Weaving the Fabric of Quantum Chemistry: Hungarians' Contributions at Home and Abroad

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Abstract

After a short introduction, we present five selected well-known "second generation" quantum chemists, working either in Hungary or abroad. We continue enumerating their contemporary followers in an *ad hoc* order.

Keywords: Widely known Hungarian quantum chemists, Pauncz, Balint-Kurti, Szabo, Kapuy, Mezey, quantum chemistry groups

Contents

1 Introduction

The intent of this chapter is to discuss, or at least to mention, the names of Hungarian scientists who had significant contribution to quantum chemistry at the time when it became a mature field. The author is aware that such a venture can not be complete. We are sure that in spite of much effort of locating our countrymen working in the field, some will slip through the net and remain unmentioned, and the weights of the scientific contributions will remain unbalanced. Admitting these discrepancies, it is our hope that the cross-section presented illustrates how many quantum chemists of Hungarian origin became widely recognized internationally, either working in their home country or abroad.

Scientists who have their own contributions in this Volume intentionally are not discussed in this chapter. We also skip here the results of some others, like Pál Gombás, Rezső Gáspár, Camille Sándorffy, Imre Csizmadia, János Ladik, István Mayer, János Ángyán, etc., who are presented in more detail in other Chapters of the book.

2 Reputed Scientists of the Field, Active in the Second Half of the XX$^{\mathbf{th}}$ Century

2.1 Ruben Pauncz

Ruben Pauncz (in Hungarian: Pauncz Rezső) started his extremely successful scientific career in Hungary, at the University of Szeged, in the city where he was born. Surviving the holocaust, he found a position at the University of Szeged from 1948 till 1956, when he emigrated to Israel. He became there "the founding father of quantum chemistry in Israel", as is written in his necrology. His CV, entitled *"Many Handicaps and a Lot of Good Luck. A Scientific Autobiography"*, is a touching and captivating reading.[1]

Attention of Pauncz soon turned to difficult problems of quantum chemistry. This branch of science was not really cultivated in Szeged at that time, thus he started to work alone for a while, until he convinced a talented former high school teacher Ferenc Berencz to join (actually, return) to the University. Together they published several important papers (mostly in Hungarian journals) on difficult problems concerning electron correlation and spin operators[2, 3, 4], for example[1]

After emigration, Pauncz continued this line of research, and became a world respected scholar of the field (see e.g. the recollection of Bácskay about Pauncz in Chapter 6. of Part I.). The Alternant Molecular Orbital (AMO)

[1]Ref.[3] is a science-historical curiosity: to my best knowledge, this is the only common publication of the famous Polish quantum chemist, Włodzimierz Kolos and Pauncz.

method is also associated to his name.[5] Celebrated books by Pauncz inspire us through his legacy[6, 7, 8].

Ruben Pauncz was a very open, friendly person, never being supercilious in spite of his broad knowledge and his important results. The present author vividly remembers taking part on a boat excursion of a scientific conference as young scientist with only a dozen of publications. A kindly smiling man suddenly approached him at this event, and started to speak in Hungarian: "Hi Péter, I am Pauncz Rezső. I have read your papers with interest, I am glad to see you in person!"

2.2 Gabriel Balint-Kurti

Finishing his bachelor studies in Cambridge, Balint-Kurti went for MSc and PhD studies to the Columbia University, USA, where he received his PhD in 1969. His first scientific paper, written with Karplus[9] about VB (valence bond) and AIM (atoms in molecules) calculations on small molecules, touched on a topic that remained in his interest throughout his scientific career. After a postdocing with Levine, Balint-Kurti found a position at Bristol University, where he was promoted to Professor of Theoretical Chemistry in 1998, and became a well respected expert of his field in the UK. In addition to the subjects mentioned above, he has been continuously working in the field of molecular collisions and scattering, an interest that probably was originated in cooperating with Levine.

Apart from studying and postdocing, Balint-Kurti stayed in the UK, keeping an awareness of his Hungarian origin. Occasionally, he hosted young Hungarian researchers, e.g. Laszló Füsti-Molnár (who graduated with Péter Szalay, later settled down in the USA and founded there the Quantum Future Scientific Software Company), or Ágnes Vibók, who became professor of physics at the University of Debrecen, Hungary (some of her work is reviewed in Chapter 10. of Part III. of this Volume).

