Supplementary information for 'Prediction of Superconductivity in Sandwich XB_4 (X=Li, Be, Zn and Ga) Films'

Shuming Zeng,[1,*] Yinchang Zhao,[2] Muhammad Zulfiqar,[3,†] and Geng Li[4,5,‡]

[1]*College of Physics Science and Technology, Yangzhou University, Jiangsu 225009, China*

[2]*Department of Physics, Yantai University, Yantai 264005, People's Republic of China*

[3]*Department of Physics, University of Sargodha, 40100 Sargodha, Pakistan*

[4]*School of Materials Science and Engineering, National Institute for Advanced Materials, Nankai University, Tongyan Road 38, Tianjin 300350, China.*

[5]*National Supercomputer Center in Tianjin, Tianjin 300457, China.*

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* zengsm@yzu.edu.cn

† muhammadżulfiqar@uos.edu.pk

‡ ligeng@nscc-tj.cn

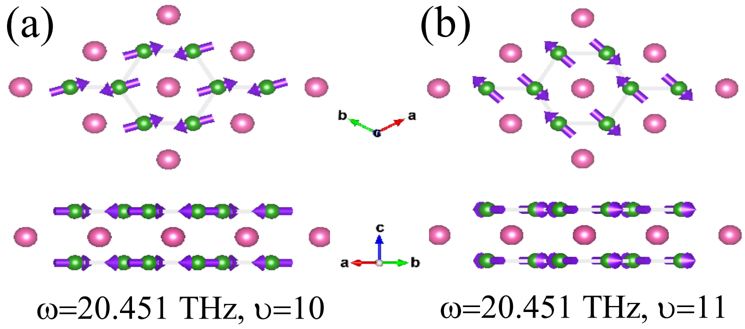

FIG. S1. Schematic diagram of the phonon modes of LiB_4 at the Γ point. ω and ν are the frequency and phonon band index, respectively. The length of the arrows is proportional to the amplitude of vibration. The top is the top view and the bottom is the side view in each subgraph.

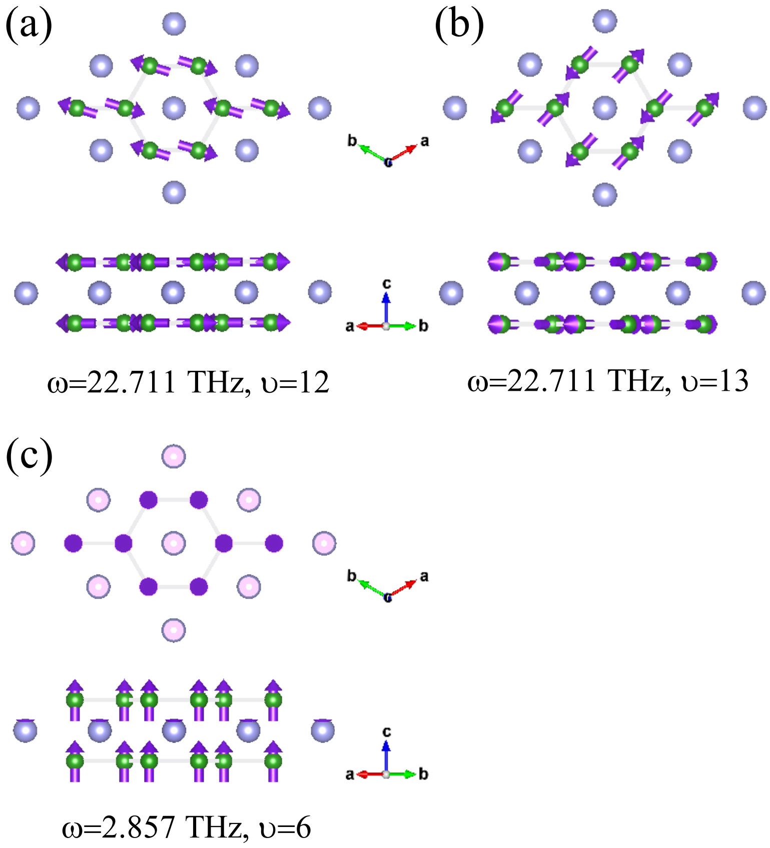

FIG. S2. Schematic diagram of the phonon modes of BeB_4 at the Γ point. ω and ν are the frequency and phonon band index, respectively. The length of the arrows is proportional to the amplitude of vibration. The top is the top view and the bottom is the side view in each subgraph.

