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ROOTS OF QUANTUM AND COMPUTATIONAL CHEMISTRY AND MOLECULAR MODELING AT THE DEPARTMENT OF CHEMISTRY OF WROCŁAW UNIVERSITY OF SCIENCE AND TECHNOLOGY

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ABSTRACT

Development of quantum and computational chemical research as well as molecular modeling at the Department of Chemistry of Wrocław University of Science and Technology has been presented in the historical perspective

1. INTRODUCTION

After the foundations of quantum mechanics were laid by Max Planck and Erwin Schroedinger's, first calculations for a hydrogen molecule made by Heitler and London inaugurated the era of quantum chemistry in 1927. It is worth to mention that Fritz London was born in 1900 in the pre-war Wrocław (Breslau). Before Schroedinger proposed in 1926 his famous equation HV = E'Ɨ', he had been a professor of theoretical physics earlier, in the years 1920-21 of the local university. He lived in Grabiszynek at today's 11 Saperów Street. In 2004, at the request of Professor Lucjan Piela, the author reached the in the university archives of the manuscript of Erwin Schroedinger's biography. It was possible thanks to the courtesy of Professor Zdzisław Latajka, the then rector of the University of Wrocław. The translation of the manuscript was published by Prof. Lucjan Piela in his best-selling book entitled "Idee Chemii Kwantowej" [l] and its English-language edition „Ideas of Quantum Chemistry" [2]. Although in 1929 Paul Dirac claimed that all the equations were already known necessary to describe the whole of chemistry, the main difficulty was to solve them. This became possible after the construction of digital machines, which happened only after World War II, giving rise to the applications of quantum chemistry for the analysis of properties of larger molecular systems. Spectacular proof of the potential of this new field of chemistry were the results obtained by Prof. Włodzimierz Kołos (1928-1996) and Professor Lutosław Wolniewicz (1930-2020) [3]. Undoubtedly this was influenced by their scientific internships at the University of Chicago in the years 1964-1968 in the group of Nobel laureate Professor Robert Mulliken (1896-1986). Calculations of the value of dissociation energy for the H_2 molecule in the ground state were found to be more accurate than the experimental values of the Energy dissociation previously obtained by Nobel Prize winner Prof. Gerhard Herzberg (1904-1999). A correction of the experimental results was published only in 1970 [4].

2. THE FIRST POLISH QUANTUM-CHEMICAL PUBLICATIONS

The first paper in the field of quantum chemistry was published in 1955 by Prof. Włodzimierz Kołos, then an employee of the Institute of Nuclear Research of the Polish Academy of Sciences in Warsaw [5]. It is worth noting that the supervisor of his doctoral dissertation was Professor Leopold Infeld, a student of Albert Einstein. At the Jagiellonian University research in this field was initiated in 1961 by Professor Alojzy Gołębiewski (1927-1987) [6]. This was facilitated by his stay in the United Kingdom at Oxford University, as part of the Rockefeller Foundation's scholarship and work in the team of Prof. Charles A. Coulson (1910-1974), a student of Rutherford and Lennard-Jones. A year later, in 1962, the first works at the Nicholas University Copernicus in Toruń were created with the participation of

Professor Lutosław Wolniewicz [7] and a bit later, in 1964, Prof. Wiesław Woźnicki (1933-1995), Prof. Karol Jankowski, Professor Jacek Karwowski and Professor Stanisław Kwiatkowski (1936-2000) [8]. Also associated later with the Nicolaus Copernicus University in Toruń, Prof. Andrzej J. Sadiej (1941-2010) published his first paper in 1965 [9] together with Prof. Alojzy Gołębiewski from the Jagiellonian University. It is worth mentioning that Andrzej Sadlej, still an undergraduate fourth-year student, wrote a very accessible, first textbook in Polish, entitled "Elementary methods of quantum theory", published by PWN in 1966.

In Wrocław, research in the field of quantum chemistry was initiated by Professor Henryk Chojnacki (1934-2012)[10]. As a graduate of Jagiellonian University, he was employed in 1955 at Wrocław University of Technology. There, initially under the supervision of Professor Krzysztof Pigoń, he experimentally studied the electrical conductivity of organic molecular crystals. After his habilitation in 1969, he devoted himself entirely to the emerging quantum chemistry in Poland. He initially collaborated with Professor Alojzy Gołębiewski. The first publications in this field began to appear in 1968 and concerned, among other things, the band structure in imidazole aggregates [11-12]. The calculations were conducted using software authored by Professor Henryk Chojnacki, prepared in the Mark language and executed on the ELLIOTT 803b computing machine (British production), which was installed in the Department of Numerical Methods at the Mathematical Institute of Wrocław University.

3. ACCESS TO COMPUTING HARDWARE AND COMPUTER NETWORKS IN WROCŁAW

Given the presence of an active scientific community in the field of applied mathematics, which originated in large part from prewar Lwów (now Lviv in Ukraine) , the serial production of digital mainframe computers was located in ELWRO in Wrocław [13]. One of the first mass-produced models was the ODRA 1204 equipped with the ALGOL language translator developed by Dr. J. Jerzy Szczepkowicz (1940-1997) from the team of Prof. Stefan Paszkowski [14, 15]. This was one of the best computers produced in this period in the countries Eastern and Central Europe. A valuable undertaking that has contributed to the to promote the use of computers to representatives of various disciplines, was the Postgraduate Study of Numerical Methods University of Wrocław. Particularly valuable lectures were given by by Dr. Jerzy Szczepkowicz, who was able to reveal the technical secrects of ODRA 1204 and Prof. Stanisław Lewanowicz, who lectured on numerical methods. That's where the author met representatives of other scientific disciplines for the first time,

who were the first large generation of computer users in Wrocław, who later in 1994 helped to organize first supercomputer center in Wrocław. Produced in Wrocław in the 70s and 80s of the twentieth century, digital machines ODRA 1204, ODRA 1305 and RIAD 32 allowed to carry semiempirical calculations at most. This required independent software development, which was used, m.in others, to interpret electron spectra obtained by Dr Aleksandra Lewanowicz [16], Dr Andrzej Olszowski [17] and Dr. Krystyna Palewska [18] from Prof. Zdzisław Ruziewicz research group and the analysis of the reactivity of heterocyclic compounds analyzed by the team of Prof. Jacek Młochowski [19].