Balint-Kurti, with his more than 180 research papers and several dozens of invited conference talks and seminars, has had an outstanding scientific career. He was also particularly active in organizing science, and took pride in conducting continuously high-level teaching. Quoting from his autobiography: *"I enjoy teaching and have taught many courses within the Physical Chemistry area... I have always attached great importance to teaching and take great care in the preparation and presentation of courses, workshops and classes."* – A nice mission statement, or rather an *ars poetica*, that is worth suggesting to follow for the young generation of scientists.

2.3 Attila Szabó

Born in Hungary, emigrated in 1956 at his age of 9 with his parents, Attila Szabó has an extraordinary role in quantum chemistry. At the be-

ginning of his scientific career, he published several important papers with quantum chemical subjects. For an example, the present author, at about the time when he was working for his PhD, remembers reading an important paper by Szabó, Langlet and Malrieu about the length-dependence of excitation energies in polyenes[10]. Later, although remaining theoretically oriented, Attila's scientific interest shifted from traditional quantum chemistry. However, in 1982, with Neil Ostlund, he published a fantastic book entitled *"Modern Quantum Chemistry"*[11], which served as a fundamental textbook for generations of quantum chemists, and is still very much in use[2]. The book aims, and succeeds, to explain complicated issues in a transparent manner, e.g. coupled cluster theory, the diagrammatic technique in many-body perturbation theory, or the Green functions. The content is possible to grasp for everyone who went through the mathematical introductory chapters of the same book.

2.4 Ede Kapuy

Ede Kapuy was renowned as the greatest quantum chemist in Hungary for decades. He had an undisputed authority in this field.

Kapuy was born on September 21, 1928 in Győr (Hungary). His family directed him toward becoming a priest. This was perhaps due to the influence of his uncle, who had been a priest-teacher at the local Gergely Czuczor Roman Catholic Gymnasium of the Benedictine Order, whose presence in Hungary exceeds 1000 years. It is not surprising, therefore, that he attended the Czuczor Gymnasium.

After finishing high school, Ede Kapuy chose a different future from what his parents suggested by deciding to become a chemist and entering the Péter Pázmány University of Budapest, named after the founder of our university[3]. He graduated in 1952 from the same institution.

Ede Kapuy received his first higher degree in physics (Candidate of Physics) as a co-worker of Gombás at the Technical University of Budapest. In 1958 he joined the Research Group for Theoretical Physics (later renamed the Quantum Theory Group of the Hungarian Academy of Sciences). He completed his second higher degree (Doctor of Physics) in 1971, became a

[2]The Szabó–Ostlund book is one of the official textbooks in the Theoretical Programme of the George Hevesy Chemistry Doctoral School at ELTE (Eötvös Loránd University), Budapest.

[3]Cardinal Pázmány has founded the University in Nagyszombat (now Trnava in Slovakia) in 1635. It was ordered to move to Buda (part of the present Budapest) by Queen Maria Theresa in 1777. Its name was Péter Pázmány University from 1921 to 1950. From this date it is called Eötvös Loránd University, ELTE. Chemists know the name of Roland Eötvös mainly from the Eötvös law, which describes the temperature dependence of surface tension. His most important contribution was perhaps the construction of a high-precision gravitational pendulum, by which he showed the proportionality of the inertial and gravitational mass with 13 digit accuracy in 1891.

senior research scientist, and Research Professor in 1977. From 1983 he was a full professor of Theoretical Physics at the University of Szeged, where he chaired the Department of Theoretical Physics.

Kapuy was a fellow of the World Association of Theoretically Oriented Chemists (WATOC). Between 1981 and 1985 he served as a member of the Editorial Board of the Journal of Molecular Structure (THEOCHEM).

The main contribution of Ede Kapuy to quantum chemistry is the development of the separated pair theory in the late fifties and early sixties. Later, his interest turned to the electron localization problem. He published some 80 papers, most of them are in English. He was author or co-author of 4 books, including perhaps the best Hungarian textbook on quantum chemistry, titled Quantum Theory of Atoms and Molecules (co-authored by Ferenc Török). He was a visiting professor at major universities in England, Germany, and Canada. He frequently served as a member of organizing committees of international conferences on quantum chemistry.

The academic interests of Ede Kapuy were not limited to his own field of research, quantum physics and quantum chemistry. His knowledge of physics at large was remarkably broad. His extensive reading was only surpassed by his extraordinary memory -– if he declared that he had not read anything about a particular problem, it was unnecessary to check the literature. On the other hand, if he read something important about the topic, he could name not only the year but the location of the contribution.

