

Supplemental Material for
High-throughput structure searches of ambient-pressure
superconductors in boron-carbon clathrates

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TABLE S1: The bond lengths, ICOHP values of the B-C, B-B, and C-C bonds of the intrinsic structure of B_8C_4 and $X_2B_8C_4$ ($X=Rb, Ca, Sr, Ba, La, Ce$), as well as the bader charge transfer amounts of the metal atoms doped at the apex and center were calculated.

| Structure | B-C (Å) | -ICOHP (eV/atom pair) | B-B (Å) | -ICOHP (eV/atom pair) | C-C (Å) | -ICOHP (eV/atom pair) | Bader(in) (eV) | Bader(out) (eV) |
|--------------|------------|--------------------------|------------|--------------------------|------------|--------------------------|-------------------|--------------------|
| B_8C_4 | 1.603 | 3.68 | 1.770 | 2.95 | 1.473 | 4.85 | - | - |
| $Rb_2B_8C_4$ | 1.729 | 6.88 | 1.897 | 5.72 | 1.583 | 8.88 | 0.678 | 0.659 |
| $Ca_2B_8C_4$ | 1.679 | 5.41 | 1.800 | 4.25 | 1.574 | 7.77 | 1.418 | 1.378 |
| $Sr_2B_8C_4$ | 1.719 | 6.75 | 1.835 | 5.18 | 1.604 | 8.17 | 1.386 | 1.367 |
| $Ba_2B_8C_4$ | 1.783 | 3.31 | 1.888 | 2.87 | 1.639 | 4.13 | 1.318 | 1.283 |
| $La_2B_8C_4$ | 1.734 | 2.52 | 1.825 | 1.79 | 1.632 | 3.37 | 1.716 | 1.672 |
| $Ce_2B_8C_4$ | 1.703 | 3.32 | 1.805 | 2.71 | 1.608 | 3.97 | 1.751 | 1.665 |

TABLE S2: The elastic and mechanical properties of the intrinsic B_8C_4 structure and the Rb-doped compound $Rb_2B_8C_4$ were calculated. All elastic constants and moduli are in units of GPa.

| Structure | C_{11} | C_{12} | C_{44} | B | G | E | ν |
|--------------|----------|----------|----------|---------|---------|---------|-------|
| B_8C_4 | 453.960 | 37.552 | -43.135 | 200.990 | 48.1600 | 133.860 | 0.390 |
| $Rb_2B_8C_4$ | 426.003 | 72.303 | 120.684 | 202.046 | 120.572 | 301.702 | 0.251 |

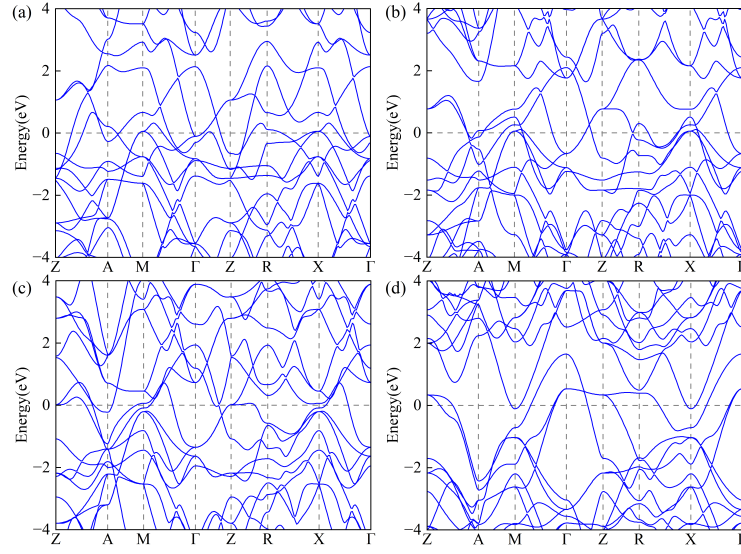


FIG. S1: The band structure for boron-carbon clathrates under ambient pressure. (a) $\text{In}_2\text{B}_8\text{C}_4$, (b) $\text{Pb}_2\text{B}_8\text{C}_4$, (c) $\text{Bi}_2\text{B}_8\text{C}_4$ and (d) $\text{Pr}_2\text{B}_8\text{C}_4$.

