Creating nanostructures within alloyed bulk thermoelectric materials can greatly decrease the lattice thermal conductivity of the material and sometimes increase the electronic power factor, thereby increasing the thermoelectric figure of merit (ZT). This nanostructuring paradigm has yielded ZTs upwards of 2 within PbTe-SrTe and similar materials. However, the rational design of thermoelectric alloys with even larger figures of merit will require a quantitative knowledge of the phase stability and electronic structure of nanoscale precipitates within a bulk phase. We demonstrate a first-principles computational approach that has helped, in conjunction with experimental efforts, to accelerate the discovery of more efficient thermoelectric materials. We give examples of how computations have provided key information about phase stability in these nanostructured systems, as well as thermodynamic and electronic properties of the matrix/nanostructure interfaces.1-6

References: