

Curriculum vitae

Lubomír Rulíšek

born 10 January 1972

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Titles: Mgr. (*MSc. equivalent*), CSc. (*PhD. equiv.*), DSc. (*Doctorate of science*, defended in January 2013), Doc. (*Assoc. Prof.*, since February 2019)

Position: Head of the Theoretical Bioinorganic Chemistry Group (Senior Research Group Leader), Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences (IOCB)

Education: MSc. in Physical Chemistry at the Faculty of Natural Sciences, Department of Physical Chemistry, Charles University, Prague, Czech Republic (Diploma Thesis: ‘*A Comparative Study of Planar and Spatial Aromaticity*’, defended in May 1995)

Ph.D. studies at the Dept. of Theoretical Chemistry, IOCB under the supervision of Dr. Zdeněk Havlas (Thesis ‘*Theoretical Studies of Interactions of Transition Metal Ions with Amino Acids and Proteins*’, defended in February 2001)

Chronology of Employment:

2012–	Head of the Theoretical Bioinorganic Chemistry Group (Senior Research Group Leader position), IOCB
2007–2012	Head of the Theoretical Bioinorganic Chemistry Group (Junior Research Group Leader position; in the 2012 evaluations by the Int. Advisory Board ranked as ‘ <i>I–Excellent</i> ’ and promoted to the senior position), IOCB
2004–2006	Head of the Theoretical Chemistry Group under the Dept. of Molecular Modelling, IOCB
2002–2004	Postdoctoral Fellow at the Dept. of Theoretical Chemistry, Lund University, Sweden, under the supervision of Prof. Ulf Ryde
2001–2002	Junior Researcher at the Dept. of Theoretical Chemistry, IOCB

Main Scientific Interests:

Theoretical bioinorganic chemistry, quantum chemistry, quantum and molecular mechanical (QM/MM) methods, organic reactivity, computational homogeneous catalysis, biomolecular design, protein–ligand interactions, computational electrochemistry, theoretical spectroscopy, conformational sampling

Scientific Community Activities:

Member of the IOCB Board (2009–2011)

Chairman of the IOCB Board (2012– 2017)

Member of the Board of the Institute of Molecular Genetics (2017–2018)

Member of the COST External Evaluation Panel (CMST Domain, September 2012)

Leader of the ‘IOCB at EXPO2010’ team (Molecules for Life) in Shanghai, China.

Member (2017–2021) and Chairman (2020–2021) of the P208 (Physical and Analytical Chemistry) Panel of the Czech Grant Agency

Editorial Board of Scientific Journals

Associate Editor in *RSC Advances* (2021–)

Associate Editor national peer-reviewed journal *Collection of Czechoslovak Chemical Communications* (2008–2011; in 2012 CCCC transformed into Wiley’s *ChemPlusChem*)

Reviewing Activities

Peer-reviewing for major international journals (e.g. *J. Am. Chem. Soc.*, *J. Phys. Chem.*, *J. Org. Chem.*, *Inorg. Chem.*, *J. Inorg. Biochem.*, *Biochemistry*, *Chem. Eur. J.*, *Phys. Chem. Chem. Phys.*, *Coord. Chem. Rev.*, *PCCP*, *JBIC*), and several foreign or domestic grant agencies (incl. ERC), foreign universities (e.g. Ph.D. opponent Univ. Stockholm, 2017, Univ. Bayreuth, 2017, Lausanne 2019); currently with a frequency of ~40 ms/projects/grants/year. In 2009, among the top 20% of the reviewers for *J. Phys. Chem.*

Organisation of Conferences:

Main organiser of the 4th and 7th *Japan-Czech-Slovak Symposium in Theoretical Chemistry* (Liblice, 2011; Prague 2018)
Main organiser of the *Quantum Bioinorganic Chemistry Conference* (Český Krumlov, June 2011)
Chairman of weekly '*IOCB Theoretical Chemistry Seminars*' (2004-2014)
Main organiser of the *ECOSTBio "Spin States in Biochemistry"* conference (Prague, April 2016)

Teaching:

MSc. Courses '*Computer Modelling of Chemical Reactions in Condensed Phase and Biomolecules*', (2008-) and '*Chemical Structure B*' (2016-2020) Faculty of Science, Charles University, Prague

Mentoring:

Supervisor of six Ph.D. students (Martin Srnec, Vojtěch Klusák, both defended in 2010; Ondrej Gutten, defended 2018, Daniel Bím, defended 2019, Agnieszka Stanczak, Tadeáš Kalvoda, both since 2020), ten postdoctoral fellows (Tibor András Rokob, Martin Lepšík, Jaccob Madhavan, Cristina Trujillo, Goar Sánchez, Haunani Thomas, Prokopis C. Andrikopoulos, Zahra A. Tehrani, Martin Culka, Sindrila Dutta Banik, Monika Stas, Erik Andris), and four diploma (MSc.) students (Ondrej Gutten, Václav Navrátil, Daniel Bím, defended 2010, 2009, and 2014, respectively; Tadeáš Kalvoda, defended 2020); co-supervisor of two Ph.D. (Jakub Chalupský, Ivana Beššeová), one diploma (Pavel Beran) and one bachelor students (Lucie Tučková)

