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Computational Materials Design for High Efficiency Photovoltaic Solar Cells and Transparent Conducting Sulfides HIROSHI KATAYAMA-YOSHIDA, YOSHIMASA TANI, KAZUNORI SATO, Osaka University — Based on the first-principles electronic structure calculations we propose computational materials design for high efficiency and low price (In free) solar cell materials based on CuInSe2. Firstly, to avoid the use of In, we try to substitute In by Zn and Sn, or by Ga. The electronic structure calculations are performed by using the KKR-CPA method. To calculate band gap energy correctly, we use self interaction corrections proposed by Filippetti et al. It is found that the direct band gap does not collapse and there appears no deep impurity state in the gap, thus it should be possible to avoid In without any deterioration of photovoltaic effect. From the calculations of mixing energy, we predict that the present system favors the spinodal decomposition and we can expect the formation of nano-wire by two dimensional spinodal nano-decomposition. When the nano-wires are formed, we can expect Type 2 band alignment between host material and the nano-wires. Due to this band alignment, efficient electron hole separation is expected leading to highly efficient photovoltaic effect. As an extension of the present design, we also propose a new class of n-type and p-type transparent conducting sulfides with the negative activation energy for the application of high-efficiency photovoltaic solar-cells.

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