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Quantum chemical modeling of the solid-state B_4X structures containing tetrahedral B_4 units with X = B, C, Al, Si

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Table S1 Cartesian coordinates (in Å) of atoms of primitive unit cell and its basis vectors for crystal structure *cF*-B_5.

Atom or vector	x	y	z
B	0.00000	0.00000	0.00000
B	0.95729	0.95729	0.95729
B	0.95729	2.17028	2.17028
B	2.17028	0.95729	2.17028
B	2.17028	2.17028	0.95729
$\vec{a}_1$	0.00000	3.12757	3.12757
$\vec{a}_2$	3.12757	0.00000	3.12757
$\vec{a}_3$	3.12757	3.12757	0.00000

Table S2 Cartesian coordinates (in Å) of atoms of primitive unit cell and its basis vectors for crystal structure *cF*-B_4C.

Atom or vector	x	y	z
C	0.00000	0.00000	0.00000
B	0.90300	0.90300	0.90300
B	0.90300	2.09860	2.09860
B	2.09860	0.90300	2.09860
B	2.09860	2.09860	0.90300
$\vec{a}_1$	0.00000	3.00160	3.00160
$\vec{a}_2$	3.00160	0.00000	3.00160
$\vec{a}_3$	3.00160	3.00160	0.00000

Table S3 Cartesian coordinates (in Å) of atoms of primitive unit cell and its basis vectors for crystal structure *cF*-B_4Al.

Atom or vector	x	y	z
Al	0.00000	0.00000	0.00000
B	1.22872	1.22872	1.22872
B	1.22872	2.43167	2.43167
B	2.43167	1.22872	2.43167
B	2.43167	2.43167	1.22872
$\vec{a}_1$	0.00000	3.66039	3.66039
$\vec{a}_2$	3.66039	0.00000	3.66039
$\vec{a}_3$	3.66039	3.66039	0.00000

Table S4 Cartesian coordinates (in Å) of atoms of primitive unit cell and its basis vectors for crystal structure *cF*-B_4Si.

Atom or vector	x	y	z
Si	0.00000	0.00000	0.00000
B	1.15169	1.15169	1.15169
B	1.15169	2.34570	2.34570
B	2.34570	1.15169	2.34570
B	2.34570	2.34570	1.15169
$\vec{a}_1$	0.00000	3.49739	3.49739
$\vec{a}_2$	3.49739	0.00000	3.49739
$\vec{a}_3$	3.49739	3.49739	0.00000

