# Curriculum vitae

# Jiří Pittner

# Address for Correspondence:

J. Heyrovský Institute of Physical Chemistry; Academy of Sciences of the Czech Republic; Dolejškova 3 CZ–18223 Prague 8; Czech Republic

 $phone: +420\text{-}266052015; \ fax: +420\text{-}286582307; \ e\text{-mail: jiri.pittner@jh-inst.cas.cz}$ 

Born: 1968; Marital Status: married, 2 children

# Employment:

Post-doc in the group of Prof. Dr. V. Bonačić–Koutecký, Humboldt University Berlin (1997) Researcher at the J. Heyrovský Institute of Physical Chemistry, AV ČR (Nov. 1997 - August 2005). Head of the Department of Theoretical Chemistry at the J. Heyrovský Institute of Physical Chemistry, AV ČR (since Sept. 2005)

# Education:

- 1986-91 Undergraduate studies: Department of Chemistry, School of natural Sciences, Charles University Prague, Czechoslovakia;
- 1991-96 Ph. D. study with Prof. Dr. V. Bonacic–Koutecky, at the Free University Berlin and Humboldt University Berlin. Thesis titled "Ab Initio Study of Optical Properties of Neutral and Charged Pure and Mixed Alkali Metal Clusters" was defended in December 1996 with result "summa cum laude".
- 2013 DSc. (Research Professor) title, Academy of Sciences of the Czech Republic Thesis entitled: "Multireference Hilbert Space Coupled Cluster Methods"
- 2015 Habilitated as Docent of Physical Chemistry, Faculty of Science, Charles University Prague

# Foreign stays:

University of Florida, Gainesville, USA: 3 months, 2000, 1 month, 2004. Humboldt University, Berlin, Germany: 1-2 months per year, 1998–2006. University of Waterloo, Ontario, Canada: 1 month, 2004,2006.

#### Scientific Awards:

Carl-Ramsauer Prize for the Dissertation, Berlin, 1997.Josef Hlávka Award for Junior Scientists, Prague, 1999.Award of the Czech Learned Society for Junior Scientists, Prague, 2001.Otto Wichterle Award for Junior Scientists, Prague, 2003.

#### Memberships and conference organizations:

Member of the Editorial Board of the Collection of Czechoslovak Chemical Communications, 2001-2011. Member of the Scientific Council of the J. Heyrovský Institute, 2004-2006.

Member of the American Chemical Society, 2011.

Member of the Board of the J. Heyrovský Institute, 2012-2021

Co-organizer of the Central European Symposium of Theoretical Chemistry (CESTC) in Hejnice, 2008. Co-organizer of the Czech-Slovak-Japan Symposium on Theoretical Chemistry (JCS) in Liblice, 2011. Co-organizer of the Central European Symposium of Theoretical Chemistry (CESTC) in Znojmo, 2013. Member of the scientific board of the Central European Symposium of Theoretical Chemistry (CESTC) conference series 2015-

Member of the Physical Chemistry Evaluation Panel of the Czech Science Foundation, Praha 2016-2019 Member of the scientific comitee of the Mariapfarr Workshops on Theoretical Chemistry 2017-

Co-organizer of the Central European Symposium of Theoretical Chemistry (CESTC) in Srni, 2018.

Member of the User Council of the Czech e-infrastructure for research and development (e-infra.cz) 2021-

Member of the Gremium of the Czech Academy of Sciences for the scientific degree DSc. (Research Professor) 2021-

# <u>Research Interests:</u>

Development and implementation of accurate quantum chemical methods for strongly correlated systems. Non-adiabatic molecular dynamics of systems undergoing photochemical reactions. Algorithms for quantum chemical calculations on quantum computers.

