	cF4	0	0	0.0004	4.318							1
B         R3m         hR36         0         0         4,901         12,500         12,500         1           L3BC         P6,mm         hP4         0         0         0         2,468         6,608         1           L3BC         P6,mm         hP13         0         0         0         2,468         6,6075         1           L3C         P6/mm         hP13         0         0         0         3,333         4,822         5,351         1         1           L4C3         C2/m         mS14         0         0         6,566         3,797         6,20         118.05         1         1           L4G3         C2/m         mS14         0         0         0,373         10.05         118.05         1         1           L4B3         P6,mm         hP3<	bcc-Li	$\mathrm{Im}\overline{3}\mathrm{m}$	tI2	0.002	0.001	0	3.431							1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	В	$R\overline{3}m$	hR36	0	0	0	4.901		12.540					1
LiBC         P63/mm         H°6         0         0         2.749         6.975	$\mathbf{C}$	$\mathrm{P}_{3}\mathrm{mmc}$	hP4	0	0	0	2.468		6.608					1
	LiBC	$P6_3/mmc$	hP6	0	0	0	2.749		6.975					1
LiC6 LiC6 ImmP6/mmhP70004.3273.603	$\mathrm{LiC}_{12}$	P6/mmm	hP13	0	0	0	4.299		6.936					1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	${\rm LiC}_6$	P6/mmm	hP7	0	0	0	4.327		3.603					1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	LiC	Immm	oI8	0	0	0	3.593	4.822	5.351					1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	${\rm Li}_4{\rm C}_3$	C2/m	mS14	0	0	0	6.566	3.797	6.220		118.05			1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	${\rm Li}_9{\rm B}_8$	$P6_3/mmc$	hP34	0	0	0	3.974		25.174					1
LiBP63/mmhP80.0380.0420.0573.05010.76010.76011LiB3P4/mbmtP160.0090.0080.0065.9664.14811LiB34P4tP1600010.7688.76811B4CCmmS300008.7745.6055.052118.781LiBa5CImmaol640004.7048.9875.64811LiBa6CAmm2oS320004.7048.9875.6486.27[4]1, 6B_0.5C"P1aP414015.58415.5867.680110.54[4]1, 6B_0.67C"CmmS92016.5285.6587.680110.54[4]1, 6B_0.67CCmmS9200.2178.1826.5398.954110.54[4]1, 6B_0.67CFmmm0.232**5.1736.8968.10.54[6]5eBC3Fmm0.980.1960.1985.1725.1776.8818.2167.996.0.665eBC3Pima0.780.1890.1977.3321.7176.8818.216.7.996.0.665eBC3FomPi120.233*2.5685.6094.4491.5111b-BC3Pima0.1040.233**2.5686.717	${\rm Li}_8{\rm B}_7$	$P\overline{6}m2$	hP15	0	0	0.0009	3.973		11.035					1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	LiB	$P6_3/mmc$	hP8	0.038	0.042	0.057	3.050		10.760					1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	${\rm LiB_3}$	P4/mbm	tP16	0.009	0.008	0.006	5.966		4.148					1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\mathrm{Li}_3\mathrm{B}_{14}$	$P\overline{4}$	tP136	0	0	0	10.768		8.768					1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$B_4C$	Cm	mS30	0	0	0	8.774	5.605	5.052		118.78			1, 6
LiBaCAmm2oS320004.7048.9875.648	${\rm LiB_{13}C_2}$	Imma	oI64	0	0	0	5.672	10.826	8.040					1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	${\rm LiB_6C}$	Amm2	oS32	0	0	0	4.704	8.987	5.648					1
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$B_{10.5}C^a$	P1	aP414	0			15.584	15.586	15.597	66.23	66.24	66.27	[4]	1, 6
g-BC3P63/mmhP160.232**5.1736.896[1][5]5e-BC3Fmmm05320.2170.211*0.202*5.1826.3598.954553r-BC3PĪaP160.2150.208*0.199*5.1725.1776.88188.2167.9960.0653a-BC3PmmaoP80.1960.1830.1902.5092.5147.81556666b-BC3PmmaoP80.2042.4852.5237.900576.881867.9960.065c-BC3IĀ3mc1640.2000.1890.1977.332556.71755h-BC3P\bar{ma}hP40.431**2.5656.717555h-BC3+xP\bar{6}hP1120.293*13.6216.4885555h-LiBC3Pmn21oP100.223**2.6187.4814.4065556h-LiBC3Pmc21oP100.0310.0280.0253.6965.2004.4945522222222222222222222222222222222222222232523	$B_{6.67}C^a$	Cm	mS92	0			16.528	5.658	7.680		110.54		[4]	1, 6
e-BC3FmmmoS320.2170.211*0.202*5.1826.3598.9545.1735.1735.1736.88188.2167.9960.0653a-BC3PmmaoP80.1960.1830.1902.5092.5147.8155567.9960.0653b-BC3PmmaoP80.2042.4852.5237.90057.815566.915c-BC3I43mcI640.2000.1890.1977.3327.90057.90057.9135h-BC3P6m2hP40.431**2.5656.71757.91355h-BC3P6m2hP40.431**2.6187.4814.406556.7175h-BC3+xP6hP1120.293**2.6187.4814.406556h-LiBC3Pmm21oP100.0310.0280.0253.6965.2004.4945577h-LiBC3Pm21oP100.2110.1950.1842.7247.0564.6115577h-LiBC3Pmm2oP100.2217.9272.7124.6795.2004.4945.228.59422li0.5BCP11aP150.2250.2090.1974.6877.0435556.71555li0.5BCP11aP150.208	$g-BC_3$	$P6_3/mmc$	hP16	0.232	*	*	5.173		6.896				[1][5]	5
