SUMMARY OF PROFESSIONAL ACCOMPLISHMENTS

Artur Piotr Durajski

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Table of Contents

I. Personal information

A) Name and surname

PhD. Eng. Artur Piotr Durajski

B) Education, scientific diploma and degrees

2011 - 2014 **PhD studies** - Częstochowa University of Technology, The Faculty of Production Engineering and Materials Technology.
The academic degree of PhD in Physics obtained at the Faculty of Physics and Astronomy of the University of Zielona Góra on 29th April 2014.
The title of the doctoral thesis: *Thermodynamic Properties of High -Pressure Superconductivity in Hydrogenated Compounds.*
Thesis supervisor: dr hab. Radosław Szczęśniak.
The thesis was awarded a distinction by: The Scientific Council of the Faculty of Physics and Astronomy of the University of Zielona Góra, Polish Physical Society and the Rector of Częstochowa University of Technology.

2010 - 2012 **Facultative pedagogical studies** - Częstochowa University of Technology, Inter-faculty Teacher Training and Development Unit.

2007 - 2011 **MA studies in Technical Physics** - Częstochowa University of Technology, the Faculty of Process and Material Engineering and Applied Physics.
MA thesis title: *The Analysis of Superconductivity Properties in selected High-Pressure Physical Systems: Formalism of the Eliasberg equation.*
Thesis supervisor: dr Radosław Szczęśniak.
The thesis was awarded a distinction by : Polish Physical Society in the national contest for inventive MA theses in Physics.

2006 - 2011 **MA studies in Management and Production Engineering** - Częstochowa University of Technology, The Faculty of Management.
MA thesis title: *Production and Quality Management in a Company Producing Automobile Components.*
Thesis supervisor: dr inż. Marek Krynke.

2003 - 2006 Jan Kochanowski Secondary School in Bełchatów

C) Employement in scientific institutions

2014 - now   **Associate Professor** at the Institute of Physics of Częstochowa University of Technology.

- Since 2016 I am the Head of the Solid State Physics Department

- From 26.07.2018 to 27.08.2018 I had a one-month scientific internships at the School of Physics and Electronic Engineering, Jiangsu Normal University, China (the group of professor Yinwei Li).

- From 01.06.2015 to 31.08.2015 I had a three-month scientific internships at the Department of Physics, University of Rome La Sapienza, Italy (the group of professor Luciano Pietronero).

II. Presentation of scientific achievements according to art. 16 section 2 of act of law as of March 14, 2003 on scientific degrees and scientific title and about scientific degrees and scientific title in art (Dz. U. 2016 item 882 with changes in Dz. U. from 2016 item 1311)

A) Title of the scientific achievement

As scientific achievement defined by art. 16 sec. 2 of the act of law as of March 14, 2003 on scientific degrees and scientific title and about scientific degrees and scientific title in art (Dz. U. 2016 item 882 with changes in Dz. U. from 2016 item 1311), I present a series of thematically related ten publications entitled:

High-temperature superconducting state in systems with conventional and unconventional pairing mechanism

B) The list of publications constituting scientific achievement (listed according to the order in which they are discussed)

[A1]. **A. P. Durajski**, R. Szczęśniak, Y. Li, 2015, *Non-BCS thermodynamic properties of H_2S superconductor*, Physica C **515**, 1-6.

Impact factor: 0.835 (released in 2015). Number of citations: 38.

My contribution to this paper consisted in planning the research, writing a part of analysis packages, performing these calculations, interpreting the results obtained and writing the manuscript. I assess my contribution to be 65%.

[A2]. **A. P. Durajski**, R. Szczęśniak, L. Pietronero, 2016, *High-temperature study of superconducting hydrogen and deuterium sulfide*, Annalen der Physik **528**, 358-364.

Impact factor: 3.039 (released in 2016). Number of citations: 29.

My contribution to this paper consisted in planning and conducting the numerical analysis, determining the thermodynamics of superconductivity of the systems analysed and writing the manuscript. I assess my contribution to be 65%.

[A3]. **A. P. Durajski**, 2016, *Quantitative analysis of nonadiabatic effects in dense H_3S and PH_3 superconductors*, Scientific Reports **6**, 38570.

Impact factor: 4.259 (released in 2016). Number of citations: 28.

[A4]. **A. P. Durajski**, R. Szczęśniak, 2017, *First-principles study of superconducting hydrogen sulfide at pressure up to 500 GPa*, Scientific Reports **7**, 4473.

Impact factor: 4.122 (released in 2017). Number of citations: 12.

My contribution to this paper consisted in planning and conducting the DFT calculations with the help of the Quantum-ESPRESSO software, solving Eliashberg equations, determining critical temperature, interpreting the results obtained and writing the manuscript. I assess my contribution to be 70%.

[A5]. R. Szczęśniak, **A. P. Durajski**, 2018, *Unusual sulfur isotope effect and extremely high critical temperature in H_3S superconductor*, Scientific Reports **8**, 6037.

Impact factor: 4.122 (released in 2017). Number of citations: 2.

My contribution to this paper consisted in planning and conducting the DFT calculations with the help of the Quantum-ESPRESSO software, solving Eliashberg equations, interpreting the results obtained and writing the manuscript. I assess my contribution to be 50%.

[A6]. **A. P. Durajski**, R. Szczęśniak, 2018, *Gradual reduction of the superconducting transition temperature of H_3S by partial replacing sulfur with phosphorus*, Physica C **554**, 38-43.

Impact factor: 1.453 (released in 2017). Number of citations: 0.

My contribution to this paper consisted in planning and conducting all DFT calculations with the help of the Quantum-ESPRESSO software, determining critical temperature, interpreting the results obtained and writing the manuscript. I assess my contribution to be 80%.

[A7]. **A. P. Durajski**, R. Szczęśniak, 2018, *Structural, electronic, vibrational, and superconducting properties of hydrogenated chlorine*, The Journal of Chemical Physics **149**, 074101.

Impact factor: 2.843 (released in 2017). Number of citations: 0.

My contribution to this paper consisted in planning and conducting all DFT calculations with the help of the Quantum-ESPRESSO software, modifying the software available for solving classic and extended Eliashberg equations, determining the thermodynamic properties of the investigated systems, interpreting the obtained results and writing the manuscript. I assess my contribution to be 80%.

[A8]. R. Szczęśniak, **A. P. Durajski**, 2014, *Anisotropy of the gap parameter in the hole-doped cuprates*, Superconductor Science and Technology **27**, 125004.

Impact factor: 2.325 (released in 2014). Number of citations: 19.

My contribution to this paper consisted in performing partial analytical calculations and numerical analysis, interpreting the results obtained and co-writing the final version of the manuscript. I assess my contribution to be 50%.

[A9]. **A. P. Durajski**, 2016, *Anisotropic evolution of energy gap in superconducting Bi2212*, Frontiers of Physics **11**, 117408.

Impact factor: 2.579 (released in 2016). Number of citations: 5.

[A10]. R. Szczęśniak, **A. P. Durajski**, A. M. Duda, 2017, *Pseudogap in the Eliashberg approach based on electron-phonon and electron-electron-phonon interaction*, Annalen der Physik **529**, 1600254.

Impact factor: 2.557 (released in 2017). Number of citations: 4.

My contribution to this paper consisted in performing partial analytic calculations and numerical analysis, discussing the results obtained and writing an draft version of the manuscript. I assess my contribution to be 45%.

- Total impact factor for the papers from [A1] to [A10] according to the JCR list: **28.134**
- Total number of quotations for the papers from [A1] to [A10] according to the WoS database: **137** (**118** without self-citations)

C) Discussing the scientific aim of the above mentioned papers and the obtained results, together with their potential applications

1. Introduction

The phenomenon of superconductivity, observed for the first time in 1911 by Heike Kammeringh-Onnes, consists in total vanish of electrical resistance and appearance of zero induction of the magnetic field in the material cooled below a certain characteristic temperature called the critical temperature (T_c). This discovery is considered nowadays to be one of the most important ones in the history of physics. The first microscopic theory providing a proper description of the superconductivity phenomenon observed in metals such as Pb, Hg, Sn, Nb and their alloys was BCS theory proposed in 1957 by Bardeen, Cooper and Schrieffer [1, 2]. The basis of this theory is an assumption that below critical temperature electrons couple (the so-called Cooper pairs), creating superconductive condensate. Generally, from the 80s of the last century, the BCS theory was regarded as the basic theory of superconductivity. A new period of research in superconductivity began in 1986 together with the discovery of ceramic superconductors synthesized based on the copper oxides [3]. These materials were characterized by substantially higher critical temperatures than conventional superconductors with the electron-phonon pairing mechanism. Unfortunately, there arose a serious problem concerning a proper description

of thermodynamics and electrodynamics of their superconductivity within the classic BCS model. It turns out that nowadays there is no complete, generally accepted theory that would explain the pairing mechanism in these systems and show the path of further search for materials that could be superconductors at room temperature [4, 5]. If critical temperature could be raised till the level at which superconductors could be cooled with the help of cheaper solutions than liquid helium or nitrogen, it would undoubtedly lead to a revolution and a huge technological breakthrough, similar to inventing electricity or constructing a computer. It is one of the reasons why wide-ranging research in this field has been conducted for over 100 years.

2. Conventional high-temperature superconductivity

The main aim of scientific research conducted by me was a theoretical analysis of high-temperature superconductivity induced by interaction of electrons with crystal lattice. I particularly focused on selected physical systems, in which hydrogen plays a key role in the process of reaching zero resistance in higher temperature than boiling temperature of liquid nitrogen (77 K).

In 1968, Ashcroft for the first time, paid attention to the possibility of inducing high-temperature superconductivity in metallic hydrogen under high pressure [6]. Recently, this trend in research has been extremely popular, which resulted in numerous theoretical papers [7–11]. Unfortunately, due to limited possibilities of equipment, the existence of superconductivity in hydrogen has not been proved experimentally till today. Although the year 2017 saw the publication of an experimental paper on hydrogen metallization around the pressure of 500 GPa [12], these results were severely criticized by scientific environment, which means they cannot be treated as credible enough [13, 14]. It might turn out that superconductivity in hydrogen does not exist at all, but this requires performing more precise observations. On the basis of his previous research on superconductivity, in 2004 Ashcroft predicted that introducing hydrogen into the crystal lattice of heavier elements would lead to chemical precompression [15], which would substantially lower the pressure value of metalizing such a system in comparison to the pressure required to metallize pure hydrogen. At the same time Ashcroft suggested that we can expect superconductivity in such a type of materials to occur at a high value of critical temperature and within pressure values obtained in laboratories. Numerous theoretical research papers [16–20] confirmed the above mentioned predictions, which inspired further experimental research. The results obtained by Li and his co-workers [17] deserve our special attention. They conducted wide-ranging structural research on the compound H_2S within the pressure values of $\sim 10 - 200$ GPa. The results obtained show that growing compression leads to the following series of structural changes: $Pbcm \rightarrow P2/c \rightarrow Pc \rightarrow Pmc2_1$ respectively for pressure of 8.7 GPa, 29 GPa and 65 GPa. It is worth considering the fact that the theoretical results obtained comply with previous experimental data obtained with the use

of the X-ray diffraction (XRD) [21, 22]. Two last structural changes occur at the pressure of 80 GPa ($Pmc2_1 \rightarrow P$-1) and 160 GPa (P-1 $\rightarrow Cmca$). Interestingly, the results obtained in the research [17] contravene previous theoretical prognoses suggesting that H_2S dissociates into sulphur and hydrogen at high pressure [23]. However, it should be noticed that partial dissociation of H_2S was noticed above 27 GPa during the research conducted with the use of Raman spectroscopy [24] and XRD [25] at room temperature. The calculations of the electronic structure performed in the paper [17] clearly suggest that the compound H_2S is a insulator till the pressure value of 130 GPa. This result correlates quite well with the value of metallization pressure equalling about 96 GPa, determined experimentally [26]. What is more, Li and his co-workers proved that within the pressure range of 130 to 180 GPa, the compound H_2S shows the existence of superconductivity with maximum critical temperature of ∼80 K.

In December 2014, first experimental results [29] were presented (updated in June 2015 [27] and confirmed in May 2016 [28]), which show that the sample H_2S prepared at low temperature $T < 100$ K and compressed to high pressure obtained in a diamond anvil cell (DAC) has high values of critical temperature. Especially when it comes to the pressure range from 115 to 200 GPa, T_c rises from 31 to 150 K [27]. As it was shown in Fig. 1, the experimental results correlate very well with theoretical predictions of Li and his co-workers [17]. Interestingly, the sample prepared at room temperature, above the pressure of 43 GPa, is subject to dissociation of the original compound according to the following scheme: $3H_2S \rightarrow 2H_3S + S$ [30–32]. In a newly formed system H_3S, under the pressure of 150 GPa, superconductivity is induced at critical temperature of 203 K. Moreover, one
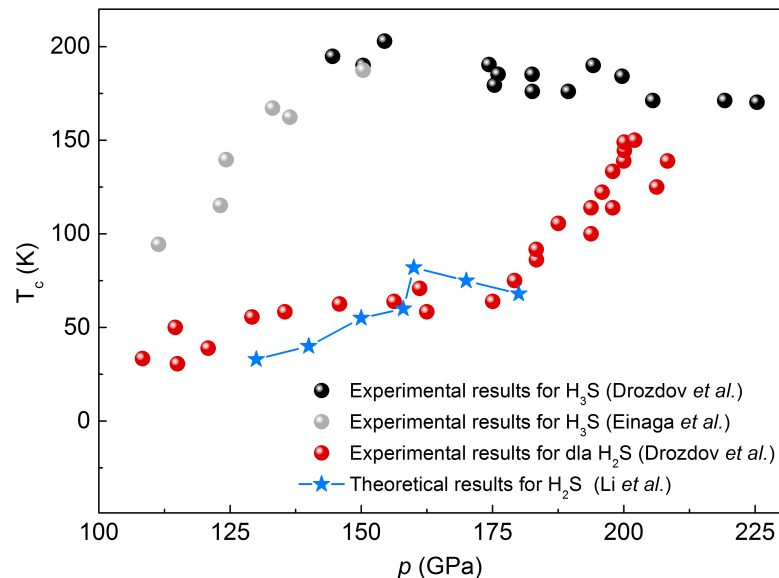
Fig. 1: Critical temperature as a function of pressure for the sample of H_2S prepared at low temperature (red balls) and the sample prepared at room temperature, which, due to pressure, was subject to dissociation and formation of H_3S (grey and black balls) [27, 28]. Theoretical results come from the research [17].

should emphasise the fact that for H_3S a strong isotope effect coming from hydrogen was observed, which clearly suggests the electron-phonon character of superconductivity. From the physical point of view, the obtained result means that a superconductor of the highest value of critical temperature known so far has been discovered. Thus, the experimental results discussed can be regarded as groundbreaking from the point of view of research on widely-comprehended high-temperature superconductivity.

