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Machine Learning and First-Principles Predictions of Materials with Low Lattice Thermal Conductivity CHIA-MIN LIN, CHENG-CHIEN CHEN, University of Alabama at Birmingham — Data-driven machine learning (ML) approaches have recently become popular and powerful in materials discovery. Here, we use combined ML and density functional theory (DFT) simulations to search for materials with low lattice thermal conductivity, which is crucial for improving the energy conversion performance of thermoelectric devices. Several compounds formed by cadmium as well as elements from the alkali metal and carbon groups are predicted to exhibit low lattice thermal conductivity (¡ 1 W/mK). Our DFT calculations of electronic structures and transport properties further indicate that the figure of merit ZT value for thermoelectric performance can be greater than 1 near 400 K in compounds like K2CdPb, where are thereby promising candidate materials for low-temperature thermoelectric applications.

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