Most of the ab initio calculation programs in the world at that time required the use of high-performance systems · computer or supercomputers such as IBM, CYBER, VAX and CRAY, which, due to the embargo on Coordinating Committee for Multilateral Export Control (COCOM) [20] until 1990 could not be sold to the Warsaw Pact countries. Few the exceptions were the aforementioned ELIOTT 803b machines installed in the in 1963 in Warsaw, Gdańsk and Wrocław and CYBER-75 installed in 1975, at the Institute for Nuclear Research in Świerk. In the case of the latter machines, limited access, via the terminal in the Palace of Culture and Science, was used mainly by the Warsaw scientific

community. Only there advanced quantum-chemical programs were installed, enabling ab initio calculations. Much later, in the late 1980s three Yugoslav clones of the VAX machine were installed in Poland. In 1994, Dr. Susan Caldwell from the University of Cambridge was invited to Wrocław on the author's initiative to participate in the Computers in Chemistry conference, organized by the Faculty of Chemistry of the Wrocław University of Science and Technology. This visit resulted in, m.in, the transfer of the source version of the MICROMOL (CADPAC for IBM PCs), and the most active the user of this program was a PhD student at the time, Krzysztof Strasburger. Thanks to this, he developed the first unique software in the country that enabled analysis of interactions between chemical molecules and positrons. Using the Linux f2c to convert code from Fortran to C he compiled the first version of Gaussian running on IBM PC in the country, and installed Cambridge Structural Database. However, most of the publications of Wrocław quantum chemists were written during internships in foreign research centres, which have access to supercomputers and appropriate software. Prof. Chojnacki's doctoral students had to create software, first using the MOST autocode and the languages ALGOL and Fortran. The experience gained in this area became later invaluable for the development of new methods or the modification of the standard software. This allowed them to be implemented and operated also during the short internships in foreign centres. At that time, in the so-called Western countries, there were already networks BITNET and EARN computer systems. In view of the above-mentioned provisions COCOM, officially it was not possible for Polish Universities to join these networks. First steps in creating computer-to-computer connections between the Institute and the Computing Center of the Wrocław University of Science and Technology were not easy. Teletype obtained thanks to courtesy of Prof. Wacław Kasprzak, installed at that time in the Institute of Physical and Theoretical Chemistry in room 405, located in the A-3 , facilitated contact with the Computing Center of the University of Technology Wrocławska. Remote calculations consisted only of loading data from paper tape and the use of conversational mode under the control of the GEORGE 3. In 1988, on the initiative of the author and with the support of the Vice-Rector Wrocław University of Science and Technology for International Cooperation, prof. Jarosław Juchniewicz, an attempt to gain access to the American BITNET network has been met with diplomatic refusal directing us to the the Western European EARN (European Academic Research Network). At the same time, however, a recommendation was sent from the US to the EARN headquarters in Ireland denying us access to the Western European network, citing the embargo COCOM [20]. Even if such access were granted, it would be necessary to overcoming technical problems related to incompatibility various network protocols used in Western European countries and problems related to the inconvertibility of the Polish currency. COCOM hurdles faded After President George Bush visit in Poland, in July 1989. By using one of the first personal computers installed at the then Institute of Physical and Theoretical Chemistry and a modem brought from the USA by Prof. Marek Samoć In 1990, it became possible to exchange correspondence in the form of e-mail via UNIPOL1@NEUVMl box in Denmark.

The first e-mails were sent from room 405 of the A-3 Building (today Professor Krzysztof Pigoń building) located at 23 Smoluchowskiego Street. The Faculty of Chemistry of the Wrocław University of Science and Technology became, next to the Institute of Physics, University of Warsaw - the first academic institution in Poland which has had an e-mail since 1990. A little later, thanks to another exchange of correspondence with EARN edited by Prof. Marek Samoć, and Józef Janyszek, PhD, in the autumn of 1990, the Wrocław University of Science and Technology was officially connected to the BITNET network (PLPWRTUll node), as the second University in Poland , after the University of Warsaw.

Another breakthrough in the access of academic institutions in Wrocław to worldwide computer networks and high computing power was due to establishment in 1995 of the Wrocław Networking and Supercomputing Center [21]. The most important part of the first application submitted on 2 July 1994 by the by Prof. Daniel Bem was a list of 223 publications made by Wrocław residents in foreign

supercomputing centers; most of them concerned calculations quantum-chemical systems. However the funds obtained in 1994 were only sufficient for the construction of the city's fibre optic network. Municipal Coordination Committee, which included representatives of academic institutions Wrocław, entrusted the editing of the second proposal of a committee chaired by Prof. Zdzisław Latajka, assisted by his students, m.in. Dr. Dariusz Bieńko. The author representing the Wrocław University of Science and Technology chaired the committee analyzing possible variants of the selection of high-performance computers. The funds obtained in 1995 made it possible to purchase the first Wrocław IBM SP2 high-power computer. To date, the main users of high-performance computers in WCSS are quantum chemists using about 95% of resources. There were periods when Wrocław computational chemists engaged about 40% of the power computing at the nearby Poznan Supercomputing and Networking Center.