The hobbies of Ede Kapuy included history and geography. He acquired such a distinguished knowledge in these subjects that he was considered an expert on these matters, as well. As the present author wrote in the introduction of the book "Correlation and Localization (Topics in Current Chemistry, a tribute to Ede Kapuy):

> *...His illness prevented him to join us* [to the WATOC'96 Congress in Jerusalem] *but he gave us advice with pertinent details about important historical sights in various small cities some of which I had never heard of. He has himself never been to the Holy Land, however[12].*

In recognition of the contributions and legacy of this remarkable scientist, a series of annual lectures in quantum chemistry was established at Eötvös University, known as the "Kapuy lectures"[4]. The Kapuy Lecture Series has became by now a prestigious scientific event at ELTE. Kapuy lecturers through a quarter of a century were: Henry F. Schaefer (2000), Rodney J. Bartlett (2001), John F. Stanton (2002), Josef Paldus (2003), Debashis Mukherjee (2004), Jürgen Gauss (2005), Ingvar Lindgren (2006), Mark Hoffmann (2007), Hiroshi Nakatsuji (2008), Enrico Clementi (2009), Wilfried Meyer (2010), István Mayer (2011), Hans Lischka (2012), Werner

[4]The text at the beginning of this Section is an abbreviated version of the blurb on the invitation card for Kapuy Lectures.

Kutzelnigg (2013), Paul G. Mezey (2014), Paul Ayers (2015), Trygve Ulf Helgaker (2016), Jerzy Ciosłowski (2017), Jean-Paul Malrieu (2018), Markus Reiher (2019), Jozef Noga (2021), Barney Ellison (2022), Gustavo Scuseria (2023), and Peter Knowles (2024).

Ede Kapuy was a great scholar, too. Of his students, we mention here Ferenc Bogár(vide infra in Section 3.4), Zoltán Csépes (many-body theory), János Pipek (Section 3.2), and Cornelia Kozmutza, who later became the wife of Ede.

2.5 Paul Mezey

Traditional chemistry was thought to be very far from mathematics. Born in 1943, Paul (in Hungarian: Pál) Mezey was an exceptional young chemist with having a deep affection of true math. In fact he has a double degree from Eötvös University: he completed the MSc requirements both in chemistry and in mathematics[5]. His scientific interests reflected this background from the beginning of his career to date – it is quite natural that he assisted in founding the *Journal of Mathematical Chemistry* in 1987, became a member of the Editorial Advisory Board from the very beginning, and became Editor-in-Chief of this journal in 1990. Among Hungarian quantum chemists, to our knowledge he was, for a long time, the only person who was both chemist and mathematician[6].

The present author started his work for MSc Thesis by obtaining an ALGOL computer code of the Linderberg equation motion to compute optical rotatory strengths. It was written by Paul Mezey before he emigrated from the communist Hungary at the end of the seventies. The code was professionally written, but in a compiler language that was getting obsolete. Computing ORD and CD spectra was the subject of PRS' thesis, so he started his work by translating Mezey's code to FORTRAN. That was, before being acquainted personally. Their interaction later developed to a scientific friendship and cooperation.

Quantum Chemical interest of Paul Mezey, all mathematically inspired, is very wide. It ranges from purely theoretically results that are often surprising and interesting but may be less "useful" from the practical point of view, to quite practical models. An example for the former is his theorem for inequalities for the electronic energies of isoelectronic systems[13], for the latter is his ADMA (adjustable density matrix assemble) method[14] which has been put in practice, and resulted many publications (see e.g. Ref.[15]). His long list of publications (more than 400 items) can certainly

[5]Ferenc Török, the chemist (MSc: 1951) and founder of quantum chemistry education at ELTE, has also obtained an MSc in applied mathematics in 1969. He studied math as a grown-up, after realizing that this is important to understand quantum chemistry.

