The high throughput approach in the search for novel materials

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The search for novel materials with improved tailored properties can be substantially accelerated with the help of ab initio high throughput computation. This is especially interesting in high priority fields like renewable energies or micro/nano electronics. After a brief introduction to the high throughput modeling philosophy, and some prior research in several fields, I will discuss how the high throughput approach has been applied to the search of novel materials for thermoelectric energy conversion. We have concentrated on half Heusler compounds. Our search through 79,057 different compositions has yielded 75 thermodynamically stable ternary compounds. We have calculated the bulk thermal conductivity for these compounds, employing a fully ab-initio approach. We find a considerable fraction of compounds for which the bulk thermal conductivities are much lower than those of known half Heuslers. We have also developed several machine learning techniques that considerably reduce the computation time, while still yielding efficient screening. We have also estimated the thermoelectric figure of merit (ZT) of the compounds within the small grain approximation. When compared with common semiconductors like Si, Ge, or the III-V compounds, half-Heuslers stand out due to having higher power factors. Estimated ZT's suggest that for some of the nanograined half-Heuslers the figure of merit might reach values above 2.