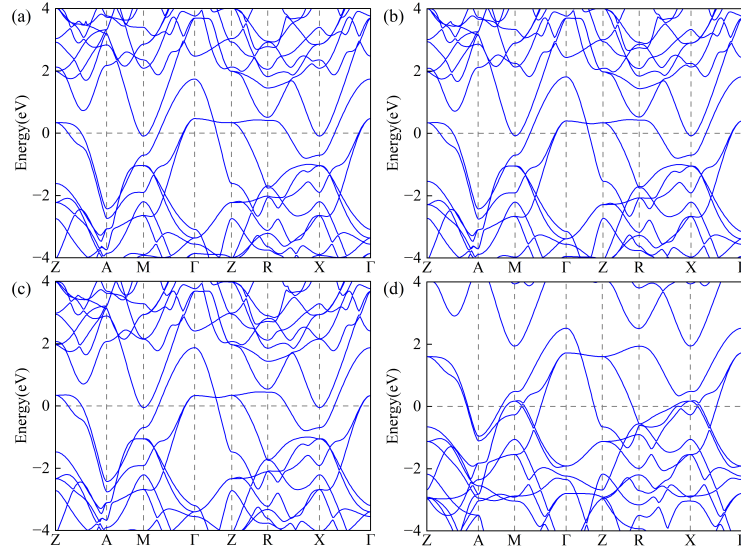


FIG. S2: The band structure for boron-carbon clathrates under ambient pressure. (a) $\text{Nd}_2\text{B}_8\text{C}_4$, (b) $\text{Pm}_2\text{B}_8\text{C}_4$, (c) $\text{Sm}_2\text{B}_8\text{C}_4$ and (d) $\text{Eu}_2\text{B}_8\text{C}_4$.

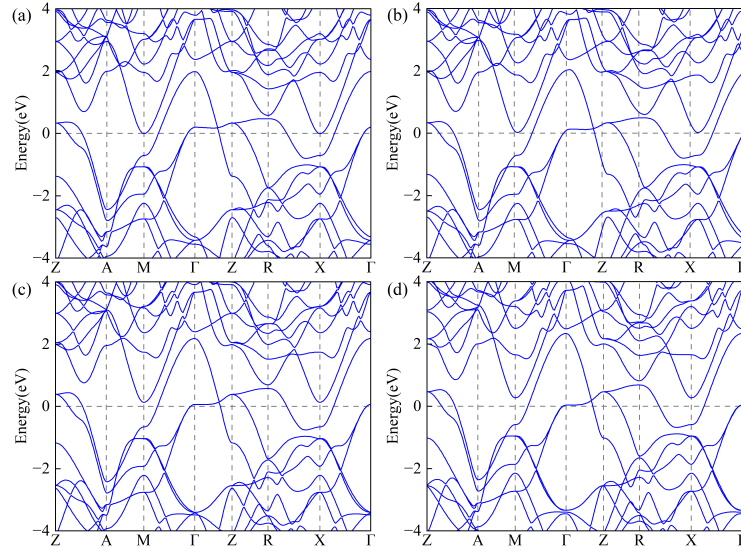


FIG. S3: The band structure for boron-carbon clathrates under ambient pressure. (a) $\text{Gd}_2\text{B}_8\text{C}_4$, (b) $\text{Tb}_2\text{B}_8\text{C}_4$, (c) $\text{Ho}_2\text{B}_8\text{C}_4$ and (d) $\text{Er}_2\text{B}_8\text{C}_4$.

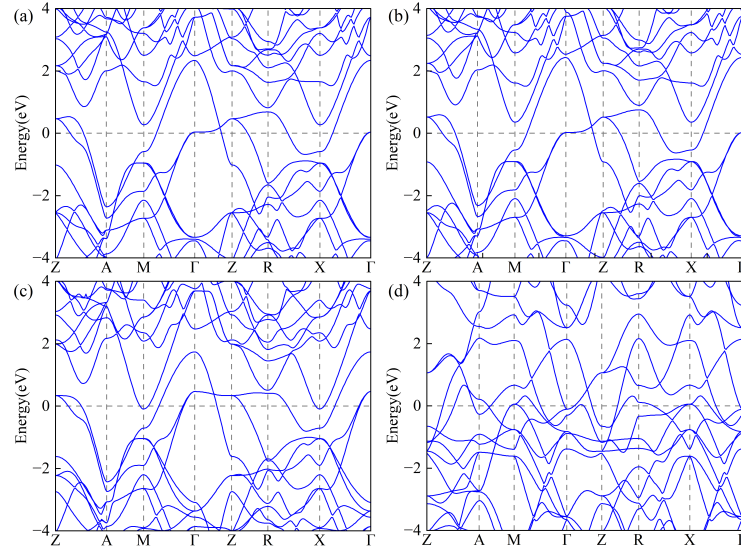


FIG. S4: The band structure for boron-carbon clathrates under ambient pressure. (a) $\text{Tm}_2\text{B}_8\text{C}_4$, (b) $\text{Yb}_2\text{B}_8\text{C}_4$, (c) $\text{Lu}_2\text{B}_8\text{C}_4$ and (d) $\text{Ce}_2\text{B}_8\text{C}_4$.