In the light of the experimental facts above and theoretical data, a natural direction of my scientific research was enlarging knowledge about superconductivity in the family of compounds H_2S and H_3S, twin systems of H_3Cl and H_3P and the mixture $H_3S_{1-x}P_x$. First and foremost, I was looking for a way to raise the value of critical temperature in those systems and getting as close as possible to room temperature. From the physical point of view, the description of superconductivity of the compounds in question is based on the idea proposed by H. Fröhlich [33, 34], i.e. on the interaction of electron gas with the vibrations of crystal lattice, which, within the framework of second quantization, can be modelled with the following statistical operator [35]:

$$H = H^{(0)} + H^{(1)}, \tag{1}$$

where:

$$H^{(0)} = \sum_{j\mathbf{k}\sigma} \bar{\varepsilon}_{j\mathbf{k}} c_{j\mathbf{k}\sigma}^\dagger c_{j\mathbf{k}\sigma} + \sum_{\nu\mathbf{q}} \omega_{\nu\mathbf{q}} b_{\nu\mathbf{q}}^\dagger b_{\nu\mathbf{q}}, \tag{2}$$

$$H^{(1)} = \frac{1}{\sqrt{N}} \sum_{jl\nu} \sum_{\mathbf{kq}\neq 0\sigma} g_\nu^{j\mathbf{k+q},l\mathbf{k}}(\mathbf{q}) c_{j\mathbf{k+q}\sigma}^\dagger c_{l\mathbf{k}\sigma}(b_{\nu\mathbf{q}} + b_{\nu-\mathbf{q}}^\dagger). \tag{3}$$

The values $c_{j\mathbf{k}\sigma}^\dagger$ and $c_{j\mathbf{k}\sigma}$ are accordingly the operator of creation and annihilation of the electron state in j-band at momentum $\mathbf{k}$ and spin $\sigma \in \{\uparrow, \downarrow\}$. Symbol $\bar{\varepsilon}_{j\mathbf{k}}$ is defined by the formula: $\bar{\varepsilon}_{j\mathbf{k}} = \varepsilon_{j\mathbf{k}} - \mu$, where $\varepsilon_{j\mathbf{k}}$ is band energy of electrons and μ signifies chemical potential. $b_{\nu\mathbf{q}}^\dagger$ and $b_{\nu\mathbf{q}}$ represent accordingly the operator of creation and annihilation for a phonon whose mode is ν and whose momentum is $\mathbf{q}$, $\omega_{\nu\mathbf{q}}$ determines the value of phonon energy. The energy of electron-phonon interaction is expressed by $g_\nu^{j\mathbf{k+q},l\mathbf{k}}(\mathbf{q})$.

Eliminating phonon degrees of freedom, with the help of a canonical transformation, from the above statistical operator we get Hamiltonian of BCS theory, which can be subsequently analysed within the framework of the mean-field approximation. Unfortunately, this approach does not allow for a quantitative description of superconductivity of the systems in which the value of electron-phonon coupling (λ) is bigger than ~ 0.5 (conventional limit of weak coupling). In most hydrogenated superconductors, we deal with strong $\lambda > 1$ or very strong $\lambda > 2$ electron interaction with crystal lattice. The compounds such as SiH_4, SnH_4 and H_2S would belong to the first group [17, 36, 37]. On the other hand, the systems characterized by very strong electron-phonon coupling are among others CaH_6, YH_6, YH_{10},

SrH$_{10}$ and H$_3$S [20, 36, 37]. Considering the facts above, my analysis of thermodynamic properties of the above mentioned materials was based on the formalism of Eliashberg equations [38] constituting the generalization of BCS theory for the systems characterized by the strong electron-phonon coupling [39]. Contrary to BCS theory, the results obtained within the framework of the Eliashberg formalism, at their quantitative level, comply with experimental measurements, regardless of the fact whether the analysed system is characterized by strong or weak electron-phonon coupling. There are even some premises saying that Eliashberg formalism might be used for the analysis of thermodynamic properties of high-temperature oxygen-copper superconductors. [40, 41].

In order to develop the Eliashberg system of equations, firstly one should write the operator (1) in matrix notation with the use of the Nambu spinor [42]. Next, to obtain an Dyson-type equation [43], a Matsubara Green function is defined [44], where diagonal elements describe thermodynamic properties of normal state above critical temperature, and non-diagonal elements characterize superconductivity [45]. In the last calculation stage, the procedure of self-consistent procedure for the formula of self-energy is used.

In case of superconductors having wide energy bands, such as hydrogenated compounds under high pressure, the Eliashberg system of equations for the function of the order parameter $\varphi_n = \varphi\left(i\omega_n\right)$ and the wave function renormalization factor $Z_n = Z\left(i\omega_n\right)$ takes the following form (one-band, isotropic version):

$$\varphi_n = \pi T \sum_{m=-M}^{M} \frac{\Lambda_{n,m} - \mu^\star \theta\left(\omega_c - |\omega_m|\right)}{\sqrt{\omega_m^2 Z_m^2 + \varphi_m^2}} \varphi_m, \tag{4}$$

$$Z_n = 1 + \frac{\pi T}{\omega_n} \sum_{m=-M}^{M} \frac{\Lambda_{n,m}}{\sqrt{\omega_m^2 Z_m^2 + \varphi_m^2}} \omega_m Z_m, \tag{5}$$

where ω_n is n-th fermionic Matsubara frequency: $\omega_n = \left(\pi/\beta\right)\left(2n - 1\right)$, θ is the Heaviside step function, whereas ω_c signifies the cut-off frequency. Conventionally, it is assumed that the value of ω_c falls within the range from $3\omega_D$ to $10\omega_D$, where ω_D is the Debye frequency [46], whose value, in case of the hydrogenated systems analysed by me, falls within the range from 200 to 350 meV, depending on the value of applied pressure. The pairing kernel for electron-phonon interaction is defined in the following way:

$$\Lambda_{n,m} = 2 \int_0^{\omega_{\mathrm{D}}} d\omega \frac{\omega}{\omega^2 + \left(\omega_n - \omega_m\right)^2} \alpha^2 F\left(\omega\right). \tag{6}$$

The Eliashberg function $\left(\alpha^2 F\left(\omega\right)\right)$, being one of two input elements for Eliashberg equations, plays the role of a bridge between theory and experiment. It is calculated most often with the help of quantum-mechanical (DFT) methods [47–49]. It can be also determined experimentally in the tunnel experiment [50, 51] or with the use of the ARPES method, i.e. angle-resolved photoemission spectroscopy [52]. From the theoretical point of view, an experimental approach is crucial as it ensures the possibility of direct comparison

of obtained experimental and numerical results, which constitutes a test for the accuracy of theoretical calculations [53]. In Eliashberg formalism, in the situation where the experimental value of T_c is known, the Coulomb pseudopotential $\mu^\star$ (the second input element for the Eliashberg equations) modelling decoupling interaction between electrons is selected so that critical temperature obtained from the numerical analysis complies with its value obtained from experimental calculations. In case there are no experimental data, an approximate value of the parameter $\mu^\star$ can be assessed with the help of Morel-Anderson formula [54, 55]:

$$\mu^\star = \frac{\mu}{1 + \mu \ln\left(\frac{\varepsilon_F}{\omega_{\ln}}\right)}, \tag{7}$$

where $\mu = \rho(\varepsilon_F) U_c$. The symbol U_c represents the Coulomb potential, $\rho(\varepsilon_F)$ signifies the density of states (DOS) at the Fermi level (ε_F). The symbol $\omega_{\ln}$ signifies logarithmic frequency:

$$\omega_{\ln} = \exp\left(\frac{2}{\lambda} \int_0^{\omega_D} d\omega \frac{\alpha^2 F(\omega) \ln(\omega)}{\omega}\right). \tag{8}$$

Professional literature usually accepts the value between 0.1 and 0.2 for the parameter $\mu^\star$. It can be proven in a relatively simple way that the assumption is correct in case of hydrogenated compounds investigated by me. Let us notice that the maximum value of $\mu^\star$ can be defined once it is assumed that $\mu \to +\infty$ (the limit of infinite U_c), which lets us write the formula (7) in the following form [55]:

$$\mu^\star_{\max} = \frac{1}{\ln\left(\frac{\varepsilon_F}{\omega_{\ln}}\right)}, \tag{9}$$

For example, for the compound of H_3S under the pressure of 200 GPa, we get $\varepsilon_F = 17.506$ meV and $\omega_{\ln} = 131$ meV [56], which gives us as a result $\mu^\star_{\max} \approx 0.2$. Additionally, the paper [56] confirms that the above mentioned result complies with the estimate of the critical value of $\mu^\star$ obtained with the help of Eliashberg equations, on the basis of providing the experimental value of critical temperature ($\mu^\star_c = 0.204$).

Taking a broader view at the issue, one should pay attention to the fact that $\varepsilon_F \gg \omega_{\ln}$, thus within Morel-Anderson approach implemented, the value of the Coulomb pseudopotential usually equals $0.1 - 0.2$ and $\mu^\star \ll \mu$. The result above creates a certain problem as in many cases high-pressure superconductivity is characterised by $\mu^\star \geq 0.3$. This situation occurs, for example, in lithium where the Coulomb pseudopotential rises together with pressure rise till the value of 0.36 for $p = 29.7$ GPa [57]. This issue was solved by Bauer, Han and Gunnarsson, who made calculations up to second order in U_c [58]. On the basis of these calculations, they stated that retardation effects, also in this case, lead to the decrease in the value of $\mu \to \mu^\star$, however, not as significant one as in case of Morel-Anderson

formula. In the case in question, the following formula was obtained:

$$\mu^{\star} = \frac{\mu + a\mu^2}{1 + \mu \ln\left(\frac{\varepsilon_F}{\omega_{\ln}}\right) + a\mu^2 \ln\left(\frac{\alpha\varepsilon_F}{\omega_{\ln}}\right)}, \tag{10}$$

where the constant a equals 1.38 and $\alpha \simeq 0.10$. Within the range of infinite U_c we obtain:

$$\mu^{\star}_{\max} = \frac{1}{\ln\left(\frac{\alpha\varepsilon_F}{\omega_{\ln}}\right)}. \tag{11}$$

In case of H_3S, the value of the Coulomb pseudopotential obtained with the help of the formula above ($\mu^{\star}_{\max} \approx 0.38$) is clearly too high in relation to numerical analyses. Nevertheless, the analysis performed for H_5S_2 shows that in extreme cases for hydrogenated compounds $\mu^{\star}$ can take values bigger than 0.4 [59].

During the research conducted, I solved Eliashberg equations on an imaginary axis and in mixed representation (the equations defined simultaneously on an imaginary axis and the real one). I used iterative methods described, for example, in [60]. In particular, the equations defined on an imaginary axis let me determine quantitatively the value of critical temperature, the difference of free energy between normal and superconductive states, thermodynamic critical field, specific heat for superconductivity and estimate values for band gap at the Fermi level and electron effective mass. The exact values of the two last parameters were determined with the help of Eliashberg equations in mixed representation [46, 61]:

$$\begin{aligned}
\varphi(\omega + i\delta) = & \frac{\pi}{\beta} \sum_{m=-M}^{M} \left[\lambda(\omega - i\omega_m) - \mu^{\star}\theta(\omega_c - |\omega_m|)\right] \frac{\varphi_m}{\sqrt{\omega_m^2 Z_m^2 + \varphi_m^2}} \\
& + i\pi \int_0^{+\infty} d\omega' \alpha^2 F(\omega') \left[\left[N(\omega') + f(\omega' - \omega)\right]\right. \\
& \times \left.\frac{\varphi(\omega - \omega' + i\delta)}{\sqrt{(\omega - \omega')^2 Z^2(\omega - \omega' + i\delta) - \varphi^2(\omega - \omega' + i\delta)}}\right] \\
& + i\pi \int_0^{+\infty} d\omega' \alpha^2 F(\omega') \left[\left[N(\omega') + f(\omega' + \omega)\right]\right. \\
& \times \left.\frac{\varphi(\omega + \omega' + i\delta)}{\sqrt{(\omega + \omega')^2 Z^2(\omega + \omega' + i\delta) - \varphi^2(\omega + \omega' + i\delta)}}\right]
\end{aligned} \tag{12}$$

and

$$Z\left(\omega+i\delta\right) = 1+\frac{i}{\omega}\frac{\pi}{\beta}\sum_{m=-M}^{M}\lambda\left(\omega-i\omega_m\right)\frac{\omega_m Z_m}{\sqrt{\omega_m^2 Z_m^2+\varphi_m^2}} \tag{13}$$

$$+\quad\frac{i\pi}{\omega}\int_0^{+\infty}d\omega'\alpha^2 F\left(\omega'\right)\left[\left[N\left(\omega'\right)+f\left(\omega'-\omega\right)\right]\right.$$

$$\times\quad\frac{\left(\omega-\omega'\right)Z\left(\omega-\omega'+i\delta\right)}{\sqrt{\left(\omega-\omega'\right)^2 Z^2\left(\omega-\omega'+i\delta\right)-\varphi^2\left(\omega-\omega'+i\delta\right)}}\right]$$

$$+\quad\frac{i\pi}{\omega}\int_0^{+\infty}d\omega'\alpha^2 F\left(\omega'\right)\left[\left[N\left(\omega'\right)+f\left(\omega'+\omega\right)\right]\right.$$

$$\times\quad\frac{\left(\omega+\omega'\right)Z\left(\omega+\omega'+i\delta\right)}{\sqrt{\left(\omega+\omega'\right)^2 Z^2\left(\omega+\omega'+i\delta\right)-\varphi^2\left(\omega+\omega'+i\delta\right)}}\right],$$

where the symbols $N\left(\omega\right)$ and $f\left(\omega\right)$ mean the Bose-Einstein and Fermi-Dirac distribution accordingly.

$$N\left(\omega\right)=\left(\frac{1}{e^{\beta\omega}-1}\right)\qquad\text{oraz}\qquad f\left(\omega\right)=\left(\frac{1}{e^{\beta\omega}+1}\right). \tag{14}$$

Below, I present the exact results concerning high-temperature superconductivity in systems with the purely electron-phonon pairing mechanism, included in the publications **[A1]** – **[A7]** constituting scientific achievement.