[6]Interestingly, his example was recently followed by two young scientists, Zsuzsanna Tóth and Zsuzsanna É. Mihálka, who both were students of the present Volume editors, and have had diplomas in both subjects.

not be cited here. Any citation is therefore a result of a subjective selection. Nevertheless, we pick a few important results of him:

- The so-called holographic theorem of the electronic density[16]. Mezey proved that, in spite of the molecular density not being analytic at every point in space (cf. the cusp theorem), it can be reconstructed from any finite part of it, where it is analytic. It has the corollary that non-identical molecules cannot have identical densities in any finite domains.
- Rigorous mathematical theory of the topology of potential energy hypersurfaces[17]
- Catchment regions on potential energy surfaces[17]
- Shape Group Analysis of Molecular Electron Density Clouds based on Topology[18]
- The elaboration of the quantum chemical Le Chatelier principle[19]

In addition to his devotion to science, Paul is always looking for connections to arts, as well. Sometimes he does this with a great humor[7]. For example, once, when discussing connections between math and statuary, he started to indicate parabolic, elliptical, and hyperbolic points on the surface of a human (actually, female) body... It has, however, been connected to quantum chemistry, too: such an analysis may also be useful on a density or an energy surface.

In connection with his holographic theorem, he often mentions, that *"a theoretical chemist without a theorem is like an organic chemist without an organ."*

Even since from their university years, Paul Mezey is in a good friendship with Gábor Náray-Szabó, see Chapter 2. in Part I. in this Volume.

3 The Fabric is Getting Dense

3.1 Groups at ELTE

Initiated by Ferenc Török, here, at ELTE was formed the largest and longest-operating group in Hungary, in which the cultivation and application of quantum chemistry was the primary task. Though for now this old laboratory has been split to several parts, it is still functioning and conducts mainstream scientific research. One of its daughter laboratories, the "Laboratory of Theoretical Chemistry" at ELTE, writes in its mission statement (http://coulson.chem.elte.hu/tchlab/mission.html):

[7]Making humor is not far from him at any area of the human life.

The Laboratory represents the continuation of the former theoretical chemistry group (laboratory, department) at Eötvös University (previous leaders: F. Török, P. Pulay, G. Fogarasi), with the mission of preserving its international reputation.

This was the laboratory where Péter Pulay started his scientific carrier. Soon joined Géza Fogarasi, Pál Császár and Gábor Pongor. (See Chapter 4. in Part I.) Later, Attila Császár and Péter Szalay joined, then Péter Surján was invited in 1990. After Pulay leaving Hungary, Fogarasi became the head of the Laboratory (later: Department) of Theoretical Chemistry at ELTE.

Gábor Magyarfalvi had MSc in 1994, PhD in 1999, both supervised by Péter Pulay, who, however, settled down at the University of Arkansas in the meantime. The subject of these theses were focused on calculating magnetic and vibrational properties and implementing computational methods. Gábor has also dealt with NMR shieldings (calculations and theoretical developments), and VCD spectroscopy. Later, his professional focus shifted towards education including talent development: He is the chair of the Hungarian National Olympiad Board (2010-), mentor and organizer of the Hungarian teams at the International Chemistry Olympiad (IChO), chair (2016, 2018-23) of the Steering Committee of the IChO.

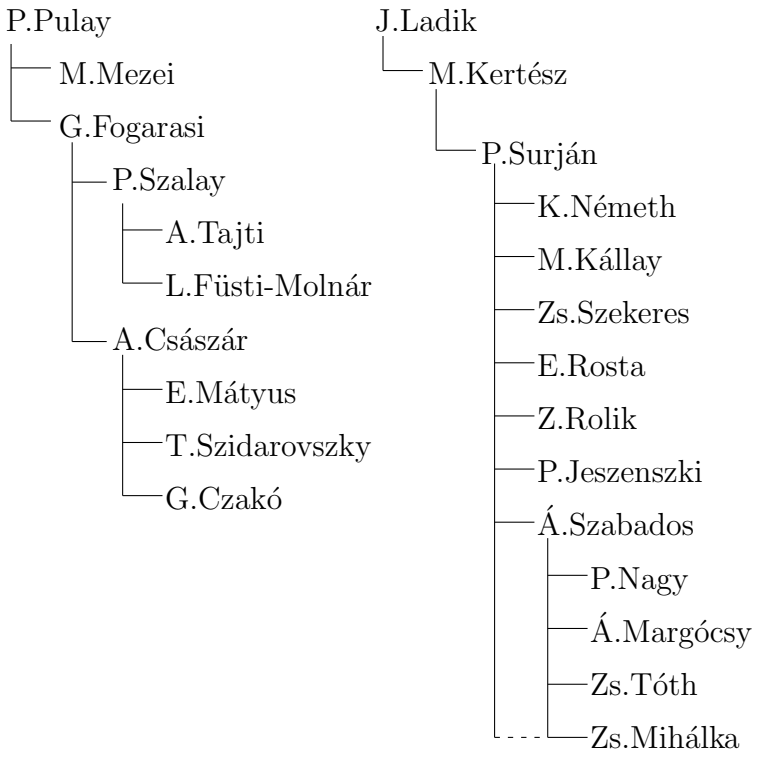
For other details of cultivating quantum chemistry at ELTE, see also Chapter 4. of Part I. by Péter Pulay of this book.

