Project Title: **Influence of pressure on the structural and optical properties of perovskite materials for fotovoltaic and optoelectronic applications**

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Research project objectives. The main objective of this research project is to study all aspects of high pressure influence on the structure and physical properties of perovskite materials applicable in solar cells and other optoelectronic devices. We are planning to perform high-pressure experiments for hybrid organic-inorganic metal halides as well as for all-inorganic compounds, which presently belong to the hottest topics in solid-state physics, chemistry and materials science. High pressure is a very efficient and *clean* way of the crystal structure modifications without any chemical interference. By employing X-ray diffraction on single-crystals squeezed in diamond-anvil cell we expect to obtain precise information on the changes of structural parameters induced by pressure. This data will be correlated with pressure-dependent variations of spectroscopic properties, relevant to the photovoltaic and other optoelectronic parameters.

A large part of the project is devoted to the careful examination of phase relations in the metal-halide perovskites under pressure. We are going to collect new data on the pressure-induced phases, including their symmetry, the stability pressure regions, the coexistence of phases, and the amorphization thresholds. These data is necessary because there is either a lack of such information or the inconsistent results are disseminated in the literature. In particular, we will undertake the pioneering studies of slow-kinetics pressure-induced transformations. Such transformations, extending into weeks or even months, have been recently observed for the first time in our laboratory. The transitions occurring at relatively low pressure and associated with dramatic changes in optical properties have to be thoroughly examined, as they can affect the optoelectronic properties of devices. We expect to clarify the mechanism of these transitions and to obtain information on the most intriguing questions: (i) if such transitions are characteristic for all hybrid perovskites and (ii) if they can also occur in all-inorganic materials? We would like also to collect high-pressure data for selected 2D perovskites (like for example Cs_2PbBr_5) and to compare the response to pressure of 3D and 2D materials.

Research project methodology. The hybrid and all-inorganic compounds will be fabricated using the low-cost methods based on the crystallization from solutions. A special care will be focused on the growing of truly single crystals. Most of the high-pressure experiments will be carried out in the modified Merrill-Basset diamond anvil cell (DAC) in hydrostatic conditions. The single-crystal X-ray diffraction experiments are aimed at detailed examination of the compression characteristics of the perovskite materials. We expect to obtain precise structural information, and in particular, the pressure dependence of bonds and angles, as these changes are crucial for the strain-induced modifications of the electronic structure and optical characteristics of perovskite materials. These studies will be supported by the high-pressure powder diffraction experiments and microscopic observations of the squeezed crystals in normal and polarized light. The collected structural data will be analyzed using the standard crystallographic tools.

The absorption edge and fluorescence of the crystals placed in the DAC will be measured with microscopic spectrophotometer because of the limitation of the crystal size by the cell diameter (0.2-0.4 mm). The spectroscopic parameters will be determined as a function of pressure, but also for the selected values of pressure, as a function of time.

For selected materials their dielectric properties will be studied as a function of pressure and temperature, which should provide additional information for the construction of phase diagrams.

Expected impact of the research project on the development of science. The perovskite materials reveal under pressure their general structure-property relations, allowing a rational search for new chemical compositions of materials of improved performance. The reliable structural data are crucial for interpretation of the structure-property relations, theoretical modeling, and predicted directions of chemical synthesis research. Moreover, the discovery of the slow-kinetics transformations in the hybrid perovskites opens a new area of research. In the optoelectronic devices the strain can be generated at the interfaces, when the flexible device is bent, or by temperature changes in extremal conditions. It is evident that such pressure- or stress-induced effects can lead to the undesirable modifications of the optoelectronic characteristics in the time scale of weeks or months after the device fabrication. We expect that the results of this high-pressure project should provide valuable scientific information and will motivate further experimental and theoretical exploration of this scientifically interesting and technologically important field.