Supplement

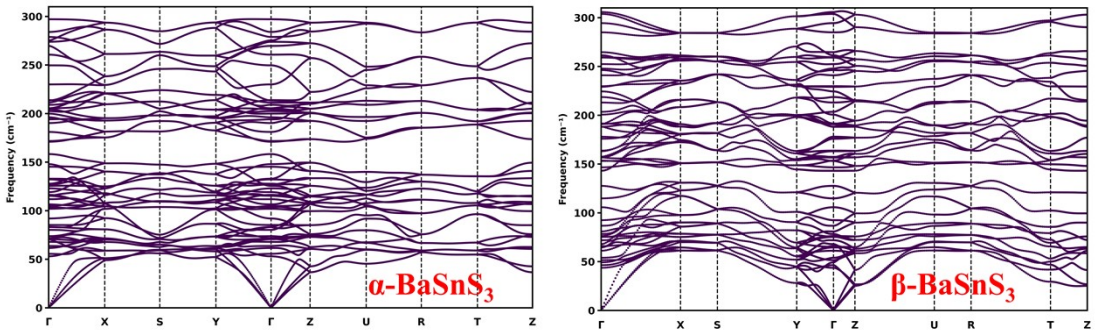

Figure S1: Phonon dispersion of the two structures at 0 K

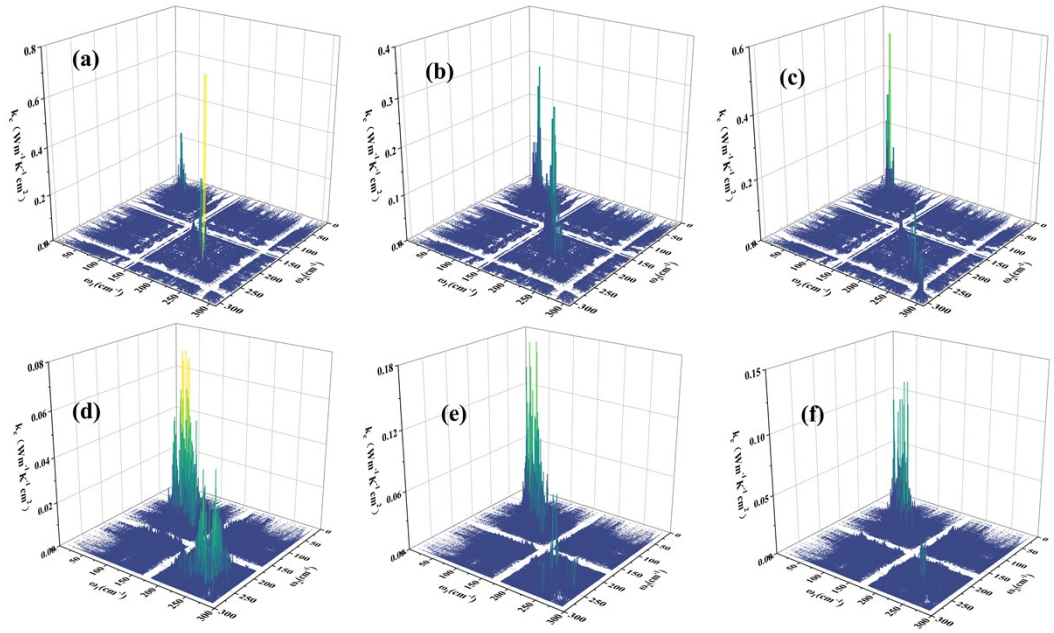

Figure S2：The mode $\kappa_c(\omega_1, \omega_2)$ of the contribution of the interbranch coherence term is calculated using the frequency of the anharmonic phonon and the eigenvector at 300 K. The points on the diagonal correspond to the quasidegenerate eigenstates ($\omega_1 \approx \omega_2$). Panels (a)-(c) represent the results for α-$BaSnS_3$ along the three Cartesian directions a, b, and c, respectively, while panels (e)-(g) show the results for β-$BaSnS_3$.

