Contribution ID: **39** Type: **Oral contribution**

Tunable bonding in the incipient metal thermoelectric GeTe

Monday, March 15, 2021 3:25 PM (20 minutes)

The group IV-VI chalcogenides have important thermoelectric applications. GeTe has emerged as a promising non-toxic candidate, especially when the high-temperature cubic phase is suppressed to room temperature. However, even the mechanism of phase transition is disputed, as is the presence of disorder. Here we combine ab initio MD with synchrotron X-ray and dynamic neutron pair distribution function (PDF) analysis. We show that previous reports of disorder and symmetry breaking are entirely due to highly damped and anharmonic phonons. As predicted by metavalent bonding theories, this arises due to a softening in local bonding on heating, which strengthens long-range <100>c correlations. This picture is consistent with reported changes in resistivity and dielectric constant, and shown to be ubiquitously present in other polarisable binary chalcogenides and hR6 structured elements. Our results unify the results of local probes and spectroscopy as applied to binary chalcogenides, and should inspire a re-examination of other highly anharmonic energy materials such as hybrid perovskites and 'rattling' thermoelectrics.

Primary authors: KIMBER, Simon (Université Bourgogne Franche-Comté); Dr ZHANG, Jiayong (Brookhaven National Laboratory); Dr CHENG, Yongiang (Oak Ridge National Laboratory); Dr ABERNATH, Douglas (Oak Ridge National Laboratory); Dr RAMIREZ-CUESTA, Timmy (Oak Ridge National Laboratory); Dr HUDSPETH, Jessica (ESRF); Dr LUO, Zhong-Zhen (Northwestern University); Prof. KANATZIDIS, Mercouri (Northwestern University); Prof. BILLINGE, Simon (Columbia University); Dr CHATTERJI, Tapan (Institut Laue Langevin)

Presenter: KIMBER, Simon (Université Bourgogne Franche-Comté)

Session Classification: Disordered Materials, complex crystal structures and aperiodic crystals, diffuse scattering and 3D-PDF

Track Classification: Disordered Materials, complex crystal structures and aperiodic crystals, diffuse scattering and 3D-PDF