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Aikinite systems:

ultra-low thermal conductivity for thermoelectric applications

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- Distance between Cu and Pb : smaller than the sum of their van-der Waals radii.
- Bonding environment around the Bi³⁺ cation is heterogeneous.

Conclusion



LOW THERMAL CONDUCTIVITY in aikinite:

- Higher U_{iso} of Cu and Pb: weak interatomic bonding and 'rattling'-like vibrations.
- Weakly bonded channels of Pb, larger mode-resolved Grüneisen parameter for Pb.
- Low frequency phonon modes observed from INS: attributed to optical modes for Pb.
- Low phonon lifetime for Pb mode: indicate increased phonon-phonon scattering.
- Pb mode hardening with increasing temperature: evidence of high anharmonicity.
- Short Cu-Pb distance: Interaction between Cu⁺ and 6s² lone pairs of Pb²⁺.
- TUNABLE SEMICONDUCTING TYPE: p-type CuPbBiS₃ to n-type via halide doping and stoichiometric changes.

References

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HPC-MSU: computation facility