Rulíšek's Group:

In total, more than 30 scientists (incl. students and postdoctoral fellows) worked in the group in the 2007–2021 period; the average size of the group has been 7-8 scientists

Key Scientific Collaborations (2011-2020):

IOCB: Petr Beier, Michal Hocek, Pavel Hobza, Ullrich Jahn, Jan Konvalinka, Josef Michl, Jan Řezáč, Ivo Starý

Domestic: Pavel Kočovský, Petr Hermann (*Charles University, Prague*), Martin Srnec (*J. Heyrovský Inst. Phys. Chem. AS CR, Prague*), Aleš Růžička (*Univ. Pardubice*)

International: Edward I. Solomon (*Stanford Univ., U. S. A.*), Ulf Ryde (*Lund Univ., Sweden*), Jana Roithová (*Radboud University Nijmegen, Netherlands*), Aleš Svatoš (*MPI Chemical Ecology, Jena, Germany*), Takeshi Yanai (*Institute for Molecular Science, Okazaki, Japan*), Tibor András Rokob (*Chem. Res. Institute, Hungary*), František Tureček (*Univ. Washington, U. S. A.*), Sergey Shleev (*Malmö Högskola, Sweden*)

Bibliographic Overview:

~120 research articles, mostly in leading international journals. LR is the *first* or *corresponding* (*senior*) author of 65 papers. 27 papers have been published in top-ranked journals, e.g. *J. Am. Chem. Soc.* (8), *Chem. Eur. J.* (11), *Chem. Sci.* (2), *Angew. Chem. Int. Ed.* (3) and *Proc. Natl. Acad. Sci. U. S. A.* (3), whereas recent contributions include one invited perspective (*Dalton Trans.* **2012**) and two invited reviews (*Coord. Chem. Rev.* **2013**, *J. Biol. Inorg. Chem.* **2016**). The work has been cited ~3450 times (with ~2700 independent citations, i.e. with all forms of self-citations excluded; source: ISI WoS Core Collection, April 8, 2021). LR's H-index is 36 (the 'independent' H-index is 29).

Patents:

'*Rationally designed MALDI matrices for analysis of metabolites and other small molecules*' (WO2010031588) with MPI for Chemical Ecology, Jena, Germany (PI contribution 10%)

Invited (Plenary or Keynote) Lectures at International Conferences (approx. 20 in total):

'Modelling Interactions in Biomolecules' conference series (Prague, Czech Republic (CZ) 2005, Prague, CZ, 2007, Mariánské Lázně, CZ, 2013, Průhonice, CZ, 2015)

Japan-Czech-Slovak Symposium in Theoretical Chemistry' series (Prague, CZ, 2005, Kyoto, Japan, 2007, Bratislava, Slovakia, 2009, Nara, Japan, 2013, Smolenice, Slovakia, 2015)

'Biomaterials Research School', Lund University, Lund, Sweden (2008)

'8th European Conference on Computational Chemistry', EUCCO-CC8, Lund, Sweden (2010)

'Computational Homogeneous Catalysis' conference, Stockholm, Sweden (2011)

'X Girona Seminar on Theoretical and Computational Chemistry', Girona, Spain (2012)

'Spin States in Biochemistry and Inorganic Chemistry' conference, Zaragoza, Spain (2012)

'Current Trends in Theoretical Chemistry VI' conference, Krakow, Poland (2013)

'Central European Symposium on Theoretical Chemistry', Znojmo, CZ (2013)

Department of Chemistry Seminar, University of Washington, Seattle, U. S. A. (2014)

Department of Chemistry Seminar, Stanford University, Stanford, U. S. A. (2014)
ACS Meetings (Boston, 2015, San Diego, U. S. A., 2016)
Department of Chemistry Seminar, Stockholm University, Sweden (2017)
Department of Chemistry Seminar, Universität Bayreuth, Germany (2017)
Department of Chemistry Seminar, ETH Zurich, Switzerland (2017)
Department of Chemistry Seminar, Lund University, Sweden (March 2018)
Quantum Bioinorganic Chemistry IV, Bath (United Kingdom (September 2018)
School on Molecular Computational Biochemistry, Krakov, Poland (March 2019)

Research Sabbaticals:

09/2014-11/2014 Stanford University, CA, U. S. A. (Edward I. Solomon) – Fulbright scholar
06/2014-07/2014 Gilead Sciences, Inc., Foster City, CA, U. S. A. (Uli Schmitz/William A. Lee)

Prizes, Awards, Titles:

Hlavka Foundation Prize (2001) – an annual award for outstanding Ph.D. students in the Czech Republic
Wichterle Prize of the ASCR (2006) – an award of the Academy of Sciences of the Czech Republic for an outstanding young researcher
Fulbright Fellowship (2014) – Stanford University
Werner von Siemens Award (2021) – the best achievement in basic research in Czechia in 2020

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Doc. Mgr. Lubomír Rulíšek, CSc. DSc.