Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental material for "prediction of potential hard sodium carbaboride compounds assuming sp^3-bonded covalent clathrates"

Ailing Liu[a], Xiaoran Cheng[a], Xingyu Wang[a], Yutong Zou[a], and Miao Zhang[a]*

Department of Physics, School of Sciences, Beihua University, Jilin 132013, China

E-mail: zhangmiaolmc@126.com

Table S1 Structural information of the predicted $NaBC_{11}$, $Na_2B_2C_{10}$, NaB_2C_{10}, $Na_2B_4C_8$, NaB_4C_8, and $Na_2B_6C_6$ at 0 GPa.

	Space group	Lattice parameters(Å)	Atomic positions
$NaBC_{11}$	$Pmm2$	$a = 4.4930$	Na 1c (0.5, 0.0, 0.00878)
		$b = 4.4984$	B 1d (0.5, 0.5, 0.25111)
		$c = 4.4736$	C 1d (0.5, 0.5, 0.74653)
		$\alpha = \beta = \gamma = 90°$	C 1a (0.0, 0.0, 0.25037)
			C 1a (0.0, -0.0, 0.74863)
			C 2f (0.24283, 0.5, 0.99141)
			C 2h (0.5, 0.24322, 0.50709)
			C 2e (0.75143, -0.0, 0.50595)
			C 2g (-0.0, 0.74949, 0.99284)
$Na_2B_2C_{10}$	$P4_2/mmc$	$a = b = 4.6107$	Na 2d (0.0, 0.5, 0.5)
		$c = 4.5306$	B 2f (0.5, 0.5, 0.25)
		$\alpha = \beta = \gamma = 90°$	C 2e (0.0, 0.0, 0.25)
			C 4m (0.23486, 0.5, 0.0)
			C 4l (0.75060, 0.0, 0.5)
NaB_2C_{10}	$Pmmm$	$a = 4.6024$	Na 1a (0.0, 0.0, 0.0)
		$b = 4.6134$	B 2r (0.0, 0.5, 0.25424)
		$c = 4.3318$	C 2s (0.5, -0.0, 0.25117)
		$\alpha = \beta = \gamma = 90°$	C 2k (0.73064, 0. 5, -0.0)
			C 2j (0.24649, -0.0, 0.5)
			C 2o (0.5, 0.74478, -0.0)
			C 2n (0.0, 0.23103, 0.5)
$Na_2B_4C_8$	$I4/mmm$	$a = b = 4.8159$	Na 2a (0.5, 0.5, 0.5)
		$c = 4.3080$	B 4d (0.0, 0.5, 0.25)
		$\alpha = \beta = \gamma = 90°$	C 8j (0.72871, 0.5, 0.0)
NaB_4C_8	$P4/mmm$	$a = b = 4.8079$	Na 1a (0.0, 0.0, 0.0)
		$c = 4.1223$	B 4i (0.0, 0.5, 0.25249)
		$\alpha = \beta = \gamma = 90°$	C 4n (0.72316, 0.5, 0.0)
			C 4m (0.22659, 0.0, 0.5)
$Na_2B_6C_6$	$Pm-3n$	$a = b = c = 4.7326$	Na 2a (1.0, 0.0, 1.0)
		$\alpha = \beta = \gamma = 90°$	B 6c (0.25, 1.0, 0.5)
			C 6d (0.25, 0.5, 1.0)

Table S2 Calculated elastic constants C_{ij} (in GPa), bulk modulus B (GPa), shear modulus G (GPa), ratio of G/B, and Vickers hardness H_v (GPa) of $NaBC_{11}$,$Na_2B_2C_{10}$, NaB_2C_{10}, $Na_2B_4C_8$, and NaB_4C_8 at 0 GPa.

	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}	B	G	G/B	H_v^{Chen}
$NaBC_{11}$	775	774	704	297	291	315	74	73	78	300	315	1.05	58.28
$Na_2B_2C_{10}$	718	718	619	252	252	282	67	75	75	276	278	1.01	51.43
NaB_2C_{10}	789	795	574	277	263	303	60	77	78	285	296	1.04	55.43
$Na_2B_4C_8$	730	730	456	229	229	255	36	78	78	251	253	1.01	48.51
NaB_4C_8	801	801	424	220	220	288	37	73	73	256	261	1.02	50.07

