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Thermal conductivity and lattice dynamics in structurally complex materials

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The lattice thermal conductivity of many different materials are displaying a 'glass like behavior' [1], with a relatively small value of the lattice thermal conductivity at ambient temperature and an almost independent temperature dependence in the range 20 to 300 K. This is the case for disordered crystals [1], for clatharates [2], but also for aperiodic crystals [3] such as the icosahedral quasicrystal i-AlPdMn [4], and the Rb_2ZnCl_4 phase that displays an incommensurately modulated phase between 190 and 300 K [5]. The detailed understanding of this behavior and the relationship between the phonon spectrum/phonon lifetime and the thermal conductivity is still a matter of debate.
In this presentation I will introduce the two main aspects of structural complexity, namely number of atom in the unit cell and disorder. On one hand, the structural complexity may be characterized by the number of atoms in the unit cell, which goes to infinity in the case of aperiodic crystals. On the other hand disorder may occur as chemical site disorder or lattice displacement. By reviewing some recent results in this field I will show the relative importance of structure and disorder [6]. A simple model of a phonon lattice gaz, as developed for Ge based clathrates [2] will be used to interpret some of the data.

[1] D. G. Cahill, S. K. Watson, and R. O. Pohl, Physical Review B **46**, 6131 (1992).
[2] P.-F. Lory *et al.*, Nature Communications **8**, 491 (2017).
[3] T. Janssen, G. Chapuis, and M. de Boissieu, *Aperiodic Crystals. From modulated phases to quasicrystals (second edition)* (Oxford University Press, Oxford, 2018), Vol. 20, IUCr Monographs on Crystallography.
[4] M. A. Chernikov, A. Bianchi, and H. R. Ott, Physical Review B **51**, 153 (1995).
[5] D.-M. Zhu and A. C. Anderson, J. Low Temp. Phys. **94**, 117 (1994).
[6] P. F. Lory *et al.*, Physical Review B **102**, 024303, 024303 (2020).