In the paper **[A1]**, based on Eliashberg spectral functions determined by Li and his co-workers [17], I analyse the system of H_2S under the influence of pressure from the range of 130 to 180 GPa. For the value of the Coulomb pseudopotential equaling 0.15, I reconstructed the experimental dependence of critical temperature on pressure, $T_c \in \langle 31, 88 \rangle$ K, and I determined other crucial thermodynamic values of superconductivity, such as band gap on Fermi surface, specific heat and thermodynamic critical field. Due to the strong electron-phonon coupling and retardation effects, the results obtained substantially differ from predictions of classical BCS theory. By generalising the results obtained, I estimated the maximum value of critical temperature possible to be observed in compounds of H_nS type, where $n = 1, 2, 3$. At the beginning I noticed that the contributions for the Eliashberg function coming from sulphur and hydrogen are most clearly separated. In particular, in the range of low frequency, electron-phonon interaction coming from sulphur is crucial, whereas for higher frequencies the contribution of hydrogen becomes important [17]. The situation in question is illustrated in Fig. 2 which presents the results for the pressure of 160 GPa at which Li and his co-workers [17] notes the highest critical temperature equalling $\sim$80 K.
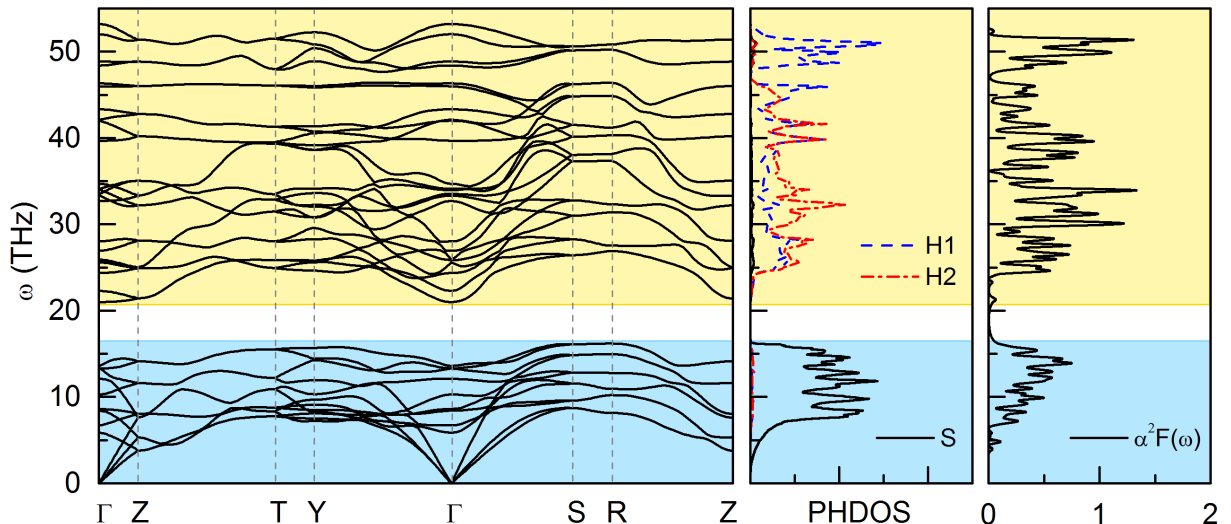
Fig. 2: Phonon spectrum, phonon density of states (PhDOS) and the Eliashberg function $\alpha^2 F(\omega)$ for H_2S under the pressure of 160 GPa [17].

Taking into account the fact above, a model Eliashberg function can be written as follows:

$$\alpha^2 F(\omega) = \lambda_0^{\mathrm{S}} \left(\frac{\omega}{\omega_{\mathrm{max}}^{\mathrm{S}}}\right)^2 \theta\left(\omega_{\mathrm{max}}^{\mathrm{S}} - \omega\right) + \lambda_0^{\mathrm{H}} \left(\frac{\omega}{\omega_{\mathrm{max}}^{\mathrm{H}}}\right)^2 \theta\left(\omega_{\mathrm{max}}^{\mathrm{H}} - \omega\right), \qquad (15)$$

where λ_0^{S} and λ_0^{H} constitute input for the constant of electron-phonon coupling, from sulphur and hydrogen accordingly. Furthermore, the symbols $\omega_{\mathrm{max}}^{\mathrm{S}}$ and $\omega_{\mathrm{max}}^{\mathrm{H}}$ signify maximum phonon frequencies. On the basis of the previous research, I assumed the following input parameters: $\lambda_0^{\mathrm{S}} \in \langle 0.3, 0.8 \rangle$ and $\omega_{\mathrm{max}}^{\mathrm{S}} = 70$ meV [62] and $\lambda_0^{\mathrm{H}} \in \langle 0.5, 2.0 \rangle$ and $\omega_{\mathrm{max}}^{\mathrm{H}} = 220$ meV [8].

As a result of the analysis performed I found out that the maximum value of critical temperature for $\mu^\star = 0.1$ equals 290 K. It should be emphasised that the Coulomb pseudopotential taken for the calculations complies with the estimation performed in Ashcroft's fundamental publication [15]. From the physical point of view, the value T_c obtained constitutes a very important result as it shows that there is a real possibility to achieve superconductivity at critical temperature close to room temperature. This result is always a direct motivation for my further research aiming at finding a way to raise T_c.

In a similar way I determined non-dimensional parameters linked with the band gap, specific heat and thermodynamic criticalfield: $R_\Delta = 2\Delta(0)/k_B T_C$, $R_C = \Delta C(T_C)/C^N(T_C)$ and $R_H = T_C C^N(T_C)/H_C^2(0)$. It should be noticed that the relations above, within classic BSC theory, take universal values: $R_\Delta = 3,53$, $R_C = 1,43$ and $R_H = 0,168$. In the case of H_nS compounds maximum values of the parameters R_Δ and R_C and the minimum value of the parameter R_H clearly diverge from classic BCS theory and equal 6.53, 3.99 and 0.093 accordingly. Complete results in the function of the constant of the coupling λ_0^{S} and λ_0^{H} for selected values of the Coulomb pseudopotential are gathered in Fig. 3.

(a) Temperatura krytyczna

(b) Parametr R_Δ

(c) Parametr R_C

(d) Parametr R_H
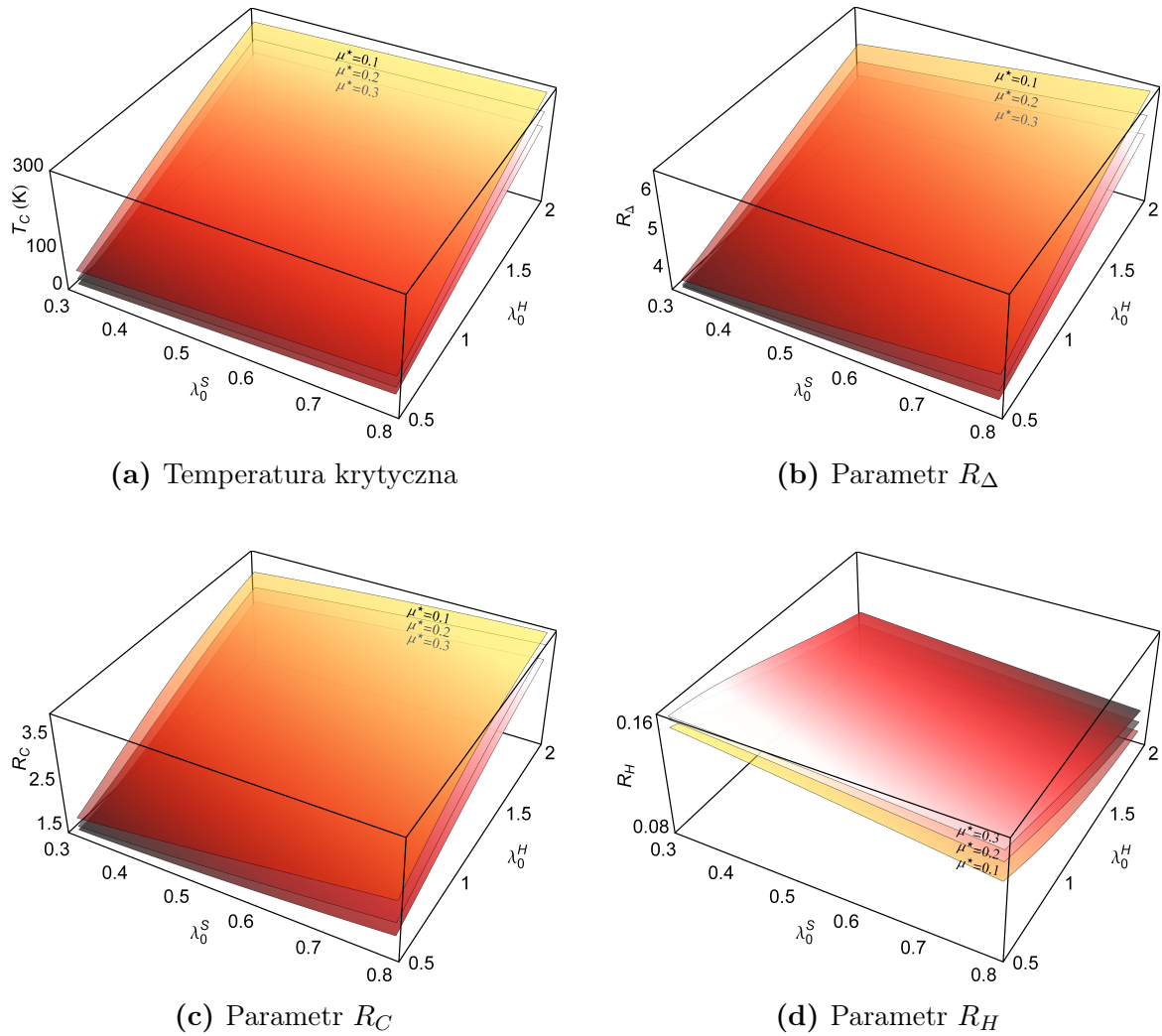
Fig. 3: Critical temperature and non-dimensional parameters R_Δ, R_C and R_H in the function of coupling constant λ_0^S and λ_0^H for selected values of the Coulomb pseudopotential.

The results presented, and in particular those for T_c suggest that it is possible to obtain superconductivity at room temperature in the family of hydrogenated compounds built on the basis of sulphur. This conclusion led to the publications of **[A4]** – **[A7]** which analyse selected options that might lead to obtaining critical temperature higher than 203 K.

Initially, I devoted the publication **[A2]** to a detailed analysis of H_3S compound and its isotope counterpart D_3S. Based on spectral functions determined in the work of [63], for the pressure of 150 GPa, I reconstructed the experimental value of critical temperature equalling 203 K for H_3S and 147 K for D_3S. What is more, I thoroughly discussed the fact of change in the value of the isotope coefficient α together with pressure. For pure metals, there is a relation $T_c M^\alpha = const$, where M is the atomic mass of the isotope contained in the lattice structure of the superconductor, and the exponent α approximately equals 0.5 [64]. On this basis, the exponent α can be described for the compounds analysed by the

following formula:

$$\alpha = -\frac{\ln[T_c]_{\mathrm{D_3S}} - \ln[T_c]_{\mathrm{H_3S}}}{\ln[M]_{\mathrm{D}} - \ln[M]_{\mathrm{H}}}, \tag{16}$$

where $[T_c]_{\mathrm{H_3S}}$ ($[T_c]_{\mathrm{D_3S}}$) is critical temperature of the hydrogen (deuterium)-based system and $[M]_{\mathrm{H}}$ ($[M]_{\mathrm{D}}$) is hydrogen (deuterium) atomic mass.

In the publication in question, on the basis of linear matching of experimental data $T_c(p)$ for $\mathrm{H_3S}$ and $\mathrm{D_3S}$ and by analysing the value of the Coulomb pseudopotential with the help of Morel-Anderson formula [54, 55], I suggested that the experimental value of T_c for $\mathrm{D_3S}$ is underestimated and should really equal about 159 K, which would allow for achieving the value of α equalling 0.35 (the value observed under higher pressure from 170 to 220 GPa). Otherwise, the coefficient in question is 0.47. Moreover, thermodynamic properties of the analysed systems were compared to properties of other conventional superconductors. It turned out that regardless of substantial deviations from BCS theory predictions, $\mathrm{H_3S}$ and $\mathrm{D_3S}$ compounds ideally match the trend set by other conventional superconductors. It is illustrated in Fig. 4 by the overview of the non-dimensional parameters obtained R_Δ, R_C and R_H in the function of T_c/ω_{ln}. It has to be recognized that the publication in question was recognized by the editor of Annalen der Physik (Editor's Choice) and placed on the cover of its May issue in 2016 [65]. What is more, it was regarded as one of the most interesting publications of 2016 [66].
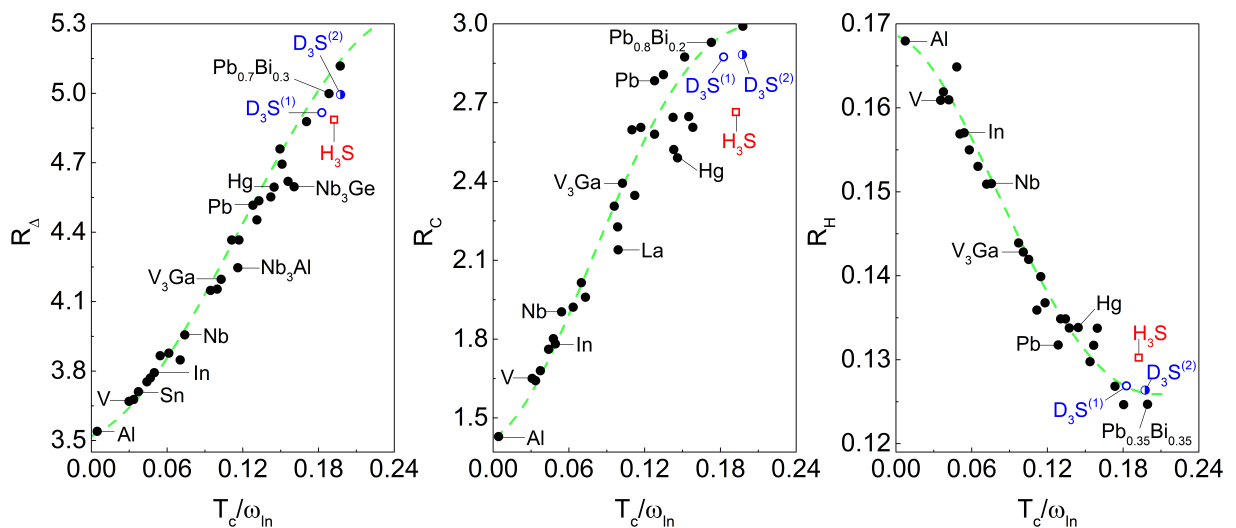
Fig. 4: Non-dimensional parameters R_Δ, R_C and R_H in the function of T_c/ω_{ln}. Experimental points taken from the work of [39]. The results for $\mathrm{D_3S}^{(1)}$ and $\mathrm{D_3S}^{(2)}$ correspond to critical temperature which equals 147 K and 159 K.

