Nowadays, people faced the problem of declining amount of fossil fuels, while increasing the demand for electricity (Fig. 1). About two-thirds of power generated from fossil fuels is delivered to the environment as a waste heat. Recovering even a small amount of lost heat would allow for large fossil fuel savings and a reduction in carbon dioxide emissions into the atmosphere. Therefore, proper use of thermoelectricity, which involves the conversion between thermal and electrical energy, can certainly be one of many ways to solve this problem. The thermoelectric effect can also be used in Peltier cooling devices that do not contain any harmful to the environment liquids or gases. The lack of moving parts, making devices quiet, durable and reliable is certainly on of the advantage of thermoelectric devices over classic ones. Recent progress in materials development and computing tools shows that thermoelectric devices can compete with traditional refrigeration technologies and power generation.

Thermoelectric materials are able to work in different temperature ranges depend on their applications, thus different materials are required for different purposes. For low and middle temperatures usually chalcogenides (S, Se, Te) and antimonides are used. Sulphur is one of the cheapest material, which makes it attractive for bulk thermoelectric materials. Furthermore, sulphur is one of the by-products of oil exploration. For this reason, its production is much higher than its consumption. Companies are piling up sulphur in the forms of pyramids, posing a huge potential threat to the environment. Hence, it is vital to utilize sulphur by making some valuable products such as thermoelectric materials.

This project is devoted to the study of the thermoelectric effect and projects' main goal is to find a suitable magnetic semiconductor, which consists of sulfur. The usefulness of the material for thermoelectric applications describes the efficiency coefficient defined as $ZT = \sigma S^2/\kappa$, where σ is the electrical conductivity, S is the Seebeck coefficient, T is the temperature and κ is the thermal conductivity. Fabrication of materials with a high ZT is a big challenge, because the values of σ, S and κ are determined by the same physical phenomena. Therefore, understanding the physical phenomena responsible for the electron and phonon transport in bulk materials is very important to develop the new strategies improving the thermoelectric efficiency ZT. One of the possibilities to increase ZT is to improve the electrical properties of the material.

Within the project two natural magnetic semiconductors will be studied: $CuCr_2S_4$ and $CuFeS_2$. The spinel $CuCr_2S_4$ is interesting due to its magnetic properties discovered recently – the bulk material has a metallic nature, while even a small addition of antimony changes its character to semiconductor, which significantly improves its thermoelectric properties. On the other hand, the second proposed material, chalcopyrite $CuFeS_2$, shows an interesting temperature dependence of the Seebeck coefficient – at low temperatures a peak appears, and in the temperature range above the peak, this coefficient remains unchanged. Moreover, the described dependence has been mapped in calculations at the atomic scale using the *ab initio* calculation methods. However, the experimental values of Seebeck coefficient differ from the first principle calculations values.

The main goal of the project is to study with *ab initio* methods the thermoelectric properties of the para-, ferro- and antiferromagnetic phases of magnetic semiconductors mentioned before: $CuCr_2S_4$ and $CuFeS_2$ and to find p- and n-type of dopants (antimony and halogen additives, respectively) that would significantly improve the thermoelectric properties of the proposed materials. The first task of the project will be carried out *ab initio* calculations. Next, the most promising doped materials will be verified experimentally. Based on the results obtained in the project, it will also be possible to analyze the correlation between thermoelectric properties and magnetism.

The technological challenge of the project is to create materials with a high thermoelectric efficiency. The scientific problem is to understand and develop the ability to predict and optimize thermoelectric properties. The results of this project can be helpful in identifying technologically relevant strategies to improve the efficiency of thermoelectric materials based on magnetic semiconductors.