4. ESTABLISHMENT OF THE FIRST QUANTUM CHEMICAL RESEARCH GROUP IN WROCŁAW

The first group of quantum chemistry at Polish technical universities was established in 1971 at the Institute of Organic and Physical Chemistry of the Wrocław Technical University. In the same year author began an assistant internship under the supervision of prof. Henryk Chojnacki, and two undergaduate students Józef Lipiński (1948-2016) and Andrzej Nowek started to work on their MSc theses. In 1972, all three started doctoral studies. Other doctoral students later joined the group: Jerzy T. Jodkowski (1950-2013), Szczepan Roszak, Tomasz Wójcik, Stanisław Styrcz, Robert Tobola, Krzysztof Strasburger and Lech Schulz. In 1984, the Department of Quantum Chemistry separated from the Department of Chemistry Physics and functioned until 2015 as the Department of Molecular Modelling and Quantum Chemistry . The Department was headed by Prof. Chojnacki, and since 2004 - by the author. In 2008 Department of Theoretical Chemistry headed by Prof. Wojciech Bartkowiak has been established. In 2015, the Department of Molecular Modeling and Quantum Chemistry has been included included in the Department of Engineering and Materials Modelling which has been later renamed as Institute of Advanced Materials in 2018.

34 people forming three generations of Prof. Henryk Chojnacki students obtained a doctoral degree, 7 - habilitated doctor and 3 - the title of professor. Between 1969 and 2020, more than 700 publications were published, which have already been cited over 12000 times. Among them is the most frequently cited over 3384 times!), in the over 75-year history of the Wrocław University of Science and Technology, the work of three doctoral students from Wrocław University of Science and Technology, Stanford University and Cambridge University: "cclib: A library for paekage-independent eomputational ehemistry algorithms" [22]. The diverse subject matter of the group's publications was often inspired by experimental work carried out first at the Institute of Physical Chemistry and Organic Chemistry (I4), and later at the Institute of Physical and Theoretical Chemistry (I30), in fields such as UVis spectroscopy, molecular electronics, chemistry organophosphorus compounds, biochemistry and molecular biology.

5. TOPICS AND RESULTS OF THE RESEARCH

The most important mission of theoretical research teams is to develop new methods to expand the range of applications of quantum chemistry. Another important trend of research is the molecular modelling of not fully understood and extraordinary properties of biomatter resulting from evolution and processes taking place with their participation. Their full interpretation opens the way to rational design of new materials like drugs or catalysts. The work carried out using the original computational methods, software and databases developed in the team have become a permanent part of the literature of the subject, as evidenced by their numerous citations. New directions of research in the

field of spectral theory were developed (dr hab. Józef Lipiński, prof. PWr) [23], molecular optics nonlinear and hyperpolarizability calculations (prof. Wojciech Bartkowiak) [24], cumulative atomic multipole expansion CAMM (Cumulative Atomie Multipole Moments) [25] later implemented by Dr. Karol M. Langner in the publicly available GAMESS software system (options $ELMOM IAMM=n) and earlier, by Dr. Andrzej Sawaryn, in the GAUSSIAN 82/86 [26], hybrid variation-perturbation decomposition of intermolecular interaction energy Hybrid Variation Perturbation Theory (HVPT) [27]. Thanks to this, it became possible to obtain the first non-empirical potential functions of the atom-atom type for individual energy components of the interaction Energy [28], used in the analysis of molecular crystal packing [29]. Software developed by Andrzej Nowek, PhD, Eng., and later by Robert Góra, PhD, DSc, enabled - starting from 1998 - the study of relatively large molecular systems and analysis of the physical nature of inhibitory activity [30, 31] and catalytic activity [32] in the active centers of proteins, in molecular crystals [33], compensation exchange and dispersion interactions in layered complexes [34] and analysis of the covalent character of the and analysis of the covalent nature of strong hydrogen bonds [35]. The recently developed MED method [36], using non-empirical dispersion functions and the multipole component of interactions electrostatic radiation, allows a much better assessment of inhibitory activity than most of the commercial empirical scoring functions. This applies even to approximate structures obtained as a result of the docking [36]. Given the predominant share of the electrostatic in enzymatic catalysis [32] static field technique catalytic converters, including a publicly available atomic multipole moments database CAMM for amino acid rotamers [37] can be used for design of theozymes [38], and dynamic catalytic fields - for analysis the effect of the proton transfer reaction in hydrogen bond chains on the catalytic activity of enzymes [39]. Adaptation of the HVPT method taking into account solvent effects [40] and induced intermolecular interactions of electro-optical properties allowed for a breakdown into capacities derived from different components for electronic [41] and oscillatory [42] properties. Krzysztof Strasburger, Professor of Wrocław University of Technology, developed from scratch the chemistry of antimatter in Poland and in particular the interactions of positrons with chemical molecules [43]. Prof. Wojciech Bartkowiak together with Dr. Robert Zaleśny developed the theory of one- and two-photon spectra [44] and the first non-empirical simulation method of the band shape function for one- and two-quantum spectra [45] and the theory of transport of charge carriers in molecular materials [46]. Professor Robert Góra, together with Bartosz Błasiak, PhD, Eng., developed simulation methods of solvatochrome shifts [47-48], the methodology of effective single-electron potentials [49] and the method of determining theexciton coupling constants [50,51], including the TrCAMM method based on cumulative atomic multipole moments CAMM [25]. Currently, R. Góra, PhD, DSc, Eng., in cooperation with Rafał Szabla, PhD, Eng are investigating new mechanisms of photochemical processes, m.in. photoanomerization in prebiotic chemistry [52] and photoredox processes[53]. The above methods often go beyond classical quantum chemistry and fall within the broader defined areas of computational chemistry and molecular modelling. An important characteristic trend of the theoretical research conducted at the Faculty of Chemistry of the Wrocław University of Science and Technology is the analysis of chemical properties and processes based on the theory of intermolecular interactions obtained from the first principles of quantum mechanics. The main goal is to obtain simpler nonempirical models that allow for the theoretical design of thenew molecular materials, such as new drugs, biocatalysts, components of molecular electronics and photonics. This is in line with the vision of the in the nineteenth century by J. W. Gibbs „the role of theoretical research to find the simplest possible tools for experimentalists". The fundamental importance intermolecular interactions to describe the properties of matter has been expressed in the introduction to the legendary textbook by Nobel Prize winner Richard Feynman: „If All current science was to be destroyed in some cataclysm and could be saved just one sentence, it should read: Everything is made up of atoms - small particles, moving in a disorderly manner, attracting each other when they are a little

