

PROCEEDINGS

High-Throughput Discovery of Crystalline Thermal Insulators Using Machine-Learning Interatomic Potentials

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ABSTRACT

Crystalline materials with intrinsically low lattice thermal conductivity (κ_L) are of great interest for thermal barrier coatings and thermoelectric applications, yet their discovery remains challenging due to the limitations of conventional trial-and-error approaches. Herein, we develop a high-throughput computational framework that integrates universal machine-learning interatomic potentials [1] with temperature-dependent lattice dynamics [2] and advanced phonon transport theory [3,4] to enable efficient and accurate prediction of thermal transport properties. Applying this approach to a diverse set of crystalline compounds, we identify multiple candidate materials exhibiting ultralow κ_L . Detailed lattice dynamics and bonding analyses reveal that such behavior originates from a hierarchical bonding framework, in which weakly bonded and highly coordinated polyhedra coexist with comparatively stronger sublattices. This bonding heterogeneity gives rise to reduced phonon group velocities and pronounced vibrational mismatch between coordination environments. As a result, both particle-like phonon propagation and wave-like coherent transport channels are effectively suppressed, leading to strongly reduced heat conduction. These findings highlight the critical role of bonding hierarchy and anharmonicity in governing thermal transport and provide physically interpretable design principles for crystalline thermal insulators. More broadly, this work demonstrates a scalable data-driven strategy for accelerating the discovery of materials with tailored thermal transport properties.

KEYWORDS

Machine-learning interatomic potentials; lattice dynamics; thermal conductivity; chemical bonding

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