Ab ca c a e a ce e a c d c a d e d c e e thermoelectric materials.

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Within the last few years it has been possible to compute the lattice thermal conductivity of bulk materials using ab initio methods. The interactions between the phonons are obtained from density functional theory and this information is incorporated into the Boltzmann to obtain the thermal conductivity. The good accuracy obtained from those calculations allows trying to use them to find new materials.

We present several strategies that we used performing such a search. The first method we used is datamining. We screened the entire MPD library to find materials with ultra low thermal conductivity using a Bayesian algorithm based on kriging with gaussian regression processes. We were able to evidence new crystalline structures, some of them with a thermal conductivity lower than wood! Among these compounds some have good electronic properties that could make them exceptional thermoelectric materials.

The second method we used is based on polymorphism. Starting from the experimentally known crystalline phase of the thermoelectric Zn-Sb compound, we reconstructed the energy surface using the Minima Hopping Method and discovered that the ground state is not the experimentally known phase. Computing the physical properties we realized that this new ground state has even better thermoelectric properties than the known ZnSb phase.

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