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Anomalous Lattice Dynamics in PbTe and Its Implications to Low Intrinsic Lattice Thermal Conductivity YI ZHANG, Department of Physics and HiPSEC, University of Nevada, Las Vegas, XUEZHI KE, Department of Physics, East China Normal Univeristy, Shanghai, China, PAUL KENT, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, CHANGFENG CHEN, Department of Physics and HiPSEC, University of Nevada, Las Vegas, JIHUI YANG, Materials Science and Engineering Department, University of Washington — Recent experiments on PbTe-based high performance thermoelectric materials raise fundamental questions about the nature of low intrinsic lattice thermal conductivity and underlying lattice dynamics. We show by first-principles calculations that the reported results can be attributed to abnormally large-amplitude thermal vibrations that stem from a delicate competition of dual ionicity and covalency, which puts PbTe near ferroelectric instability. It produces anomalous properties such as partially localized low-frequency phonon modes, a soft transverse optical phonon mode, and a positive temperature coefficient for the band gap. These results account for experimental findings and resolve the underlying atomistic mechanisms. The relation between these anomalies and the low intrinsic lattice thermal conductivity will be discussed.

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