distant, but repelling each other when they are too tight" [54]. This refers to the to potential energy curves sufficient to describe the properties of all the forms of matter that can be used to design new materials , unknown in nature, with the desired properties. Research In the field of the theory of interactions has been proposed to author by Prof. H. Chojnacki. The result was a doctoral dissertation on the exchange perturbation theory of intermolecular interactions using semi-empirical wavefunctions. The derived analytical formulas for the the individual components of the energy of the interactions [55] later made it possible to construct simpler models of the properties of large molecular systems associated mainly with long-range effects related to inhibitory [30-31,36] and catalytic [32,38,39] activity of enzymes. However, the verification of such models required calculation of the exact non-empirical values of the energy components obtained by ab initio methods.

A significant influence on undertaking further, non-empirical research in this area was the author's three-month internship in 1974 at the Laboratory of Quantum Chemistry at the University of Warsaw. It should be added that the systematic non-empirical research initiated in Warsaw in the 1970s in the field of intermolecular interaction theory based on perturbation theory with adapted symmetry (SAPT - Symmetry Adapted Perturbation Theory) contributed to the leading role of students of Professor Kołos (including Professor Bogumił Jeziorski, member of the Polish Academy of Sciences, and Professor Grzegorz Chałasiński, member of the Polish Academy of Sciences) in this field on a global scale [1,2,56,57]. The application of the hybrid variational-perturbational method (HVPT) [27], which is significantly less costly than perturbational methods, enabled the verification of developed models of catalytic or inhibitory activity for large active centers of enzymes [30-32,36,38-39] or zeolites [58]. Some doctoral students from Prof. Kołos's team were involved in interdisciplinary research with Prof. David Shugar (1915-2015) from the Department of Biophysics at the University of Warsaw. As a result of this, an incidental outcome of the author's internship at the University of Warsaw, where he had the opportunity to conduct calculations using the CDC CYBER-73 computer, became a publication concerning the dramatic impact of zero-point vibrations on the probability of the double proton transfer process in systems with double hydrogen bonds [59]. Its authors were doctoral students from three different universities: the Wrocław University of Technology, the University of Warsaw, and the University of Wrocław. According to a hypothesis put forward by Prof. Per Olof Löwdin from the University of Uppsala in Sweden, this phenomenon was considered until recently as a possible source of mutations in DNA. According to Prof. Shugara's suggestion, however, over 50% of experimentally observed DNA mutations result from the deamination of cytosine. This topic later became the subject of cooperation between the author and the team of Prof. Raymond Poirier from Newfoundland University in Canada [60].

It is worth adding that until 1970, part of the Faculty of Chemistry at the University of Wrocław was located in the Old Chemistry building at 23 Smoluchowskiego Street (currently named after Professor Krzysztof Pigoń) together with the Department of Physical Chemistry of Wrocław University of Technology, and the employees of both universities shared scientific and social relationships while occupying the same building. In 1969, Dr. Henryk Ratajczak, after returning from an internship at the Institute of Quantum Mechanics Applications in Paris, gave a lecture entitled "Quantum Theories of Intermolecular Interactions" at a seminar of the Polish Chemical Society held at the Technical University. Since 1969, a group of students of Professor Henryk Ratajczak began conducting research in quantum chemistry at the Department of Theoretical and Physical Chemistry at the Institute of Chemistry at the University of Wrocław: Dr. Krystyna Mazur, Professor Zdzisław Latajka, Professor M. Małgorzata Bryant-Szczęśniak (employed until the end of 2020 as a Distinguished Professor at Oakland University in the USA), Dr. Krzysztof Skowronek, Dr. Jerzy Moc, and Professor Piotr Piecuch (currently employed as a Distinguished Professor & MSU Foundation Professor at Michigan State University in the USA). The first publications of the team appeared in 1972 [61-62], and currently, the research in

the field of quantum chemistry is continued by the students of Prof. Zdzisław Latajka: Dr. Agnieszka Gordon, Prof. Dr. Hab. Robert Wieczorek, Dr. Małgorzata Biczysko (currently working at Shanghai University in China), Dr. Hab. Sławomir Berski, Dr. Krzysztof Mierzwicki, Dr. Hab. Jarosław Panek, Dr. Hab. Andrzej Bil, Dr. Hab. Piotr Durlak, and Dr. Przemysław Dopieralski.

Some of Prof. Chojnacki's students took up work in other research teams after defending their doctoral dissertations. Dr. Hab. Jerzy Jodkowski (1950-2013) joined Prof. Emil Ratajczak's team, specializing in experimental studies of gas-phase reactions at the Pharmaceutical Faculty of the Medical University of Silesia in Wrocław and initiated theoretical research on gas-phase reaction kinetics there. Dr. Stanisław Styrcz [45] began working at the Świętokrzyski University in Kielce in 1979, while Dr. Eng. Andrzej Nowek worked at the Jan Długosz Academy in Częstochowa, Jackson State University, and Opole University after defending his doctoral thesis.

In the years 1979-1983, biochemist Dr. Andrzej Sawaryn joined Professor H. Chojnacki's group, who actively participated in the implementation of CAMM in the Gaussian system [26]. Thanks to his inspiring influence, the author became interested in the relationship between intermolecular interaction theory and enzymatic catalysis [32,38-39].

