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Doping studies of alkali-metal rocksalt based I-V-VI_2 compounds with intrinsically minimal thermal conductivity MICHELE NIELSEN, Department of Mechanical Engineering, The Ohio State University, VIDVUDS OZOLINS, Department of Materials Science, UCLA, JOSEPH HEREMANS, Department of Mechanical Engineering, Department of Physics, Ohio State University
— Past research has shown that rocksalt-based I-V-VI compounds have intrinsically low thermal conductivity as a result of the lone-pair electrons on the group V element. Theoretical calculations have revealed the presence marginally stable acoustic phonons which have extremely large Grüneisen parameters. These result in a strong anharmonicity in heat-carrying acoustic phonon branches of select I-V-VI_2 compounds. Here, we extend this work to the electronic properties of the materials, which all have similar valence band structures. As a result of these two material properties, we are able to explore if the excellent zT observed in $AgSbTe_2$ extends to materials with cheaper starting elements and better high-temperature stability. Here we introduce new doping studies in I-V-VI_2 compounds where the group I element is an alkali-metal atom.

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