Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

**Impact of Lone-Pair Electrons on Thermal Conductivity in CuSbS2 Compound**[1] BAOLI DU, RUIZHI ZHANG, KAN CHEN, MICHAEL REECE, Queen Mary University of London, MATERIAL RESEARCH INSTITUTE TEAM — Compounds with intrinsically low lattice thermal conductivity are of practical importance for thermoelectric energy conversion. Recent studies suggest that s2 lone pair orbital electrons are a key contributing factor to the anomalously low lattice thermal conductivity of chalcogenide compounds that contain a nominally trivalent group VA element. CuSbS2 has an orthorhombic structure with space group Pnma. The pyramidal SbS5 units are separated by CuS4 tetrahedron so that the base of the square pyramidal units are aligned to face one another, thus directing the Sb lone pair electron density into the void separating the SbS5 units. Different from tetrahedrite, all the Cu atoms are bonded in the CuS4 tetrahedron. So, it has a perfect structure to study the influence of electron lone pair on thermal conductivity without the impact from trigonal coordinated Cu. In this work, the trivalent transition metal atom Fe and IIIA atom Ga without lone-pair electrons were chosen to substitute Sb in CuSbS2. The changes in the bonding environment by foreign atoms and their influences on the thermal properties have been studied and correlated.

[1]Marie Curie International Incoming Fellowship of the European Community Human Potential Program under Contract no. PIIF-GA-2013-622847

Baoli Du
Queen Mary University of London

Date submitted: 03 Nov 2015 Electronic form version 1.4