The former ***Laboratory of Theoretical Chemistry*** has split already into three labs. One with the same name, in which Péter Surján, Péter Szalay and Ágnes Szabados (the head of the Lab) are working, another one lead by Attila Császár ***Laboratory for Molecular Spectroscopy,*** and the ***Research Group for Molecular Quantum Dynamics*** (head: Edit Mátyus). Apart from these, in the Institute of Chemistry, quantum chemistry is cultivated also in the Laboratory of Chemical Informatics, head: László Túri. Ödön Farkas, Imre Jákli, Zoltán Novák, and András Perczel occasionally do quantum chemical calculations in the Department of Organic Chemistry. János Daru is also working at the Organic Chemistry Department, he is a theoretician, focusing on transferring the accuracy of state-of-the-art local electron correlation methods to atomistic path integral molecular dynamics simulations of condensed phase systems[20].

András Baranyai is a professor in the Department of Physical chemistry at ELTE. He is not a "quantum chemist" in the narrower sense. He was involved in research on non-equilibrium thermodynamics, a very difficult field cultivated only by a few scientists in the world. However, during the second half of his scientific carrier, Andras changed his interest and did research simulating water structures, by which he received notable scientific reputation (*sapienti sat*).

It is perhaps not an overstatement that the Theoretical Chemistry Labo-

ratory has been functioning as a successful theoretical school[8]. To illustrate this, consider the following two-rooted genealogy tree[9]:



The lines indicate supervisions (either for PhD or for MSc, or both), the dashed line means co-supervision. The above names are known for quantum chemists, mainly for their theoretical developments.

It is evident that the results of such a successful school must originate from several reasons. Here we would like to point out just one important factor. From the 1990-s the Institute of Chemistry at ELTE introduced a reform in the education of mathematics for chemistry students. The present author was asked to develop and teach a course in higher applied mathematics. The course (which was later split into several shorter courses) summarized advanced analysis including the theory of complex functions, methods for solving differential equations including Sommerfeld polynomial method, Laplace transformation and the concept of Green's functions, using Dirac's δ, properties of Fourier transformation, elements of probability theory, variational calculus, theory of coordinate systems (metric tensor, etc.), elements of functional analysis (linear spaces and operators), bra–ket for-

[8]The present author published a paper recently in Hungarian, reviewing the history and results of quantum chemists at ELTE[21]

[9]This is only a small subpart of the scientific genealogy tree of the mentioned researchers.

malism, non-orthogonal bases and orthogonalization procedures, orthogonal polynomials, and a rather involved introduction into the theory of point groups and their representations. A thorough summary of the physics and formalism of quantum mechanics was also included. All this was taught already at the BSc level. Some of the courses being compulsory, others were optional. This material was quite exhausting to teach and to learn, and in fact, it created a cross-link between the two branches of the above genealogy tree: the present author has taught all members of the younger generation, when they were undergraduate. Elements of quantum chemistry were taught by Fogarasi, Császár and Szalay again for all students. As advanced graduate courses, students could choose among many options. The present author e.g. was teaching formalisms to be used in methodological developments in quantum chemistry, including second quantization, partitioning technique, Bloch-type equations, and the use of Green's operators for obtaining energy differences directly. Péter Szalay had PhD courses on electronic structure methods, while Attila Császár taught the theory of high-resolution ro-vibrational spectroscopy. To my best knowledge, the level of the above math teaching is quite high even on international standards. Therefore, it is perhaps not just by chance that the students in the above tree came to like theoretical research and later achieved substantial results in this field.

Applied Quantum Chemistry is also important for physicists working in material science. At ELTE, we mention Jenő Kürti, János Koltai, Andor Kormányos and László Oroszlány, who work at the Institute of Physics and Astronomy, and study materials of strong current interest (polymers, fullerenes, nanotubes, graphene and novel 2D materials).

3.2 Groups at BME

Quantum chemistry at the Technical University of Budapest (BME) was actively used and developed at three places. The Institute of Physics was one of these, in which Gombás founded the Quantum Theory Group, where Ede Kapuy, and his former student János Pipek, became members.

