Abstract Submitted
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Giant thermal resistivity of interlaced nanoparticles[1] YEVGENIY PUZYREV, XIAO SHEN, SOKRATES PANTELIDES, Vanderbilt University — We present a theoretical study of thermal resistivity of "interlaced crystals," recently discovered in hexagonal-$CuInS_2$ nanoparticles [1]. Interlaced crystals exhibit a perfect global Bravais lattice with two cations and multiple ordering patterns within the cation sublattice. The interlaced crystal consists of interlaced domains and phases where the corresponding phase/domain boundaries are not uniquely defined. Since there are no structural defects or strain, the interlacing has a minimal effect on electronic properties, but causes a large increase in phonon scattering at the boundaries. The size of domains reaches down to one nanometer, resulting in a high density of the boundaries, making interlaced crystals an attractive candidate for thermoelectric applications. Large-scale molecular dynamics calculations show orders of magnitude increase in the thermal resistivity caused by a high density of boundaries. This is a general effect, arising due to a mass disparity of the cations present in interlaced crystals.

[1] "Interlaced crystals having a perfect Bravais lattices and complex chemical order revealed by real-space crystallography." X. Shen, et. al, Nature Comm. 10.1038/ncomms6431.

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