# Predicting Thermal Conductivity and Classifying Chemical Bonds using DFT and Machine Learning

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This talk details our development of computational tools for accurately predicting thermal conductivity from first-principles calculations. We utilize harmonic and anharmonic force constants, extracted from supercell DFT calculations, to model phonon transport. Applying this methodology to lanthanum-pnictides, we demonstrate a counterintuitive result: LaBi's thermal conductivity surpasses that of LaP, despite the lighter mass of phosphorus. We attribute this discrepancy to the strong anharmonicity in LaP, a consequence of its more metavalent La-P bonds. In the second part, we explore the nature of metavalent bonding itself. To remove any bias, we employ unsupervised machine learning classification on a broad material dataset. We identify four descriptors that effectively categorize five distinct bonding types, excluding weak Hydrogen and van der Waals interactions. This analysis provides new insights into chemical bonding beyond traditional classifications.