In 2003, as a result of an open competition, Dr. Paweł Lipkowski, a graduate of the University of Wrocław, who is engaged in topological analysis of electron densities [63], joined the quantum chemistry group.

In 2005, as a result of obtaining a European reintegration grant (ERG), after completing research internships in the USA, France, and Italy, Professor Tadeusz Andruniów, a graduate of the Jagiellonian University, joined the team, conducting advanced research on photoinduced processes in proteins such as rhodopsin [64], fluorescent proteins [65-66] , or azurin [67]. In 2007, in collaboration with the team of Prof. Massimo Olivucci (University of Siena, Italy), he proposed a mechanism of photoisomerization in rhodopsin, using advanced hybrid calculations CASPT2//CASSCF/MM as a research tool [68]. This mechanism, confirmed experimentally three years later, contributed to the design of a biomimetic molecular photo-switch based on the structure of the rhodopsin chromophore [69-70]. In 2009, Prof. T. Andruniów was awarded the national competition "Stay with us" by the weekly Polityka, and from 2010 to 2014 he led a large project at the Wrocław EIT+ Technology Center, which resulted in over 15 publications.

In 2017, Dr. Eng. Bartosz Błasiak, after defending his doctoral thesis at Korea University, took a position at our department under the Polonez grant; he is working on the development of new methods for calculating molecular properties [41,47-49]. In the spring of 2021, Dr. Eng. Rafał Szabla (PhD in 2017 from the Institute of Biophysics of the Czech Academy of Sciences in Brno), specializing among other things in theoretical research on the photostability of nucleic acids [52-53], will join our department, collaborating with experimental teams at Harvard University and the Medical Research Council in Cambridge. It is worth noting that both Dr. Błasiak and Dr. Szabla are graduates of the Bioinformatics specialization, and they completed their theses under the supervision of Dr. Hab. Robert Góra, professor at Wrocław University of Technology.

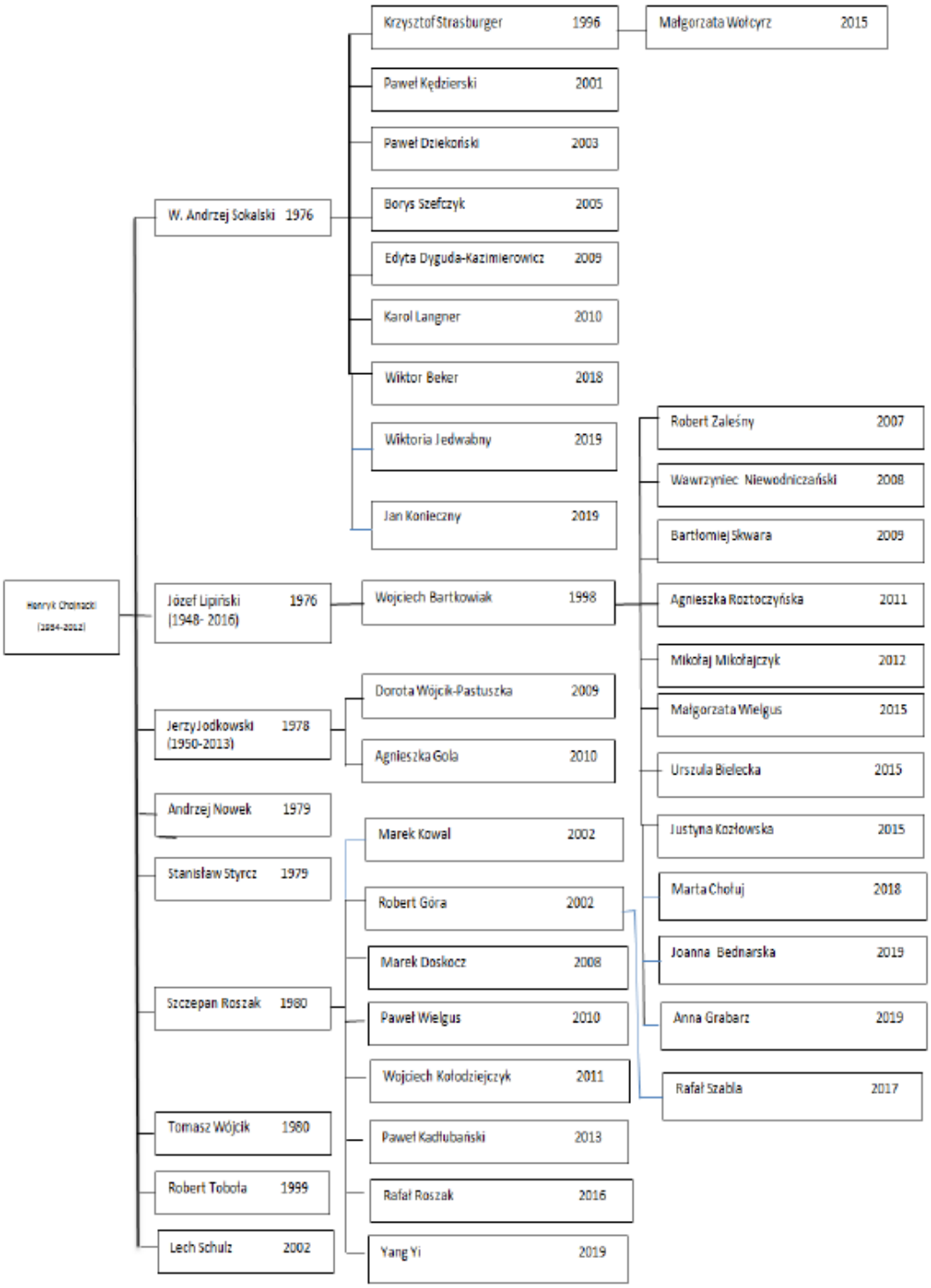
6. INTERNATIONAL COOPERATION

Since the late 1970s, international cooperation has been developed, resulting in many publications. Within this framework, 52 joint publications were produced with The Johns Hopkins University in Baltimore, 33 publications with Arizona State University, and 140 publications with Jackson State University. Cooperation was also conducted with the National Institute of Standards and Technology (Gaithersburg, USA), Lawrence Livermore National Laboratory (Berkeley, USA), Roswell Park Cancer