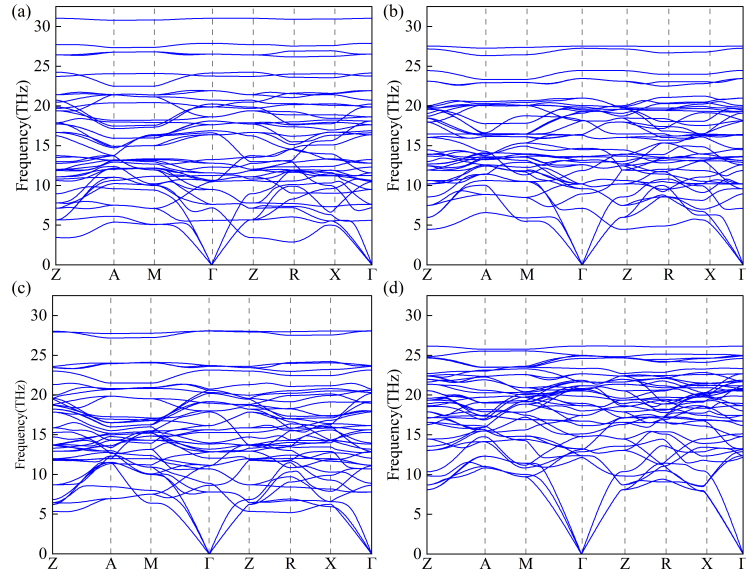


FIG. S5: The phonon spectrum for boron–carbon clathrates under ambient pressure. (a) $\text{In}_2\text{B}_8\text{C}_4$, (b) $\text{Pb}_2\text{B}_8\text{C}_4$, (c) $\text{Bi}_2\text{B}_8\text{C}_4$ and (d) $\text{Pr}_2\text{B}_8\text{C}_4$.

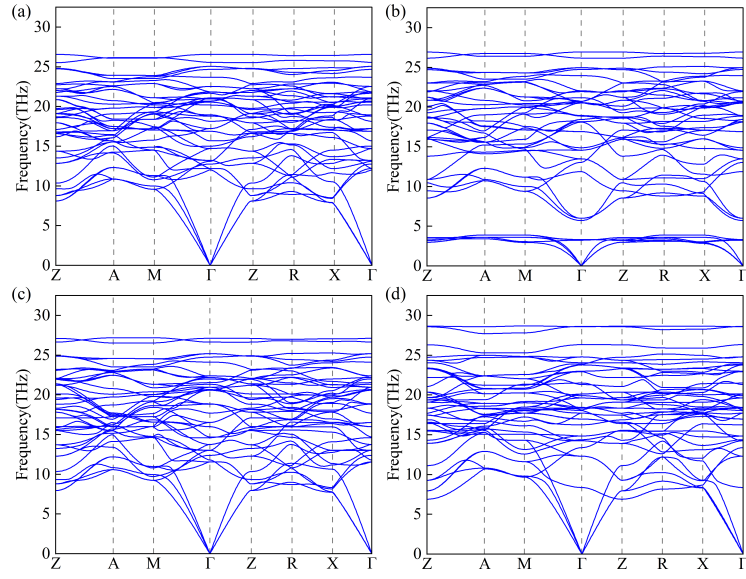


FIG. S6: The phonon spectrum for boron-carbon clathrates under ambient pressure. (a) $\text{Nd}_2\text{B}_8\text{C}_4$, (b) $\text{Pm}_2\text{B}_8\text{C}_4$, (c) $\text{Sm}_2\text{B}_8\text{C}_4$ and (d) $\text{Eu}_2\text{B}_8\text{C}_4$.