János Pipek was interested originally in many-body perturbation theory, also in a localized MO basis. While visiting Paul Mezey in Canada, he developed the *Pipek-Mezey localization*, one of the most popular iterative *a posteriori* localization schemes[22]. János' interest later turned to various problems in solid state physics and material structure, that we cannot detail here. In the latest part of his scientific career he became engaged with the quantum chemical application of wavelet theory, cooperating with Szilvia Nagy[23, 24, 25].

István László and László Udvardi (see Chapter 4. in Part III.), as well as Barna Apagyi, Károly Ladányi, Sándor Kugler, Imre Varga, were all members of this group, together with some further theoreticians, whose field

of research was tangentially related to quantum chemistry.

The second quantum chemistry center at BME was the Physical Chemistry Department, where Ferenc Billes, András Grofcsik, Árpád Kiss, and Miklós Kubinyi were applying quantum chemistry with an orientation toward molecular spectroscopy. This is the department to which Mihály Kállay joined later (see Chapter 1. in part II.)

The third group doing also successful applied quantum chemistry at BME has been formed within the Department of Inorganic and Analytical Chemistry. Some names (in alphabetic order) are Zoltán Benkő, Gábor Csonka, Oldamur Hollóczky, József Nagy, László Nyulászi, Julianna Oláh, Gábor Pongor (before joining to ELTE), and Tamás Veszprémi. An interesting relation between theory and experiment was realized by István and Magdolna Hargittai, who used to do experimental research collecting and analyzing electron diffraction spectra. In parallel with the decline of this experimental technique, they realized the importance of applied quantum chemistry, and published many important papers in that field, some of them processing electron diffraction measurement data collected earlier. While István has retired form the Department of Inorganic and Analytical Chemistry at BME, it is also interesting to note that much earlier, after the emigration of János Ladik to Germany in the 1970-s, Hargittai was the superintendent of the Ladik's orphaned group for a while.

3.3 Groups in Debrecen

Settled down in Debrecen as the head of the Department of Theoretical Physics, Rezső Gáspár established an active quantum chemical research there. All members of his department are not listed here, we just mention Ágnes Nagy, who became well known in density functional theory (cf. Chapter 6. in part III. of this book), and Ágnes Vibók, who, together with his husband Gábor Halász, achieved notable results in various fields of quantum chemistry. (Some of their works are discussed in part III., Chapter 10.)

Oldamur Hollóczki, emitted from BME, found a position at Debrecen, in the Institute of Chemistry. He thus opened the door for quantum chemistry to be cultivated in Debrecen not only by physicists *(vide supra)*, but by chemists, too.

3.4 Groups in Szeged

Following Rezső Pauncz's emigration from Hungary in 1956, the Department of Theoretical Physics in Szeged continued its quantum chemistry research, albeit with less intensity. The research mainly followed the Gombás' school in the atomphysical many-body problem, with contributions from János Horváth, Ferenc Berencz, and Vilmos Maráz. The next generation of researchers turned their attention to the field of solid-state physics (Iván

Gyémánt, György Papp, and Zsuzsa Varga). At the same time, chemists began to contribute significantly to the field of quantum chemistry, especially Miklós Bán, Gyula Dömötör, Gyula Tasi and Márta Révész (who later became István Mayer's wife).

Following the invitation of Ede Kapuy to the Department of Theoretical Physics in Szeged, a new phase of quantum chemical research began. First Ferenc Bartha and later, in 1987, Ferenc Bogár were appointed as members of Ede Kapuy's research group. Their main research interest was the application of localized orbitals in Møller-Plesset perturbation calculations, with special emphasis on the double perturbation formulation of the problem, the convergence of localization corrections, and the application of this theory to spatially extended systems. In 1994, Ferenc Bogár joined János Ladik in Erlangen, where he worked on the calculation of the electron structure of quasi-1D polymers, including electron correlation through the quasiparticle approach. Their results were published in several papers on the conductivity of single-stranded DNA[26]. From 2003 onwards, he became involved in computer-aided drug design research at the Institute of Medical Chemistry of the University of Szeged.

Gábor Paragi, from the current staff of the Theoretical Physics Department, revitalized quantum chemical research and contributed to the development of the DFT-based Ziegler-Rauk energy decomposition analysis and its application to biomolecular systems.