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$e-BC_3$	Fmmm	oS32	0.217	$0.211^{*}$	$0.202^{*}$	5.182	6.359	8.954					S3
a-BC3PmmaoP80.1960.1830.1902.5092.5147.815[6]5b-BC3PmmaoP80.2042.4852.5237.900[6]5c-BC3I $\overline{43}$ mcI640.2000.1890.1977.332[7]5h-BC3P $\overline{6}$ m2hP40.431**2.5656.717[3]5h-BC3+xP $\overline{6}$ hP1120.293*13.6216.48855h-LiBC3Pmn21oP100.223**2.6187.4814.406[3]8g-LiBC3Pmc21oP100.0310.0280.0253.6965.2004.49488Li_0.5BCImm2o1100.2100.1950.1842.7247.0564.61122Li_0.5BCP $\overline{1}$ mhP150.2250.2090.1974.6877.04322Li_0.5BCPImaoP100.2217.0272.7124.67922Li_0.5BCPIm2oP290.2836.7328.0964.69622Li_0.5BCPIaP150.2084.4504.5976.56986.4165.2285.942Li_0.5BCPIaP150.2084.1397.106[8]9Li_0.67BCP $\overline{6}$ hP80.1180.1090.1044.7043.5405.40Li_2B_2CP $\overline{4}$ mR2tP100.438*	$r-BC_3$	$P\overline{1}$	aP16	0.215	0.208*	$0.199^{*}$	5.172	5.177	6.881	88.21	67.99	60.06		S3
b-BC3PmmaoP80.2042.4852.5237.900[6]5c-BC3I $\overline{4}3m$ cI640.2000.1890.1977.332[7][7]5h-BC3P $\overline{6}m2$ hP40.431**2.5656.717[3]5h-BC3+xP $\overline{6}$ hP1120.293**2.6187.4814.406[3]8g-LiBC3Pmn21oP100.223**2.6187.4814.406138g-LiBC3Pmc21oP100.0310.0280.0253.6965.2004.494141414Li0.5BCImm2oI100.2100.1950.1842.7247.0564.611141212Li0.5BCP $\overline{3}$ 1mhP150.2250.2090.1974.6877.043121212Li0.5BCPImaoP100.2217.0272.7124.67912121212Li0.5BCP1aP150.2086.7328.0964.69612 <td><math>a-BC_3</math></td> <td>Pmma</td> <td>oP8</td> <td>0.196</td> <td>0.183</td> <td>0.190</td> <td>2.509</td> <td>2.514</td> <td>7.815</td> <td></td> <td></td> <td></td> <td><b>[6</b>]</td> <td>5</td>	$a-BC_3$	Pmma	oP8	0.196	0.183	0.190	2.509	2.514	7.815				<b>[6</b> ]	5
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$b-BC_3$	Pmma	oP8	0.204			2.485	2.523	7.900				<b>[6</b> ]	5
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$c-BC_3$	$I\overline{4}3m$	cI64	0.200	0.189	0.197	7.332						[7]	5
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$h-BC_3$	$P\overline{6}m2$	hP4	0.431	*	*	2.565		6.717				[3]	5
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$h-BC_{3+x}$	$P\overline{6}$	hP112	0.293			13.621		6.488					5
g-LiBC3Pmc21oP100.0310.0280.0253.6965.2004.4948Li_{0.5}BCImm2oI100.2100.1950.1842.7247.0564.6112Li_{0.5}BCP31mhP150.2250.2090.1974.6877.0432Li_{0.5}BCPmmaoP100.221 $\cdot$ 7.0272.7124.6792Li_{0.42}BCPmm2oP290.283 $\cdot$ 6.7328.0964.6962Li_{0.5}BCP1aP150.208 $\cdot$ 4.4504.5976.56986.4165.2285.942Li_{0.67}BCP62mhP80.1180.1090.1044.7043.540 $\cdot$ [8]9Li_2B_2CP4m2tP100.772 $\cdot$ 4.1397.106[8]9Li_2B_2CP4m2tP100.438**4.3057.1579	$h-LiBC_3$	$Pmn2_1$	oP10	0.223	*	*	2.618	7.481	4.406				[3]	8
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	g-LiBC <sub>3</sub>	$Pmc2_1$	oP10	0.031	0.028	0.025	3.696	5.200	4.494					8
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\mathrm{Li}_{0.5}\mathrm{BC}$	Imm2	oI10	0.210	0.195	0.184	2.724	7.056	4.611					2
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	${\rm Li}_{0.5}{\rm BC}$	$P\overline{3}1m$	hP15	0.225	0.209	0.197	4.687		7.043					2
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	${\rm Li}_{0.5}{\rm BC}$	Pmma	oP10	0.221			7.027	2.712	4.679					2
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\mathrm{Li}_{0.42}\mathrm{BC}$	Pmm2	oP29	0.283			6.732	8.096	4.696					2
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	${\rm Li}_{0.5}{\rm BC}$	P1	aP15	0.208			4.450	4.597	6.569	86.41	65.22	85.94		2
Li2B2C $P\overline{4}m2$ tP100.7724.1397.106[8]9Li2B2C <sup>b</sup> $P\overline{4}m2$ tP100.438**4.1245.3429Li2B2CP42/mmctP100.4184.3057.1579	${\rm Li}_{0.67}{\rm BC}$	$P\overline{6}2m$	hP8	0.118	0.109	0.104	4.704		3.540					
$Li_2B_2C^b$ $P\overline{4}m2$ $tP10$ $0.438$ *       * $4.124$ $5.342$ 9 $Li_2B_2C^b$ $P\overline{4}m/c$ $tP10$ $0.418$ $4.305$ $7.157$ 9	${\rm Li}_2{\rm B}_2{\rm C}$	$P\overline{4}m2$	tP10	0.772			4.139		7.106				[8]	9
$Li_{0}B_{0}C = P4_{0}/mmc + P10 = 0.418 = 4.305 = 7.157 = 0.0000000000000000000000000000000000$	${\rm Li}_2{\rm B}_2{\rm C}^{\rm b}$	$P\overline{4}m2$	tP10	0.438	*	*	4.124		5.342				-	9
1.220 $1.2/1000$ $0.10$ $0.10$ $0.10$ $1.00$ $1.00$	${\rm Li}_2{\rm B}_2{\rm C}$	$P4_2/mmc$	tP10	0.418			4.305		7.157					9
$Li_2B_2C$ Pm mS20 0.190 4.256 10.647 4.190 117.77 9	${\rm Li}_2{\rm B}_2{\rm C}$	$\rm Pm$	mS20	0.190			4.256	10.647	4.190		117.77			9
$Li_2B_2C$ Cmcm oS40 0.106 2.818 4.873 26.377 9	${\rm Li}_2{\rm B}_2{\rm C}$	Cmcm	oS40	0.106			2.818	4.873	26.377					9