For the Tetragonal crystals, the mechanical stability requires that the elastic constants satisfy the following mechanical criteria:$C_{11}> 0$, $C_{33} > 0$, $C_{44} > 0$, $C_{66} > 0$, $(C_{11}$ - $C_{12}) > 0$, $(C_{11} + C_{33}$ - $2C_{13}) > 0$, $[2(C_{11} + C_{12}) + C_{33} + 4C_{13}] > 0$. For the Orthorhombic crystals, the mechanical stability requires that the elastic constants satisfy the following mechanical criteria: $C_{11} > 0, C_{22} > 0, C_{33} > 0$, $C_{44} > 0$, $C_{55} > 0$, $C_{66} > 0$, $[C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})] > 0$, $(C_{11} + C_{22}$ - $2C_{12}) > 0$, $(C_{11} + C_{33}$ - $2C_{13}) > 0$, $(C_{22} + C_{33}$ - $2C_{23}) > 0$

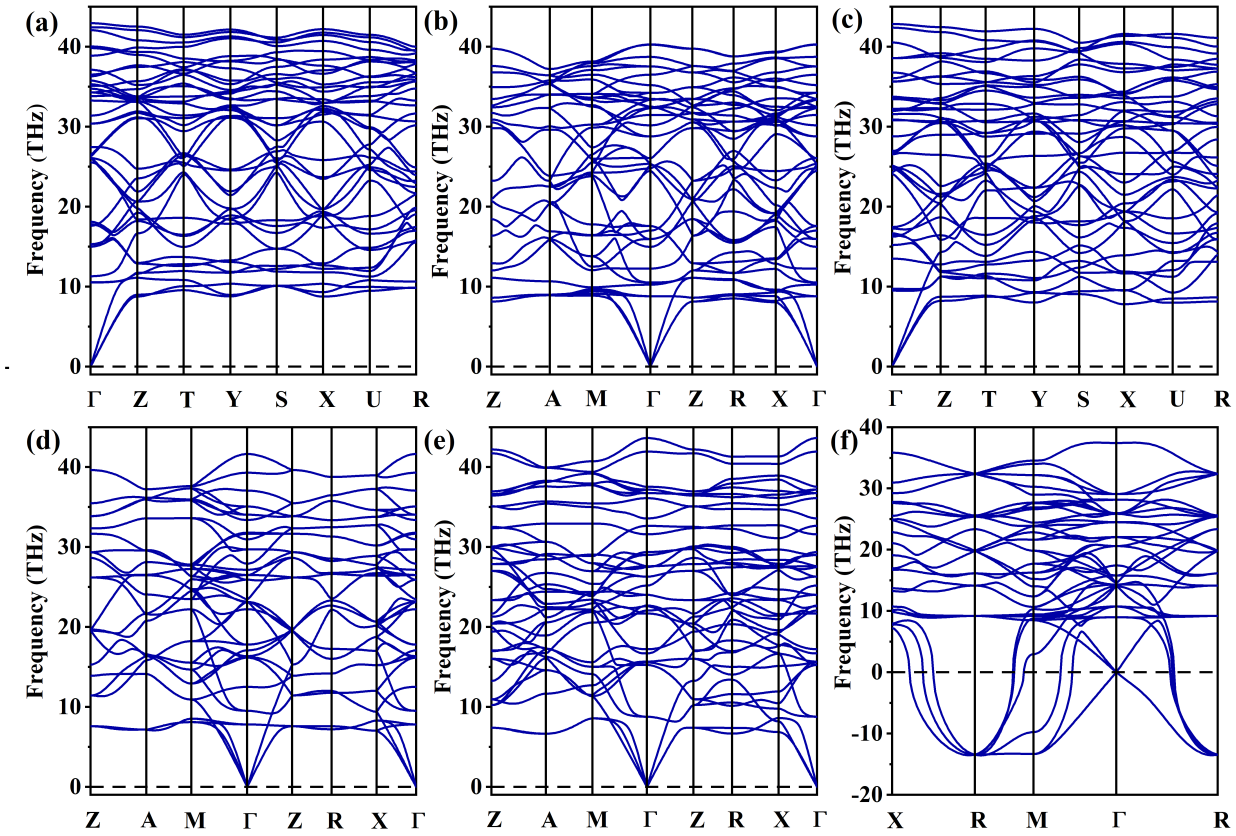

Fig. S1 Calculated phonon dispersion curves for (a) $NaBC_{11}$ (b) $Na_2B_2C_{10}$ (c) NaB_2C_{10} (d) $Na_2B_4C_8$ (e) NaB_4C_8 (f) $Na_2B_6C_6$ at 50 GPa.

