Project No. 02417

Report form of Joint Research Project at ZAIKEN (FY2024)

Title of Project	Development of stable inorganic lead-free halide perovskites for the solar cells		
Priority Area	II-A(4R & Processes), II-B(4R & Structure), II-C(4R & Properties)		
	New proposal		
Name of Main Applicant	Farhod Shokir		
Institution	Physical Technical Institute, National Academy of Sciences of Tajikistan	**title**	Dr./ Head of Department

Aim of the research project

Inorganic and organic-inorganic hybrid halide perovskites have attracted extensive attention of researchers around the world for numerous technological applications such as solar cells, catalysts, light emitting diodes (LEDs), lasers, X-ray detectors, photodetectors, and field-effect transistors. Among the several types of clean energy sources available around the world, solar energy is the most promising and efficient system. According to NREL, in recent years, the efficiency of perovskite solar cells (PCE) has increased quite significantly from 3.8% to more than 26.1% [1]. However, these materials exhibit instability under environmental conditions caused by humidity, high temperature and ultraviolet (UV) light irradiation. In addition, the materials used in the light absorption layers of these solar cells typically contain a toxic element, i.e., Pb. Our target of the current project is to find stable lead-free materials for the use in light absorption layer of the perovskite type solar cells, which contribute to all three priority areas proposed in the call for the current project by ZAIKEN, but our major goals are to “replace” conventional Si-based solar cells by a new perovskite type of solar cells and to “replace” toxic Pb by other elements.

[1] https://www.nrel.gov/pv/cell-efficiency.html

Contents and results of the research

In the current project, we have tried synthesizing lead-free inorganic halide perovskites by the spin-coating method and analyze their geometrical and electronic structures both experimentally and theoretically. For the theoretical understandings of these properties, first principles calculations have been conducted within a density functional theory (DFT). In addition to further DFT calculations, density of states of phonons and dispersion curves in k-space will be obtained by the direct method with phonopy package [3]. From the calculated phonon DOSs, influence of anion and cation mixing on the temperature dependent phase stability have been discussed.

The followings have been carried our with Prof. Yamamoto
(a) sample preparations
Thin films of lead-free inorganic halide perovskites with various kinds of cation and anion mixing were prepared by spin-coating method at Waseda.
(b) XRD
Crystal structures and the phase stability under ambient condition were monitored by XRD at Waseda.
(c) UV-Vis
Electronic structures of the synthesized films were examined by UV-Vis spectrometer at Waseda.
(d) SEM-EDX, SEM-AES
The morphology of the sample surface is characterized by SEM, and EDX and/or AES mapping will be also performed for the elemental analysis at Waseda.
(e) first-principles calculations
In order to study electronic structure and stability, the first-principles calculations were performed within a density functional theory. In addition, phonon density of states and dispersion curves in k-space were calculated by combined use of the results of the above calculations and phonopy code.

References
[2] G. Kresse, J. Furthmuller, Comput. Mater. Sci. 6 (1996) 15.
[3] A. Togo, I. Tanaka, Scr. Mater., 108 (2015) 1.

Outputs of the project (publications, presentations, patents)

Results of the current joint project have been partially presented as an invited talk [4] and oral talks [5, 6] in the international conference and been published in the international journal [7, 8].

[4] T. Yamamoto et al., 12th International Conference on Luminescent Detectors and Transformers of Ionizing Radiation, June 16-21, 2024, Riga, Latvia
[5] T. Yamamoto et al., 7th International Conference on the Physics of Optical Materials, August 26-30, 2024, Becici, Montenegro
[6] T. Yamamoto et al., PRiME2024, October 6-11, 2024, Honolulu, USA
[7] D. D. Nematov et al., J. Electron. Mater. 54 (2025) 1634-1644
[8] M.S. Kurboniyon et al., Inorg. Chem. 63 (2024) 21212-21221.