The validity of applying classical formalism of Eliasberg equations for the description of hydrogenated compounds was confirmed in the work of **[A3]** with the analysis of the influence of lowest-order vertex correction for electron-phonon interaction on superconductivity in $\mathrm{H_3S}$ and its twin system $\mathrm{H_3P}$, for which the experimental results confirm the occurrence of a superconductive phase below the temperature of 103 K [67]. In particular,

using the density functional theory (DFT) methods implemented in Quantum-ESPRESSO software, I determined electron and phonon properties of the compounds in question and Eliasberg functions defined as follows [47, 48]:

$$\alpha^2 F(\omega) = \frac{1}{2\pi\rho\left(\varepsilon_F\right)} \sum_{\nu\mathbf{q}} \delta(\omega - \omega_{\nu\mathbf{q}})\frac{\gamma_{\nu\mathbf{q}}}{\omega_{\nu\mathbf{q}}}, \tag{17}$$

where the symbol $\gamma_{\nu\mathbf{q}}$ defines the width of phonon lines:

$$\gamma_{\nu\mathbf{q}} = 2\pi\omega_{\nu\mathbf{q}} \sum_{ij} \int \frac{d^3k}{\Omega_{BZ}} |g_\nu^{j\mathbf{k}+\mathbf{q},l\mathbf{k}}(\mathbf{q})|^2 \delta(\varepsilon_{i\mathbf{q}} - \varepsilon_F)\delta(\varepsilon_{j\mathbf{k}+\mathbf{q}} - \varepsilon_F). \tag{18}$$

Then, on the basis of the determined functions $\alpha^2 F(\omega)$ for the pressure of 200 GPa, I reconstructed the experimental values of critical temperature (178 K for H$_3$S and 81 K for H$_3$P) using classic Eliasberg equations and extended equations complemented by vertex corrections, which take the following form [68, 69]:

$$\begin{aligned}
\varphi_n &= \pi T \sum_{m=-M}^{M} \frac{\Lambda_{n,m} - \mu^\star\theta\left(\omega_c - |\omega_m|\right)}{\sqrt{\omega_m^2 Z_m^2 + \varphi_m^2}}\varphi_m \\
&- \frac{\pi^3 T^2}{4\varepsilon_F} \sum_{m=-M}^{M} \sum_{m'=-M}^{M} \frac{\Lambda_{n,m}\Lambda_{n,m'}}{\sqrt{\left(\omega_m^2 Z_m^2 + \varphi_m^2\right)\left(\omega_{m'}^2 Z_{m'}^2 + \varphi_{m'}^2\right)\left(\omega_{-n+m+m'}^2 Z_{-n+m+m'}^2 + \varphi_{-n+m+m'}^2\right)}} \\
&\times \left[\varphi_m\varphi_{m'}\varphi_{-n+m+m'} + 2\varphi_m\omega_{m'}Z_{m'}\omega_{-n+m+m'}Z_{-n+m+m'} - \omega_m Z_m\omega_{m'}Z_{m'}\varphi_{-n+m+m'}\right]
\end{aligned} \tag{19}$$

and

$$\begin{aligned}
Z_n &= 1 + \frac{\pi T}{\omega_n} \sum_{m=-M}^{M} \frac{\Lambda_{n,m}}{\sqrt{\omega_m^2 Z_m^2 + \varphi_m^2}}\omega_m Z_m \\
&- \frac{\pi^3 T^2}{4\varepsilon_F\omega_n} \sum_{m=-M}^{M} \sum_{m'=-M}^{M} \frac{\Lambda_{n,m}\Lambda_{n,m'}}{\sqrt{\left(\omega_m^2 Z_m^2 + \varphi_m^2\right)\left(\omega_{m'}^2 Z_{m'}^2 + \varphi_{m'}^2\right)\left(\omega_{-n+m+m'}^2 Z_{-n+m+m'}^2 + \varphi_{-n+m+m'}^2\right)}} \\
&\times \left[\omega_m Z_m\omega_{m'}Z_{m'}\omega_{-n+m+m'}Z_{-n+m+m'} + 2\omega_m Z_m\varphi_{m'}\varphi_{-n+m+m'} - \varphi_m\varphi_{m'}\omega_{-n+m+m'}Z_{-n+m+m'}\right].
\end{aligned} \tag{20}$$

The results obtained allow to notice a considerable reduction of the Coulomb pseudo-potential value once vertex corrections are taken into account. It is a crucial result as it decreases the contribution of the parameter whose function, in fact, is to match theoretical results to experimental data. However, my further analysis showed that regardless of the change in the value of the depairing parameter by -9.3% in the case of H$_3$S and by -5.7% in the case of H$_3$P, the course of the order parameter obtained within the framework of classic Eliasberg equations does not differ from the one obtained with the help of the equations extended by vertex corrections. It means that the thermodynamic properties of the systems in question can be successfully analysed within classical Migdal-Eliashberg approach provided that the Coulomb pseudopotential is appropriately matched. In the

same year, the research concerning the impact of vertex corrections on superconductivity in the compound of H_3S was also conducted by Sano et al. [35]. They proved that once the value of $\mu^\star$ is determined beforehand, lowest-order vertex corrections, similarly to anharmonic effects [70], substantially reduce (by about 20%) the value of critical temperature. The negative influence of vertex corrections on the value of T_c was also confirmed by the results of my latest research conducted for the compound of H_3Cl [71]. However, it should be noticed that observed reductions amount to merely about 2%. The existence of such big discrepancies derives from the difference in the method of analysing vertex corrections. My calculations are based on ignoring momentum dependency and solving Eliasberg equations with vertex correction in a self-consistent way. On the other hand, Sano does not omit momentum dependency but introduces a series of additional approximations and finally does not obtain his result in a self-consistent way. It is worth emphasising that both the first and the second method have their imperfections. That is why the best solution would be introducing and solving complete equations in a self-consistent way. From the mathematical point of view, it is quite a complex issue, but worth our attention, like the analysis of high-order vertex corrections. I shall come back to these issues in my further research.

The paper **[A4]** presents systematic research which aimed at obtaining critical temperature close to room temperature. It focused on the increase of pressure as one possible factor allowing for the achievement of the desired effect. External pressure can be regarded as a parameter which allows for controlling the properties of researched materials. A change in pressure leads to a change in the distance between atoms, which in some conditions can cause metallization of the system and transition into the superconductivity state. It also has influence on the increase of such key values as the constant of electron-phonon coupling or critical temperature. The best example is calcium which, while exposed to compression, experiences a series of structural transformations while its T_c grows till the value of 29 K, which so far has been the highest critical temperature obtained experimentally for an element [72]. In case of hydrogen, theoretical research suggests that the increase in pressure to an extremely high value of 2000 GPa might cause transition from the normal o superconductive state at the temperature of 600 K [8, 73]. Of course, it is not a rule that pressure increase causes T_c increase. In certain circumstances, it can lead to T_c decrease and even to superconductivity loss. Such a situation takes place, for example, in the case of lithium [74] or the compound of MgB_2 [75]. In the light of the information above, I found it very important to check how the system H_3S behaves at conditions of very high pressure. The initial stage of the research encompassed the procedure of optimization of lattice constants and atom location in an elementary cell by minimizing the system's enthalpy due to the value of assumed pressure. The minimum obtained allowed for further simulations which were subsequently completed by calculations performed within the frame of Eliashberg theory. The results obtained show that in the pressure range from 250 to 500 GPa, the system

H_3S of lattice structure $Im\bar{3}m$ is dynamically stable, which manifests itself in lack of imaginary frequencies in the phonon spectrum. The enthalpy diagram in the function of pressure also confirms a tendency to keep the cubic structure of the system above the value of 180 GPa. Moreover, for all the pressure values analysed, one can notice a clear maximum in electron density of states near the Fermi surface, which, to a large extent, is responsible for inducing high-temperature superconductivity in H_3S [35, 76, 77]. The analysis performed leads to the conclusion that increasing pressure to the limits of laboratory possibilities (~500 GPa) does not allow for obtaining the superconductivity state in the compound of H_3S above the temperature of 200 K. Fig. 5 illustrates the course of T_c in the function of pressure. It is worth paying attention to the fact that the
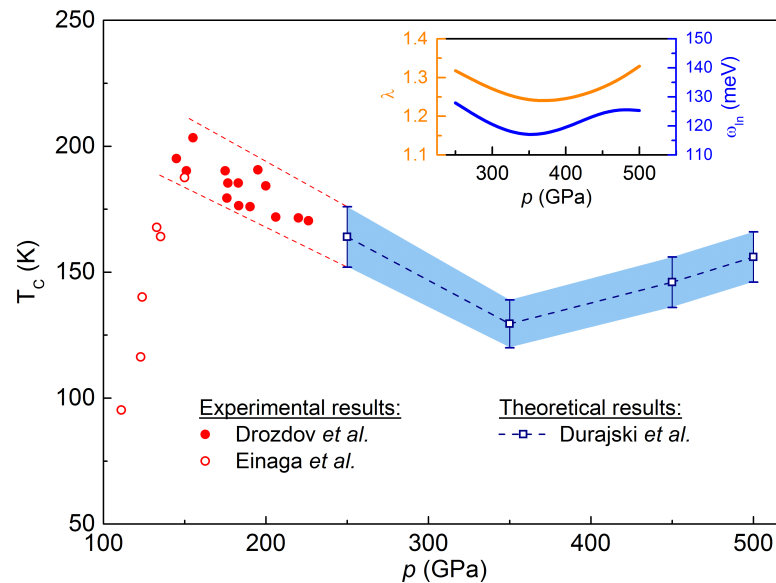

Fig. 5: Critical temperature in the function of pressure for H_3S. Deviations from set values of T_c were obtained for $\mu^\star = 0.11 - 0.15$.

results obtained in the range from 250 to 350 GPa correspond very well to experimental data for lower pressure values, marked in the diagram by red symbols [27, 28]. On the other hand, over 350 GPa, there is an opposite trend and critical temperature begins to rise systematically till its maximum value equalling 155 ± 10 for the pressure of 500 GPa. The course described strongly correlates with the function of electron-phonon coupling constant $(\lambda = 2 \int_0^{\omega_D} d\omega \alpha^2 F(\omega)/\omega)$ and the course of logarithmic phonon frequency $(\omega_{\ln})$. The calculated values of λ and $\omega_{\ln}$ were drawn in the function of pressure in inset of Fig. 5. The results above strongly suggest that experimenters should look for a different method which would allow them to achieve the superconductivity state in room temperature.

Following that path, in my work **[A5]** I examined the influence of sulphur isotopes on the superconductivity state in H_3S. In case of replacing hydrogen with deuterium in an elementary cell, the reduction of critical temperature was experimentally proved, whereas, in case of sulphur, professional literature does not contain any information on this topic.
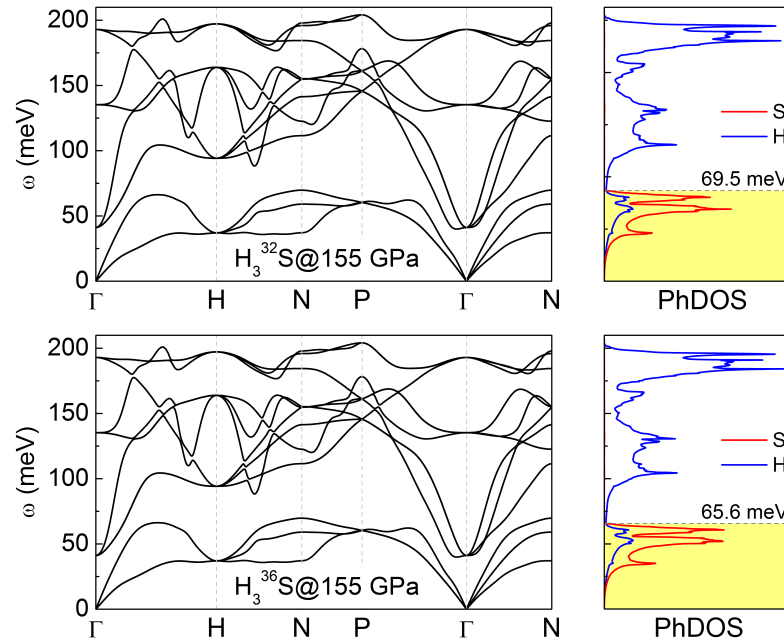
Fig. 6: The influence of sulphur isotope change on the phonon structure of H_3S.

