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Computational Design of Photovoltaic Materials with Self Organized Nano Structures KAZUNORI SATO, Graduate School of Engineering Science, Osaka University and PRESTO-JST, HIROSHI KATAYAMA-YOSHIDA, Graduate School of Engineering Science, Osaka University — Chalcopyrite and II-VI semiconductors, such as Cu(In, Ga)Se_2, $Cu_2ZnSn(S, Se)_4$ and Cd(S, Te), are one of the most promising materials for low cost photovoltaic solar-cells. In this paper, based on first-principles calculations, we propose that self-organized nano-structures in these compounds will enhance the conversion efficiency. Our calculations are based on the KKR-CPA-LDA [1] with the self-interaction correction [2]. We also use VASP package [3] for calculating mixing energy and effective interactions of the systems by using the cluster expansion method [4]. For phase separating systems, we simulate nano-structure formation by using the Monte Carlo method. 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. Moreover, we can expect multiplication of generated carriers due to the multi-exciton effects in nano-structures [5].

[1] H. Akai, http://sham.phys.sci.osaka-u.ac.jp/kkr/
[2] A. Filippetti and N. A. Spaldin, PRB 67 (2003) 125109.
[3] G. Kresse and J. Hafner, PRB 47 (1993) 558.
[4] A. Zunger, NATO ASI B 319 (1994) 361.
[5] Y. Tani et al., APEX 3 (2010) 101201, 4 (2011) 021201, JJAP 51 (2012) 050202.

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