Table S1. Stability and lattice parameters of select Li-B-C phases obtained in our DFT calculations. References are given for phases most relevant to this study and full structural information is provided in CIF files. At T = 0 K, we constructed the full convex hull and indicated the distance to the convex hull ( $\Delta E_{c. hull}$  in eV/atom). For key phases, we performed phonon calculations and showed the distance to the convex hull constructed at T = 0 K with zero point energy (ZPE) and at T = 600 K. Phases found to be dynamically unstable are marked with asterisks; in cases with negligible contribution of imaginary modes to the phonon density of states, we provided estimates of the distances to the convex hull with ZPE and at T = 600 K as well. <sup>a</sup>Since Jay et al.'s study [4] did not explicitly specify the particular distribution of atoms on partial occupancy sites in each block, we considered several possible decorations and used aP414-B<sub>10.5</sub>C as OPO1 and mS92-B<sub>6.67</sub>C as OPO2. <sup>b</sup>Structure from Ref. [8] after our full DFT relaxation.

Parameter	DFT	Experiment	Description	Reference
m		13.88 au	mass of 2 Li atoms	
a	2.73863 Å	2.672 Å	bond length	[10]
u	$333.01 \ {\rm cm}^{-1}$	$351.43 \text{ cm}^{-1}$	oscillation frequency	[10]
$\mathrm{D}_0^{\mathrm{mol}}$	0.464  eV/atom	0.53  eV/atom	dissociation energy	[11]
$\mathrm{D}_0^{\mathrm{bcc}}$	1.595  eV/atom	1.63  eV/atom	cohesive energy	[11]
$\mathrm{D}_{0}^{\mathrm{bcc-mol}}$	1.131  eV/atom	1.10  eV/atom	$\mathrm{D}_0^\mathrm{bcc}$ - $\mathrm{D}_0^\mathrm{mol}$	

