Thermoelectric materials are solid compounds, which can directly transform energy between heat and electricity, due to their unique transport properties. In practice, thermoelectric materials are widely used *i.a.* for construction of cooling devices or thermoelectric generators designed to recover waste energy or even to power devices operating in extreme conditions, *e.g.* space area. The efficiency of these devices is directly related to efficiency of constituent materials and their work temperature and nowadays it does not exceed 5 %. For these reasons, new thermoelectric materials, characterized by higher efficiency and higher work temperature, in comparison to currently applied solutions, are intensively studied. However, creation of such materials is extremely hard due to interdependence of transport and structural properties (*e.g.* problems with obtaining high electrical conductivity and low thermal ones at the same time). One of the most promising thermoelectric materials are copper based compounds which are characterized by ultrahigh thermoelectric efficiency, possibility of working in high temperature range and also relatively low price and low toxicity. Over the last 7 years, a few Cu-based materials with very high thermoelectric performance and working temperature of about 750–1000 K have been developed. Among them, binary Cu_2X compounds (where X = S or Se) are characterized by the best properties. However, excellent thermoelectric parameters of these materials are strongly related to their poor stability, particularly under electric current and temperature gradient, which create working conditions of thermoelectric materials.

Literature review indicates, that there a few new techniques, which can influence the stability of Cu-based materials. Among them, one of the most promising proposals is doping Cu_2X structures by *e.g.* iron (Fe) or antimony (Sb) ions. However, literature data lacks a comprehensive analysis focused on different chemical compositions of Cu_2X compounds doped by Fe or Sb atoms. Also a lack of an attempt of doping these materials by any other impurities can be observed. In my project, I decided to study this problem in much wider, methodical way. I am going to obtain Cu_2X thermoelectric materials by means of various methods (*i.a.* self-propagating high-temperature synthesis SHS, hydrothermal method) and sintering techniques (high-temperature isostatic pressing HIP, spark plasma sintering SPS) and thus determine the influence of the synthesis conditions on the final properties of the materials. Furthermore, in my project Fe, Sb, Zn and Mg dopants, will be introduced into Cu_2X structures, in order to reduce excessive copper ions migration, which is responsible for their low stability, and at the same time to keep high thermoelectric properties. The dopants will be introduced to these materials in various molar ratio and by using two different methods. Obtained materials will be characterized in terms of structural and transport properties (electrical conductivity, thermal conductivity or Seebeck coefficient). At the end, the representative samples with known chemical composition, taken from different measurement cycles will be mechanically tested in temperature range of 300–1000 K. Proposed approach will allow determination of the stability of studied materials.

In parallel with experimental studies, the theoretical analysis focused on *ab initio* calculations will be carried out. By means of FP-LAPW method within framework of density functional theory (DFT) I'll perform calculations aimed at geometry optimization of model structures. Optimized structures will be used in calculations of electrical and thermal properties, which then will be compared with experimental ones.

The main purpose of my project is to expand current state of knowledge of the transport mechanisms (electrical and thermal ones) in Cu-based materials and also to obtain chemically and mechanically stable thermoelectric materials characterized by high efficiency. In the bigger picture, the obtained materials may significantly influence development of the thermoelectric technologies designed to, *i.a.* recover waste energy.