Prototype perovskite photovoltaic materials, $CH_3NH_3PbI_3$ and $CH_3NH_3PbBr_3$, are cheap in production and their efficiency grows – it is 22% at the moment. They are supreme with respect to other solar cells if one compares the voltage generated at the electrodes – 1.3 V. However, there are some industrial problems which do not allow the production: lack of the resistivity to moisture and a degradation during the work of the device. The first problem can be solved using the transition metal oxides, such as ZnO doped with B, Al, Ga, In. It is believed that the second problem is connected to the charge accumulation at the junctions – we plan to work on it.

The advantage of ZnO over more popular, nowadays, TiO_2 is much lower electrical resistivity of the former, and easier and cheaper production of this crystal, especially at elastic polymers; in order to build the devices which are easy to roll. There is one property which makes difficult to use it in the heterojunctions with the perovskites, namely a decomposition from PbI_3 to PbI_2. Chemical reaction responsible for this is dependent on the atomic structure of the interface. Therefore, we will work on achoice of various surfaces of the investigated materials and ways of doping, such that the unwanted phenomenon diminishes.

Recombination of charges in the interface depletion region depends on the band levels alignment; of the valence and conduction manifold. We will tailor the energetic positions of these bands by means of the doping and the structural modifications of the surfaces.

In the solar cells which are industrially produced, there are charge selective layers introduced before the cathode and anode. The n-type doped ZnO might undertake the role of the electron collecting layer and restrict the holes transport. Design of the interfaces with such parameters that efficient perovskite solar cell could be produced without the charge blocking layers is our priority.

This project will be performed by means of *ab initio* modeling of the atomistic structures and material properties such as optical transparency, absorption of light and electronic conductivity. We will use the open source codes which are efficiently parallelized for hundreds of processors and allow the simulations of systems consisting of thousand of atoms.