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Ferroelectric Phase Transition and the Minimal Lattice Thermal Conductivity of (Pb,Ge)Te Alloys RONAN MURPHY, Tyndall National Institute, Cork, Ireland, EAMONN MURRAY, Departments of Physics and Materials, Imperial College, London, UK, STEPHEN FAHY, IVANA SAVIC, Tyndall National Institute, Cork, Ireland — Exploiting the fascinating properties of materials near soft mode phase transitions is an emerging concept in the quest to increase thermoelectric efficiency [1,2]. The underlying idea is that soft phonons lead to intrinsically low thermal conductivity, while possibly preserving electronic transport properties. Here we investigate how tuning the proximity to the ferroelectric phase transition via chemical composition affects the lattice thermal conductivity of $Pb_{1-x}Ge_xTe$ alloys [3]. Using first-principles virtual-crystal simulations, we show that the anharmonic contribution to the lattice thermal conductivity is minimized at the phase transition due to the maximized acoustic-optical interaction. The interplay between anharmonicity and mass disorder shifts the conductivity minimum towards the composition at which the scattering due to mass disorder is maximized. Our results suggest that tuning soft optical modes in $Pb_{1-x}Ge_xTe$ and similar alloys may be a promising strategy to enhance their thermoelectric efficiency. [1] D. T. Morelli, V. Jovovic, and J. P. Heremans, Phys. Rev. Lett. 101, 035901 (2008). [2] L.-D. Zhao et al, Nature 508, 373 (2014). [3] R. M. Murphy, E. D. Murray, S. Fahy, and I. Savic, Phys. Rev. B 93, 104304 (2016).

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