



Research interests in theoretical quantum chemistry, multireference methods, tensor networks, quantum algorithms for chemistry, quantum information theory, computer science

Personal Details

Date of birth: May 16, 1984
Marital st.: married, two children

Education

- 2008–2012 **Ph.D. in physical chemistry**, Charles University in Prague, Faculty of Science
Thesis: "Quantum computing approach to non-relativistic and relativistic molecular energy calculations",
Supervisor: Dr. J. Pittner (J. Heyrovský Institute of Physical Chemistry, AS CR).
- 2010 **RNDr. degree**, Charles University in Prague, Faculty of Science
- 2006–2008 **MSc. in physical chemistry**, Charles University in Prague, Faculty of Science, *summa cum laude*
- 2003–2006 **BSc. in general chemistry**, Charles University in Prague, Faculty of Science, *summa cum laude*

Professional Activities

Employment

2012–present **Researcher, group leader (since 2018)**, J. Heyrovský Institute of Physical Chemistry, AS CR

Research experience

- 2016, 2017 **Visiting researcher**, Group of Prof. A. Aspuru-Guzik, Harvard University, Cambridge USA
(5 months)
- 2014–2015 **Postdoctoral stay**, Group of Prof. Ö. Legeza, Wigner Research Centre for Physics, Hungarian Academy of Sciences, Budapest
- 2014 (Jun - Jul) **Research visit**, Group of Prof. T. Yanai, Institute for Molecular Science, Okazaki, Japan
- 2010 (Dec) **Study visit**, Winter School in Theoretical Chemistry, Finland
- 2010 (Jul) **Study visit**, Sostrup Summer School in Quantum Chemistry, Denmark

Invited Lectures

- UCT& IOCB Theoretical Chemistry Seminars 2025 (Nov), Prague, Czech Republic.
- Computational Molecular Science Seminar, RIKEN R-CCS, Kobe, Japan, 2025 (Jun).
- American Chemical Society Fall meeting 2024 (Aug), Denver, USA.
- 8th JCS Symposium on Theoretical and Computational Chemistry 2024 (Jun), Sapporo, Japan.
- 5th FR – CZ Barrande workshop on Nanotechnologies, Prague, Czech Republic, 2024 (June).
- Sanibel Symposium 2024 (invited hot topic presentation), St. Augustine, USA, 2024 (Feb).
- Algorithmiq company invited seminar, 2023 (Nov).
- Virginia Tech Quantum Summer Workshop, Riva San Vitale, Switzerland, 2023 (Jun).
- 3rd Quantum international Frontiers 2023, Lodz, Poland, 2023 (Jun).
- Sanibel Symposium 2023 (invited hot topic presentation), St. Augustine, USA, 2023 (Feb).

- Chemistry + Materials HPC/AI seminar series, Intel, 2022 (Nov).
- Seminar at CATRIN-RCPTM, Palacký University, Olomouc, Czech Republic, 2022 (Sep).
- WATOC Congress 2020 (organized in 2022), Vancouver, Canada.
- American Physical Society Meeting 2022 (March), Chicago, USA.
- Autumn School on Correlated Electrons, Jülich, Germany, 2021 (Sep).
- Lorentz-CECAM workshop on 'Useful Quantum Computing for Quantum Chemistry', 2021 (Feb).
- Seminar of the Department of Physical and Theor. Chemistry, University of Graz, Austria, 2019 (Oct).
- 7th JCS Symposium on Theoretical and Computational Chemistry 2018, Prague, Czech Republic.
- Aspuru-Guzik group seminar, Harvard University, Cambridge, USA, 2016 (Jun).
- Winter School on Quantum Computing for Quantum Chemistry 2012, Indian Wells, USA.
- 4th JCS Symposium on Theoretical and Computational Chemistry 2011, Liblice, Czech Republic.

Pedagogical activity

- 2025–present **Lectures**, *Introduction to quantum computing in physics*, Charles University in Prague, Faculty of Mathematics and Physics
- 2024–present **Exercises for lectures**, *General Chemistry*, Charles University in Prague, Faculty of Mathematics and Physics
- 2022 (Oct) **Workshop**, *Autumn School of Quantum Chemistry*, J. Heyrovský Institute of Physical Chemistry, AS CR
- 2016–present **Lectures**, *Tensor network methods and DMRG in quantum chemistry*, Charles University in Prague, Faculty of Mathematics and Physics
- 2008–2014 **Exercises for lectures**, *Theoretical and Computational Chemistry*, Charles University in Prague, Faculty of Science
- 2010, 2013 **Exercises for lectures**, *Quantum Computers*, Charles University in Prague, Faculty of Mathematics and Physics

Supervised students

- 3 supervised Ph.D. (J. Brandejs, defended 2022, M. Matoušek, defended 2025, P. Beran), 1 co-supervised Ph.D. (A. Antalík, defended 2021), and 1 MSc. (M. Matoušek, defended 2020) students at Charles University in Prague, Faculty of Mathematics and Physics. 1 MSc. student (P. Begy) at Palacky University in Olomouc.

Awards

- J. Heyrovský Young Scientist fellowship (2017-2022).
- Post-doc fellowship for perspective young scientists provided by the Academy of Sciences CR (2014/2015).
- Prize for the best poster presentation at the conference Molecular Quantum Mechanics 2010, May 24-29, 2010, University of California, Berkeley, USA.

Grant projects

- Ministry of Education of the Czech Republic, Project “Efficient DMRG-Based Methods for Advancing Polaritonic Chemistry in Strongly Correlated Regimes” (2025-2028).
- Grant agency of the Czech Republic, Project “MULTiscale chemical Simulations on noisy Quantum computers (MUSIQ)” (2025-2027).
- Grant agency of the Czech Republic, Project “Accurate and efficient DMRG-based methods for extended molecules” (2023-2025).
- Grant agency of the Czech Republic, Project “On-surface synthesis and characterization of multiradical molecules” (2023-2025), co-PI.
- SPEC project, U.S. Dep. of Energy, Office of Science, Office of Basic En. Sci. (2022-2026), co-PI.
- Grant agency of the Czech Republic, Project “Massively parallel tensor network methods for strongly correlated quantum chemistry” (2018-2020).
- Grant agency of the Charles Univ., Project “Quantum chemistry on quantum computers” (2010-2012).

Publications

- 59 peer-reviewed publications, over 2400 citations, h-index 23