Abstract Submitted
for the SHOCK19 Meeting of
The American Physical Society

Electronic transport properties of Li_2SnX_3(X=S, Se) from first principles calculation ENAMUL HAQUE, MD. ANWAR HOSSAIN, Mawlana Bhashani Science and Technology University — Lithium-based materials usually exhibit very attractive properties such as fast ionic conduction and high thermal stability. Here, the calculated electronic transport properties of fast ion conductors using the first-principles method will be presented. All the calculations have been performed by using Tran-Blaha-modified Becke-Johnson (TB-mBJ) potential. The obtained indirect bandgap of Li_2SnS_3 is 2.14 eV, which fairly agrees with the measured value of 2.38 eV. But Li_2SnSe_3 shows direct bandgap (1.95 eV). The energy bands of both materials are flat that lead to high Seebeck coefficient approaching ˜326 V K^{-1} at 700 K. The combination of high Seebeck coefficient and conductivity leads to high power factor (reaching ˜6 mW m^{-1} K^{-1} at 700 K). Because of their high thermal stability and high power factor, both materials are the potential candidate for thermoelectric device applications. The electronic structure and physical mechanism behind high power factor will be explained in details.

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Date submitted: 01 Apr 2019 Electronic form version 1.4