Artur Durajski - description for the general public

The material that would be able to conduct electricity with absolutely zero resistance at room temperature is like *The Holy Grail* sought by the scientists for more than 100 years. Its discovery would undoubtedly lead to a revolution in electronics, energy, transportation and many other areas of our lives. Until recently, the highest critical temperature equal to 164 K (-109^{o}C) characterized copper-oxide compound on the basis of mercury (HgBaCaCuO). After 20 years since its discovery, the first experimental results were presented in December 2014 (updated in June 2015 and confirmed in May 2016), which prove that H_2S compound placed under high pressure has extremely high values of the critical temperature. In particular, in the range of the pressures from 115 GPa to 200 GPa, the critical temperature increases from 31 K to 150 K. In addition, it should be emphasized that the strong isotope effect was observed, which clearly suggests the electron-phonon origin of the superconducting state. Interestingly, as a result of a dissociation of the initial compound ($3H_2S \rightarrow 2H_3S + S$), the superconducting state with a critical temperature equal to as much as 203 K (-70^{o}C) was induced under the pressure at 150 GPa. From a physical point of view, the result obtained indicates that it was discovered a superconductor with the highest value of the critical temperature known so far. Except that dry ice is enough for cooling it instead of liquid nitrogen, it is characterized also by the fact that it is easy and inexpensive to produce. The problem is only associated with the high pressure required for the metallization and the transitions of the hydrogen sulfide into superconducting state. From the application point of view, however, it is desirable to find a way to reduce the pressure to the atmospheric value.

In light of the above experimental facts, the natural direction for further scientific work is to widen the knowledge of the superconducting state in the family of the hydrogen-rich compounds. My previous theoretical studies on the thermodynamic properties of these materials were based on the Eliashberg equations formalism, which is the generalization of Bardeen-Cooper-Schrieffer theory (the BCS theory) on the systems characterizing with the strong electron-phonon coupling. Performed analysis allowed for the quantitative determination of the critical temperature, the free energy difference between the normal and the superconducting state, the thermodynamic critical field, the specific heat for the superconducting state, the value of the energy gap at the Fermi level and the electron effective mass. Through the generalization of the results I estimated the range of the values of the critical temperature observable in the compounds of H_nS type, where $n = \{1, 2, 3\}$. As a result of the above analysis, it was found that the maximum value of the critical temperature may be as high as 290 K (17^{o}C), which gives the hope for another breakthrough and suggests further exploration to the experimenters.

An exploration will be carried out as a part of this project, in order to determine whether, as a result of doping H_3S compound with elements of *p-block* or *s-block* of the periodic table, there is a possibility to decrease the pressure and increase the critical temperature to the level allowing the application use of the tested materials. The necessary *ab-initio* calculations of the electronic structure, the phonon structure and the electron-phonon coupling will be conducted with an use of the Quantum-Espresso software. Besides its effect of dopant concentration on the stability of the superconducting state, the impact of the unit cell's compression and the structural transitions present as its result will be also investigated. Conducting a comprehensive theoretical study is important from the point of view of the future experimental studies. The correctness of the finding above may be evidenced by the fact that the first experimental studies on compounds consisted of sulfur and hydrogen were preceded and directly inspired by *ab-initio* calculations conducted by Yinwei Li *et al.*