Project No. 02516

Report form of Joint Research Project at ZAIKEN (FY2025)

Title of Project	**Development of stable inorganic lead-free halide perovskites for the solar cells**		
Priority Area	**II-A, II-B, II-C**		
New proposal or Continuation of 2024			
Name of Main Applicant	**Farhod Shokir**		
Institution	**Physical Technical Institute, National Academy of Sciences of Tajikistan**	**title**	**Dr./ Head of Department**
Name of partner applicants (if any)	**Dilshod Nematov, Amondullo Burkhonzoda, Zafari Umar, Makhmadzoir Kayumov**		
Name of the host faculty at Waseda	**Prof. Tomoyuki Yamamoto**		

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
(Please indicate to which extent the expected objectives in your proposal have been achieved.)

In the current project, we attempted to synthesize lead-free inorganic halide perovskites using the spin-coating method and to analyze their geometric and electronic structures both experimentally and theoretically. To gain a theoretical understanding of the properties of perovskite materials, we performed first-principles calculations within a density functional theory.

The followings have been carried out with Prof. Yamamoto,

-This study uses DFT to analyze the effect of halogen substitution in $CsSnI_3$ perovskites upon transition to chlorine-containing $CsSnI_{3-x}Cl_x$ compositions.

-Partial substitution of iodine with chlorine (x = 1) in the β-phase results in a minimum band gap of 0.83–1.33 eV, close to the Shockley–Queisser limit.

-Optical properties are significantly improved: the absorption coefficient in the visible range exceeds 10^5 cm^{-1}, significantly higher than that of the original $CsSnI_3$.

-The dependence of the band gap on chlorine concentration is nonlinear due to changes in interatomic distances and the redistribution of electron states.

-Complete halogen substitution leads to the formation of $CsSnCl_3$ and causes a lattice compression of approximately 10.3%.

-At hydrostatic pressures of 0–30 GPa, compression of the crystal structure and an increase in the elastic modulus are observed.

-Most compounds of the β-$CsSnX_3$ (X = I, Br, Cl) system retain mechanical stability over the studied pressure range.

-The compound $CsSnBr_2Cl$ exhibits signs of elastic instability at pressures above 20 GPa.

-Pressure promotes a narrowing of the band gap and enhancement of optical absorption, which offers potential for photovoltaic and optoelectronic devices.

-These results indicate the potential of chlorination, doping, and strain engineering to optimize lead-free perovskites for solar energy applications.

Outputs of the project (publications, presentations, patents)

Parts of the results from the current joint project have been published in the international journals [1-3].

[1] A. Burhonzoda et al., Comp. Conden. Matter 46 (2026) e01253
[2] A. Burhonzoda et al., Comp. Conden. Matter 45 (2025) e01130-e01130
[3] Z. Umar et al., Comp. Conden. Matter 44 (2025) e01062