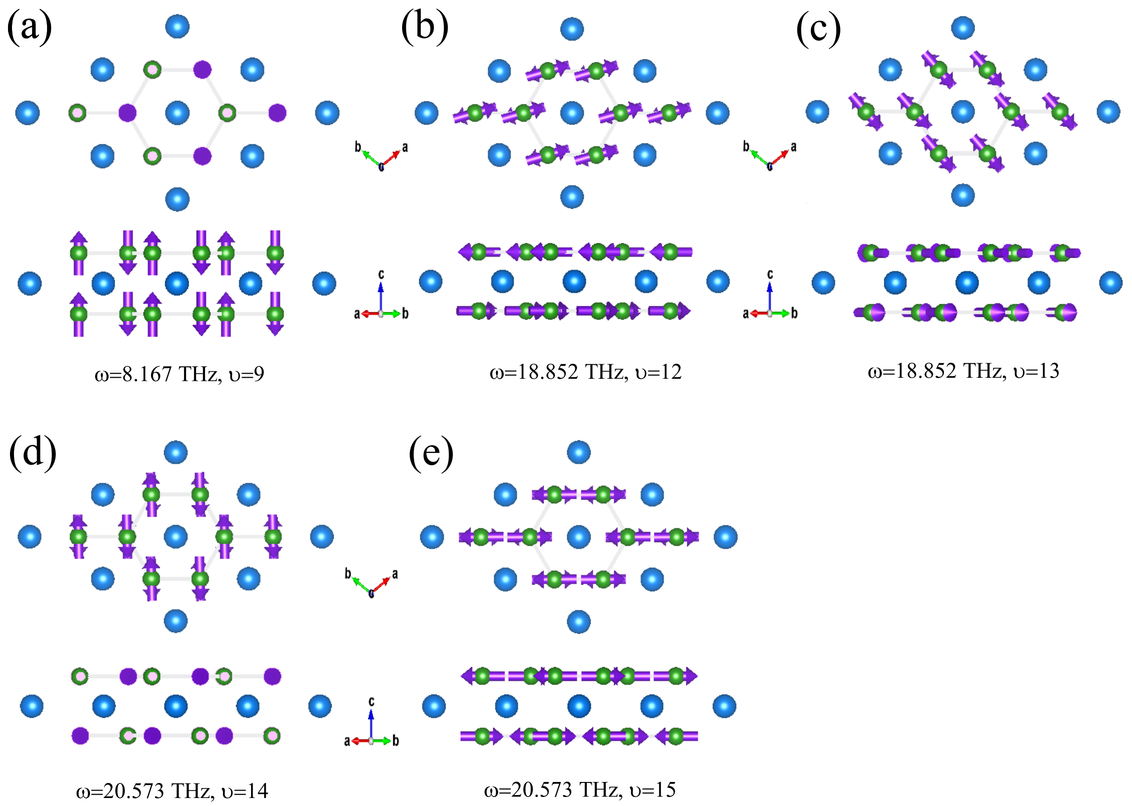

FIG. S3. Schematic diagram of the phonon modes of ZnB_4 at the Γ point. ω and ν are the frequency and phonon band index, respectively. The length of the arrows is proportional to the amplitude of vibration. The top is the top view and the bottom is the side view in each subgraph.

