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DEFECTS AND THEIR INFLUENCE ON THE THERMOELECTRIC PROPERTIES OF MATERIALS: AN *AB INITIO* STUDY

Alexandre BERCHE and Philippe JUND

ICGM, Univ. Montpellier, CNRS, ENSCM, Montpellier, France
philippe.jund@umontpellier.fr

For thermoelectric applications, *ab initio* methods generally fail to predict the transport properties of materials because of their inability to predict properly the carrier concentrations that control the electronic properties. Concerning the thermal properties, the study of the impact of defects is mainly hindered by the huge computer resources needed to consider the large supercells necessary for this kind of study.

In this presentation, a methodology based on the thermodynamics of defects and the phase stability supposed to fill in this gap (especially concerning the electronic properties) is presented. It is then applied to several thermoelectric materials belonging to the Heusler family. We show for the NiTiSn [1] half-Heusler compound that by taking into account the scattering of phonons by the grain size boundaries (*i.e.* nanostructuring), a good agreement of the calculated thermal conductivity with experiments can be obtained. Similarly in the Fe_2VAl Heusler compound [2], the existence of cubic Al-V antiphase clusters around an Iron atom permits to explain the peculiar measured electronic properties of this material.

[1] P. Hermet and P. Jund, J. Alloy. Compd. **688**, 248-252 (2016)
[2] A. Berche, M. Talla Noutack, M.-L. Doublet and P. Jund, Materials Today Physics **13**, 100203 (2020)