Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

The way to enhance thermoelectric properties of Bi_2O_2Q (Q=S and Se) system by introducing chalcogen mixture net.[1] CHANGHOON LEE, JISOOK HONG, Pohang University of Science and Technology, WANG RO LEE, Chonbuk National University, DAE YEON KIM, 4Agency for Defense Development (ADD), JI HOON SHIM, Pohang University of Science and Technology — First principles density functional theory calculations were carried out for the series of bilayered semiconducting Bi_2O_2Q (Q=S, Se) and hypothetically constructed Bi2O2S0.5Se0.5 compounds in which chalogen square net of pure Bi_2O_2Q compound is replaced with having stripe type structure of chalcogen mixture net to explore their electronic structures, the change in their electronic structures under the chalcogen mixing, and the possibility for improving in their thermoelectric properties. By introducing chalcogen mixture net in pure Bi_2O_2Q, the band gap should be adjusted, and the indirect band gap in pure Bi_2O_2Q compound is changed to direct band gap. According to the analysis of calculated thermoelectric properties of Bi_2O_2Q and $Bi_2O_2S_{0.5}Se_{0.5}$ compounds, thermoelectric properties are strongly enhanced in $Bi_2O_2S_{0.5}Se_{0.5}$ compound. It seems to be due to the fact that the electrical conductivity is strongly enhanced by the decrease of dimensionality of its electronic structure and the broadening of sharpness of density of states near the Fermi level. Therefore, we believe that band modulation by introducing chalcogen mixture net in its pure compound Bi_2O_2Q compound gives a help to improve their thermoelectric properties.

[1]2013R1A1A2060341

Changhoon Lee
Pohang University of Science and Technology

Date submitted: 05 Nov 2015 Electronic form version 1.4