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Computational Design of Co-Doping Method for Indium-Reduced Chalcopyrite-Type Photovoltaic Materials KAZUNORI SATO, Graduate School of Engineering Science, Osaka University, PRESTO-JST, YOSHIMASA TANI, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University — Chalcopyrite-type semiconductor $CuInSe_2$ (CIS) is one of the most promising materials for low cost photovoltaic solar-cells. However, from the point of resource security, high concentration of In in CIS is serious disadvantage. In this paper, we propose co-doping method to reduce the concentration of In in CIS-based photovoltaic materials, i.e., 2In are replaced by Zn and Sn. According to the electronic structure calculations by the KKR-CPA-LDA [1] with the self-interaction correction [2], the substitution of Zn and Sn for In does not alter the electronic structure of CIS so much. We extend our co-doping method to enhance the efficiency of solar energy conversion. In addition to Zn+Sn co-doping, we introduce S impurities at Se sites. Due to the phase separation it is found that nano-structures with high concentration of S are self-organized under the layer-by-layer crystal growth condition. Since type-II band alignment is expected between Cu(Zn, Sn)Se_2 and Cu(Zn, Sn)S_2, we can expect efficient electron-hole separation in decomposed Cu(Zn, Sn)(Se, S)$_2$ [3].

[1] H. Akai, http://sham.phys.sci.osaka-u.ac.jp/kkr/
[2] A. Filippetti and N. A. Spaldin, Phys. Rev. B 67 (2003) 125109.
[3] Y. Tani et al., Appl. Phys. Express 3 (2010) 101201.

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