Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Superhard B_2CO phases deriving from carbon allotropes

Chao Liu[a], Mingwei Chen[b], Julong He[c], Shuangshuang Yu[a], Tongxiang Liang*[a]

a School of Materials Science and Engineering, Jiangxi University of Science and Technology, Ganzhou 341000, China

b Institute of Engineering Research, Jiangxi University of Science and Technology, Ganzhou 341000, China

c State Key Laboratory of Metastable Materials Science and Technology, Yanshan University, Qinhuangdao 066004, China

Author to whom correspondence should be addressed. E-mail address: liang_tx@126.com.

In order to compare the differences of results based on LDA and GGA, the lattice parameters, mechanical property, and electrical property have been calculated.

Table S1 lattice parameters *a*, *b*, *c* (Å) for *o*P16-, and *o*C16-B_2CO at zero pressure and 80 GPa.

	*o*P16		*o*C16	
	0 GPa	80 GPa	0 GPa	80 GPa
LDA	*a* = 8.847; *b* = 4.364; *c* = 2.603;	*a* = 8.264; *b* = 4.111; *c* = 2.451;	*a* = 6.142; *b* = 6.421; *c* = 2.601;	*a* = 5.663; *b* = 6.067; *c* = 2.460;
GGA	*a* = 8.985; *b* = 4.425; *c* = 2.643;	*a* = 8.363; *b* = 4.151; *c* = 2.478;	*a* = 6.263; *b* = 6.500; *c* = 2.639;	*a* = 5.740; *b* = 6.116; *c* = 2.486;

The maximum difference is 2%, the minimum difference is 0.8%.

Table S2 Independent elastic constants C_{ij}, and mechanical property parameters as *B*, *G* of *o*P16-, and *o*C16-B_2CO based on GGA-PBE. C_{ij}, *B*, and *G* are expressed in GPa.

	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}	*B*	*G*
*o*P16	665.3	724.0	715.2	252.7	280.8	256.7	92.9	89.0	61.9	288.0	280.8
*o*C16	511.5	630.2	744.1	289.6	216.2	245.0	160.0	39.31	109.1	275.2	251.1

*o*P16-, and *o*C16-B_2CO are both mechanical stable.

Table S3 Calculated volume *V* for unit cell (Å^3), bond parameter as bond-type μ, bond length d^{μ} (Å), bond number n^{μ} and *Hv* (GPa) for *o*P16-, and *o*C16-B_2CO based on GGA-PBE.

	V	μ	d^{μ}	n^{μ}	N_e^{μ}	f_i^{μ}	H_V^{μ}	*Hv*
*o*P16	105.103	B-C (I)	1.560	8	0.591	0.313	55.859	44.513
		B-C (II)	1.600	4	0.547	0.161	59.655	
		B-C (III)	1.607	4	0.541	0.110	62.346	
		B-O (I)	1.624	4	0.673	0.785	31.353	

		B-O (II)	1.650	4	0.642	0.831	27.674	
		B-O (III)	1.655	8	0.636	0.529	39.123	
*o*C16	107.414	B-C (I)	1.541	8	0.599	0.351	55.510	41.342
		B-C (II)	1.614	8	0.521	0.276	49.335	
		B-O (I)	1.633	8	0.647	0.495	42.555	
		B-O (II)	1.663	8	0.613	0.873	25.065	

Whether based on LDA or GGA, the *o*P16-, and *o*C16-B_2CO are both superhard.

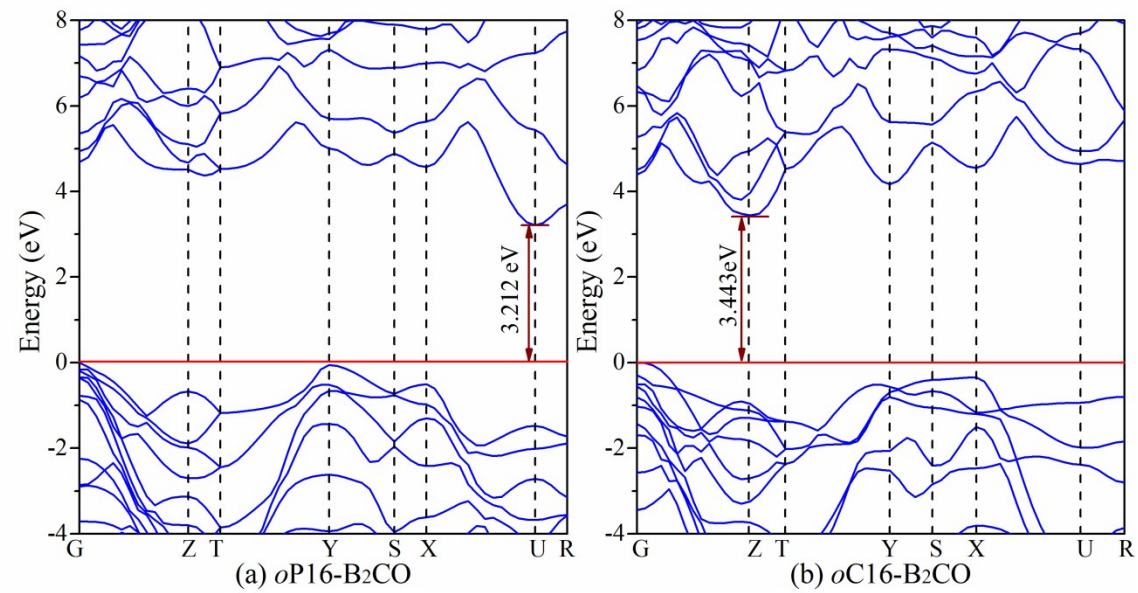

Figure S1 Calculated electronic band structures for *o*P16-, and *o*C16-B_2CO at zero pressure based on GGA-PBE. The Fermi level is represented by a horizontal red line.

The band structures deviations of *o*P16-B_2CO and *o*C16-B_2CO are 1.65% and 0.91%, respectively.

The results indicated that the LDA and GGA have little influence on the system we studied. The trend obtained by LDA is correct and validated.