Materials based on silicide, selenide and telluride phases are continually under study because of valuable functional properties. They may find application in devices for energy conversion and storage, such as thermoelectric modules or batteries. For illustration, magnesium silicide modified with germanium and/or tin and doped with antimony or bismuth has good thermoelectric properties as n-type material (thermoelectric figure of merit ZT = 1.4). The p-type counterpart, doped with silver or gallium has much worse properties (ZT = 0.4). As for efficient thermoelectric modules good quality p-type and n-type materials are both necessary, a lot of work is being done to improve the performance of p-type materials. In many cases the results reported in the literature refer to theoretical calculations and characterisation of real systems is limited to electrical and thermal properties without due consideration of compositional and microstructural effects. The best n-type derivatives of magnesium silicide are, however, multiphase with clearly hierarchical structure. Similarly, the p-type materials have complex microstructure and composition, which may account for the observed erratic changes in electrical properties upon heating and cooling.

The core concept of this project revolves around developing p-type layers based on Mg-Si, Sn-Se/Te, Cu-Se/Te, Sb-Te systems, characterisation of their composition and microstructure with special focus on the architecture of interfaces, electrical and thermal properties and their evolution as a function of temperature. Thermochemical calculations, will underpin the results of experiments. An entirely innovative idea is that of executing comparative studies on layers with the same composition but different microstructure. Layers deposited by pulse magnetron sputtering may have controlled structures ranging from fully amorphous to fully crystalline depending on process parameters. The proposed approach will contribute to better understanding interrelations between the transport properties, composition and microstructure. Experimental results will be confronted with the calculations for the multiphase systems with different proportions of components.

The acquired knowledge may provide guidelines for designing devices which in an eco-friendly manner covert waste heat into electricity.