Generally, we can distinguish four stable, naturally occurring sulphur isotopes: ^{32}S (31.972 u), ^{33}S (32.971 u), ^{34}S (33.968 u) and ^{36}S (35.967 u). For all the cases above I conducted numerical analyses within the pressure range from 155 to 225 GPa. The pressure range was not chosen at random, it strictly corresponds to the experimental results obtained for the structure $Im\bar{3}m$, which makes it possible to perform a comparative analysis of the results obtained with the experimental data. Like it was anticipated, my performed research let me conclude that sulphur isotope change does not have any influence on the electron structure of a system analysed. However, there are interesting outcomes in the phonon structure. Increasing mass of the sulphur isotope makes the boundary of the input coming from sulphur shift to the constant of electron-phonon coupling towards lower values, which means that the percentage input coming from hydrogen increases. Fig. 6 presents phonon structures and PhDOS for two extreme cases: the isotope with the minimum atomic mass (^{32}S) and the isotope with the maximum atomic mass (^{36}S). The area marked yellow shows the range of frequencies in which vibrations coming from sulphur are of primary importance. Due to the above mentioned shift, we can notice an untypical isotopic effect reflected in the critical temperature increase to the value of 242 K at the pressure of 155 GPa and the isotope of ^{36}S. Fig. 7 presents the detailed results. The value of the Coulomb pseudopotential was matched in such a way as to make it possible to reconstruct experimental results for average sulphur mass. Analysing the T_c change graph in the function of pressure, one has to pay attention to the fact that despite reversed and non-trivial isotope effect, pressure growth is accompanied with a general decrease in critical temperature, in accordance with the trend set by experimental points. The results presented in the work **[A5]** show that the growth in the value of critical temperature by
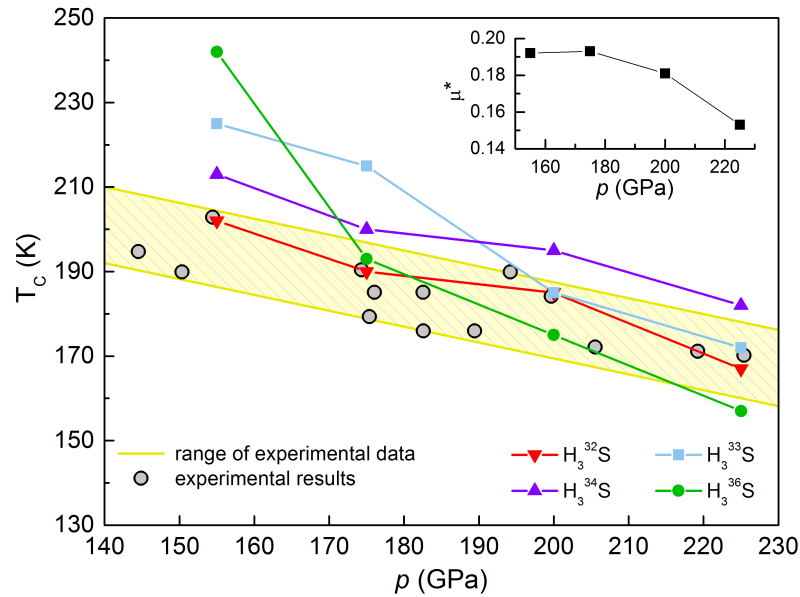
Fig. 7: Critical temperature in the function of pressure for H3S with different sulphur isotopes.

almost 40 K, in relation to a record-like experimental result, is possible. It is one more proof of electron-phonon pairing character in the compounds of hydrogen and sulphur, provided that theoretical results are experimentally proven.

In 2016, a record value of T_c equalling 280 K was predicted in the compound $H_3S_{0.925}P_{0.075}$ [78]. The authors of this paper performed a widely-ranged numerical analysis based on the method of Virtual Crystal Approximation (VCA). In this method, in an elementary cell of H_3S, atom S is replaced with pseudopotential which is specially constructed superposition of two atoms, S and P in the proportions corresponding to the assumed chemical composition. This method is much more effective than the supercell method as calculations are performed on a primitive cell, though in some situations it might turn out much less credible. Analysing in detail the results presented by [78], it can be noticed that critical temperature for the system $H_3S_{0.925}P_{0.075}$ grows systematically, together with pressure from the value of 224 ± 18 K for 150 GPa to 260 ± 20 K for 250 GPa. This result goes against the trend set by experimental data for H_3S which show T_c decrease accompanied by pressure growth in the range beyond 150 GPa [27]. Due to this fact, the work **[A6]** focuses on the verification of the method consisting in partial replacement of sulphur with phosphorus atoms, based on calculations of supercells measuring $2 \times 2 \times 2$ and containing 64 atoms. Fig. 8 presents a set of three analysed supercells which correspond to the following configurations a) $H_3S_{0.875}P_{0.125}$, b) $H_3S_{0.5}P_{0.5}$ and c) $H_3S_{0.375}P_{0.625}$. For each presented cell, I performed calculations of electronic and phonon structure, electron-phonon interaction for the pressure of 155, 180, 205 and 230 GPa. The dynamic stability of the analysed systems was confirmed. Next, critical temperature calculations performed with the use of formalism of Eliasberg equation for a wide range of the Coulomb pseu-
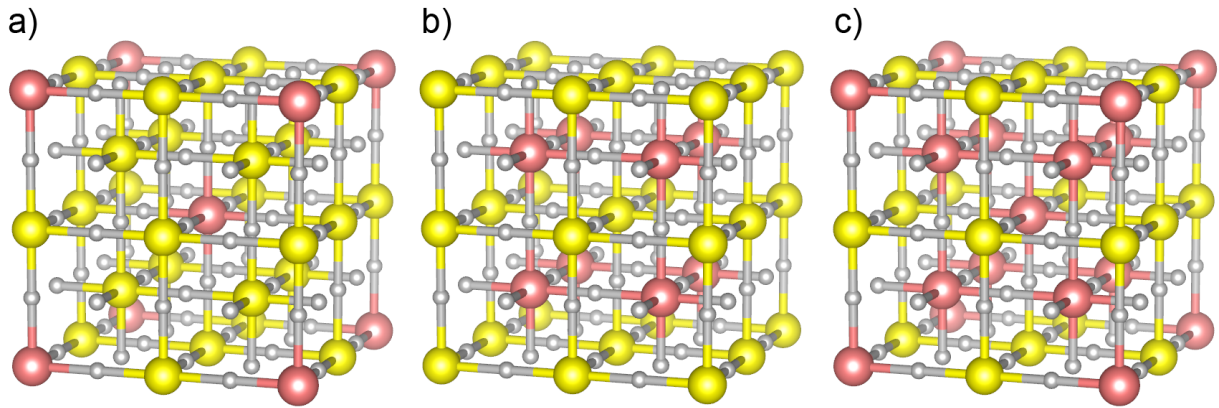
Fig. 8: Supercells formed by doubling an elementary 8-atom cell in each direction. Grey balls represent hydrogen atoms, yellow ones stand for sulphur atoms, and red ones correspond to phosphorus atoms.

dopotential, from 0.1 to 0.2, showed that doping the compound of H_3S with phosphorus negatively influences on superconducting state. In particular, one could notice a smaller value of critical temperature in the whole range of analysed pressure values. Interestingly enough, similarly to the case of the work mentioned before, it was possible to reconstruct a trend observed in the experiment, consisting in the decrease in T_c values accompanied with pressure growth (Fig. 9). In my opinion, it proves very big inaccuracy of the VCA
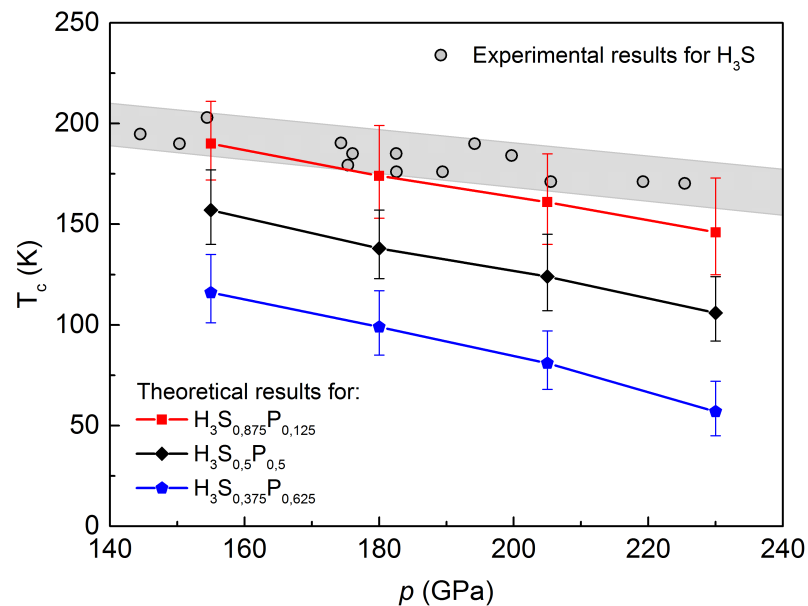
Fig. 9: Critical temperature in the function of pressure for $H_3S_{1-x}P_x$.

method used in the publication [78] to determine superconductivity characteristics. The result obtained in the paper by [78] does not lead to the conclusion that partial replacement of sulphur atoms with phosphorus atoms in an elementary cell of H_3S would allow for achieving superconductivity at the temperature close to room temperature.

In the publication **[A7]**, the last one from the series of papers concerning the description of the superconductivity state in systems of classical electron-phonon pairing mechanism, I analysed the system of H_3Cl. During the analysis of experimental data it is not difficult to notice that phosphorus and sulphur, which in their coupling with hydrogen display the highest critical temperature values, are neighbours in the periodic table of elements (elements of the third period, group VA and VIA). Taking it into account, it may be assumed that also the compound of chlorine and hydrogen might display superconductivity properties (chlorine - an element of the third period, group VIIA). One more hypothesis also seems correct. It says that as electronegativity of an element X in the cell H_3X grows, also critical temperature of the system rises [79]. Chlorine, sulphur's neighbour, shows higher electronegativity than phosphorus and sulphur, thus, it is a potential candidate for analysis. Considering the facts above, I performed a complete calculating procedure, which consisted in finding a potential crystal structure for which the enthalpy of the system H_3Cl reaches the lowest value, in determining electron and phonon properties and in determining constant values for electron-phonon interaction for pressure values from 150 to 250 GPa. I showed that for the compound H_3Cl, the structure $Im\bar{3}m$ is the most advantageous energetically and dynamically stable in the pressure range analysed. What is more, it allows for transition into superconductivity characterized by very strong electron-phonon coupling $\lambda = 2.21$ at the pressure of 150 GPa. Subsequently, pressure growth makes the value of λ drop to 0.91 for $p = 250$ GPa. On the basis of determined spectral functions, critical temperature for H_3Cl was determined alongside with the use of classic Eliashberg equations and their extended versions, enriched with lowest-order vertex corrections. Additionally, the results obtained were compared with the results calculated with the help of the analytical McMillan formula [80]. Due to lack of any experimental data, the above mentioned calculations were performed with the assumption of a constant value of the Coulomb pseudopotential ($\mu^\star = 0.13$). It made it possible to determine the influence of vertex corrections on T_c. It turns out that for a fixed value of $\mu^\star$, vertex corrections only slightly reduce the value of critical temperature and band gap. As Fig. 10 shows, pressure has a significant influence on the order parameter and on T_c as it makes critical temperature drop from 198 to 77 K in the range of 150 to 250 GPa. Thus, the highest obtained result is close to the record value of critical temperature, experimentally observed in H_3S and may constitute a departure point for further high-pressure experimental measurements. Additionally, the paper tackles the issue of the isotope effect, which clearly confirms the classic pairing mechanism in the system of H_3Cl, provided it is experimentally verified.

Finally, it should be clearly emphasised that the topic concerning hydrogenated compounds is still open. Intensive research carried out in many leading scientific centres all over the world aims not only at increasing critical temperature but also at decreasing external pressure required for metallization and transition into superconducting state, which could
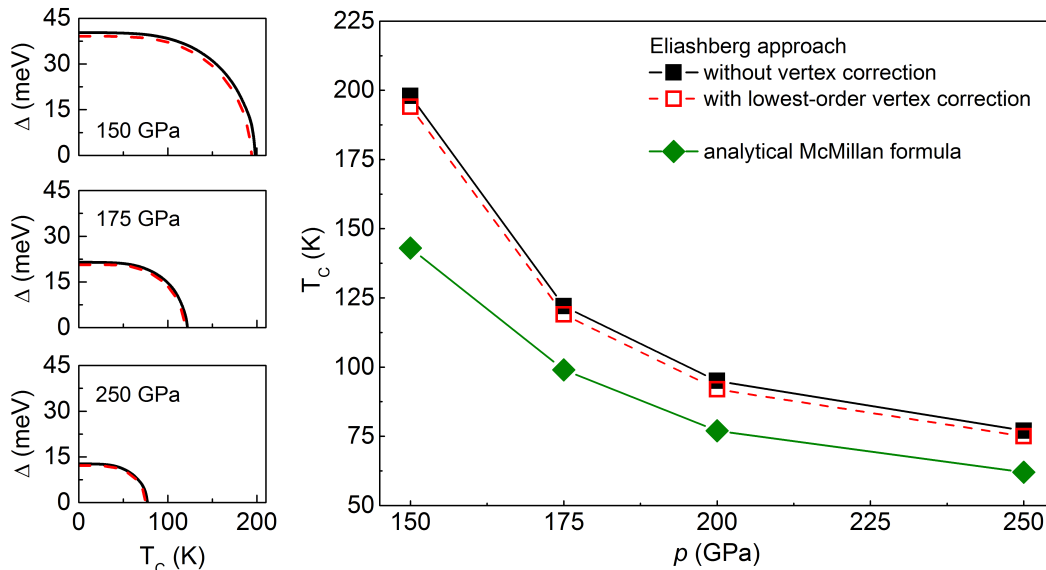
Fig. 10: Order parameter in the temperature function and critical temperature in the function of pressure for H_3Cl.

ensure practical use of such superconductors in the future. One possible way to achieve that seems to be increasing the concentration of hydrogen atoms in the elementary cell. There are many hopes concerning the systems analysed in last years, in which one heavy atom matches six or ten hydrogen atoms. In particular, the following compounds should be mentioned: CaH_6 ($T_c = 235$ K) [16], YH_6 ($T_c = 247$ K) [36], MgH_6 ($T_c = 270$ K) [81] and YH_{10} ($T_c = 291$ K) [36]. Unfortunately, currently all we have are theoretical predictions. Lack of experimental verification hinders further progress in analysing these superconductors.

3. Unconventional high-temperature superconductivity

Superconductivity with a high value of critical temperature is also observed in compounds of copper oxides (so-called cuprates). In 1986, on the basis of their measurement of electrical resistance, Georg Bednorz and Alex Müller noticed that their analysed sample LaBaCuO reaches zero resistance at the temperature about 30 K [3]. Soon several other superconductors based on copper-oxygen planes were discovered (among others, $YBa_2Cu_3O_{7-\delta}$ [82] and $Bi_2Sr_2CaCu_2O_{8+x}$ [83]), whose critical temperature exceeded the boiling temperature of liquid nitrogen. Let us notice that apart from H_2S and H_3S, these are materials characterized by the highest experimentally verified values of T_c. For example, for the $HgBa_2Ca_2Cu_3O_{8+y}$ (Hg1223) compound, the achieved $T_c \simeq 135$ K. This value can grow to over 150 K if the sample is exposed to external pressure of $11 - 15$ GPa [84, 85]. Further compression to ~ 31 GPa can lead to critical temperature equalling even 164 K [86]. Contrary to conventional superconductors with the electron-phonon pairing

mechanism, the mechanism responsible for the formation of Cooper pairs and the existence of superconductivity in cuprates is still under discussion [64, 87–90]. In 2012, it was suggested that superconductivity induced in these materials might be at least partially modelled with the use of extended Fröhlich Hamiltonian [91]. This general approach consisted in taking into account an additional constant of compression for electron-electron-phonon interaction linked with the Coulomb potential of diagonal interactions [92]. The suggested approach is based, in particular, on three fundamental postulates saying that as far as high-temperature superconductors are concerned: i) the electron system of copper-oxygen planes plays a very important role (quasi-two-dimensionality of the electron system), ii) there is classic electron-phonon interaction, whose constant of compression does not have to be high (the pairing mechanism given by Fröhlich) and iii) there are strong electron correlations, but electron-electron interaction is inseparably linked with phonon absorption or emission. Two first postulated describe classical van Hove's scenario [93]. The third one generalises Hubbard correlations, i.e. classic two-body interaction is replaced with the three-body one (electron-electron-phonon).

