



# Libor Veis

## Curriculum Vitae

*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 status: 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

2003–present **Researcher, group leader**, J. Heyrovský Institute of Physical Chemistry, AS CR.

#### Research experience

- 2017 (Jul - Aug) **Visiting researcher**, Group of Prof. A. Aspuru-Guzik, Harvard University, Cambridge USA.
- 2016 (Sep - Nov) **Visiting researcher**, Group of Prof. A. Aspuru-Guzik, Harvard University, Cambridge USA.
- 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

- 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 Theoretical Chemistry, University of Graz, Austria, 2019 (Oct).
- 7<sup>th</sup> Japan-Czech-Slovak (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.
- 4<sup>th</sup> Japan-Czech-Slovak (JCS) Symposium on Theoretical and Computational Chemistry 2011, Liblice, Czech Republic.

## Pedagogical activity

- 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, P. Beran, M. Matoušek), 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.

## 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

- Grant agency of the Czech Republic, Project "Accurate and efficient DMRG-based methods for extended molecules" (2023-2025).
- SPEC project, U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences (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 University, Project "Quantum chemistry on quantum computers" (2010-2012).

## Publications

- 41 peer-reviewed publications, about 1000 citations, h-index 16