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Atomic-Level Lattice Chemistry for High-Performance Bulk Thermoelectrics

In Chung

Department of Chemical and Biological Engineering, Seoul National University, South Korea

Email: inchung@snu.ac.kr

The deliberate introduction of foreign atoms and vacancies into bulk crystal lattices generates atomic-scale defects whose structure depends on local coordination chemistry and size matches with host atoms. These defects can evolve into higher-order configurations, from one-dimensional dislocations to multidimensional nanostructures, which interact with charge carriers and phonons in unique ways. By tailoring these interactions, defect engineering provides a powerful route to manipulate key physical properties of bulk solids and achieve otherwise unattainable functionalities. Establishing the formation mechanisms of such defects is therefore essential for developing predictable design principles that enable precise control of target structures within crystals. Extending this atomic-level understanding to mesoscopic and macroscopic lattice chemistries further allows stabilization of heterostructured nanohybrid materials with emergent properties.

In this work, I present our recent progress on predictive design principles for multiscale defect architectures across diverse crystal systems. These strategies allow decoupled control of fundamental parameters governing the thermoelectric figure of merit (ZT), including carrier mobility, carrier concentration, electrical conductivity, and Seebeck coefficient, ultimately leading to a series of record-performance thermoelectric materials capable of converting waste heat into usable electrical energy.