Depletion of reserves of natural fuels, and hence rising energy costs, focus attention on ways to allow for a more rational use of energy. A large part of the energy wasted is the waste heat generated in various processes. For example, if we look at the energy balance of the car with a combustion engine, almost 30% of the energy is dissipated by the hot exhaust gases. The recovery of even a small part of the heat, in the global scale will allow giant economic savings, and what may be even more important, it will reduce the amount of pollutants emitted into the environment, poisoning us and causing the greenhouse effect. One of the technologies that are well-suited for the recovery of the waste heat are thermoelectric generators. They allow for the direct conversion of heat into electricity utilizing thermoelectric effects occurring in materials, but do not have any moving parts and thus are virtually maintenance free. These advantages were appreciated by using thermoelectric generators as a source of electricity in lasting over 30 years space missions of Voyager and many others space crafts. If the thermoelectric material is heated on the one side, and on the other is cooled, an electric potential difference is created on its ends. In order that such thermoelectric pile can operate effectively, the thermoelectric material must be a good electrical conductor, it must have a large thermoelectric effect and conduct heat poorly. These requirements from the point of view of material properties are in contradiction to each other. A compromise of these properties are a combination found in semiconductor materials. Unfortunately, most of thermoelectrics used in current thermoelectric generators have a moderately high thermoelectric figure-of-merit $ZT \cong 1$ allowing only to achieve generator efficiency of about 5%. So there is a need for new and better thermoelectric materials.

In recent years, a widely studied materials are crystalline semiconductors with ultralow thermal conductivity. One of the most promising groups are superionic copper chalcogenides Cu_2X (X=S, Se, Te) having a thermal conductivity of 0.3 $W \cdot m^{-1} \cdot K^{-1}$, and with appropriate modifications providing maximum ZT value above 2, for p-type conductivity. The main issues are a lack of equally good materials of *n*-type conductivity, necessary to create a high performance generator, and high mobility of copper ions in the structure, decreasing the durability and stability of the thermoelectric properties. Therefore, the aim of the project is to optimize the thermoelectric properties of the new superionic thermoelectric materials based on Cu_2X (X = S, Se, Te) by selection of the appropriate method of synthesis and selection of the optimal concentration of charge carriers, through the introduction to the Cu_2X structure of selected dopants, and modification of the structure by transition metal doping, toward reduction of material degradation associated with the migration of copper ions.

Three methods of Cu_2X synthesis are planned to be used in the project, leading to different types of material microstructure: i) synthesis by direct reaction of a stoichiometric mixture of the elements without melting of the reaction product, ii) melting and crystallization of the compound from the melt, iii) hydrothermal reaction of appropriate precursors leading to nanopowders. Synthesized powders will be densified by using a modern electrical current assisted sintering method. The resulting materials will be thoroughly characterized in terms of chemical composition, microstructure and phase composition using advanced research methods, with an emphasis on diffraction structural studies. In order to determine their thermoelectric properties, measurements of thermal conductivity, electrical conductivity, thermoelectric power, concentration and mobility of charge carriers will be carried out, which will be used then to determine ZT parameter as a function of temperature. At the same time thermodynamic durability of the obtained materials will be determined using methods of thermal analysis, based on observation of weight changes and thermal effects accompanying the heating of samples. In parallel, based on the obtained structural data, supercomputer calculations of the electronic structure will be carried out and the models of crystal structure of the tested materials will be created. These results will allow us to predict the impact of the planned modifications of the structure on a number of material properties, including thermoelectric properties, as well as make easier to understand and explain the changes observed experimentally. The complementary use of experimental and theoretical techniques will greatly facilitate research and significantly increase its scientific value.

It is expected that the results of research will permit for a considerable improvement of the thermoelectric properties of the materials from the Cu_2X group, while increasing their durability. Looking at the potential efficiency of the thermoelectric generator based on these materials, it should allow to obtain an efficiency value exceeding 10%. This extended knowledge will also help to better explain the sources of extremely low thermal conductivity of these materials and set new directions for research of potentially better thermoelectric materials.