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First-Principles Materials Design of Chalcopyrite-Type Photovoltaic Materials with Self-Organized Nano-Structures YOSHIMASA TANI, Graduate School of Engineering Science, Osaka University, KAZUNORI SATO, Graduate School of Engineering Science, Osaka University, PRESTO-JST, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University
— Cu(In, Ga)Se_2 (CIGS) is a chalcopyrite-type semiconductor and one of the most promising materials for low cost photovoltaic solar-cells. In this paper, based on first-principles calculations, we propose that spinodal decomposition will enhance the conversion efficiency in CIGS. Our calculations are based on the KKR-CPA-LDA [1] with the self-interaction correction [2]. From the calculated mixing energy of CIGS, it is found that the system favors the spinodal decomposition. We also perform Monte Carlo simulations and find that quasi-one-dimensional nano-structures with high concentration of impurities are formed under the layer-by-layer crystal growth condition in CIGS [3]. It is expected that the photo-generated electron-hole pairs are efficiently separated by the type-II interface and then effectively transferred along the quasi-one-dimensional structures in CIGS. Moreover, we can expect multiplication of generated carriers due to the multi-exciton effects in nano-structures [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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