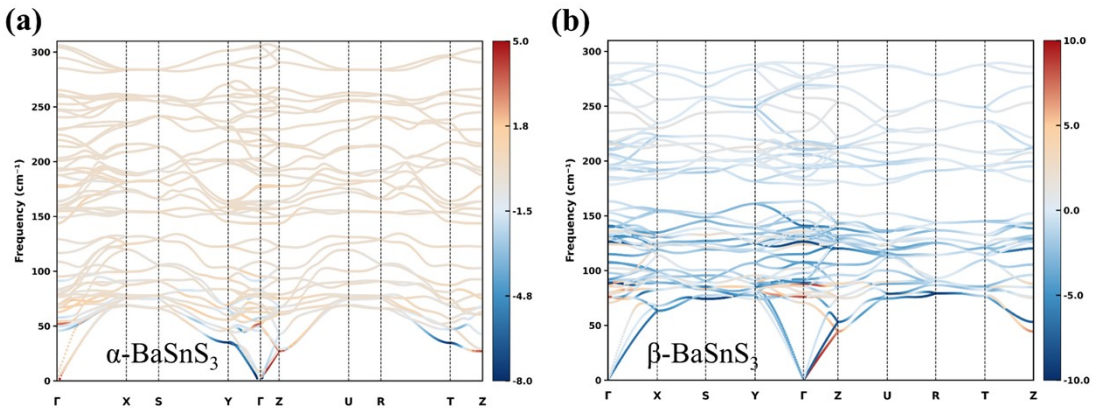

Figure S3: Grüneisen parameter projections on the phonon dispersion along high-symmetry paths at 300 K.

AMSET input：

settings = {

general settings

"scattering_type": ["IMP", "ADP","POP"],

"doping": [-1e18, -2e18, -3e18, -4e18, -5e18, -6e18, -7e18, -8e18, -9e18, -1e19, -2e19, -3e19, -4e19, -5e19, -6e19, -7e19, -8e19, -9e19, -1e20, -2e20, -3e20, -4e20, -5e20, -6e20, -7e20, -8e20, -9e20, -1e21, 1e18, 2e18, 3e18, 4e18, 5e18, 6e18, 7e18, 8e18, 9e18, 1e19, 2e19, 3e19, 4e19, 5e19, 6e19, 7e19, 8e19, 9e19, 1e20, 2e20, 3e20, 4e20, 5e20, 6e20, 7e20, 8e20, 9e20, 1e21],

"temperatures": [300,600],

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"bandgap": 1.629,
# electronic_structure settings
"interpolation_factor": 35,
# materials properties
"deformation_potential": "deformation.h5",
"elastic_constant": [
[     67.787,     30.859,     41.268,     -0.000,     -0.000,     -0.000 ],
[     30.859,     96.578,     30.470,      0.000,      0.000,     -0.000 ],
[     41.268,     30.470,     80.091,     -0.000,     -0.000,      0.000 ],
[     -0.000,      0.000,     -0.000,     29.539,     -0.000,      0.000 ],
[     -0.000,      0.000,     -0.000,     -0.000,     26.240,      0.000 ],
[     -0.000,     -0.000,      0.000,      0.000,      0.000,     33.435 ],
 ],
"static_dielectric": [[18.116406, 0, 0], [0, 25.365648, 0], [0, 0, 13.979044]],
"high_frequency_dielectric": [[8.412952, 0, 0], [0, 8.487048, 0], [0, 0, 6.911846]],
"pop_frequency": 5.22,
# performance settings
"write_mesh": True,


settings = {
        # general settings
        "scattering_type": ["IMP", "ADP","POP"],
        "doping": [-1e18, -2e18, -3e18, -4e18, -5e18, -6e18, -7e18, -8e18, -9e18, -
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4e20, -5e20, -6e20, -7e20, -8e20, -9e20, -1e21, 1e18, 2e18, 3e18, 4e18, 5e18, 6e18,
7e18, 8e18, 9e18, 1e19, 2e19, 3e19, 4e19, 5e19, 6e19, 7e19, 8e19, 9e19, 1e20, 2e20,
3e20, 4e20, 5e20, 6e20, 7e20, 8e20, 9e20, 1e21],
        "temperatures": [300,600],
        "bandgap": 1.12,
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    # electronic_structure settings
    "interpolation_factor": 35,
    # materials properties
    "deformation_potential": "deformation.h5",
    "elastic_constant": [
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        [34.241, 101.051, 45.128, 0.000, 0.000, 0.000],
        [47.771, 45.128, 75.852, 0.000, 0.000, 0.000],
        [0.000, 0.000, 0.000, 24.887, 0.000, 0.000],
        [0.000, 0.000, 0.000, 0.000, 30.458, 0.000],
        [0.000, 0.000, 0.000, 0.000, 0.000, 29.320],
    ],
    "static_dielectric": [[40.751878, 0, 0], [0, 48.472853, 0], [0, 0, 54.157067]],
    "high_frequency_dielectric": [[12.518883, 0, 0], [0, 12.368479, 0], [0, 0,
10.894433]],
    "pop_frequency": 4.04,
    # performance settings
    "write_mesh": True,
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