The analysis of thermodynamic properties of high-temperature superconductivity performed in the publication [91] consisted in developing a quotation for the order parameter, although its basis was a canonical transformation eliminating phonon degrees of freedom. Regardless of further approximations related to the negligence of retardant and high-compression effects or using the approximation of the so-called Mean Field Theory to the element describing effective four-fermionic interaction, very interesting results were obtained at the quantitative level. In particular, it was shown that the obtained equation for the order parameter makes it possible to calculate properly the band gap at the temperature close to the absolute zero once the experimental values of critical temperature and Nernst temperature or pseudogap temperature are known. Examples of results obtained for YBCO are shown in Fig. 11. In particular, one should pay attention to very good correlation of theoretical results and experimental data for the relation $2\Delta(0)/k_B T_c$.

My contribution to the development of the high-temperature superconductivity theory in cuprates consisted in implementing the scheme presented above, serving to describe hole-doped superconductors with a symmetry type of $d_{x^2-y^2}$, for which a pseudogap occurs above critical temperature. In particular, I focused on reconstructing experimental results obtained via the angle-dependent ARPES technique. Moreover, I undertook to approximate mean-field results, which can be obtained with the use of a canonical transformation, by developing complete Eliashberg equations based on the assumed Hamiltonian taking into account electron-phonon and electron-electron-phonon interaction. It resulted in three publications (**[A8]**-**[A10]**), whose characteristics I present below.

Within the framework of the scheme in question, the Hamiltonian modelling electron-phonon and electron-electron-phonon (EEPh) interaction in cuprates takes the following form [91]:

$$H = H^{(0)} + H^{(1)} + H^{(2)}, \tag{21}$$
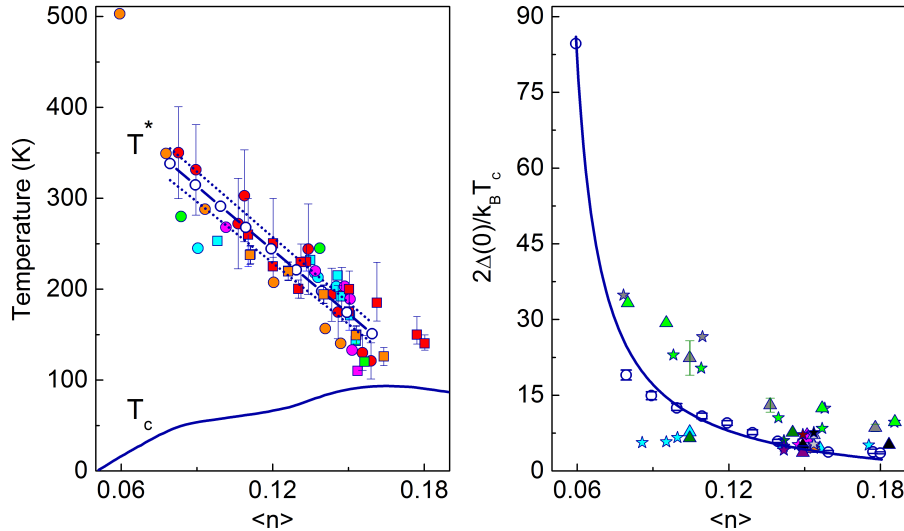
Fig. 11: Critical temperature and pseudogap temperature and the relation of $2\Delta(0)/k_B T_c$ in the function of hole doping for YBCO. Open circles signify the average $T^\star$ and numerical results for $2\Delta(0)/k_B T_c$. Other symbols stand for experimental data [94].

where the first part describes, similarly like in Fröhlich's publication, the system of non-interacting electrons and phonons (single-band case):

$$H^{(0)} = \sum_{\mathbf{k}\sigma} \overline{\varepsilon}_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}}. \tag{22}$$

The symbol $\overline{\varepsilon}_{\mathbf{k}}$ is defined by the formula: $\overline{\varepsilon}_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu$, where $\varepsilon_{\mathbf{k}}$ is electron band-energy: $\varepsilon_{\mathbf{k}} = -t\gamma(\mathbf{k})$, where $\gamma(\mathbf{k}) = 2\left[\cos(k_x) + \cos(k_y)\right]$. We assume that electrons may propagate in a square lattice with the hopping integral t. The interaction operators EPh and EEPh are expressed by the following formula, respectively:

$$H^{(1)} = \sum_{\mathbf{k}\mathbf{q}\sigma} v_{\mathbf{k}}^{(1)}(\mathbf{q}) \, c_{\mathbf{k}+\mathbf{q}\sigma}^{\dagger} c_{\mathbf{k}\sigma} \phi_{\mathbf{q}} \tag{23}$$

and

$$H^{(2)} = \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}\mathbf{l}\sigma} v_{\mathbf{k},\mathbf{k}'}^{(2)}(\mathbf{q},\mathbf{l}) \, c_{\mathbf{k}-\mathbf{l}\sigma}^{\dagger} c_{\mathbf{k}\sigma} c_{\mathbf{k}'+\mathbf{l}+\mathbf{q}-\sigma}^{\dagger} c_{\mathbf{k}'-\sigma} \phi_{\mathbf{q}}, \tag{24}$$

where: $\phi_{\mathbf{q}} = b_{-\mathbf{q}}^{\dagger} + b_{\mathbf{q}}$. $v_{\mathbf{k}}^{(1)}(\mathbf{q})$ i $v_{\mathbf{k},\mathbf{k}'}^{(2)}(\mathbf{q},\mathbf{l})$ signify the matrix for EPh interaction and the tensor for EEPh interaction.

In the article **[A8]** the above mentioned Hamiltonian was simplified by eliminating phonon degrees of freedom. Additionally, the symmetry of the order parameter of a type $d_{x^2-y^2}$ was imposed (dominant symmetry observed experimentally in case of the majority of examined cuprates). Finally, it was possible to express the analysed Hamiltonian in this form:

$$H' = H'^{(0)} + H'^{(1)} + H'^{(2)}, \tag{25}$$

where

$$H^{'(0)} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \tag{26}$$

$$H^{'(1)} = - \sum_{\mathbf{k_1 k_2}\sigma}^{\omega_0} \frac{V_{\mathbf{k_1 k_2}}}{2N_0} c^{\dagger}_{\mathbf{k_1}-\sigma} c^{\dagger}_{-\mathbf{k_1}\sigma} c_{-\mathbf{k_2}\sigma} c_{\mathbf{k_2}-\sigma}, \tag{27}$$

and

$$H^{'(2)} = - \sum_{\mathbf{k_1}\sim\mathbf{k_4}\sigma}^{\omega_0} \frac{U_{\mathbf{k_1}\sim\mathbf{k_4}}}{2N_0^3} \phi_{\mathbf{k_1}\sigma} \phi^{\star}_{\mathbf{k_2}\sigma} c_{-\mathbf{k_3}\sigma} c_{\mathbf{k_3}-\sigma} c^{\dagger}_{\mathbf{k_4}-\sigma} c^{\dagger}_{-\mathbf{k_4}\sigma}. \tag{28}$$

Functions $V_{\mathbf{k_1 k_2}}$ oraz $U_{\mathbf{k_1}\sim\mathbf{k_4}}$ represent pairing potentials for EPh and EEPh for the symmetry of a type $d_{x^2-y^2}$:

$$V_{\mathbf{k_1 k_2}} = V \eta(\mathbf{k_1}) \eta(\mathbf{k_2}) \tag{29}$$

and

$$U_{\mathbf{k_1}\sim\mathbf{k_4}} = U \eta(\mathbf{k_1}) \eta(\mathbf{k_2}) \eta(\mathbf{k_3}) \eta(\mathbf{k_4}), \tag{30}$$

where: $\eta(\mathbf{k}) = 2[\cos(k_x) - \cos(k_y)]$. Next, it was possible to define Green function of superconductivity on the basis of which we developed the equation for anomalous thermodynamic average:

$$\begin{aligned}
\varphi_{\mathbf{k}} &= \left(\frac{1}{N_0} \sum_{\mathbf{k_1}}^{\omega_0} \eta(\mathbf{k_1}) \varphi_{\mathbf{k_1}} \right) \\
&\times \left[V + U \left(\frac{1}{N_0} \sum_{\mathbf{k_2}}^{\omega_0} \eta(\mathbf{k_2}) \varphi_{\mathbf{k_2}} \right) \left(\frac{1}{N_0} \sum_{\mathbf{k_3}}^{\omega_0} \eta(\mathbf{k_3}) \varphi^{\star}_{\mathbf{k_3}} \right) \right] \eta(\mathbf{k}) \chi_{\mathbf{k}},
\end{aligned} \tag{31}$$

where: $\varphi_{\mathbf{k}} = \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle$ and

$$\chi_{\mathbf{k}} = \frac{\tan\left[\frac{i\beta}{2} \sqrt{\varepsilon_{\mathbf{k}}^2 + M_{\mathbf{k}}^2} \right]}{2i\sqrt{\varepsilon_{\mathbf{k}}^2 + M_{\mathbf{k}}^2}}. \tag{32}$$

The relationship between the amplitude of anomalous thermodynamic average ($|\varphi_{\mathbf{k}}|$) and temperature for selected values of U is presented in Fig. 12. In the case of $U = 0$ (Fig. 12(A)) $|\varphi_{\mathbf{k}}|$ systematically decreases together with temperature growth and finally disappears at $T_c \simeq 0.0231t$. In other cases where $U \neq 0$ (Fig. 12(B)-(D)) for $0 < T < T_c$, the antinodal area $|\phi_{\mathbf{k}}|$ is slightly dependent on temperature and above critical temperature it turns into anomalous normal state existing till pseudogap temperature. Contrary to antinodal areas, nodal areas of the amplitude decrease significantly together with temperature growth and, as a result, disappear at $T_c \simeq 0.0231t$. The last stage consisted in determining the equation which would allow us to analyse the anisotropic character of the order parameter: $\Delta_{\mathbf{k}} = 2\eta(\mathbf{k}) |\varphi_{\mathbf{k}}| \left[V + U |\eta(\mathbf{k})| |\varphi_{\mathbf{k}}|^2 \right]$. The publication in question demonstrates, taking as an example the compound $YBa_2Cu_3O_{7-\delta}$, that the analysed mechanism allows for reconstructing, in detail, experimental results obtained with the help of the ARPES method. In the publication **[A9]**, due to a big number of experimental data which might
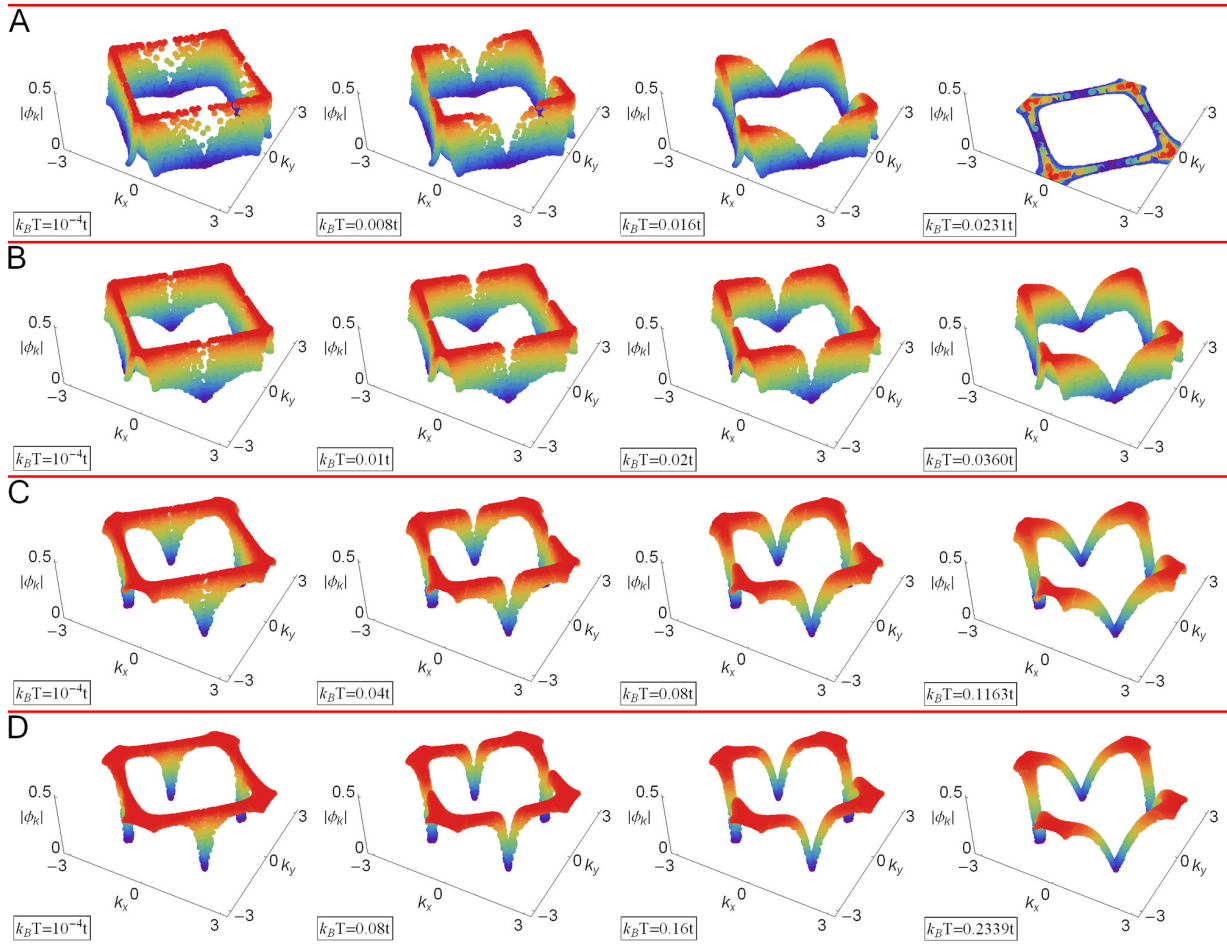
Fig. 12: The amplitude of anomalous thermodynamic average near Fermi energy for selected values of U and temperature. In particular, (A) $U = 0$, (B) $U = 0.02t$, (C) $U = 0.05t$ oraz (D) $U = 0.1t$. It was assumed that $V = 0.02t$ and $\omega_0 = 0.3$.

serve to verify the results obtained, I analysed the structure of the order parameter ($\Delta_{\mathbf{k}}$) for the superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212). The obtained results clearly show that the antinodal area $\Delta_{\mathbf{k}}$ is slightly dependent on temperature and above critical temperature it turns into pseudogap. On the other hand, the value of $\Delta_{\mathbf{k}}$ near the nodal area depends strongly on temeperature. The publication shows very good correlation between the used model and experimental data obtained for different values of doping. Apart from the influence of hole-doping, I also investigated the impact of temperature on the structure of the order parameter. The obtained results are demonstrated in Fig. 13 and Fig. 14, where grey circles signify numerically obtained values of band gap, red lines stand for averaged numerical results, whereas green squares mean experimental results taken from the publications by [95–97].