Institute (Buffalo, USA), Pacific Northwest National Laboratory (USA), University of Bristol (UK), Memorial University of Newfoundland (St. Johns, Canada), and Kyoto University (Japan). Research contracts were executed in cooperation with the National Institute of Standards and Technology (Gaithersburg, USA), Air Products and Chemicals (Allentown, USA), Jackson State University (USA), and the Wrocław EIT+ Technology Center. It is worth emphasizing that in collaboration with the team of Prof. Jerzy Leszczyński in Jackson, participated more than 20 employees, doctoral students, and students from Wrocław University of Technology. Fruitful scientific contacts were established there with the team of Prof. Andrzej Sadlej from Nicolaus Copernicus University and Prof. Sławomir Grabowski from the University of Lodz, and later with the University of Basque Country Euskal Herriko Unibertsitatea UPV EHU in the Basque Country [34,63]. In later years, Professor Bartkowiak's team expanded collaboration with the Royal Institute of Technology in Stockholm, the Institute of Macromolecular Chemistry of the Academy of Sciences of the Czech Republic (IMC) in Prague, the Institute of Biophysics of the Academy of Sciences of the Czech Republic (IBF) in Brno, the Institute of Organic and Pharmaceutical Chemistry of the National Hellenic Research Foundation in Athens, Matej Bel University in Banská Bystrica, Slovakia, the University of Girona in Spain, the MRC Laboratory of Molecular Biology, Cambridge Biomedical Campus in the United Kingdom, the University of Nantes, and Interdisciplinary Chemistry, Synthesis, Analysis, Modeling: CEISAM in France.

Quantum Chemistry Group (2007) Standing from left: Paweł Lipkowski, Tadeusz Andruniów, Szczepan Roszak, Wojciech Bartkowiak, Krzysztof Strasburger, Borys Szefczyk, Robert Góra, Paweł Kędzierski, Wojciech Kołodziejczyk, Jakub Kamiński, Edyta Dyguda-Kazimierowicz, Małgorzata Wołcyrz, Krzysztof Tajchert, Henryk Chojnacki, Andrzej Sokalski.

Research school of profesor Henryk Chojnacki



7. CONFERENCES

For the author, the first contact with quantum chemistry was the winter school of the Student Scientific Club of Chemists at the Faculty of Chemistry, organized in Szklarska Poręba in 1968 by a fifth-year student, Jerzy Mager. One of the lecturers was Prof. Henryk Chojnacki, and the Quantum Chemistry School in Wisła was organized by a friendly Student Scientific Club of Chemists at Jagiellonian University, led by Prof. Ludwik Komorowski and Prof. Małgorzata Komorowska, during which lectures were given, among others, by Prof. Ewa Brocławik, who was then a fifth-year student at UJ.

The first nationwide conference on quantum chemistry in Wrocław was organized in 1986 by Prof. Henryk Chojnacki at the headquarters of the Wrocław branch of PAN on Podwale Street. Subsequently, in 1994, 1996, and 1999, in collaboration with the Center for Advanced Research in Biotechnology in Rockville, USA, and the Institute of Inorganic Chemistry and Rare Earths Metallurgy (I-5), the author co-participated in the organization of international conferences on Computers in Chemistry, gathering many national and foreign quantum chemists. A lasting legacy of these meetings are three special issues of the journal Computers & Chemistry (Elsevier). Later organized by a team, at the initiative of the author, in the years 2004, 2006, 2008, 2010, 2012, 2014, 2016, and 2018, the international conferences Modeling & Design of Molecular Materials (MDMM) achieved the status of a leading cyclical series of meetings in the field of computational chemistry and molecular modeling in Central and Eastern Europe. A total of 790 scientists from over 30 countries around the world participated in them. Some of the presented works were published in 8 post-conference issues of the Journal of Molecular Modeling (Springer) and in the book "Molecular Materials with Specific Interactions: Modeling and Design" [71]. Since 2022, the MDMM conferences have been held alternately in Gdańsk, Kraków, and Wrocław [72].

List of conferences and workshops organized by the Department of Chemistry

National Conference "Quantum Chemistry-86", December 4-6, 1986, Wrocław.

Polish-American workshop "Computational methods for large molecular systems" affiliated with the IIIrd Computers in Chemistry conference, June 23-26, 1994, Wrocław. [160 participants from 15 countries, 45 plenary lectures and 70 posters, 25 articles in a special issue of the journal Computers & Chemistry, 19 (3) 1995].

IVth Computers in Chemistry conference, October 17-21, 1996, Polanica Zdrój. [21 articles in the special issue of Computers & Chemistry, 22 (1) 1998].

Polish-American workshop "New trends in computational methods for large molecular systems" affiliated with the V Computers in Chemistry conference, July 1-6, 1999, Szklarska Poręba. [170 participants from 20 countries, 35 lectures, 100 posters, 30 articles in a special issue of Computers & Chemistry, 24 (3-4) 2000].

Polish-American workshop 'Introduction to molecular modeling', May 15-31, 2002, Wrocław [37 participants, 15 lectures].

Ist conference on Modeling & Design of Molecular Materials, September 16-20, 2004, Wrocław. [87 participants from 14 countries, 29 lectures, 40 posters, 21 articles in the special issue of the Journal of Molecular Modeling, 11 (4-5) 2005].

IInd conference on Modeling & Design of Molecular Materials, September 10-15, 2006, Wrocław. [124 participants from 15 countries, 31 lectures and 59 posters; 25 articles in the special issue of the Journal of Molecular Modeling, 13 (6-7) 2007 and 16 chapters in the book 'Molecular Materials with Specific Interactions: Modeling and Design', Springer, 2007].

