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Computational Nano-materials Design of Self-Organized Cd(Te,S) and Cd(Te,Se)Type II Nanowire (Konbu-Phase) by Spinodal Nano-Decomposition for High-Efficiency Photovoltaic Solar-Cells
HIROSHI KATAYAMA-YOSHIDA, MASAMUNE OSHITANI, Graduate School of Engineering Science, Osaka University, KAZUNORI SATO, Graduate School of Engineering Science, Osaka University and PRESTO-JST — Based on multi-scale simulations combined ab initio electronic structure calculation (KKR-CPA) and Monte Carlo simulation (MCS) of the two-dimensional layer-by-layer crystal growth, we have designed the self-organized quasi-one-dimensional nano-structures (Konbu-Phase) fabricated by two-dimensional spinodal nano-decomposition for high-efficiency photovoltaic solar cells (PVSCs) in $Cd(Te_{1-x}S_x)$, and $Cd(Te_{1-x}Se_x)$. The Konbu-Phase enhances the nano-scale electron-hole separation in PVSCs due to their Type II band alignment. The Konbu-Phase also increases the efficiency of PVSCs by multi-exciton formation using the inverse Auger effect in the self-organized quasi-one-dimensional nanostructures. We also discuss how to fabricate Konbu-Phase starting from the uniform nano-particles made by the photo-chemical reactions. Reference: M. Oshitani, K. Sato, H. Katayama-Yoshida, Applied Physics Express 4 (2011) 022302.

Kazunori Sato
Graduate School of Engineering Science, Osaka University

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