Pedagogical Activity: Charles University Prague

Exercises to the lecture "Chemical structure", Faculty of Science, W.S. 1998–2012

Lecture "Theoretical and computational chemistry", Faculty of Science, S.S. 2003-2020

Lecture "Numerical and algorithmic methods of quantum chemistry", Faculty of Science, W.S. 2000, 2011, 2017. Lecture "Second quantization, diagrammatic methods, perturbation and CC theories", Faculty of Science, W.S. 2001, 2006, 2007, 2012, 2016, 2021

Lecture "Analytic gradient techniques in quantum chemistry", Faculty of Science, W.S. 2002, 2009, 2015, 2020 Lecture "The symmetric and unitary groups in quantum chemistry", Faculty of Science, W.S. 2003, 2004, 2013, 2019

Lecture "Introduction to density functional and density matrix functional theory", Faculty of Science, W.S. 2005, 2008, 2014, 2018, 2022

Lecture "Quantum computers and algorithms", Faculty of Mathematics and Physics, W.S. 2010,2013,2021.

# Supervised PhD. Students:

Ondřej Demel (2006); Kiran Bhaskaran-Nair (2011); Jan Šmydke (2011); Jiří Brabec (2012); Libor Veis (2012); Marek Pederzoli (2019), Jakub Lang (2019), Andrej Antalík (2021), Jakub Višňák, Wasif Baig Mirza, Richard Habrovský, Jakub Martinka

### <u>Recent Invited Lectures:</u>

World Association of Theoretically Oriented Chemists (WATOC) 2017, Munich, Germany, September 2017 Sanibel Symposium, St. Simons Island, February 2019

 $10\mathrm{th}$  Triennial Congress of the International Society for Theoretical Chemical Physics (ISTCP), Tromso, July 2019

Warsaw Molecular Electronic Structure conference, online (University of Warsaw), September 2020

Torun Astrophysics, theoretical Spectroscopy, and Quantum chemistry, mini-symposium, online (University of Torun), October 2020

Tensor product methods for strongly correlated molecular systems, online (Max Planck Institute of Complex Systems, Dresden) March 2021

57th Symposium on Theoretical Chemistry (STC2021), online (University of Wuerzburg), September 2021

25th International Workshop on Quantum Systems in Chemistry, Physics and Biology (QSCP 2022), Torun, Poland, June 2022

# Scientometric data:

109 peer-reviewed papers, 9 monography chapters, 4100 citations (3400 self-free), h-index 37.

# Awarded Research Grants:

Development of the MR BWCCSD method, Grant Agency of the Czech Republic, 2000–2002

Analytic gradient of the MR BWCCSD method, Grant Agency of the Czech Republic, 2004–2006

MR BWCC method with connected triple excitations, Grant Agency of the Academy of Sciences of the Czech Republic, 2004-2007

Computer-aided implementation of multireference coupled cluster methods, Grant Agency of the Czech Republic, 2007-2010

Efficient methods for ab-initio non-adiabatic molecular dynamics, Grant Agency of the Academy of Sciences of the Czech Republic, 2008-2011

Quantum Chemistry on Quantum Computers, Grant Agency of the Czech Republic, 2008-2012

Explicitly correlated multireference coupled cluster methods, Grant Agency of the Czech Republic, 2011-2015 Ab initio molecular dynamics with non-adiabatic and spin-orbit effects applied to time-dependent fluorescence, Grant Agency of the Czech Republic, 2012-2016

Hilbert-space multireference coupled cluster methods, their parallel implementation, and application to excited states, Czech Ministry of education, 2013-2015.

Local multireference coupled cluster methods based on the pair natural orbital approach, AVČR - DAAD, 2014-2015.

DMRG-based externally corrected coupled cluster methods, Czech Science Foundation, 2016-2018

Relativistic DMRG-based externally corrected coupled cluster methods, Czech Science Foundation, 2018-2020 New coupled cluster methods externally corrected by DMRG: Implementation for new generation of supercomputers and application to transition metal complexes, Czech Ministry of Education, 2017-2020

Time evolution of conjugated systems in excited states by surface hopping nonadiabatic molecular dynamics, (co-PI), Czech Science Foundatuion, 2019-2021

Praha, 15. listopadu 2022