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**Computational nano-materials design of high efficiency photovoltaic materials by spinodal nano-decomposition in Chalcopyrite-type semiconductors** HIDEO ASAHINA, YOSHIMASA TANI, Osaka University, KAZUNORI SATO, Osaka University, PRESTO-JST, HIROSHI KATAYAMA-YOSHIDA, Osaka University — Chalcopyrite-type semiconductor CuInSe2 (CIS) is one of the most promising materials for low cost photovoltaic solar-cells due to its self-regeneration mechanism. However, from the point of resource security, high concentration of In in CIS is serious disadvantage. Recently, Cu2ZnSnS4 (CZTS) attracts much attention to overcome this disadvantage of CIS. This material has already been investigated as a photovoltaic material but the efficiency is not high enough. Based on the first-principles calculations by the KKR-CPA method, we propose how we can enhance the efficiency of CZTS by utilizing the self-organization phenomena caused by spinodal nano-decomposition of Cu & Cu-vacancy, S & Se, and Se & Oxygen [1]. We will compare our design with the available experimental data of STEM-EDX, EELS, Atom Probe Tomography and Raman Scattering data. In addition to the above materials design, we also discuss intermediate band type solar-cells caused by the spinodal nano-decomposition, and propose Fe-doped CuFeS2-CuAlS2 (CFS-CAS), CuFeS2-CuGaS2 (CFS-CGS) and CuFeS2-CuInS2 (CFS-CIS) as promising materials with enhanced conversion efficiency up to 50%.

[1] Y. Tani et al., Appl. Phys. Express 3 (2010) 101201. Jpn. J. Appl. Phys. 51 (2012) 050202.

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