Project No. 02116 / Grant No. JPMXP0621467974

Report form of Joint Research Project at ZAIKEN (FY2021)

Title of Project	**Design of the stable light absorption layer for inorganic perovskite solar cell**		
Priority Area	**I-B, III-B, I-C, III-C**		
Continuation of joint research in 2020			
Name of Main Applicant	**Farhod Rahimi**		
Institution	**Academy of Sciences, Republic of Tajikistan**	**title**	**President (Professor)**

Aim of the research project

Lead-halide perovskites have attracted great attention these days due to their potential applications for the light absorption layers of the next generation solar cells and for light emitting devices. There are some stable polymorphs depending upon the temperature in the lead-halide perovskites, i.e., α-, δ- and γ-phases. Among them, α- and γ-phases with cubic and orthorhombic structured perovskites, respectively, have good optical properties for the above applications, while δ-phase with orthorhombic non-perovskite structure is not suitable for such purpose. Some of them crystallize in δ-phase at ambient condition, e.g., $CsPbI_3$, though such materials with α- or γ-phases are quite good for solar cells. Hence, a lot of attempts have been done to stabilize the α- and/or γ- phases at room temperature by anion and cation mixings. In the current study, influence of cation and anion mixings on the phase stability and on the electronic structures of the lead-halide perovskites are investigated by using the first-principles calculations within a density functional theory (DFT) level, which will be applied to the development of new stable and efficient light absorbing materials for the next generation solar cells.

Contents and results of the research

In this 2021 joint project with Prof. Yamamoto, ZAIKEN, Waseda University, the first principles calculations have been carried out by Tajik group and the fabrication of the inorganic lead halide perovskite and its experimental analysis were done by students in a research group of Prof. Yamamoto. For the former calculations, well established DFT package, VASP [1] was used to investigate phase stability, structure change and electronic structures of the cation and anion mixed inorganic lead halide perovskites, say $APbX_3$, where A =Cs, Rb, K, and X = I, Br, Cl. In addition to such anion and cation mixing of A and X, substitution effect of Pb by other elements, for instance, Bi3+, have also been studied both theoretically and experimentally. The first principles calculations were conducted for the super cells expanding the unit cells of the cubic and orthorhombic perovskites, in which one of the cation and/or anion were replaced by another cation or anion, respectively, to investigate phase stability by total electronic energies.
Some of the calculated results suggest candidates for the stable phase at room temperature by cation/anion mixing or substation of Pb. As one of the candidates in Pb-substitution type, a series of $CsPb_{1-x}Bi_xI_3$ was synthesized by a spin coating technique changing the concentration of Bi and synthesis conditions such as temperature and atmosphere at heat treatment. All the synthesized films were characterized by the X-ray diffraction and scanning electron microprobe. As suggested by the first principles calculations, stability of the perovskite phase is improved by Bi substitution at Pb site. From the current joint work, we will be able to contribute to the development of the stable light absorbing layer with inorganic perovskites in the next generation perovskite solar cells

[1] G. Kresse, J. Furthmuller, Comput. Mater. Sci. 6 (1996) 15.

Outputs of the project (publications, presentations, patents)

Publications

1. M. Subhoni, Z.Umar, T. Yamamoto, F. Rahimi. First principle calculations of the electronic structure of Mn doped AMO_3 (A=Ca, Sr; M=Sn, Zr, Ti, Hf). *Reports of the National Academy of Sciences of Tajikistan*, N^o.1-2 (64), 2021, pp.94-98. (in Russian)
2. Z. Umar, F.Shokir, F.Rahimi, M. Subhoni, T.Yamamoto. Electronic structure of $SrZrO_3$ and $SrHfO_3$ phosphors materials doped with Mn^{4+} ions. Proceedings of the National Academy of Sciences of Tajikistan, N^o.1 (182), 2021, pp.58-68. (in Russian)

Some more works are under preparation for the submission of joint papers to international journals

Presentations

Some of the results will be presented in the international conferences such as EMRS, Warsaw, Poland, and in FMS, Phu Quoc, Vietnam.