

## MS18. Thermoelectric materials - from fundamental science to applications

Chairs: Oliver Oeckler, Sylvie Hébert

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### MS18-O1 Structure dynamics relation of thermoelectric materials studied by neutron spectroscopy and *ab initio* calculations

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Minimizing the lattice thermal conductivity  $k_l$  is one promising way of improving the figure of merit of thermoelectric materials [1,2]. Several mechanisms are known leading to a strong reduction of  $k_l$ . The most efficient mechanisms are due to complex structures resulting in a general diminishment of heat-carrying vibrational states and to scattering of the heat-carrying acoustic phonons. Phonon scattering can be accomplished in many ways. Imperfection of a structure in the form of site and chemical disorder, presence of voids, interfaces, surfaces and dislocations open up temperature independent scattering channels. In perfectly ordered, crystalline matter umklapp-scattering and multi-phonon events establish efficient scattering mechanisms at high temperatures.

In thermoelectric materials all those mechanisms are simultaneously present. Moreover, the interplay of disorder, anharmonicity and structure deformation on temperature and pressure changes can lead to new and non-stationary features in the dynamics of the compounds which can open up additional decay channels for acoustic phonons. The anharmonic off-center motion of cations in clathrates is one example of such complex dynamics [3].

A comprehensive characterization of the interplay of acoustic phonons with scattering centres requires their discrimination and the understanding of their effect on the collective dynamics on a microscopic scale. This prerequisite is met by Inelastic Neutron Scattering (INS) and neutron diffraction. INS is a spectroscopic technique sampling the 4-dimensional phase space of energy and momentum matching the energies of collective vibrational excitations and the interatomic distances in thermoelectric compounds. We present a characterization of the dynamics of filled skutterudites [4] and of the open-framework compounds AV<sub>2</sub>Al<sub>20</sub> (A = Al, Ga, Sc, La) and AOs<sub>2</sub>O<sub>6</sub> (A = K, Rb, Cs) [5]. We discuss the aspect of collective dynamics as well as the consequences of so called ‘rattling’ modes for the lattice thermal conductivity of these compounds.

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