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$_2$ZnSn(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].


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