Abstract for the general public

Project title: Diamond-like semiconductors as low-cost thermoelectric materials for direct conversion of waste heat into electricity

Motivation

Rising energy costs, dwindling natural resources, environmental pollution, and global climate change are pressing issues facing modern society. Thermoelectric (TE) energy conversion can effectively contribute to a sustainable energy supply, while the waste heat recovery by TE generators (TEG) is a good way to reduce fossil fuel consumption and CO_2 emissions. However, the high cost, moderate efficiency, and toxicity of the best TE materials limit the possibility of the mass production of TE converters. Therefore, the search for low-cost and environmentally friendly materials with high energy conversion performance is among the main tasks of TE materials engineering and TE energy development. Diamond-like semiconductors (DLS) are a promising family of TE materials that can effectively respond to the aforementioned challenges.

Project goal

The project aims to develop new low-cost, eco-friendly, and highly efficient thermoelectric materials from the family of diamond-like semiconductors by simultaneous engineering of electronic and phonon transport. To achieve the project goals, we propose the following concepts:

1) Defect State (DS) engineering. The DS will be introduced into the bandgap of semiconductor materials aiming to establish a source of charge carriers for the enhancement of electronic transport. This approach will eliminate the negative effect of the nonoptimized bandgap and dynamically enhance the carrier concentration with the temperature rise.
2) Bonding Inhomogeneity (BI) approach. The presence of bonding inhomogeneities will be exploited to perturb phonon transport and significantly reduce the lattice thermal conductivity.

Description of the research

Within the project, we will investigate the crystal structure, microstructural properties, thermal stability, and electronic and thermal transport properties of lightweight DLS materials. We will combine the information about the crystal structure, defect formation energies, electrical conductivity activation energies, and Boltzmann transport calculations to verify the ability of the DS to produce thermally activated carriers for electronic transport. In turn, the ability to strongly disturb the phonon transport by bonding inhomogeneity approach will be investigated by analyzing the results of the electron localization function calculations, ultrasonic measurements, and Debye-Callaway calculations. The main aspects of the research can be listed as follows: i) establishing scalable and reproducible synthesis methods; ii) estimating optimal conditions for the DS and BI engineering using defect formation energies calculations and bonding analysis; iii) developing a sintering procedure for repeatable and reproducible thermoelectric properties; iv) optimization of the electronic and thermal transport properties towards high TE performance using DS and BI concepts.

The expected results

This 3-year project aims to develop new lightweight *n*- and *p*-type DLS materials with high thermoelectric performance providing a path towards mature and sustainable TE converters. The main aim of the project will be realized by the synergistic implementation of DS and BI concepts offered in the project.