The goal of the presented project is the systematic and consistent study using the density functional theory (DFT) of electronic, optic, elastic and other physical properties, as well as establishing of the relationship between the structure-property and property-property dependences of I-III-VI_2 (I = Cu, Ag, III = In, Ga, Al, VI = S, Se, Te etc) ternary chalcopyrite (CP) semiconductors for solar cells application. The I-III-VI_2 ternary CP is the group of crystals possessing the set of properties which make them interesting for fundamental and applied study. It is known, that these materials allow the composition modification by partial substitutions of cations and anions. Such substitution enables change of the chemical composition of materials leading the crystal structure and properties change. The titled materials can be used as active elements for nonlinear optics, as optical filters, LED application, high-efficiency quantum dots for photocatalysis (for example $CuGaS_2$ crystal), sensors and, most prospective-in solar cell application. Also, the possibility of producing the high-quality thin films makes CP very attractive for thin-films sensors and solar cells. The potential practical application of CP crystals requires a thorough study of properties of titled compounds. In this project, we will perform the theoretical investigation of the crystal structure and different physical properties of titled CP crystals in the framework of DFT.

The electronic band structure and other properties of pure crystals will be studied. The methodology of calculation using different types of exchange and correlation functionals together with Hubbard approach (DFT+U) as well as dispersion correction of DFT (DFT-D) in order to obtain the results for CP close to the experimental data will be developed. Since CP crystals form solid solutions, it is interesting from a fundamental point of view to study the effect of isomorphic substitution of anions and cations on the electronic structure of those materials. In the proposed project the dependencies of structural parameters and physical properties on the chemical composition of the solid solution will be investigated using the first principles simulation. The simulation of the solid solution will be based on the virtual crystal approximation (VCA) and supercell (SC) methods. Establishing the concentration dependences of properties of the compounds will allow us to find the exact chemical composition required to choose in order to get the material with the desired propertirs.

The use of impurities of alkaline and rare earth atoms leads to the emergence of additional donor levels in the band gap. The intermediate solar cells have been created on the basis of doping of pure semiconductor by ions of different types. The intermediate band solar cells (IBSC) can be created on the basis of doped CP semiconductors. Using the first-principles calculations, a study of the position of the energy levels of impurity in the forbidden band for different CP crystals will be carried out. Also, the doping of different atoms type, as well as concentration influence which will increase the absorption of light, will be established. The modification will increase the efficiency of the use of such materials in order to their use in photovoltaics.

Computer simulation of the surface of crystals, allow establishing the most favorable and stable direction for the growth of thin films from CP. The energetic characteristics of the adatoms, as well as a number of adsorbed molecules, will be also studied. Influence of defects on the structure of energy bands and properties of materials.

On the basis of theoretical calculations, a correlation analysis of various parameters of CPs will be carried out. A thorough consideration of the relation between the lattice parameters ternary CP compounds, on one side, and ionic radii, electronegativities and other parameters of the constituting ions, on the other side, will allow for establishing a simple empirical model and finding its equation, which links together the abovementioned quantities. The developed approach will be used for prediction of structural parameters for new isostructural materials. The findings of the present project will offer a systematic overview of the structural properties of CP and can serve as helpful guides for the synthesis of new CP compounds. Such studies are important for understanding the nature of physical properties and processes that arise in materials, as well as for predicting/constructing of new functional materials with predefined properties. Obtained results can be useful for development of photovoltaics as well as provide improvement of efficiency of existing semiconducting devices. The proposed project will expand information about titled CP and will have positive influence on science and technology, materials science, physics as well as fabrication process development of new technological materials.