# SUCCESS STORY: Research and Education in Theoretical Chemistry at Eötvös University of Budapest, Hungary

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Most chemists consider chemistry as a fundamentally experimental science and chemistry indeed does not have a comprehensive theory of its own. Nevertheless, over the last decades theoretical chemistry has become an integral part of research and university-level education in chemistry and in related fields of molecular and material science. Within the limits of this short article summarizing research and education in theoretical chemistry at ELTE, *i.e.*, Eötvös University of Budapest, the leading research university in Hungary, it is impossible to explain the reasons behind this paradigm shift in chemistry. It is only mentioned that by 2013 in nearly half of the publications in the prestigious *Journal of the Americal Chemical Society* theoretical (mostly quantum) chemistry is used though not the principal theme of the article.

Quantum chemistry, providing a relatively consistent theory for large parts of chemistry, is the application of quantum mechanics to chemical systems. Through its many approximations, required to make it applicable to systems of useful size and complexity, quantum chemistry has its own and distinct characteristics. Nevertheless, it must be recognized that quantum chemistry is still not able to treat all chemical systems of interest. Thus, classical mechanics (and semi-classical theory) play an important part of the armamentarium of theoretical chemistry, as emphasized vividly by the 2013 Nobel prize in chemistry. These days almost all areas of theoretical chemistry rely heavily upon computation, so the term computational chemistry also provides a good description of research in the field not only of quantum chemistry but also of theoretical chemistry.

That a single dedicated person can make a difference in the education of many is proved by the story of Professor Ferenc Török of ELTE, an inorganic chemist and spectroscopist by training, who recognized the advances lying ahead of theoretical and especially quantum chemistry in the second half of the 1960s. The dedication of Professor Török to theoretical chemistry and in particular to quantum chemistry led to the start of a teaching program in quantum chemistry which eventually led to a full set of courses in quantum chemistry at ELTE. Professor Török, together with Professor Ede Kapuy from the Technical University of Budapest, authored a book, *Quantum theory of atoms and molecules*, which appeared in 1975 in Hungarian. Since resources for high-caliber basic research were scarce before 1989 at Hungarian universities, it also made sense for many to try to excel in theoretical chemistry, a field considered to be less expensive than experimental chemistry. Furthermore, education in natural sciences has been a very strong point of the Hungarian elementary and high-school education system since about 1890; thus, many students who entered the university in the 1960s and 1970s had a thorough training in math, physics, and chemistry, subjects needed to excel in theoretical chemistry. The traditional high-level training characterizing the basic education system of Hungary resulted in a number of outstanding mathematicians and theoretical physicists of Hungarian origin in the 20$^{th}$ century, to name just a few of the best known ones we mention (in alphabetical order) Cornelius Lanczos, John von Neumann, Leó

Szilard, Edward Teller, and Eugene Wigner, as well as the molecular physicists Rezső Gáspár and Pál Gombás.

The research and education in theoretical chemistry was elevated to new heights by the outstanding achievements of a student of Professor Török, Professor Peter Pulay, the father of the "force method" of electronic structure theory. Professor Pulay became instrumental in setting up an originally small research group of theoretical chemists at ELTE. Later on a Laboratory of Theoretical Chemistry and even later a Department of Theoretical Chemistry was formed, by then without the guidance of Professor Pulay, who left for the USA. The leader of the Laboratory and the Department of Theoretical Chemistry was Professor Géza Fogarasi and the group was strengthened by Professor Imre Ruff, who represented the non-quantum-chemistry school of theoretical chemistry. By 2013 among the 70 or so faculty members of the Institute of Chemistry of ELTE there are about 10 full professors whose main research area is computational chemistry.

The scope of theoretical/computational chemistry research is unusually wide at ELTE. There are successful research groups in the fields of electronic structure theory, nuclear motion theory, reaction kinetics, molecular modeling, as well as Monte Carlo and molecular dynamics (MD) simulations. While several of the groups emphasize method development, especially in quantum chemistry, several interesting applications using the methods developed have been published. Another important characteristic of research in theoretical chemistry at ELTE, which also applies to the Hungarian quantum chemistry school in general, is the emphasis on the joint utilization of experimental and theoretical information in solving interesting chemical problems. In what follows I briefly mention a few key publications from the theoretical chemists of ELTE, focusing only on the last few years.

Developments in the group of Professor Péter Szalay related to electronic structure theory cover highly accurate configuration interaction (CI) and coupled cluster (CC) techniques. A review on some of these achievements can be found in a recent article, which appeared in *Chemical Reviews* (**2012**, *112*, 108). Members of the same theoretical chemistry group are at least partially responsible for developing several electronic structure codes, including CFOUR (http://cfour.de) and an earlier version of MRCC (http://www.mrcc.hu). Perturbative approaches to the electron correlation treatment are key elements of the research performed in the group of Professor Péter Surján.

