Machine Learning driven insight into Bonding Heterogeneity Effects on Thermal Conductivity

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Materials at both ends of the thermal conductivity spectrum are desirable for various technological applications. Despite substantial progress in modeling thermal transport within materials, identifying materials with the desired thermal conductivity remains a considerable challenge. This difficulty is partly attributable to the computationally intensive nature of such calculations and to the complexities of modeling many body interactions in solids.[1,2] Recognizing that chemical bonding within a material plays a crucial role in phonon dynamics, several studies have incorporated bonding analysis to investigate the origins of low lattice thermal conductivity. These studies have identified bonding-related features, including bonding heterogeneity, as among the important factors that induce low lattice thermal conductivity.[3–6] In this work, the investigation aims to determine whether we can find such an observation on a larger scale using machine learning techniques. To achieve this, a database of bonding analysis data obtained using the LOBSTER[7–10] program was first generated for approximately 13,000 materials[11,12] sourced from the Materials Project.[13] This data was subsequently transformed into machine-learning-ready descriptors that can numerically quantify the material's bonding heterogeneity. These descriptors were evaluated within machine learning algorithms (e.g., random forests) to assess how their inclusion, alongside traditional structure and composition-based descriptors, influences model predictive performance. The primary target property in these models is the total lattice thermal conductivity, including three-phonon interactions.[14] ML models, on average, showed a significant reduction in prediction errors, and feature importance analyses indicated that bonding heterogeneity descriptors exert a considerable influence. Finally, using SISSO,[15,16] a symbolic regression technique, a new descriptor was identified, revealing that increased bonding heterogeneity in a material correlates with a decrease in total lattice thermal conductivity.

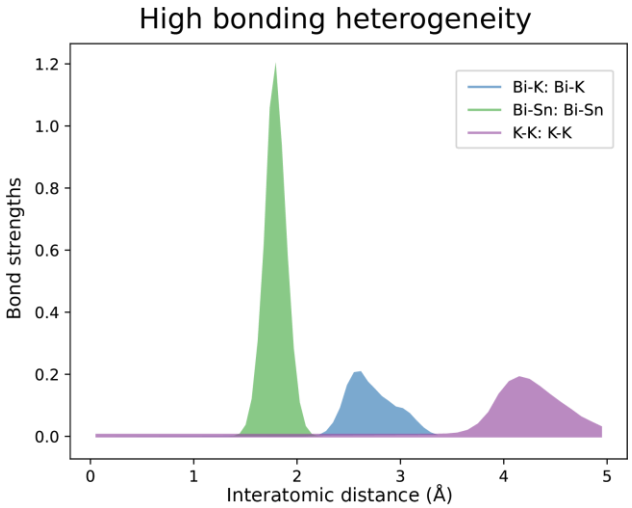

Figure 1: Illustrative example for a material with high bonding heterogeneity

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