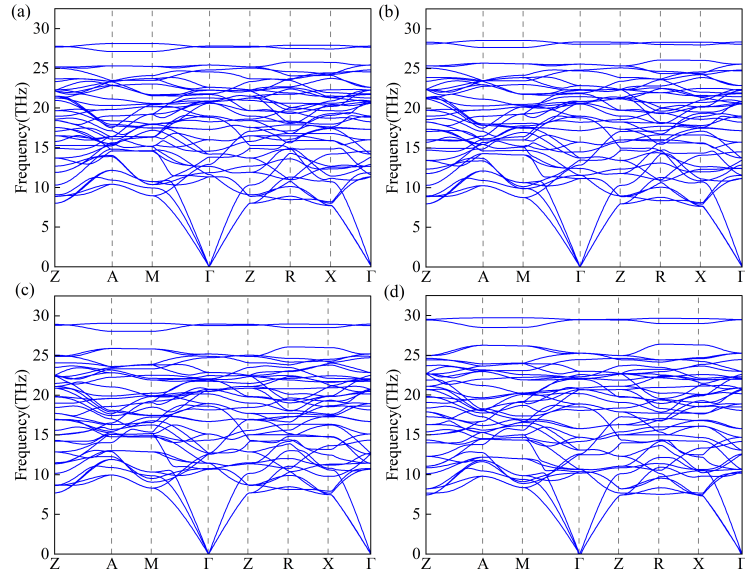


FIG. S7: The phonon spectrum for boron-carbon clathrates under ambient pressure. (a) $\text{Gd}_2\text{B}_8\text{C}_4$, (b) $\text{Tb}_2\text{B}_8\text{C}_4$, (c) $\text{Ho}_2\text{B}_8\text{C}_4$ and (d) $\text{Er}_2\text{B}_8\text{C}_4$.

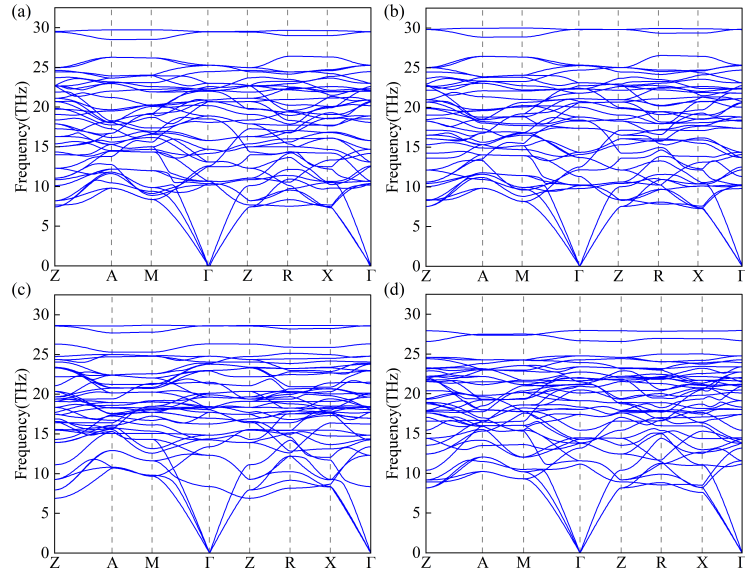


FIG. S8: The phonon spectrum for boron-carbon clathrates under ambient pressure. (a) $\text{Tm}_2\text{B}_8\text{C}_4$, (b) $\text{Yb}_2\text{B}_8\text{C}_4$, (c) $\text{Lu}_2\text{B}_8\text{C}_4$ and (d) $\text{Ce}_2\text{B}_8\text{C}_4$.