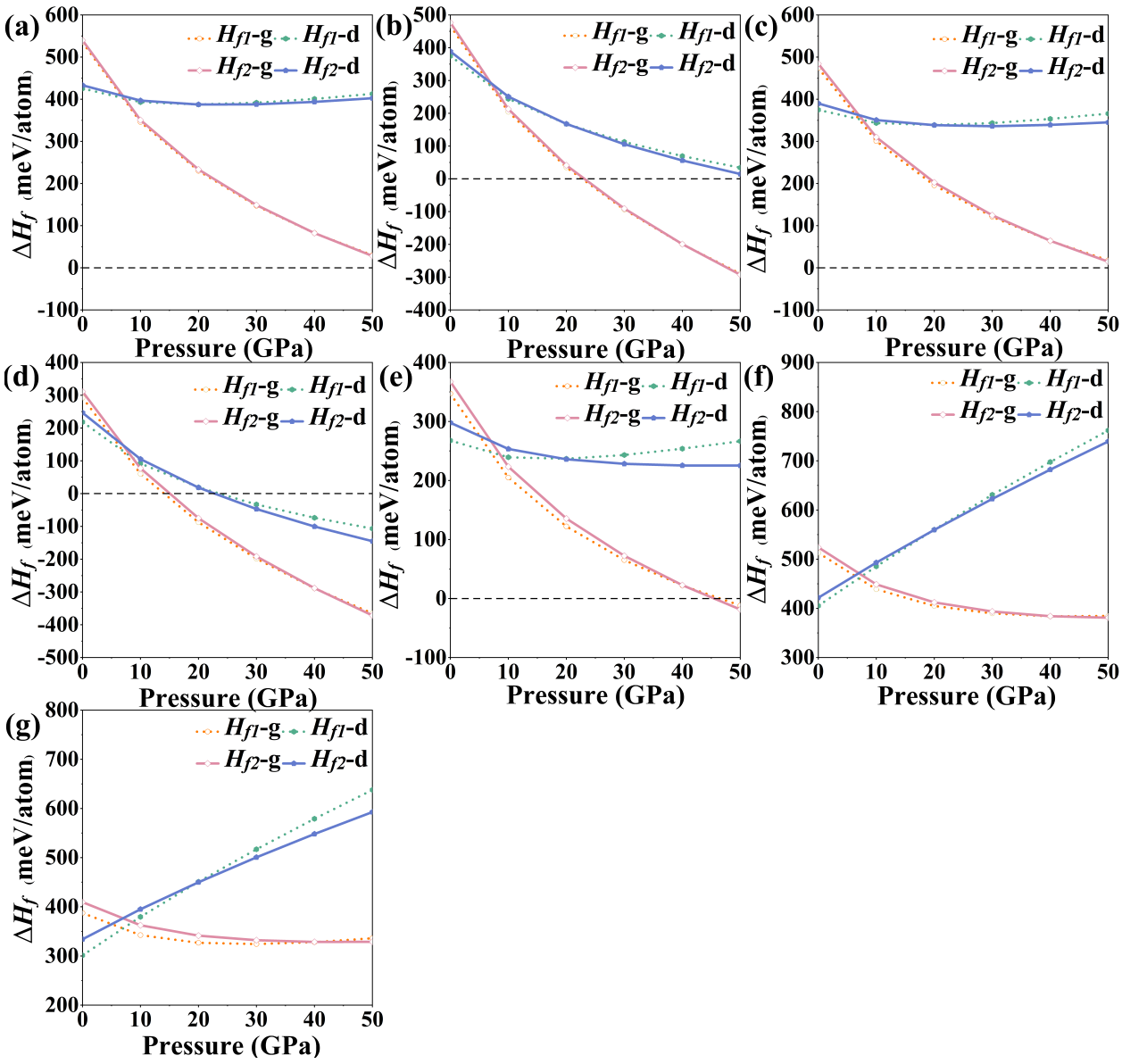

Fig. S2 Calculated formation enthalpies for ΔH_f as a function of pressure. (a) $NaBC_{11}$. (b) $Na_2B_2C_{10}$. (c) NaB_2C_{10}. (d) $Na_2B_4C_8$. (e) NaB_4C_8. (f) B_2C_{10}. (g) B_4C_8. Here, "g" and "d" represent the carbon using graphite and diamond in two possible synthesis paths, respectively.