IIIrd conference on Modeling & Design of Molecular Materials, June 23-28, 2008, Piechowice [107 participants from 20 countries, 45 lectures, 52 posters, 25 articles in the special issue of the Journal of Molecular Modeling, 15 (6) 2009].

IVth Conference on Modeling & Design of Molecular Materials, July 4-8, 2010, Wrocław [110 participants from 16 countries, 40 lectures, 66 posters, 29 articles in a special issue of the Journal of Molecular Modeling, 17 (9) 2011].

Vth Conference on Modeling & Design of Molecular Materials, September 10-14, 2012, Wrocław [136 participants from 21 countries, 39 lectures, 91 posters, 19 articles in a special issue of the Journal of Molecular Modeling, 19 (10) 2013].

VIth Conference on Modeling & Design of Molecular Materials, June 29 - July 3, 2014, Kudowa Zdrój [114 participants from 22 countries, 45 lectures, 77 posters, 12 articles in the Journal of Molecular Modeling, 21 2015].

VIIth Conference on Modeling & Design of Molecular Materials, June 26-30, 2016, Trzebnica [108 participants from 15 countries, 34 lectures, 72 posters, 13 articles in the Journal of Molecular Modeling, 23 2017].

VIIIth conference on Modeling & Design of Molecular Materials, June 24-28, 2018, Polanica Zdrój [96 participants from 11 countries, 36 lectures, 50 posters].

8. TEACHING

In the field of didactic activity, it is worth emphasizing the pioneering contribution of Professor Henryk Chojnacki, author of three textbooks devoted to the structure of atoms and molecules as well as quantum chemistry [68-70]. At the initiative of the author, a MSc program in chemical informatics was opened in 1997, which was transformed in 2009 into the first English-language MSc program of bioinformatics [71] at Polish technical universities. A large group of students of the aforementioned specialty and later doctoral candidates had the opportunity to participate in international exchange programs, such as Tempus, Erasmus, and Fulbright, based on bilateral agreements with Bristol University in the United Kingdom (Paweł Kędzierski, Robert Góra, Borys Szefczyk, Edyta Dyguda, Ewa Chydyk, Jolanta Żurek, Wiktor Beker), Erlangen-Nuremberg University in Germany (Urszula Uciechowska, K. Sokołowska), Jackson State University in the USA (Marek Kowal, Robert Góra, Marek Doskocz, Paweł Wielgus, Edyta Dyguda, Bartłomiej Skwara, Jarosław Szymczak, Robert Zaleśny, Julia Saloni, Wojciech Kołodziejczyk from Kyoto University in Japan (Paweł Szarek), Uppsala University in Sweden (Klaudia Szeler), and the University of Virginia in the USA (Kornelia Gładysz). As a result of these internships, a number of valuable publications were produced, and all participants defended their doctoral theses at Wrocław University of Technology or at the partner institution.

At that time, doctoral students Krzysztof Strasburger and Maciej Pyka launched the first student computer lab in Wrocław operating on the Linux system, equipped with, among other things, the country's first complete software package for managing the crystallographic database CSD provided by Prof. Zdzisław Gałdecki from Łódź University of Technology. Later, Dr. Paweł Kędzierski, together with doctoral student Edyta Dyguda, developed an original laboratory course in molecular modeling called Modeling Biomolecules, conducted with the author in 2006 and 2007 at Jackson State University in the USA, funded by NSF, trained 30 American professors of biochemistry. Currently, similar courses are offered in master's studies for English-speaking specialties in Bioinformatics, Medicinal Chemistry, and Pharmaceutical Biotechnology at the Faculty of Chemistry of Wrocław University of Technology. In 1998, the author's graduate, Tomasz Cierpicki, currently a professor at the University of Michigan in Ann Arbor, USA, independently solved the structure of a peptide inhibitor (subjected to experimental research by Prof. Jacek Otlewski) composed of 56 amino acids in his thesis. He used two-dimensional NMR spectroscopy and available software. This was one of the first works of its kind on a national scale. It was awarded in a nationwide competition organized by the Polish Chemical Society for the best master's thesis. Later, PTCh awards were also received by Edyta Dyguda, Wiktor Beker, and Dawid Grabarek. Numerous doctoral students from the team have received prestigious START scholarships from the Polish Science Foundation: Wojciech Bartkowiak, Robert Góra, Borys Szefczyk, Robert Zaleśny, Paweł Kędzierski and Edyta Dyguda-Kazimierowicz, who additionally received scholarships from L'Oreal and Hasco-Lek. Diamond grants were obtained by undergraduate students: Wiktor Beker, Joanna Bednarska, and Mikołaj Janicki. Recently, Prof. T. Cierpicki, together with Prof. Grembecka (a graduate of Wrocław University of Technology cooperating with the team since her doctoral studies), discovered a drug against the previously incurable childhood leukemia and prostate cancers. Dr. Ireneusz Bulik, the best graduate of Wrocław University of Technology in 2010, completed his doctoral thesis in quantum chemistry under the supervision of Prof. Gustavo Scuseria (Rice University, Houston) and is currently working at Yale University. He is the recipient of the American Harry B. Weiser Award in chemistry. Graduates of the Bioinformatics and Chemical Informatics specializations initiated by the author currently work at companies such as Vertex Pharmaceuticals in Boston, USA, Stratified Medical, the Center for New Technologies in Warsaw, Selvita SA, Biocentrum, FQS Fujitsu Poland, Nietsch Instruments in Kraków, Celther-Poland in Cieszanów, Techland, Micro Solutions, and Startfund in Wrocław. Almost half of the graduates from this elite specialization have defended their doctoral dissertations, are currently in doctoral studies, or work in academic institutions such as the Nestle Institute of Health in Fribourg, Switzerland, Korea University in Seoul, the Institute of Low Temperatures and Structural Research of the Polish Academy of Sciences in Wrocław, the Wrocław Center for Networking and Supercomputing, King Abdullah University of Science and Technology in Saudi Arabia, Institut de Biologie Structurale in Grenoble (France), the Institute of Molecular and Cell Biology in Warsaw, and the University of Edinburgh in the United Kingdom, the University of Southern California, University of California in Los Angeles (USA), Wageningen University and University of Groningen in the Netherlands, Jackson State University in the USA, Czech Academy of Sciences, Brno in the Czech Republic, Interdisciplinary Center for Mathematical Modeling in Warsaw, Munster University in Germany, University of Basel in Switzerland, University of Helsinki in Finland, and Yale University in the USA.

