Abstract for the general public in English

A superconductor is a material that below a certain temperature, called the critical temperature, exhibits some specific properties. First, it is characterized by zero electrical resistance; moreover, it is an ideal diamagnetic. The first superconductor discovered in 1911 by Kamerlingh Onnes had an extremely low critical temperature, only a few degrees above absolute zero. Ever since this discovery, scientists have dreamt of room-temperature superconductivity. However, raising the critical temperature turned out to be extremely challenging, and despite many advances (and several Nobel Prizes) over the years, the materials known would need to be cooled by liquid helium or liquid nitrogen. A room-temperature superconductor can revolutionize technology. A superconducting power grid would not lose energy via resistance, so it would result in tremendous energy savings compared with the technology we have today.

The recent discovery of hydrogen-rich materials that exhibit superconducting properties above 200 K seems to be very promising. These binary systems (combining hydrogen with heavier elements), despite having a record high critical temperature, require very high pressures, which limits their potential use on an industrial scale. Furthermore, at the moment these substances have already been studied so extensively that it seems unlikely that a groundbreaking discovery will be made without a modification of the strategy.

A recent discovery indicating the existence of a superconducting phase at 288 K in a system consisting of hydrogen, carbon, and sulfur seems very promising. Admittedly, this compound still requires high metallization pressure, however, it seems to be a good starting point for further research.

Therefore, the project aims to investigate the superconducting properties of ternary systems to find a material that exhibits better parameters than previously known substances. We assume that doping of extra electrons into known hydrogen-rich binary systems will improve their performance and make it possible to find superconductors with higher critical temperatures at a lower pressure than so far. This strategy is related to the fact that the phonon density of states of binary hydrides consists of separated regions - a region of low-frequency vibrations associated with atoms of heavy elements and a region of high frequencies originating from vibrations of hydrogen atoms. The addition of a third, intermediate-mass component may fill this gap in the phonon density of states and thus significantly change the superconducting properties of the system.

In particular, the scope of the study includes finding stable structures in systems of stoichiometry S-X-H, La-X-H, and Y-X-H, in which X represents the light elements from the p-block (C, B, N, Al, Si, P). Then, the calculations of the electronic, lattice dynamics, and electron-phonon coupling properties will be carried out within the framework of Density Functional Theory (DFT) and Density Functional Perturbation Theory (DFPT) implemented in the Quantum Espresso package. A detailed analysis of the superconducting state properties (in particular, the critical temperature values, superconducting energy gap, thermodynamic critical field, or specific heat) will be performed in the framework of the Migdal-Eliashberg theory, which takes into account the strong-coupling effects characteristic for high-temperature superconductors. Among all the superconductors analyzed theoretically, the most promising systems will be verified experimentally.

While the results of the project will greatly expand the current state of knowledge of superconductivity in previously unknown ternary systems, the most desirable outcome is the discovery of superconductivity at ambient conditions, the Holy Grail of condensed-matter physics. It is important to note that superconductor-based technology has had a profound effect on basic scientific research and offers possibilities for commercial applications that are, as yet, largely unrealized.