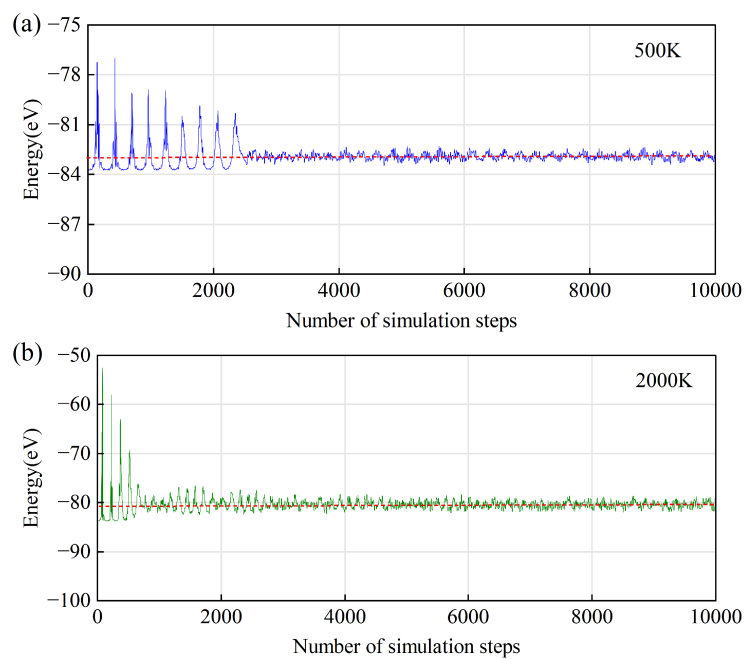


FIG. S9: The AIMD curves for $\text{Rb}_2\text{B}_8\text{C}_4$. (a) 500 k (b) 2000 K

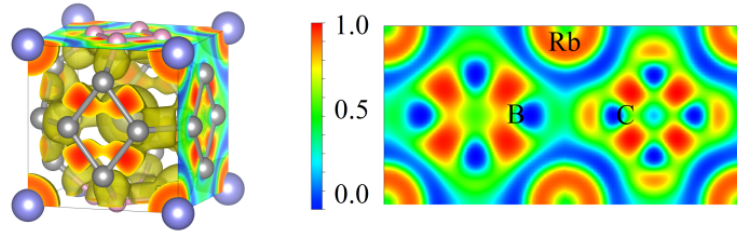


FIG. S10: 3D electron density isosurfaces and ELF plot of $\text{Rb}_2\text{B}_8\text{C}_4$ under ambient pressure.

