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Thermoelectric Materials and Novel Thermoelectric Phenomena

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Striking the balance between thermal and charge transport is a main goal when searching for optimized thermoelectric materials. This difficult task can be achieved by controlling detailed features in the band structure as well as increase the phonon scattering mechanisms. We will discuss methodologies developed in the AFLOW consortium (www.aflow.org) to improve the quality and the speed of the theoretical predictions through a set of examples. Specifically novel rattling mechanism in oxy-chalcogenides, electronic bands convergence due to Ca- and Ga-doping in SnTe, and novel thermoelectric minerals.