The other major area of quantum chemistry concerns the motion of the nuclei, *i.e.*, the vibrational and rotational motion of molecules. Professor Attila G. Császár is active in this field, he published some of his work in the magazines *Science* (**2003**, *299*, 539) and *Nature* (**2008**, *453*, 906). Last year Professor Császár declared, in a *Perspective* article which appeared in *Phys. Chem. Chem. Phys*. (**2012**, *14*, 1085), that we live in the fourth age of quantum chemistry and accurate and efficient numerical solution of not only the electronic but also the nuclear Schrödinger equation has become possible. In 2013 the first theoretical chemistry group at a university in Hungary was funded by the Hungarian Academy of Sciences, the name of the group is MTA-ELTE Research Group on Complex Chemical Systems and it is led by Professor Attila Császár. For this group complex chemical systems does not mean large (and therefore „complex") molecules, as it has to be recognized that even the smallest molecules, like the triatomic water molecule, behave much as complex systems when their nuclear motions (vibrations and rotations) are considered.

An important research area in theoretical chemistry concerns the determination and reduction of large chemical reaction mechanisms, like those characterizing combustion systems (combustion of $H_2$ as well as combustion of hydrocarbons fuels come to mind). This is the area where Professor Tamás Turányi publishes most of his work, for recent examples of his achievements see the book "*Development of detailed chemical kinetic models for cleaner combustion*" (Springer, Heidelberg, 2013).

Modeling of large molecular systems is the specialty of Professor András Perczel, who performs classical and quantum chemical calculations as well as MD simulations to model peptides and proteins and their various spectra, most importantly NMR and CD spectra. Professor Perczel is also the leader of a research group supported by the Hungarian Academy of Sciences (MTA), this MTA-ELTE research group is called Protein Modeling Group. One of their recent in silico studies made it to the cover of *Chem. Eur. J*. (**2012**, *19*, 2628).

Members of the Research Laboratory of Chemical Informatics are active in different fields of computational chemistry. Professor András Baranyai is an expert of non-equilibrium classical simulations. Lately, he focused on the development of classical model potentials of water. Their polarizable water model reproduces the most important features of solid, liquid and gas phase water and was published in *J. Chem. Phys.* (**2013**, *138*, 204507). Professor László Túri's main field of interest is the semi-classical simulation of the solvated electron. The most important findings of his research are summarized in *Chemical Reviews* (**2012,** *112*, 5641). The two associate professors of the laboratory, Dr. Ödön Farkas and Dr. Gergely Tóth are active on diverse fields of computational chemistry: classical simulations, applied quantum chemical calculations, chemometrics, application of numerical methods, and conformational analysis.

Just in 2013 three large international conferences have been organized by theoretical chemists at ELTE: the *23rd High Resolution Molecular Spectroscopy* meeting was organized by Professor Attila G. Császár, the *VIIIth Congress of the International Society of Theoretical Chemical Physics* was managed by Professor Péter R. Surján, while the *9th European Conference on Computational Chemistry* took place under the guidance of Professor Péter G. Szalay.

A successful research program must be based on a successful teaching at the graduate and postgraduate levels. As mentioned, ELTE led Hungary toward making theoretical chemistry a mandatory course in the curriculum of all chemists and high-school chemistry teachers. Unfortunately, the Bologna process reduced the possibility to train students focusing on theory, as it is expected that BSc graduates have strong practical skills. Our teaching program for students being interested in theoretical chemistry is built upon basic math (about 14 credits), physics (about 10 credits), and computer science (about 4 credits). These preliminary studies are followed by a semester-long, 6-credit study of „Mathematics of Chemistry" and another semester-long 5-credit course on „Theoretical Chemistry". Following these latter two courses special lectures and practice sessions are offered on computational chemistry, containing basic signal processing, data analysis, as well as quantum chemical and classical dynamical simulations, and bioinformatics.

Further specialization to computational chemistry is open at the MSc level. The credit sum of the optional and elective courses on theoretical and computational chemistry exceeds 100. Diversity of the courses offered is extremely high, the courses cover almost all fields of

computational chemistry. Before the Bologna process made ELTE change some of its degree programs, ELTE came up with a 5-year program yielding a MSc in Cheminformatics. Now this program is part of the MSc in Chemistry program as a specialization. The best students follow up their studies in the PhD program of the Institute of Chemistry of ELTE, where the *Theoretical and Physical Chemistry, Structural Chemistry* subprogram provides the framework for their education.

Several courses in theoretical chemistry are offered not only in Hungarian but also in English; therefore, those who would like to take part in the education opportunities offered by the theoretical chemists at ELTE have the opportunity to do this, perhaps via the Erasmus program or as full-time MSc students.