9. OTHER RESEARCH TEAMS CONDUCTING COMPUTATIONAL WORK

Quantum-chemical calculations were also carried out by experimental groups at our department, utilizing readily available software installed in national supercomputing centers. Prof. Danuta Michalska-Fąk, formerly a doctoral student of Prof. Bogusław Kędzia at the Institute of Inorganic Chemistry and Metallurgy of Rare Elements at Wrocław University of Technology, upon returning from her research internship in the USA in 1986, developed studies on infrared spectra and Raman spectra

using ab initio and DFT methods. The subjects of research include molecules of inorganic compounds and complexes with metal ions (in particular, platinum compounds with anti-cancer activity) [77-80]. Work published with her subsequent doctoral students (currently research and teaching staff at the Faculty of Chemistry): Dariusz C. Bieńko [77], Rafał Wysokiński and Wiktor Zierkiewicz have gained a significant number of citations in the global literature. The calculations of oscillatory spectra combined with experimental studies are continued by former doctoral students of Prof. Michalska-Fąk: Dr. Eng. Magdalena Malik-Gajewska and Dr. Hab. Barbara Morzyk-Ociepa [80], a professor at Jan Długosz University in Częstochowa. On the other hand, Dr. Hab. Wiktor Zierkiewicz [81-82], along with his protégé, Dr. Eng. Mariusz Michalczyk, and Dr. Eng. Rafał Wysokiński, conducts theoretical research on the structures, properties, and nature of interactions in complexes stabilized by non-covalent bonds (halogen, chalcogen, pnictogen, tetrel, triel, aerogen). In the above-mentioned institute, calculations related to oscillatory spectroscopy were carried out by Prof. Piotr Drożdzewski [83] and Dr. hab. Andrzej T. Kowal [84], as well as students of Prof. Bogusław Kędzia. It is worth adding that the promoter of the doctoral theses of Prof. B. Kędzia and the aforementioned Prof. W. Wojciechowski was Prof. Bogusława Jeżowska-Trzebiatowska from the University of Wrocław. From the Institute of Inorganic Chemistry and Metallurgy of Rare Elements also comes Prof. Jerzy Leszczyński, who obtained his doctorate under Prof. Walter Wojciechowski in 1975. After leaving Poland for the USA, he established a strong computational chemistry center at Jackson State University (JSU). Prof. Jerzy Leszczyński is the author of over 1000 original publications cited more than 23,000 times. The subject of the professor's scientific activity includes theoretical studies of nucleic acids and predicting the properties of nanomaterials, particularly their toxicity. In 1998, he founded the Computational Center for Molecular Structure and Interactions at JSU, and currently directs the Interdisciplinary Center of Nanotoxicity there. In 2001, he received a White House award for his achievements, and in 2009, he received an award from the President of the USA. In 2007, he was honored with the Marie Skłodowska-Curie Medal awarded by the Polish Chemical Society. In 2009, from the hands of the President. Since 2016, he has been an honorary doctor of the Wrocław University of Technology.

Starting from 1983, theoretical research on reactivity was also conducted by a team led by Prof. Ludwik Komorowski [88-89]. These have been presented in a separate publication in the current special issue of Wiadomosci Chemiczne [90]. Dr. hab. inż. Bartłomiej Szyja, a graduate of the chemical informatics MSc program, after returning from internships in the Netherlands and Germany, initiated computational work on the catalysis of CO2 hydrogenation processes at the Department of Chemistry and Fuel Technology [91]. Prof. Bogdan Kuchta, also employed at Université Aix Marseille in France, conducts intensive research in theoretical analysis of gas adsorption on porous materials at the Department of Bioprocess Engineering, Micro and Nanoengineering [92]. The molecular modeling techniques initiated at the former Department of Bioorganic Chemistry led by Professor Paweł Kafarski are continued at the Department of Bioorganic Chemistry, now directed by Professor Łukasz Berlicki. The main stream of research is associated with computer-aided design of enzyme inhibitors, specifically glutamine synthetase [93], aminopeptidase [94], and urease [95]. In recent years, work has also been carried out on designing inhibitors of protein-protein interactions [96]. The newly developed computational techniques are the result of extensive interdisciplinary collaboration with leading centers around the world and are increasingly becoming a working tool for experimental teams at the Faculty of Chemistry at Wrocław University of Technology, contributing an integrating input to the continually increasing scientific potential of the faculty.

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Ratajczak, Prof. Szczepan Roszak, Dr. Hab. Krzysztof Strasburger, Prof. PWr, and Dr. Hab. Bartłomiej Szyja for their valuable comments and corrections, and especially Dr. Hab. Aleksandra Lewanowicz for numerous editorial remarks. This article is an extended and updated version of the chapter "Quantum Chemistry, Computational Chemistry, and Molecular Modeling at Wrocław University of Science and Technology," which appeared in the Archives of the Institute of Physical and Theoretical Chemistry of Wrocław University of Science and Technology 1994-2014, edited by Prof. L. Komorowski, Publishing House of Wrocław University of Science and Technology, Wrocław,2019.

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