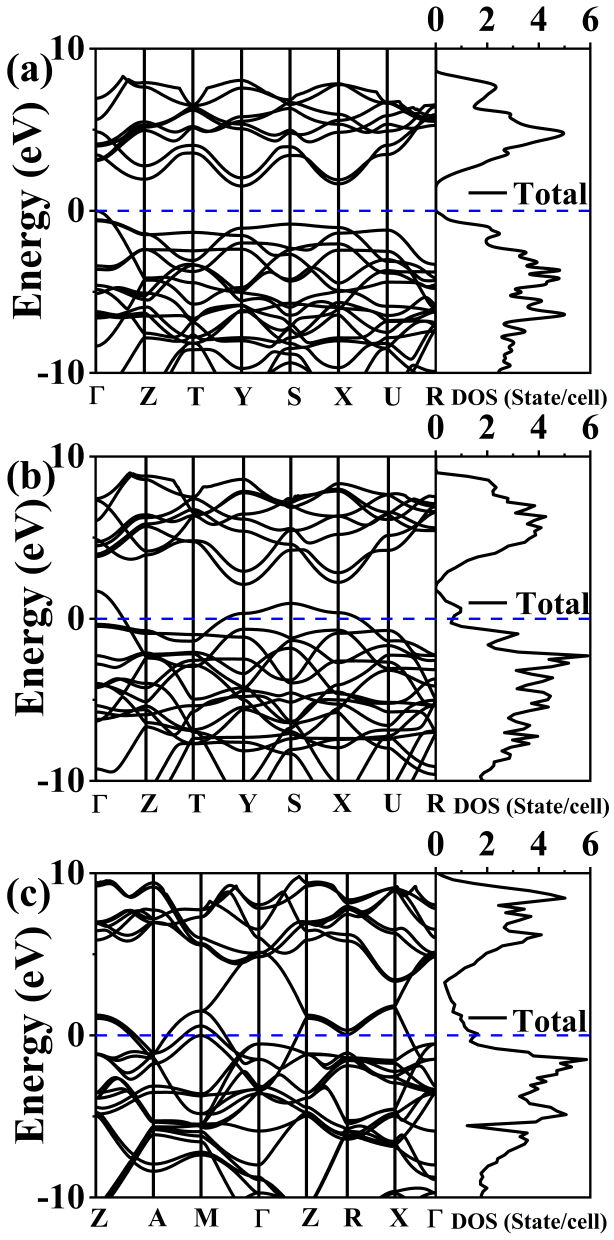

Fig. S3 Electronic band structures and density of states of (a) $NaBC_{11}$. (b) NaB_2C_{10}. (c) NaB_4C_8, at 0 GPa.

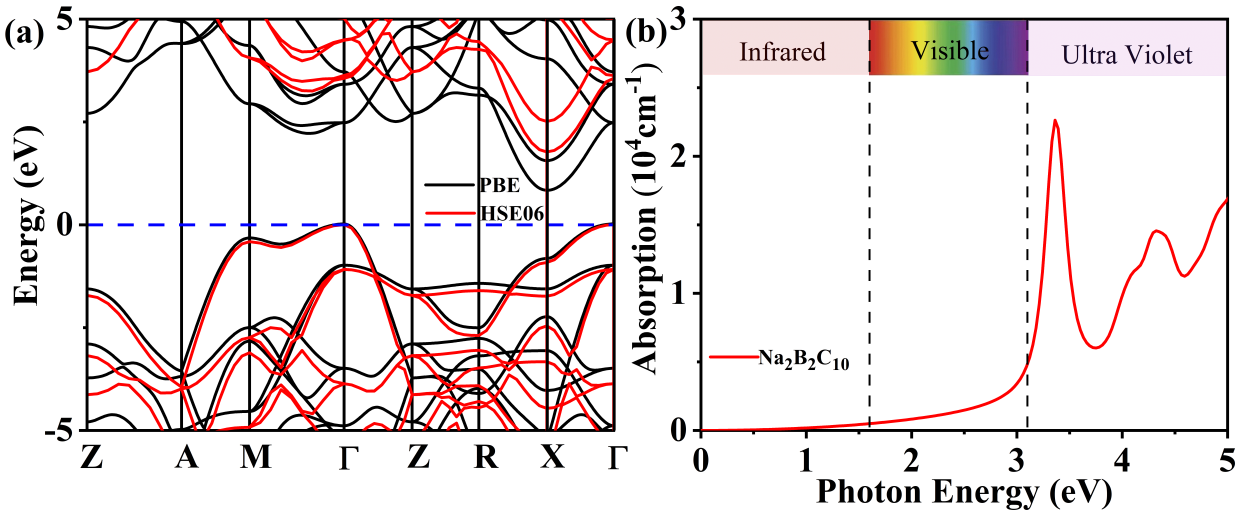

Fig. S4 Calculated (a) band structure of $Na_2B_2C_{10}$ using the PBE (black lines) and HSE06 (red lines) functionals, and (b) optical absorption spectra of $Na_2B_2C_{10}$ were simulated by HSE06 function under ambient pressure.

