Understanding and Optimizing Bulk Thermoelectric Materials
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Thermoelectric materials research continues to expand due to the need to increase energy conversion efficiencies, as well as the expanding role of thermoelectrics in niche applications. I will review several examples demonstrating the successes and limitations of semi-classical models of electron and phonon transport in the study of bulk thermoelectric materials. Single band models provide a simple starting point for analysis and optimization, and can facilitate the development of more physically-accurate models. The importance of identifying intrinsically favorable electronic structures will be demonstrated with La$_{3-x}$Te$_4$, where a heavy-band/light-band configuration leads to desirable properties. Using other chalcogenides and intermetallics as examples, I will also discuss the importance of phonon dispersions and scattering mechanisms, and how they can provide insight for materials exploration efforts. Research supported by the U. S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.