Fossil fuels like coal, oil and natural gas, are still dominating energy sources. However, they are limited, cause immense pollution by releasing harmful gases and are not available everywhere on Earth. There is a strong pressure to reduce our dependency on fossil fuels as they are unfriendly for environment and contribute to global warming. Numerous countries have already started taking steps to make use of alternative energy sources. Presently, around 20% of world's energy needs comes from renewable energy sources. Solar energy is the cleanest and most abundant renewable energy source available. Sunlight contains a surprisingly large amount of energy. On average, even after passing through hundreds of kilometers of air on a clear day, solar radiation reaches Earth with enough energy in a single square meter to run a mid-size desktop computer – if all the sunlight could be captured and converted to electricity. Photovoltaic technologies harvest some of that energy now and will grow in both usage and efficiency in the future. In solar cell the sunlight is absorbed and converted through the photoelectric effect into electric energy. The conversion efficiency depends on the properties of the absorber applied in the device.

In recent decade new organic-inorganic lead halides materials of perovskite structure have emerged as excellent absorbers for photovoltaic application. Within 7 years following the first report, the perovskite solar cells showed a very fast improvement towards the energy-conversion efficiency over 22%. This unprecedented progress, along with the ease and low cost of fabrication, strongly motivates further intense studies in this field. However, the toxic and water soluble lead compounds may be an obstacle on their way to the practical applications. Hence, there is a quest for alternative, non-toxic, and chemically stable photo harvesters. One of the possible ways is engineering of materials through doping or chemical substitution. However, such approach usually leads to some chemical and structural inhomogeneity, which can limit a control on the desired properties. The high-pressure studies proposed in this project are free from this disadvantage. High pressure can modify bond lengths and angles in perovskite materials without chemical interference. Such structural distortions affect the electronic structure of the crystal and therefore this technique offers a possibility of precise tuning basic properties of photovoltaic materials, like energy gap and carrier diffusion length.

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. 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 structural transformations 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.

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 trigger 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.