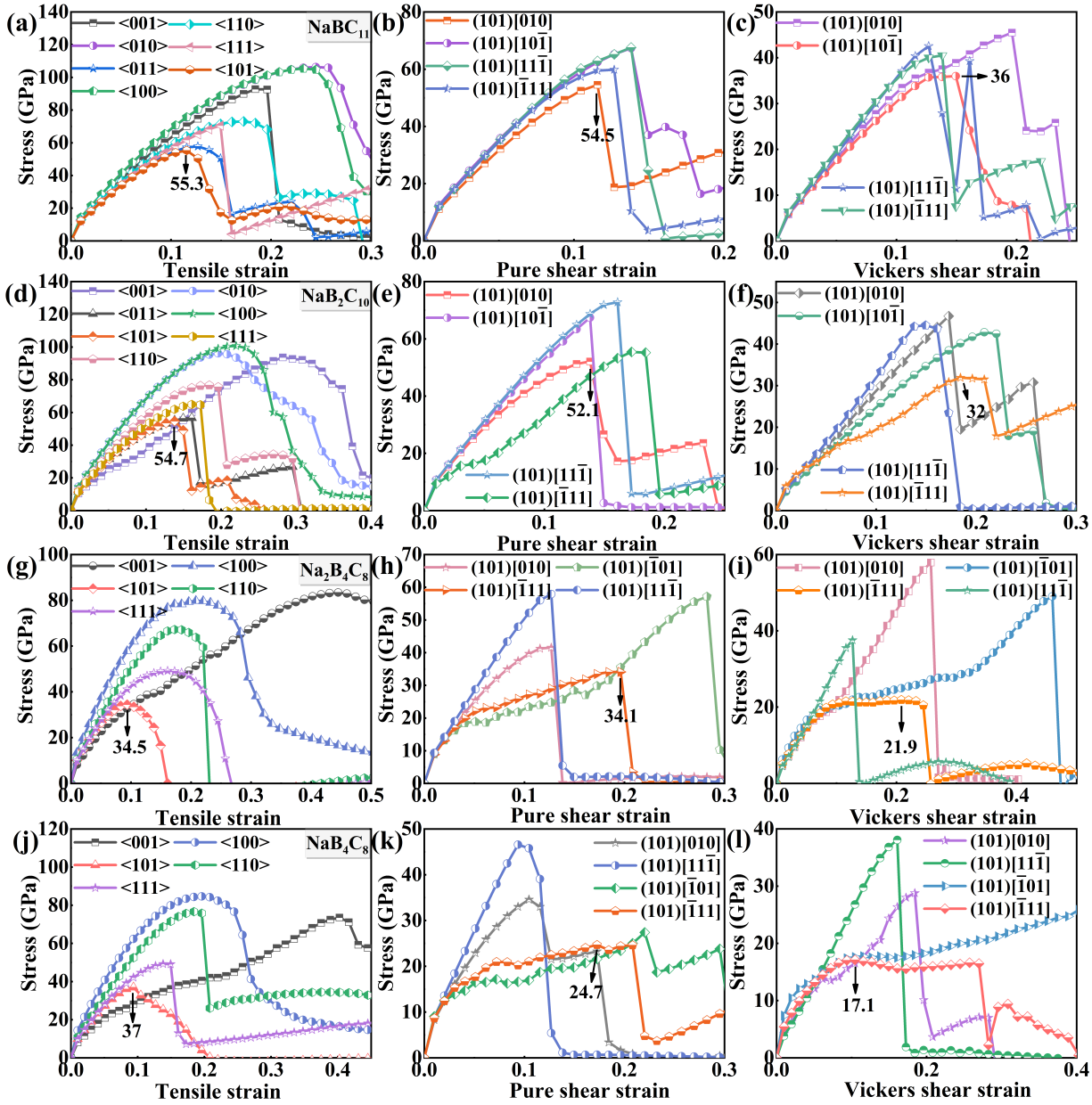

Fig. S5 Calculated tensile, pure shear and Vickers indentation shear deformation stress - strain curves of (a-c) $NaBC_{11}$, (d-f) NaB_2C_{10}, (g-i) $Na_2B_4C_8$, and (j-l) NaB_4C_8.