Table S2. Parameters obtained in our density functional theory (DFT) calculations for evaluation of the chemical potential of Li diatomic gas. The corresponding experimental values are given for reference.

The chemical potential of  $Li_2$  molecular vapor within the ideal diatomic gas model can be found as [9]

$$\mu^{\mathrm{mol}}(T, P) = E^{\mathrm{mol}} + E^{\mathrm{mol}}_{\mathrm{ZPE}} + \Delta\mu^{\mathrm{mol}}(T, P)$$
(1)

where the zero-point energy (ZPE) is  $E_{\text{ZPE}}^{\text{mol}} = h\nu/2$  and the (T, P)-dependent entropy contribution is

$$\Delta\mu^{\mathrm{mol}}(T,P) = -kT \left\{ \ln\left[ \left(\frac{2\pi mkT}{h^2}\right)^{\frac{3}{2}} \frac{kT}{P} \right] + \ln\left[\frac{8\pi^2 IkT}{2h^2}\right] - \ln\left[1 - \exp\left(-\frac{h\nu}{kT}\right)\right] \right\}.$$
 (2)

The  $\Delta \mu^{\text{mol}}(T, P)$  term combines the translational, rotational, and vibrational entropy contributions and was evaluated using the DFT parameters listed in Table S1. At 1800 K and 1 bar, these degrees of freedom contributed 78%, 27%, and 5%, respectively. Note that for comparison with experiment we used  $D_0^{\text{mol}} = E^{\text{mol}} + E_{\text{ZPE}}^{\text{mol}} - E^{\text{at}}$ . The following expression is used to calculate the moment of inertia in the above formula:  $I = 2m(a/2)^2 = ma^2/2$ .

The chemical potential of bcc-Li is found within the harmonic approximation using the DFT phonon density of states  $g(\omega)$  as

$$\begin{split} \mu^{\rm bcc}(T,P) &= E^{\rm bcc} + E^{\rm bcc}_{\rm ZPE} + \Delta \mu^{\rm bcc}(T), \\ E^{\rm bcc}_{\rm ZPE} &+ \Delta \mu^{\rm bcc}(T) = \int_0^\infty d\omega g(\omega) \frac{\hbar\omega}{2} + kT \int_0^\infty d\omega g(\omega) \ln\left[1 - \exp\left(-\frac{\hbar\omega}{kT}\right)\right] \\ &= kT \int_0^\infty d\omega g(\omega) \ln\left[2\sinh\left(\frac{\hbar\omega}{2kT}\right)\right]. \end{split}$$

We relied on the same expressions to map out the (T, P) phase boundaries for delithiation of LiBC. After calculating the phonon densities of states for LiBC and Li<sub>x</sub>BC, we determined P(T) for a set of temperatures by equilibrating the chemical potentials of Li in LiBC and the combination of Li<sub>2</sub> and Li<sub>x</sub>BC:

$$\frac{1}{1-x}\text{LiBC} = \frac{1}{2}\text{Li}_2 + \frac{1}{1-x}\text{Li}_x\text{BC}.$$

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