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

Semiconductive superhard FeB_4 phase from first-principles calculations

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Electronic Supplementary Information

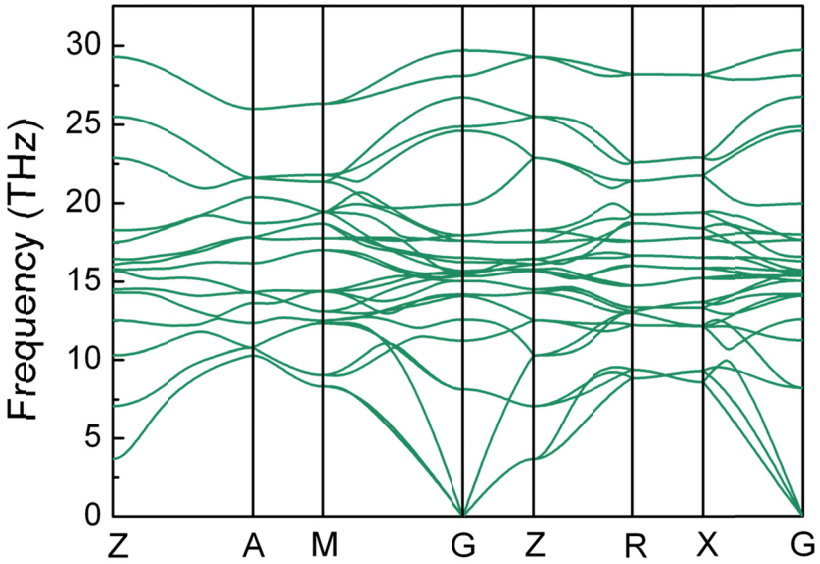

Fig. S1. Phonon dispersion curve of tP10-FeB_4 calculated at zero pressure.

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Table S1. Ionicity values applied for fitting the relationship between Philips ionicity (f_i) and Li's ionicity (f_l).

Crystal	f_l [a]	f_i [b]
Diamond	0	0
Si	0	0
Ge	0	0
c-BN	0.189	0.256
β-Si_3N_4	0.198	0.4
AlN	0.289	0.449
GaN	0.289	0.5
InN	0.328	0.578
Stishovite	0.28	0.57
Al_2O_3	0.37	0.796
SnO_2	0.328	0.78
Y_2O_3	0.453	0.843
AlP	0.164	0.307
AlAs	0.146	0.274
GaP	0.164	0.374
GaAs	0.146	0.31
GaSb	0.109	0.261
InP	0.2	0.421
InAs	0.181	0.357
InSb	0.144	0.321
ZnS	0.357	0.623
ZnSe	0.329	0.63

[a]Ref. 1, [b]Ref. 2,3

Reference:

1. K. Li, X. Wang, D. Xue, *J. Phys. Chem. A* **2008**, 112, 7894.

2. J. He, E. Wu, H. Wang, R. Liu, Y. Tian, *Phys. Rev. Lett.* **2005**, 94, 015504.

3. F. Gao, J. He, E. Wu, S. Liu, D. Yu, D. Li, S. Zhang, Y. Tian, *Phys. Rev. Lett.* **2003**, 91, 015502.