Investigations of the physical properties of advanced materials for ultrafast data recording recently attract the great attention of researchers. Also, synthesis and creations of new artificial materials for medical and technology applications become popular in the new millennium. However, the process of new materials creation and their properties optimization for the different application can be extremely expensive and not efficient without predictive theoretical guidance. Thus, the preferable initial stage of new materials design is the computer modeling and simulations of their physical properties.

The aim of proposed project is to build methodology used in theoretical study of the physical properties of chalcogenide semiconductor materials based on first principle calculations. Up to now the electronic properties of these materials were not predicted correctly by theoretical investigations. Conducting of preliminary studies using computer simulations will enable to improve the information about physical properties of the investigated materials without significant financial expenses. The proposed investigations will be implemented for a particular kind of material defined by common formula $X_n(PY_3)_m$ (X=Sn, Mn, Pb, Y=S, Se; n, m=1,2) but they can be generalized to a wider range of semiconductor materials with strongly correlated electron system.

Conducting the calculations of electronic, optical, magnetic as well as vibration properties of $X_n(PY_3)_m$ crystals using first principle approach, will give us the tool for investigation of different physical properties of the whole family of the materials. It will also explain the problem of their electron domain polarization that is important in memory devices applications. The understanding of the nonstoichiometry, presence of vacancies and defects as well as surface limitation will help to predict properties of new materials synthesized by the modification of already existing ones. It will give idea about production of advanced materials applicable in data storage FRAM memory. The theoretical prediction and experimental check of supposed physical properties will give possibility to improve the technology of ferroelectric materials synthesis. The knowledge about design of these materials, their production and characteristics will develop new technology in fast data storage. It may also give materials for mezoelectronic application, the new branch of technology giving new possibilities in solution of the energy sawing problem.