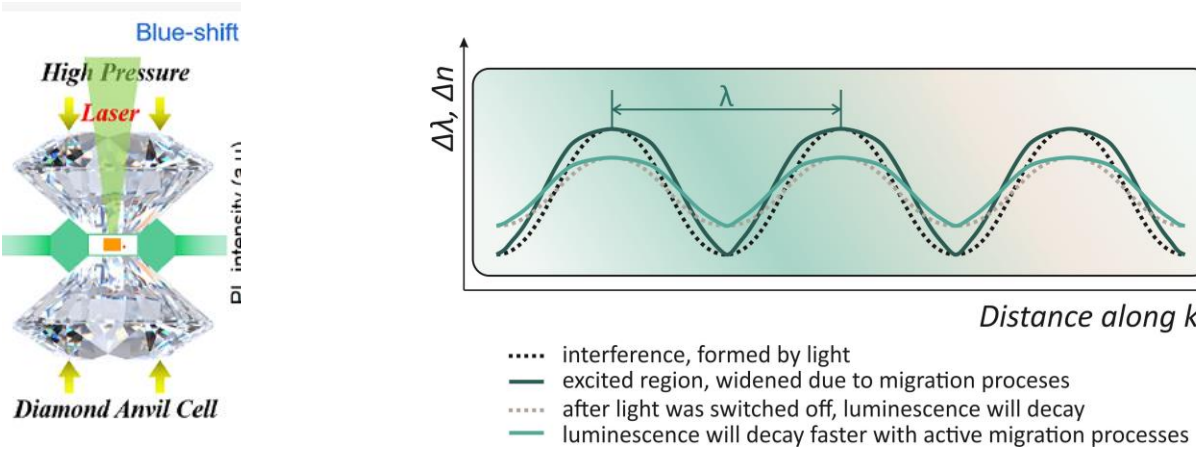
Impact of chemically and physically-induced structural phase transitions on optical properties of inorganic perovskites: theory and experiment.

Constantly growing energy consumption and limitations of non-renewable energy resources, such as oil, gas etc., create serious global challenges for the whole mankind. Development of new materials for the green-energy and/or energy-saving devices has already become one of targeted and of high priority directions of modern fundamental and applied research. Smart materials engineering supported by thoroughly selected methods of physical and chemical research implemented in various industrial and *ad hoc* designed experimental setups is a very efficient way towards resolution of those global energy problems.

Among countless crystalline materials, provided by nature or created artificially, there are large groups with identical or close crystal structures, which are already used in various applications. Perovskites – cubic, tetragonal orthorhombic – are one of those materials. Their applications for photovoltaics, scintillating, non-linear optics etc. are already known. Yet there are many fundamental questions related to the properties of those perovskites, which hinder their prospective applications. In particular, structural stability and phase transition still remain to be an important issue. Therefore, in the proposed project we are going to perform combined synergetic experimental and theoretical studies of a large number of perovskite (including lead-free ones as well).

Project predicts preparation of various types of perovskites, important form application point of view as well as fundamental one. They will be examined by sophisticated and modern methods, which include high pressures generated in diamond anvil cells, and nonlinear optical spectroscopy.



Ideas of: high-pressure experiments in diamond anvil cell (on the left), and nonlinear optical experiment: laser induced holographic gratings (on the right).

The experimental part of the project will be strongly supported by theoretical research, based on first principle's method. Already existing long-standing fruitful collaboration between the Polish and Chinese teams forms the strong ground for efficient project implementation. We anticipate that the project findings will contribute to the knowledge of physics and chemistry of perovskites and performance of devices based on those materials. The project will make a profound positive impact on the development and strengthening of research ties between both countries. It will also be beneficial for the young researchers from both sides.