Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Pressure intrinsically induced thermoelectric enhancement in the SnSe crystal YONGSHENG ZHANG, Institute of Solid State Physics, Chinese Academy of Sciences, SHIQIANG HAO, Department of Materials Science and Engineering, Northwestern University, LI-DONG ZHAO, Beihang University, CHRISTOPHER WOLVERTON, Northwestern University, ZHI ZENG, Institute of Solid State Physics, Chinese Academy of Sciences — SnSe is an excellent thermoelectric material due to its high ZT value ($\sim$2.6 along the b direction) at high temperature $\sim$923 K. However, in the temperature range of 300$-$773K, the ZT values are just 0.1$-$0.9. To make this material more efficient, its thermoelectric properties should be large in the entire temperature range. Here, we use DFT calculations to show how pressure intrinsically enhances the thermoelectric properties below 700 K along the three directions (a, b and c) of the crystal (the low-T SnSe-$Pnma$ phase) due to a significant boost in electrical transport. The estimated ZT values of p-type along the b and c directions can reach as high as 3.3 and 2.1 at 6 GPa and 700 K, respectively. At 6 GPa, the a direction shows n-type properties and its ZT value is 1.9 at 600 K. It is significant that high-performance both n-type and p-type conductors could be available in SnSe just through applying pressure. Our work on SnSe under pressure sheds light on a new mechanism for screening high efficiency thermoelectric materials.

Yongsheng Zhang
Institute of Solid State Physics, Chinese Academy of Sciences

Date submitted: 24 Nov 2015 Electronic form version 1.4