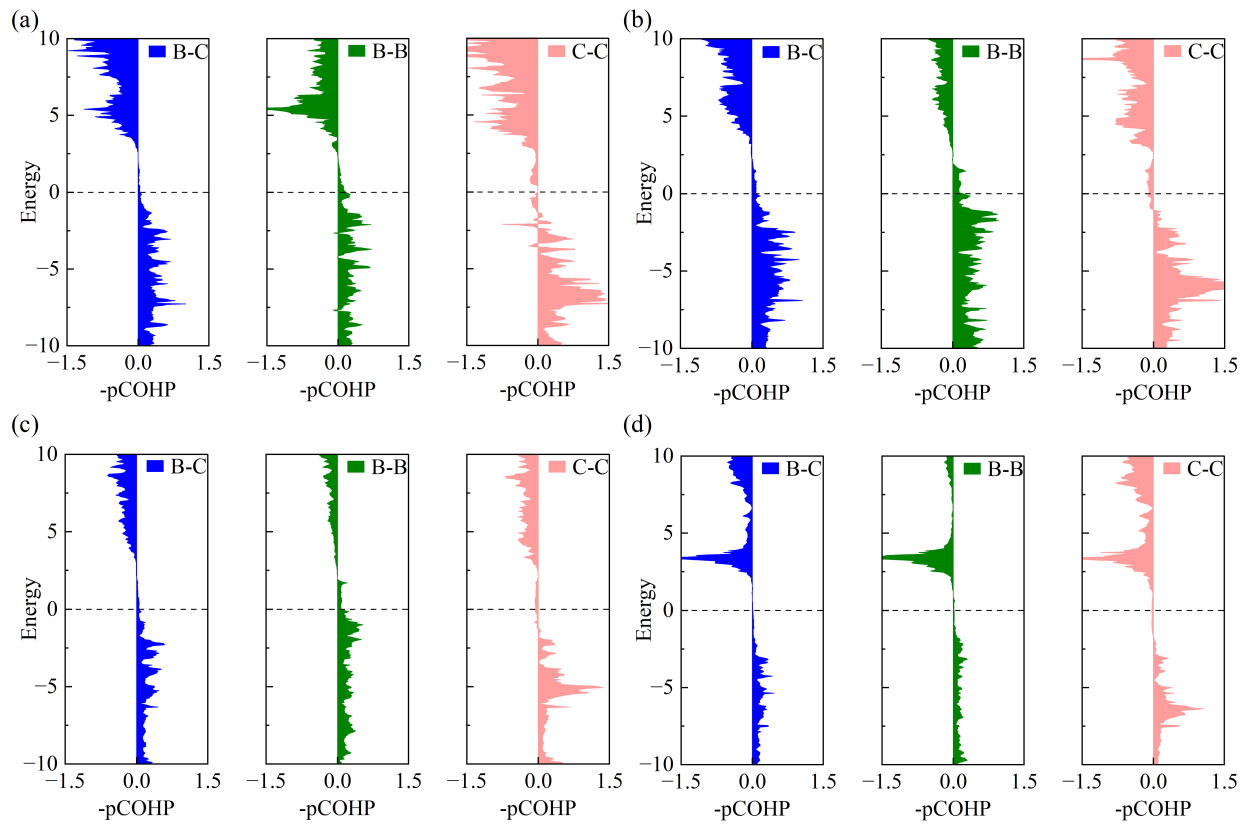


FIG. S11: The $-p\text{COHP}$ curves for boron-carbon clathrates under ambient pressure. (a) $\text{Ca}_2\text{B}_8\text{C}_4$, (b) $\text{Sr}_2\text{B}_8\text{C}_4$, (c) $\text{Ba}_2\text{B}_8\text{C}_4$ and (d) $\text{La}_2\text{B}_8\text{C}_4$.

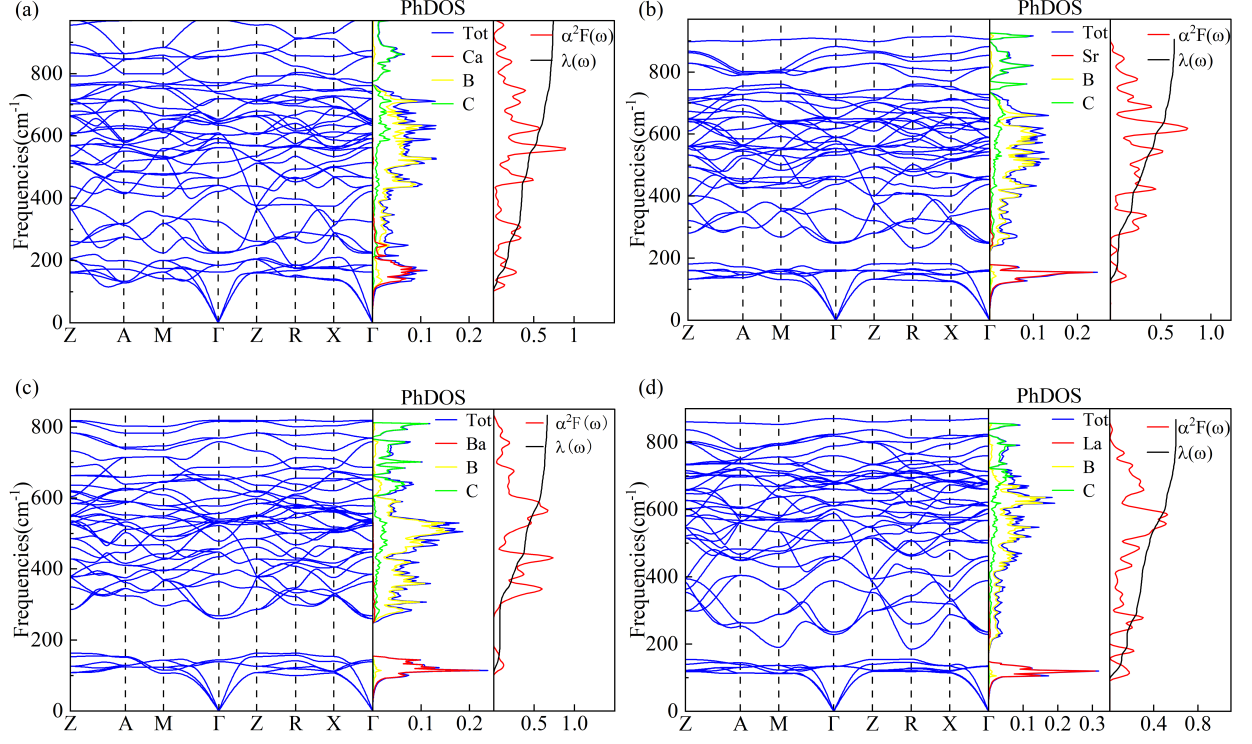


FIG. S12: The calculated PhDOS, $\alpha^2 F(\omega)$, and EPC integrals $\lambda(\omega)$ for boron-carbon clathrates under ambient pressure. (a) $\text{Ca}_2\text{B}_8\text{C}_4$, (b) $\text{Sr}_2\text{B}_8\text{C}_4$, (c) $\text{Ba}_2\text{B}_8\text{C}_4$ and (d) $\text{La}_2\text{B}_8\text{C}_4$.

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