More recently, Gábor Czakó, coming from Attila Császár's group in Budapest (see Part III, Chapter 2), settled in Szeged and established a modern computational reaction dynamics research group at the Department of Physical Chemistry and Materials Science. He has made a number of significant achievements in elucidating mechanisms of SN2 reactions.

3.5 Groups at MTA

The Hungarian Academy of Science (MTA) managed several research institutes in the country. Prominent names working at MTA groups involve Tamás Szondy, who introduced the method of moments, and, cooperating with Károly Ladányi and Mihály Mezei, published several important papers on it[27, 28]. He was also known as an expert of the evaluation of quantum chemical integrals.

In Ladik's group several researchers worked, of whom Géza Biczó, István Lukovits, and István Mayer remained in Hungary, while Miklós Kertész and Sándor Suhai moved abroad[10]. Members of the next generation, Imre Bakó, Andrea Hamza, György Lendvay, Tibor Nagy, Imre Pápai, and András Stirling worked also at MTA, now in a reorganized institution belonging to the Hungarian Research Network.

[10]For Ladik's contribution, see Chapter 5. in Part I., while Chapter 7. discusses István Mayer. Kertész and Suhai will be mentioned below in Section 3.6.

In another institute of MTA, the Wigner Research Center, physicists were active in theoretical solid state physics having some natural overlap with quantum chemistry. Of them, Örs Legeza is widely known in quantum chemical community, mainly for his effort to develop, use and popularize density matrix renormalization group (DMRG) techniques for molecular systems. For his recent works, see Chapter 5. in Part III. in this book.

3.6 Outside the Country

Several well known quantum chemists of Hungarian origin have submitted their contributions to this Book, or have been discussed in detail in one of the Chapters. A few more colleagues are listed below, to illustrate the extent of Hungarian's contributions to the field.

Albert Bartók-Pártay graduated at ELTE in 2006 (MSc in Chemistry) with the supervision of András Baranyai, he went for PhD to the University of Cambridge where he obtained PhD in physics in 2010. He works in Warwick, UK. Main areas of research interest of Albert are materials modelling on the atomistic scale, developing methods to accelerate simulations while making accurate predictions. He is also interested in electronic structure calculations, density functional theory and related developments. He is using tools from machine learning to build fast and accurate models that are based on large amounts of ab initio data.

Attila Bende. Many citizens of Romania having Hungarian nationality, living typically in Transylvania, cultivate a strong science there, some are involved in natural sciences. Quantum chemistry is only marginally represented, but its elements were thought by János Máté in Kolozsvár (Cluj-Napoca) at the Babes-Bolyai university already in the second half of the twenties century. Of the younger generation the work of Attila Bende is worth mentioning.

Attila obtained his BSc in physics from the Babeş-Bolyai University, Kolozsvár in 1996, and his MSc in 1997 at the same place. Then he came to Debrecen, Hungary, where he, supervised by Ágnes Vibók, received his PhD in 2004. He has found a position at the National Institute for Research and Development of Isotopic and Molecular Technologies, Kolozsvár, Romania, where he is currently occupying leading positions. His scientific interest covers atomic and molecular physics and quantum chemistry, having results in the fields of excited state relaxation dynamics, photochemistry, intermolecular interactions, macromolecular modeling, and band structure of biopolymers. He has published some 100 scientific papers in these fields, which received significant scientific reputations.

Gábor Csányi was born in Hungary, but grew up in Britain. He is professor of molecular modelling in Cambridge. His expertise is in atomistic simulation, particularly in multi scale modelling that couples quantum mechanics to larger length scales. He is engaged in applying machine learning

and other data intensive techniques to materials modelling problems, such as deriving force fields (interatomic potentials) from ab initio electronic structure data. Also interested in statistical problems in molecular dynamics, e.g. in enhanced sampling algorithms that can be used explore the global configuration space of materials and molecules

Péter Deák is a physicist working in computational material science. Graduated at ELTE, first became a professor at BME, finally settled down in Germany (Univerität Bremen).

László Füsti-Molnár obtained his MSc and PhD at ELTE, supervised by Péter Szalay. He visited several foreign laboratories, including that of Gabriel Bálint-Kürti in Bristol. He settled in the USA, and founded the Quantum Future Scientific Software LLC for the development of effective quantum chemical program systems based mainly on density functional theory.

