

## Looking for new thermoelectric materials among ternary intermetallic using high-throughput calculations

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Novel high-performance materials are needed for developing thermoelectric devices. One way to answer this need is to identify new materials which could exhibit promising properties. In order to screen a large number of compounds, we have decided to combine first-principles calculations and experiments.

We focus our investigation within the ternary intermetallic compounds  $T-M-X$ , with  $T$  a transition metal, a rare earth or an alkaline earth metal,  $M$  an element from the first line of the transition metal and  $X$ , a metalloid. In each prototype, all the possible  $T-M-X$  combination are investigated by DFT calculations. Among all these candidates, those which are predicted as thermodynamically unstable and metallic are dismissed. For the most promising compounds, predicted stable and semiconductor, complementary calculations as the phonon structure or additional BoltzTrap calculations can be provided to go further. After those theoretical steps, experimental investigations are done to confirm calculations and measured thermoelectric properties.

In the presentation, we will discuss our screening method through the example of several prototypes as TiNiSi [1], MgAgAs or Mg<sub>6</sub>Cu<sub>16</sub>Si<sub>7</sub>. For instance, the study of the equimolar TMX in four different prototypes lead to the investigation of 2280 possible configuration. Then our screening process allowed us to highlight more than 20 possible new semiconductors, which could be promising for thermoelectric applications.

[1] Barreteau C. *et al.*, Looking for new thermoelectric materials among TMX intermetallics using high-throughput calculations, *Comput. Mater. Sci.*, 156 (2019) 96-103