Jožef Stefan Institute
Ljubljana, Slovenia
K7 / Department for
Nanostructured Materials

VIRTUAL SEMINAR
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Advances in Thermoelectric Ternary and Quaternary Sulphides

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The design and optimization of thermoelectric (TE) materials rely on the intricate balance between thermopower (S), electrical resistivity (r) and thermal conductivity (k); perfecting such a balance is key to improve energy recovery systems and TE cooling devices. Complex copper sulfides can provide an eco-friendly high-performance low-cost alternative by using elements that are abundant in naturally occurring minerals. Most of these materials exhibit low thermal conductivity possibly determined by local structural distortions, rattling phenomena, or strong bond anharmonicity. However, the improvement of the TE performances of these materials remains a challenge, due to the interdependent and contrary effects of their parameters S, r and k. The presence of structural defects, non-stoichiometry, the nature of the chemical bonds, order/disorder phenomena in these complex structures are still a matter of debate, which is of capital importance for the optimization of their TE properties. Our investigations on some thermoelectric complex sulphides derived from natural minerals (colusite, tetrahedrite, stannoidite, germanite, mohite-derivatives) will be presented.1 Mechanical alloying, SPS sintering, as well as structural and microstructural features will be reported, together with electrical, thermal properties. Band structure and vibrational dispersions from first principles calculations will be discussed.

[1] JACS 140 (2018) 2186, Angewandte Chemie Int. Ed. 58 (2019) 15455, Adv. Energy Mater. 9 (2019) 1803249, PRM 4 (2020) 025404, Chem. Mater. 32 (2020) 830, Acta Mater. 195 (2020) 229, Appl. Mater. Today 22 (2021) 100948, J. Mater. Chem. C 9 (2021) 773 (Review article), Angewandte Chemie Int. Ed. (2021, DOI : 10.1002/anie.202108686), J. Mater. Chem. A 9 (2021) 10812, Inorg. Chem. (2021, DOI: 10.1021/acs.inorgchem.1c02105)

Kindly invited.