

Abstract Submitted
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The electrical and thermoelectric properties of isoelectronic doping in SnSe : a first principles study* DUC CUONG DO, S.H. RHIM, Department of Physics and Energy Harvest Storage Research Center, University of Ulsan, Republic of Korea, JOO-HYOUNG LEE, School of Materials Science and Engineering, Gwangju Institute of Science and Technology, Republic of Korea, SOON CHEOL HONG, Department of Physics and Energy Harvest Storage Research Center, University of Ulsan, Republic of Korea — SnSe has been well-known as an excellent thermoelectric material with the highest ZT up to 2.6 at high temperature . Recently, there has been much attention on the thermoelectric properties of SnSe-based materials. In this work, we present a first-principles study on the electrical and thermoelectric properties of SnSe by isoelectronic doping; substitutions of C, Si, and Ge for the Sn site and S and Te for the Se site, with 3.125 and 6.250% concentration. Among those dopants, C gives a big modification of band structure with the band gap reduced by the defect levels in the band gap, whereas changes in band structure by other dopants are negligible. It is suggested that the C doped SnSe can improve the Seebeck coefficient near room temperature and enhance the power factor at high temperature, because of the electrical conductivity enhanced by the localized defect state of the C doped SnSe. * This work is supported by grants from the Priority Research Centers Program (Grant No. NRF-2009-0093818) and the Basic Science Research Program (Grant No. NRF-2015R1A2A2A01003621) through NRF funded by the MOE and MSIP of Korea.

Duc Cuong Do
University of Ulsan

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