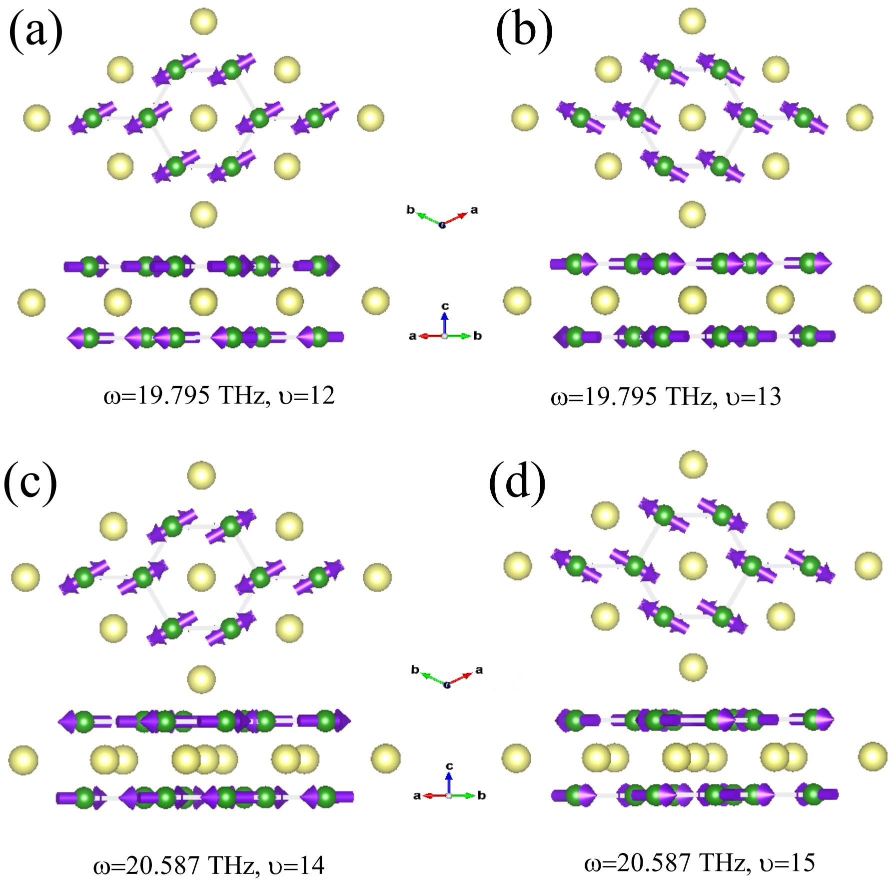

FIG. S4. Schematic diagram of the phonon modes of GaB_4 at the Γ point. ω and ν are the frequency and phonon band index, respectively. The length of the arrows is proportional to the amplitude of vibration. The top is the top view and the bottom is the side view in each subgraph.

TABLE SI. The convergence tests for the k-mesh (ZnB_4). Each test using 96 cores.

k-mesh	λ	$T_c^{\mu^*=0.10}(K)$	Times (hour)
18×18×1	1.23	38.69	15.11
36×36×1	1.24	38.77	41.45
48×48×1	1.24	38.76	103.64
60×60×1	1.24	38.76	184.56

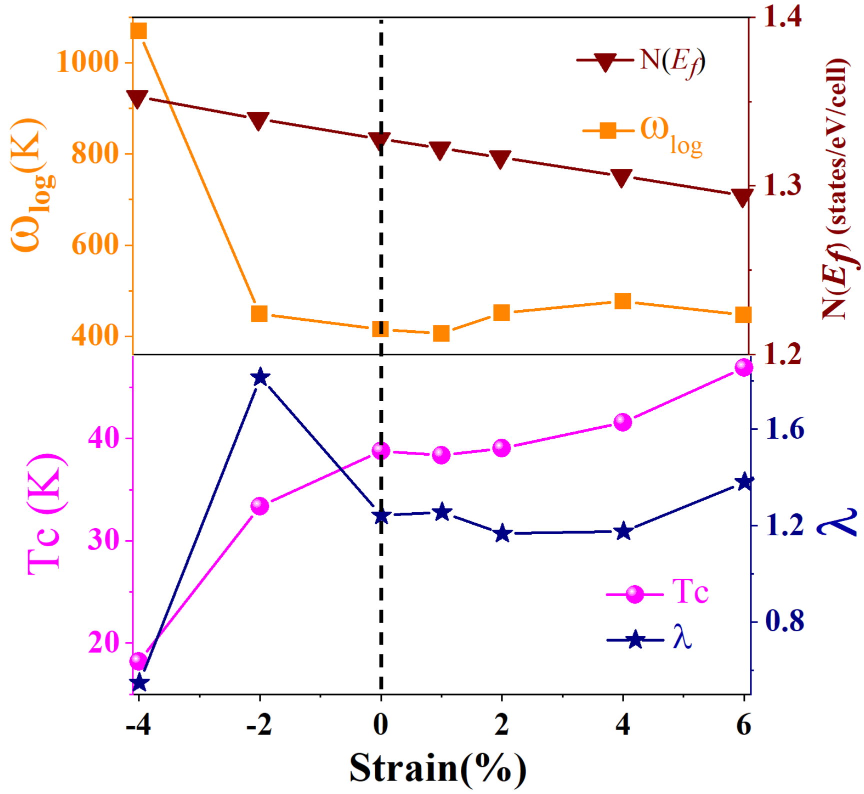

FIG. S5. Superconducting transition temperature T_c (magenta), EPC constant λ (royal), DOS of the FS N(E_f) (wine), and logarithmically averaged phonon frequency ω_{log} (orange) versus the strain ε for the sandwitched ZnB_4 film.

