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Exploring nanoscale fluctuations and ferroelectric phase stabilization in S doped PbTe thermoelectrics KEVIN KNOX, EMIL BOZIN, Brookhaven National Laboratory, CHRISTOS MALLIAKAS, MERCOURI KANATZIDIS, Northwestern University, SIMON BILLINGE, Columbia University, Brookhaven National Laboratory — PbTe is one of the most important commercial thermoelectric materials for applications above room temperature. A paraelectric phase of fluctuating ferroelectric-like Pb structural dipoles emerges in PbTe at elevated temperatures, although it adopts an average rock-salt structure at all temperatures. These intrinsic nanoscale fluctuations are believed to improve the thermoelectric properties of PbTe by limiting the lattice thermal conductivity. Additionally, alloying and chemical substitution in PbTe appreciably improve the thermoelectric figure of merit, as is the case in $PbTe_{1-x}S_x$. However, the exact mechanism for this enhancement is not well understood. It has been shown that $PbTe_{1-x}S_x$ exhibits a peak in resistivity at a doping dependent temperature. By analogy with Ge doped PbTe, this anomalous resistivity may be the signature of a ferroelectric phase stabilization. In this talk, we explore this possibility by characterizing the average and the local structure of $PbTe_{1-x}S_x$ as a function of temperature and doping using a neutron based atomic pair distribution function (PDF) approach.

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