Monika Fuxreiter graduated at ELTE. After a postdocing period Monika went to Debrecen with a prestigious starting grant of the Hungarian Academy. Later she became professor in Italy, at the University of Padova. She is committed to exploit the knowledge on context-sensitive biomolecular recognition for drug discovery. To this end, she is engaged with combining theory and experiments. We quote here merely three of her representative publications[29, 30, 31].

Gergely Gidófalvi was born in Budapest, Hungary. He received his BSc in 2002 from San Diego State University, his MSc from the University of Chicago in 2003, and PhD in 2006 from the same place, supervised by D. Mazziotti. Between 2007 and 2010, he worked with Ron Shepard as a postdoctoral fellow at Argonne. From 2010 he has been on the faculty of Gonzaga University in the Department of Chemistry and Biochemistry. His research focuses on efficient computational algorithms for modeling molecular properties and energetics of reactions.

Miklós Kertész obtained his MSc in physics in 1971 from ELTE, performing his work at the Research Institute of Chemistry of the Hungarian Academy with the supervision of János Ladik. His thesis was about the use of UHF in band structure calculations for polymers. After leaving Hungary, he was working in Gainesville in Florida at the Quantum Theory Project with Henk Monkhorst, and later with Roald Hoffmann at Cornell, Ithaca, NY. Finally, he became professor at the Georgetown University, Washington. He preserved his interest in the quantum theory of crystals, polymers, and material science in general.

Ildikó Kovách, Professor Emerita at the Catholic University of Washington (CUW), started her higher education at he Semmelweis Medical University of Budapest. Obtaining her PhD from the University of Kansas, she found a position at the Department of Chemistry at CUW. Her interest is mainly biochemistry, but her research involved molecular mechanics and dynamics.

Mihály Mezei graduated as a chemist at ELTE, in the same year as Paul Mezey and Gábor Náray-Szabó. He is working at Icahn School of Medicine at Mount Sinai in New York on computer simulation of aqueous systems. He developed Monte Carlo and free energy simulation methodology and made biomolecular applications. For representative publications, see e.g.[32, 33, 34, 35]

Károly Németh graduated at ELTE with the supervision of Péter Surján in 1996. He occupied postdoc positions with Franz Mark, János Ángyán, Gustavo Scuseria, Peter Pulay, and Matt Challacombe. He held a researcher position from 2005 to 2012 at the Argonne National Laboratory. Currently he is a research professor, Illinois Institute of Technology, Chicago, Illinois, USA. His current interest is material science, including the theory and practice of batteries related materials design[36].

Edina Rosta graduated at ELTE, Budapest with P. Surján, obtained PhD at UCLA with A. Warshel, spent some time at NIH, where she became acquainted with Attila Szabó, and became professor in London, first in King's College and later at the University College. (See her contribution, Chapter 7. in Part III. of this book.)

Sándor Suhai, emitted from Ladik's group in Budapest, settled down in Heidelberg, Germany at the German Cancer Research Center, where he became a leading researcher in the field of polymers using ab initio band structure calculations as well as density functional based methods.

Péter Szabó obtained his PhD in 2017 from the University of Veszprém, Hungary, supervised by György Lendvay. After PhD, he visited several places in Europe (Sweden, Luxembourg). He is staying currently at the Catholic University of Leuven, Belgium. His thesis was about dynamics of molecular collisions. Maintaining his interest in that field, he also has notable results in the theory of polarizability[37].

Róbert Izsák obtained an MSC diploma in 2006 from the University of Szeged, supervised by Gyula Tasi, then went to the Cardiff University where he worked under the supervision of Peter Knowles, and received PhD in 2010. After some research work at the Max Planck Institute in Germany, he went back to the UK, and currently is a group leader at Riverlane Ltd, Cambridge. His field is method development for excited states and applications of quantum computing.

Kálmán Varga received his PhD in physics from the University of Debrecen, Hungary. Currently he is a professor of physics at the Department of Physics and Astronomy in Vanderbilt University, Nashville, Tennessee, USA. He uses first principles modeling for the study light and matter interaction, and works on the description of strongly coupled light-matter systems in optical cavities, quantum plasmonics, and laser induced electron currents.

Further scientists of Hungarian origin have their own chapters in this

book (***György Bácskay,*** Sydney, Australia: Chapter 6. in Part I., ***László von Szentpály,*** Stuttgart, German: Chapter 9., Part III.). Some did not preserve their Hungarian roots, even if having undeniably Hungarian names. Some others may have remained unmentioned, a regrettable but probably unavoidable shortcoming of any endeavor of enumerating colleagues with a particular focus.

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