I. SCRIPT FOR T_c CALCULATION

1. Script to calculate electron-phonon coefficients

```
cat > elph.in <<eof
phonons of ZnB4
 &inputph
  tr2_ph=1.0d-14,   !!! effect phonon quality
  prefix=' ZnB4',
  fildvscf='ZnB4dv',
  amass(1)=65.409,
  amass(2)=10.811,
  outdir='./',
  fildyn='ZnB4.dyn',
  electron_phonon='interpolated',
  el_ph_sigma=0.005,
  el_ph_nsigma=10,
  alpha_mix=0.3,
  trans=.true.,
  ldisp=.true.,
  nq1=9, nq2=9, nq3=1
 /
eof
mpirun -np 96 ph.x < elph.in > elph.out
```

2. Script to calculate T_c

```
cat > tc.in <<eof
    30   0.5   1        ! emax (something more than highest phonon mode in THz), degauss, smearing method
      12               ! Number of q-points for which EPC is calculated,
    0.0000000    0.0000000    0.0000000 1
    0.0000000    0.1283001    0.0000000 6
    0.0000000    0.2566001    0.0000000 6
    0.0000000    0.3849002    0.0000000 6
    0.0000000    0.5132002    0.0000000 6
    0.1111111    0.1924501    0.0000000 6
    0.1111111    0.3207501    0.0000000 12
    0.1111111    0.4490502    0.0000000 12
    0.1111111    0.5773503    0.0000000 6
    0.2222222    0.3849002    0.0000000 6
    0.2222222    0.5132002    0.0000000 12
    0.3333333    0.5773503    0.0000000 2
    elph_dir/elph.inp_lambda.1
    elph_dir/elph.inp_lambda.2
    elph_dir/elph.inp_lambda.3
    elph_dir/elph.inp_lambda.4
    elph_dir/elph.inp_lambda.5
    elph_dir/elph.inp_lambda.6
```

```
        elph_dir/elph.inp_lambda.7
        elph_dir/elph.inp_lambda.8
        elph_dir/elph.inp_lambda.9
        elph_dir/elph.inp_lambda.10
        elph_dir/elph.inp_lambda.11
        elph_dir/elph.inp_lambda.12
        0.10                          ! \mu the Coloumb coefficient in the modified
                                    ! Allen-Dynes formula for T_c (via \omega_log)
    eof
    lambda.x < elph.in > elph.out
```

3. Output for T_c calculation

```
     lambda = 1.683100 (    1.682938 )  <log w>=  437.273 K  N(Ef)=
11.565178 at degauss= 0.005
     lambda = 1.318463 (    1.318304 )  <log w>=  420.748 K  N(Ef)=
9.286085 at degauss= 0.010
     lambda = 1.254620 (    1.254468 )  <log w>=  416.215 K  N(Ef)=
8.963193 at degauss= 0.015
     lambda = 1.241619 (    1.241492 )  <log w>=  415.578 K  N(Ef)=
8.974573 at degauss= 0.020
     lambda = 1.234089 (    1.233998 )  <log w>=  416.056 K  N(Ef)=
9.021735 at degauss= 0.025
     lambda = 1.228656 (    1.228600 )  <log w>=  416.901 K  N(Ef)=
9.085480 at degauss= 0.030
     lambda = 1.226354 (    1.226326 )  <log w>=  417.733 K  N(Ef)=
9.175427 at degauss= 0.035
     lambda = 1.226925 (    1.226919 )  <log w>=  418.260 K  N(Ef)=
9.289254 at degauss= 0.040
     lambda = 1.228852 (    1.228868 )  <log w>=  418.361 K  N(Ef)=
9.415892 at degauss= 0.045
     lambda = 1.230448 (    1.230489 )  <log w>=  418.016 K  N(Ef)=
9.543561 at degauss= 0.050
lambda         omega_log          T_c
   1.68310        437.273            55.214
   1.31846        420.748            42.036
   1.25462        416.215            39.306
   1.24162        415.578            38.768
   1.23409        416.056            38.534
   1.22866        416.901            38.409
   1.22635        417.733            38.399
   1.22692        418.260            38.469
   1.22885        418.361            38.551
   1.23045        418.016            38.579
```