In the last publication devoted to the issues concerning superconductivity in cuprates (publication **[A10]**), I developed Eliashberg quotation using the Hamiltonian (21), which let me go beyond the mean-field approximation. A general scheme of the procedure
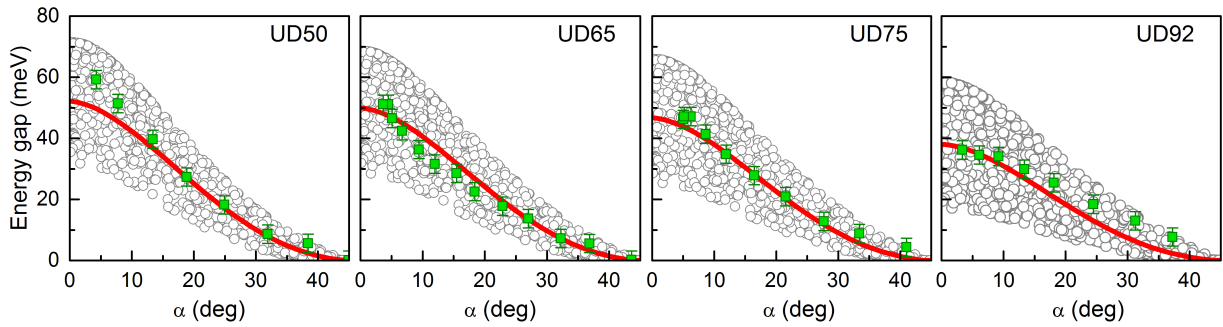
Fig. 13: The relationship between band gap of the superconductor Bi2212 and the angle for different concentrations of holes in $T = 10$ K. Markings UD50, UD65, UD75 and UD92 correspond to hole concentration equalling respectively: 0.08, 0.10, 0.12 and 0.16.
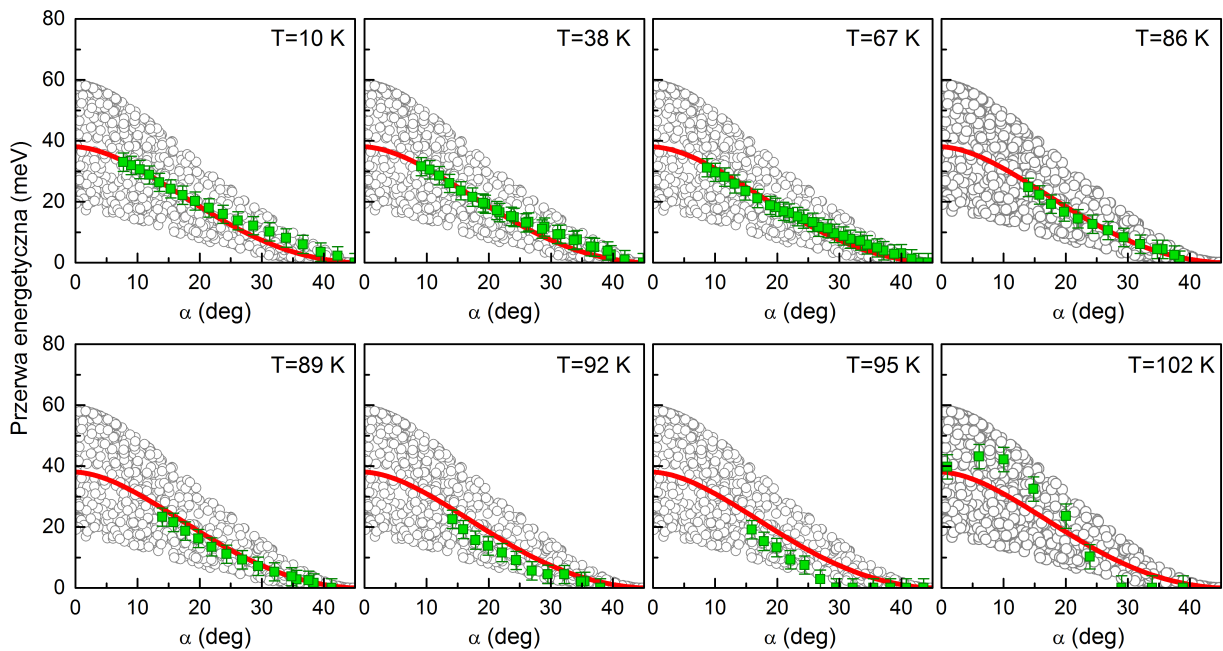
Fig. 14: The impact of temperature on band gap in Bi2212 (UD92).

generating Eliashberg equations looks as follows. First of all, Nambu spinors are defined:

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix} \quad \text{oraz} \quad \Psi^{\dagger}_{\mathbf{k}} = \begin{pmatrix} c^{\dagger}_{\mathbf{k}\uparrow} & c_{-\mathbf{k}\downarrow} \end{pmatrix}, \tag{33}$$

Thanks to them, it is possible to write down Green matrix function $G_{\mathbf{k}}(i\omega_n) = \left\langle\!\left\langle \Psi_{\mathbf{k}} | \Psi^{\dagger}_{\mathbf{k}} \right\rangle\!\right\rangle_{i\omega_n}$ in the following form:

$$G_{\mathbf{k}}(i\omega_n) = \begin{pmatrix} << c_{\mathbf{k}\uparrow} | c^{\dagger}_{\mathbf{k}\uparrow} >>_{i\omega_n} & << c_{\mathbf{k}\uparrow} | c_{-\mathbf{k}\downarrow} >>_{i\omega_n} \\ << c^{\dagger}_{-\mathbf{k}\downarrow} | c^{\dagger}_{\mathbf{k}\uparrow} >>_{i\omega_n} & << c^{\dagger}_{-\mathbf{k}\downarrow} | c_{-\mathbf{k}\downarrow} >>_{i\omega_n} \end{pmatrix}. \tag{34}$$

Diagonal elements of the matrix $G_{\mathbf{k}}(i\omega_n)$ describe the properties of normal state, whereas

non-diagonal elements describe the properties of superconductivity. Next, an equation of Dyson type should be developed for Green matrix function:

$$G_{\mathbf{k}}(i\omega_n) = G_{0\mathbf{k}}(i\omega_n) + G_{0\mathbf{k}}(i\omega_n)M_{\mathbf{k}}(i\omega_n)G_{0\mathbf{k}}(i\omega_n), \tag{35}$$

where $M_{\mathbf{k}}(i\omega_n)$ is the matrix of self-energy and $G_{0\mathbf{k}}(i\omega_n)$ denotes the propagator for the non-interacting electrons:

$$G_{0\mathbf{k}}(i\omega_n) = (i\omega_n\tau_0 - \bar{\varepsilon}_{\mathbf{k}}\tau_3)^{-1}. \tag{36}$$

The last stage consists in obtaining in a self-consistent way the set of the Eliashberg isotropic equations for the wave function renormalization factor, the band energy shift function ($\chi_n = \chi(i\omega_n)$) and the function of the order parameter:

$$Z_n = 1 + \left(v_1 + \frac{v_2}{2}\langle n\rangle\right)^2 \frac{1}{\beta\omega_n}\sum_m P(n-m)\,\omega_m Z_m \frac{1}{N}\sum_{\mathbf{q}} D_{\mathbf{q}}^{-1}(m), \tag{37}$$

$$\chi_n = -\left(v_1 + \frac{v_2}{2}\langle n\rangle\right)^2 \frac{1}{\beta}\sum_m P(n-m)\frac{1}{N}\sum_{\mathbf{q}} D_{\mathbf{q}}^{-1}(m)\left[\varepsilon_{\mathbf{q}} + \chi_m - \mu\right], \tag{38}$$

$$
\begin{aligned}
\varphi_n =\ & \left(v_1^2 + v_1 v_2\langle n\rangle\right)\frac{1}{\beta}\sum_m P(n-m)\,\varphi_m \frac{1}{N}\sum_{\mathbf{q}} D_{\mathbf{q}}^{-1}(m) \\
+\ & \frac{v_2^2}{\beta^3}\sum_{m_1\sim m_3} P(n - m_1 - m_2 - m_3 + 1)\,\varphi_{m_1}\varphi_{m_2}\varphi_{m_3} \\
\times\ & \frac{1}{N^3}\sum_{\mathbf{q}_1} D_{\mathbf{q}_1}^{-1}(m_1)\sum_{\mathbf{q}_2} D_{\mathbf{q}_2}^{-1}(m_2)\sum_{\mathbf{q}_3} D_{\mathbf{q}_3}^{-1}(m_3),
\end{aligned}
\tag{39}
$$

where: $D_{\mathbf{q}}(m) = (\omega_n Z_n)^2 + (\chi_n + \bar{\varepsilon}_{\mathbf{q}})^2 + \varphi_n^2$. The function $P(n)$ is defined as:

$$P(n) = \frac{\nu^2}{n^2 + \nu^2}, \tag{40}$$

where: $\nu = \beta\omega_0/2\pi$. The system of Eliashberg equations shown above should be complemented by the equation for the chemical potential.

It can be demostrated that extremely simplified Eliashberg equations generalise the model based on a canonical transformation, which quantitatively linked the value of critical temperature, pseudogap temperature and the order parameter for $T = 0$ K [91]. At the level of the Eliashberg equations, it was proven that for a defined value of EPh potential ($\nu_1 = 150$ meV) and low values of EEPh potential ($\nu_2 = 0.75$ eV), the relationship of the order parameter ($\Delta = \varphi/Z$) in the function of doping for $\langle n\rangle < 0.95$ looks very similar for the course occurring for classical superconductivity induced by electron-phonon interaction [60]. As it is shown in Fig. 15, the situation changes rapidly for high values of EEPh potential ($\nu_2 = 5$ eV). In the analysed case, the order parameter
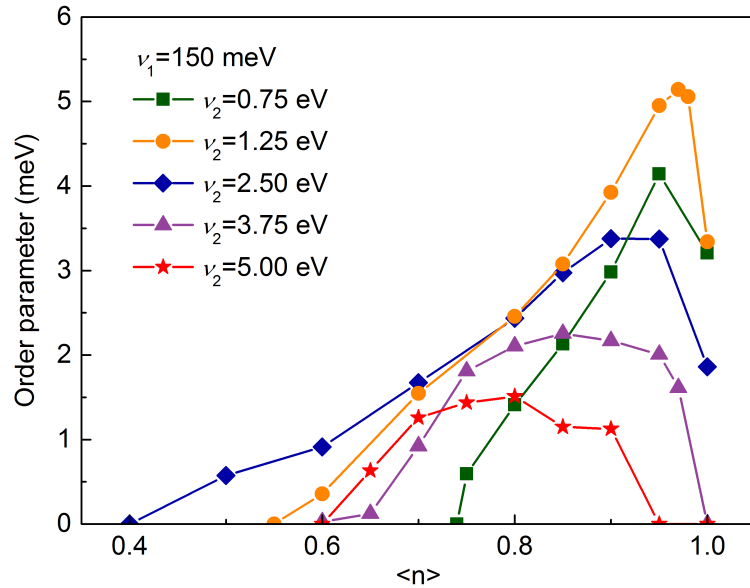
Fig. 15: The maximum value of the order parameter as a function of doping.

