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Structurally complex Zintl compounds for high temperature thermoelectric power generation ALEXANDRA ZEVALKINK, Jet Propulsion Laboratory, GREGORY POMREHN, ZACHARY GIBBS, JEFFREY SNYDER, California Institute of Technology — Zintl phases, characterized by covalently-bonded substructures surrounded by highly electropositive cations, exhibit many of the characteristics desired for thermoelectric applications. Recently, we demonstrated promising thermoelectric performance (zT values between 0.4 and 0.9) in a class of Zintl antimonides that share a common structural motif: anionic moieties resembling infinite chains of linked tetrahedra. These compounds ($A_5M_2Sb_6$ and A_3MSb_3 compounds where A = Ca or Sr and M = Al, Ga and In) crystallize as four distinct, but closely related chain-forming structure types. Their large unit cells lead to exceptionally low lattice thermal conductivity due to the containment of heat in low velocity optical phonon modes. Here, we show that chemical substitutions on the A and M sites can be used to control the electronic and thermal transport properties and optimize the thermoelectric figure of merit. Doping with alio-valent elements allows for rational control of the carrier concentration, while isoelectronic substitutions can be used to fine-tune the intrinsic properties. A combination of Density Functional calculations and classical transport models was used to explain the experimentally observed transport properties of these compounds.

Alexandra Zevalkink
Jet Propulsion Laboratory

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