COMPOSITIONAL DESIGN OF THE Pb-FREE DOUBLE PEROVSKITE AS A PROMISING LUMINESCENCE MATERIAL

The purpose of the project. The rising star of an enormous interest of the academic community is halide perovskites, $CsPbCl(Br,I)_3$, which are widely investigated due to their outstanding characteristics. There is a need of finding new elements that can replace Pb in the crystal structure owing to its toxicity, as even a low concentration of lead causes environmental hazards and is harmful to human health as potential carcinogen. Moreover, the European Union has already restricted the use of toxic and heavy metals. Halide double perovskites ($A_2B^IB^{III}X_6$) (HDPs), sharing a similar crystal structure with a pair of nontoxic heterovalent metal cations replacing two toxic lead cations, are promising alternatives [1]. Considering this, the goal of the project is to investigate the optoelectronic properties of the synthesized rare-earth HDPs, and find the possibility of their tuning relying on the connection between composition-structure-properties.

Description of the project.
The main goal of the project is to obtain stable more effective lead-free HDP material using the approach of composition engineering and different methods of synthesis to get photoluminescent (PL) materials to produce effective white light emitting diodes (WLEDs) [2].

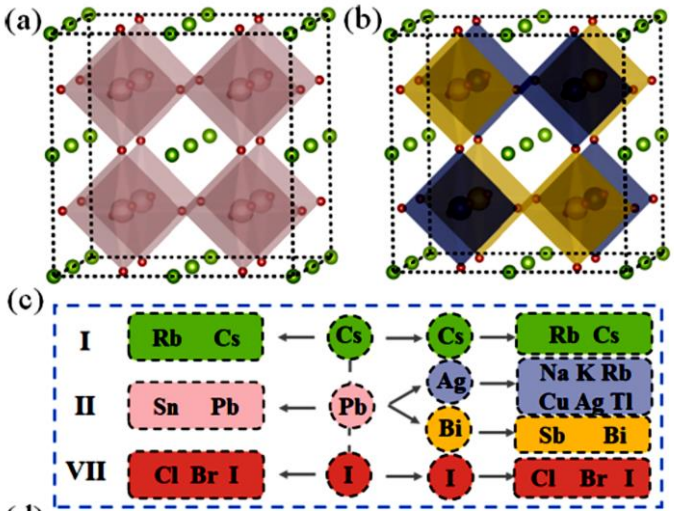

Fig. 1. A schematic crystal structure of (a) cubic perovskite and (b) double perovskite, (c;d) typical compositions of halide perovskites and HDPs [1].

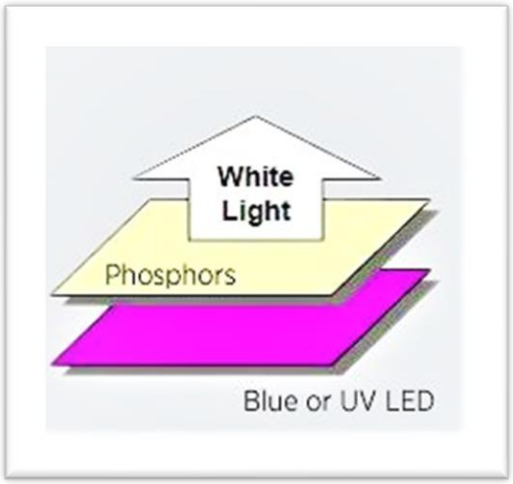

Fig. 2 Scheme of conversion of blue or near-UV light from the LED into white light [2].

Reasons for undertaking this research topic. The successful implementation of this project, because of its interdisciplinary base (chemistry, physics, computer calculations), will result in gaining deep fundamental knowledge about new perovskite materials in different forms, like nanocrystals, powders, bulk materials. Comprehensive analysis of the high number of the experimental data of HDPs, which now are a very hot topic of material sciences, may offer a further advance in properties of these materials, for LED (WLED) production. LEDs are used as a light source in home light bulbs, traffic lights, smartphone, laptop screens, or monitors. They offer a tremendous opportunity for innovation in lighting form, because they are better in color richness, contrast, and power consumption, which makes them worth the higher investment cost.

The most important expected effects. The stable lead-free HDP material will be obtained and WLEDs will be produced, which can be used in multifunctional lighting. The results of our project will be published in highly ranked journals to inform the international scientific community about our conclusions. We are going to take part in international conferences, workshops and seminars, where we will share the obtained knowledge with other scientists and PhD students.

[1] Q. Sun, W.-J. Yin Thermodynamic Stability Trend of Cubic Perovskites. *J. Am. Chem. Soc*., **2017**, 139, 14905.
[2] https://www.energy.gov/eere/ssl/led-basics