disappears for $\langle n \rangle < 1$. It also draws a curve, whose characteristic shape (superconducting dome) is experimentally observed for cuprates [98]. It is worth noticing that one can also observe a characteristic plateau of the analysed function for $\langle n \rangle \in \langle 0.85; 0.90 \rangle$. Additionally, the publication in question proves that band gap observed in the electron density of states in the temperature range from 0 K to the so-called pseudogap temperature ($T^\star$) is induced by the functions Z and χ. The input for the course of the electron density of states coming from φ seems to be slight. In particular, Fig. 16 presents the form of the function $N(\omega)$ defined for the case: $v_1 = 150$ meV, $v_2 = 5$ eV and $\langle n \rangle = 0.8$. It was stated that for temperatures lower than T_c, the half-width of the energy gap slightly decreases together with temperature growth, whereas a clear decrease is observed for maximum values of the function $N(\omega)$. What is interesting, contrary to the shape of the electron density of states linked with classical electron-phonon interaction, the curve $N(\omega)$ is clearly non-symmetrical in relation to the Fermi level. It turns out that the observed lack of symmetry derives from strong renormalisation of electron band energy. It should be additionally emphasised that the asymmetry of the electron density of states defined experimentally is clearly noticeable in the shape of experimental curves [99]. Above critical temperature, band gap disappears quite slowly. The first non-zero value of the function $N(\omega)$ at Fermi level can be observed only at the temperature of 243.7 K. Above this temperature, the course of the electron density of states displays little traces of band gap, the so-called pseudogap, which gradually disappears together with temperature growth. In the analysed case, the pseudogap finally disappears at the temperature of $T^\star = 290,1$ K. The result above explains the origins of the pseudogap, which is a crucial result from the point of view of research in superconductivity in cuprates.
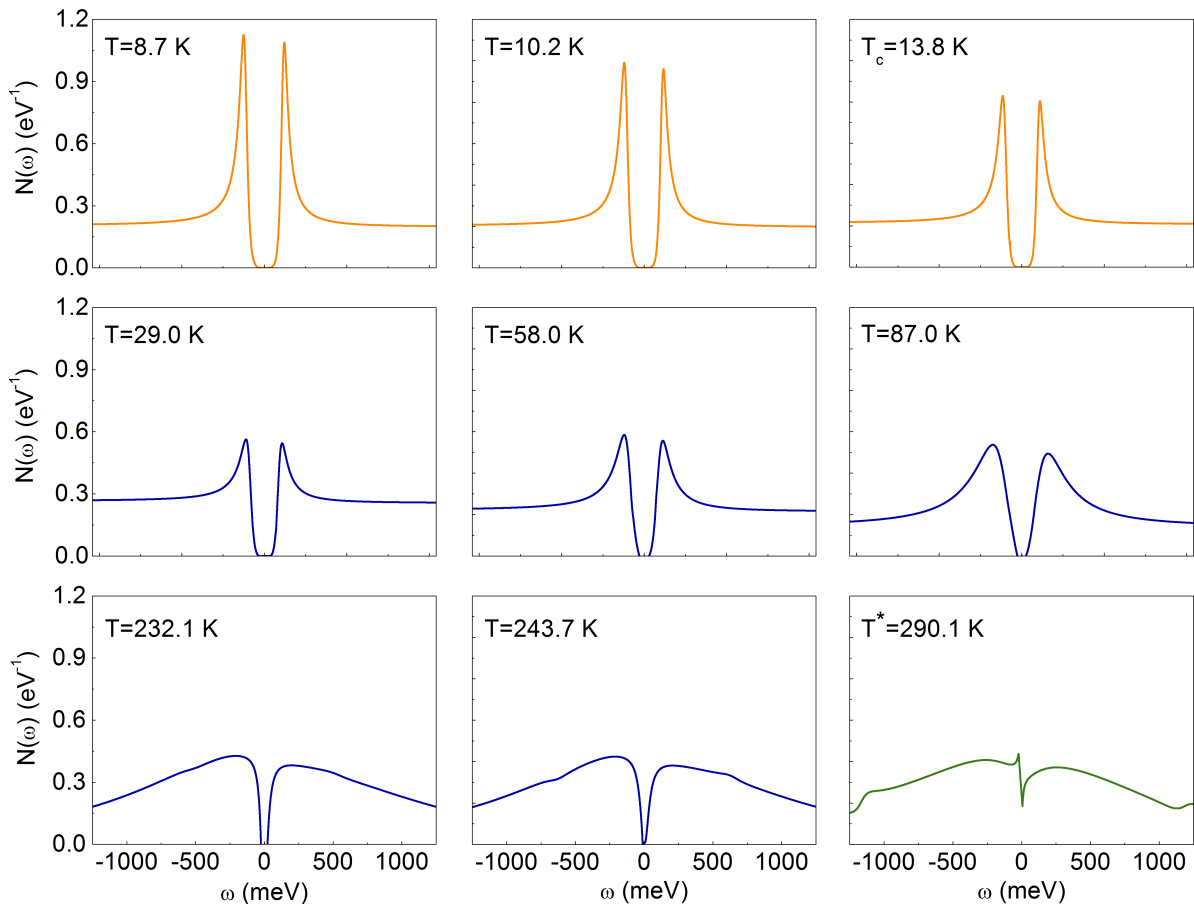
Fig. 16: The temperature evolution of the electron density of states.

Finally, it should be emphasized that although copper-oxygen compounds are characterised by critical temperatures much lower than hydrogenated compounds, they constitute a very important and interesting group of superconductors. First of all, they have an advantage of passing into superconductivity characterized by relatively high critical temperatures, already under atmospheric pressure. What is more, high sensitivity to doping makes their thermodynamic properties easy to manipulate. Research in the pairing mechanism in cuprates aims at exploring the nature of the formation of superconductivity and also at focusing on factors that might ensure its existence at room temperature.

4. Summary

The results of the analysis performed do not only show that the issue of both conventional and unconventional superconductivity still remains valid, but they also suggest that superconductivity at room temperature seems to be possible to obtain (at least under high pressure).

The publication series discussed above and constituting scientific achievement consists of two main parts. The first one concerns conventional superconductors of classical electron-phonon coupling (publications **[A1]**-**[A7]**), whereas the second one encompasses

unconventional superconductors (publications **[A8]**-**[A10]**). The common characteristics of both parts is the fact that the analysed systems are characterised by passing into superconductivity at maximally high values of critical temperature.

In case of conventional superconductors, due to the experiment showing the existence of superconductivity at the temperature of 203 K, for my analysis I selected hydrogenated compounds of the type H_3S, where the phenomenon of chemical pre-compression plays a crucial role. The aim of my analysis was to find a way to increase critical temperature to the highest value possible. The analysis performed was based on the numerical analysis of electron and phonon properties of compounds of a defined crystal structure and chemical composition. It was a springboard for a further, quantitative analysis of superconductivity parameters on the basis of formalism of Eliasberg equation. In particular, I showed that:

- increasing external pressure to which the sample H_3S is exposed to the laboratory boundaries of 500 GPa does not allow for obtaining superconductivity at temperature higher than the one obtained experimentally for the pressure of 155 GPa.

- increasing critical temperature to the value of 242 K, at the pressure of 155 GPa is possible if one takes into account the impact of sulphur isotope mass (^{36}S) on superconductivity of H_3S. I noted the inverse isotopic effect for sulphur.

- partial replacement of sulphur atoms with phosphorus (sulphur's neighbour in the periodic table of elements) atoms results in a decrease in critical temperature in the whole range of analysed pressure. This result, obtained by the supercell method, clearly shows false calculation reading occurring with the use of the virtual crystal approximation method.

- the calculations performed for the system H_3Cl rendered comparable values of T_c in relation to these obtained experimentally for H_3S. It means that introducing a more electronegative element in the place of sulphur also is not a factor triggering desired critical temperature increase.

Of course, the above mentioned results need experimental verification by critical temperature and energy gap measurement for appropriately prepared samples. In the future, I intend to continue theoretical research in superconductors of a type H_3S, taking into account aspects not analysed before. Among others, I shall try to find a way to shift the maximum of the electron density of states closer to Fermi level, which might result in increasing the electron-phonon coupling constant and subsequently lead to critical temperature growth.

In the case of unconventional superconductors (cuprates), lack of a generally accepted theory explaining the pairing mechanism makes it difficult to perform an analysis aiming at controlling superconductivity features of these systems. In my research, the part devoted to cuprates is based on the Hamiltonian modelling effective electron-phonon and electron-electron-phonon interaction. Within the framework of this approach I was, in particular,

able to reconstruct experimental results obtained by the angle-dependent ARPES technique for superconductors YBCO and Bi2212. Additionally, within the framework of the Eliasberg approach, I developed simultaneous thermodynamic equations determining the function of order parameter, the wave function renormalization factor and the function of shifting band energy. At the level of obtained Eliasberg equations, I performed model calculations which showed that in the case of a high value of electron-electron-phonon pairing potential, the order parameter in the doping function has a similar course to the one observed experimentally. Focusing on the developed equations, I also found a relationship between the factor renormalising the wave function and the function of shifting band energy and a band gap. It let me suggest a new scenario of pseudogap formation. This result constitutes substantial contribution in the development of superconductivity and motivates to continue further research. The proposed approach to cuprates description casts a new light on the character of pairing in these systems, emphasising the role of phonons. I expect that it shall let me understand more deeply the properties of the analysed materials and predict the occurrence of superconductivity in new materials on the basis of oxygen-copper planes. I shall conduct that type of analysis in the future by completing the model used with elements describing strong electron correlations.

III. Discussion of other research achievements

I began my scientific cooperation with dr. hab. Radosław Szczęśniak in 2009, during I completing my five-year M.A. course in physics. Initially, within the framework of scientific meetings, we focused on issues concerning astrophysics, quantum dots and describing the properties of magnetic systems within the Hubbard model. I became interested in superconductivity during preparations for writing my M.A. thesis. Since then, I have been dealing with the theoretical analysis of different aspects of superconductivity, beginning with determination of stability of crystal structures of superconductors exposed to high pressure, and finishing with a quantitative description of thermodynamics of superconductivity of these systems within the framework of various theoretical models. Apart from looking for a theoretical model for cuprates and describing high-pressure superconductivity in pure elements and hydrogenated compounds, recently I have been also investigating new concepts encompassing the phenomenon of electron transport in systems of non-standard geometry (cooperation with prof. A. Khater and dr. D. Szczęśniak) [100] and the phenomenon of chaos in molecular systems (cooperation with prof. W. Leoński and dr. inż. M. Jarosik) [101]. In this way, I mastered a series of advanced theoretical methods, both numerical and analytic, which help investigate new areas of physics. Below, I present a short summary of my most important scientific achievements, not constituting directly my habilitation achievement and I describe scientific cooperation with local and foreign scientific research centres. Moreover, I focus on research projects and awards for research activity. Finally, I make a synthesis of the most important bibliometric data concerning all my research conducted so far.

A) Summarising other most important scientific achievements

- *Charcteristics of semi-conductor to metal transition and inducing superconductivity in transition metal dichalcogenides*

Due to their unique electric, optical and mechanical properties, dichalcogenides of transition metals, such as MoS_2, WS_2, $MoSe_2$ and $MoTe_2$ are next to graphene the most thoroughly analysed two-dimensional systems. Interesting properties of these materials show during the reduction of a 3D to a 2D system. For example, semi-conducting MoS2 in a 3D form is characterised by an indirect band gap, whereas a single layer of MoS_2 has a direct band gap, which has a serious impact on electron properties of the systems in question. In my research, I showed that two-layer systems such as MoS_2, WS_2, $MoSe_2$ and

WSe_2, as a result of intercalation with calcium elements may display metallic and superconductive properties. I obtained the highest critical temperature of 13.3 K for the system of $(MoS_2)_2Ca$. The detailed results concerning the stability analysis and thermodynamic properties of the cases in question are included in three publications [102–104].

- *Quantum oscillations in the layers of superconducting lead and research in graphene-type systems*

Quantum size effects occur in materials measured in nanometers. After passing a certain measuring boundary, the classical system stars behaving like a quantum system and shows properties unseen previously in bulk materials. These effects are interesting both from the point of view of experimental and theoretical physics. An interesting example can be thin layers of lead, in which electron-phonon properties, including thermodynamic parameters of superconductivity, depend on the number of atomic layers constituting the system. Quantum oscillations of critical temperature are analysed both experimentally and theoretically. In my research, I determined all relevant parameters of superconductivity for the system whose thickness varied from 5 to 10 atomic layers. The detailed results can be found in the publications [105, 106]. In recent years, I have been also analysing in detail two-dimensional systems such as graphene decorated with litium [107], silicene under biaxial tensile strain [108] or hole-doped graphane [109], showing exceptionally interesting superconducting characteristics.

B) Scientific cooperation and scientific internships

I treat scientific cooperation with Polish and foreign scientific research centres as one of key ways to develop my qualifications and gain new knowledge. As far as conducting joint research and publishing papers, I cooperate with the following academic centres (in alphabetical order): AGH University of Science and Technology in Cracow, Jan Długosz University in Częstochowa, Jiangsu Normal University (China), La Sapienza University of Rome (Italy), University of Maine (France), University of Zielona Góra. In the years 2014 - 2018, within the framework of scientific cooperation, I had one long-term scientific internship at the Department of Physics, La Sapienza University of Rome (Italy), and three short-term scientific internships at the School of Physics and Electronic Engineering, Jiangsu Normal University (Chiny), at the Institute of Complex Systems, National Research Council (Italy) and at the Institute of Physics, University of Zielona Góra (Poland).

## C) Research projects and awards for research activity

The scientific research described above was financed mainly within the framework of scientific projects. In the years 2012 - 2017, I was the head of 6 institute grants linked to conducting scientific research and tasks connected with them, serving the professional development of young scientists. Grants no BS/MN-203-301/2017, BS/MN-

203-301/2016, BS/MN-203-303/2015, BS/MN-203-303/2014, BS/MN-203-302/2013 and BS/MN-203-302/2012 were financed by the Ministry of Science and Higher Education. Since 2017, I have been the head of the project entitled *Crystal structure and thermodynamic properties of new high-temperature superconductors* (2016/23/D/ST3/02109) granted within the framework of the contest SONATA 12 organised by the National Centre of Science (NCN). I have received many awards for my research activity, among others, from the Foundation for Polish Science (a scholarship for Young Scientists START 2017), the Ministry of Science and Higher Education (a scholarship for Outstanding Young Scientists in 2018 and a scholarship for outstanding achievements for the academic year 2013/2014), Polish Physical Society (awards for my M.A. and PhD theses and two scholarships for Young Physicists participating in Meetings of Polish Physicists) and the Rector of Częstochowa University of Technology (eight awards for research in superconductivity).

D) Bibliometric summary

Below, I present the bibliometric summary of my scientific achievements prepared on the basis of the Web of Science database.
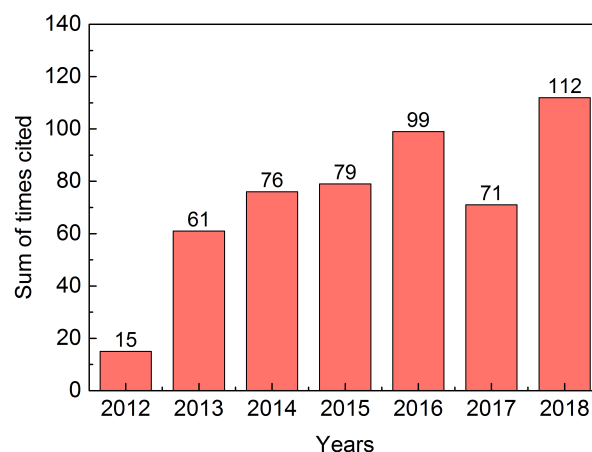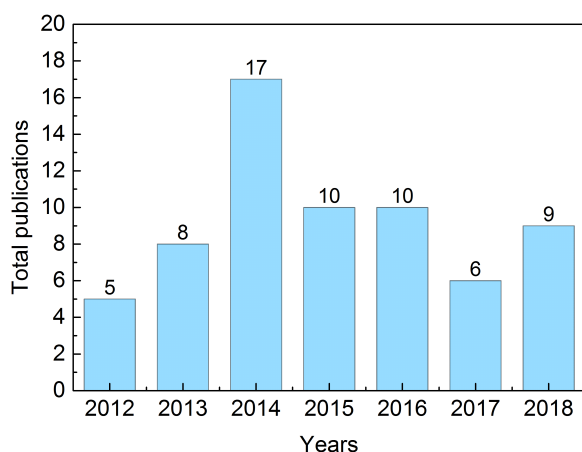
- Total number of publications: **65**
- Total number of citations: **514** (without self-citations: **289**)
- H-index: **15**
- Summary impact factor: **113.052**

Artur Durajski

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