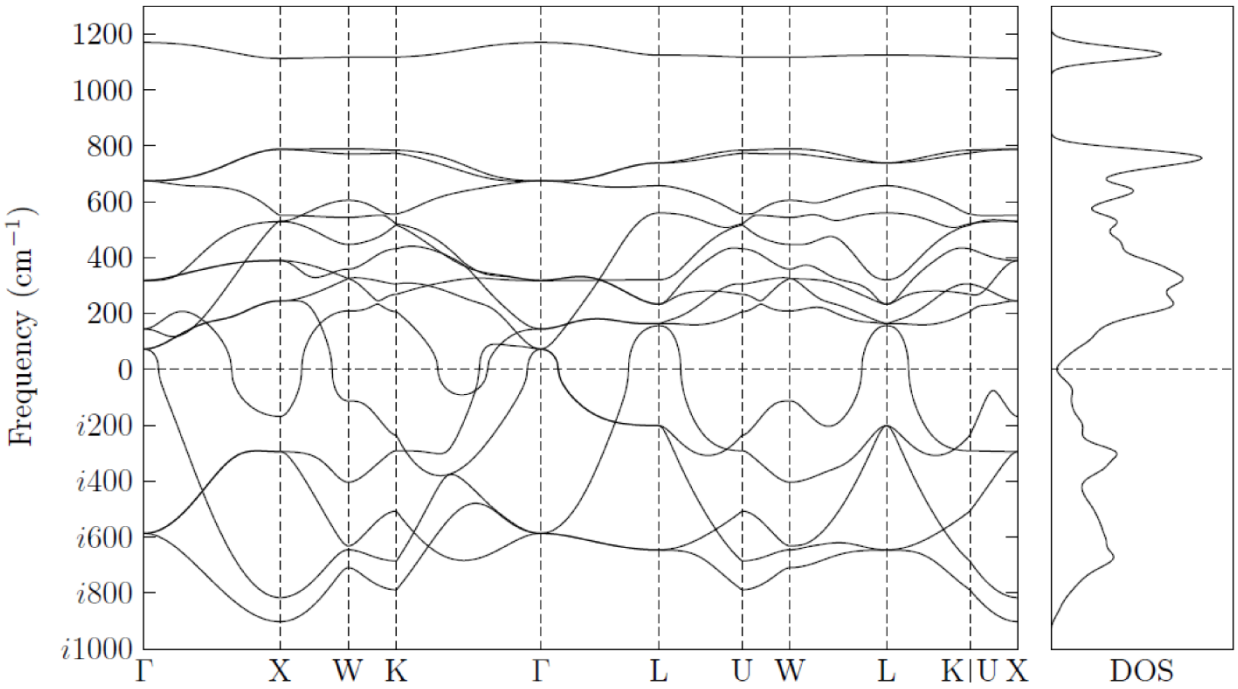

Figure S1 Calculated phonon dispersion curves along high-symmetry lines in the first Brillouin zone (left panel) and phonon density of states (right panel) for *cF*-B_5.

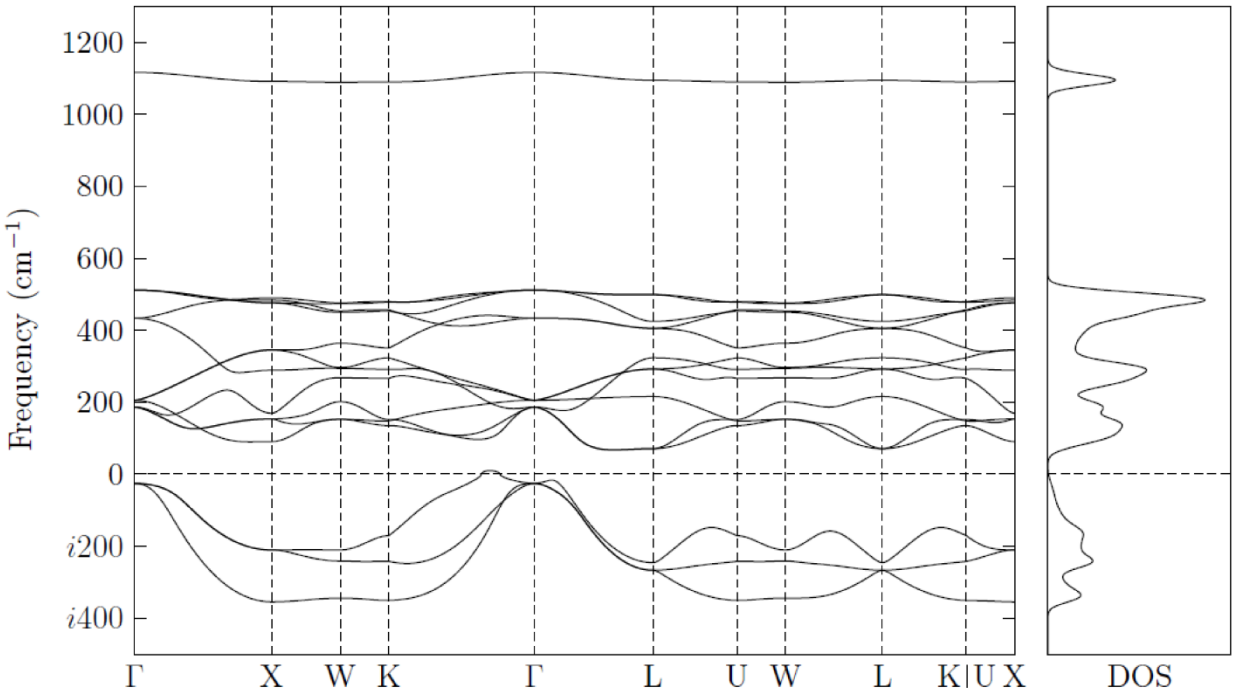

Figure S2 Calculated phonon dispersion curves along high-symmetry lines in the first Brillouin zone (left panel) and phonon density of states (right panel) for *cF*-B_4Al.