



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

- 2017 **J. Heyrovský Young Scientist position**.
- 2003–present **Researcher**, 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

- Autumn School on Correlated Electrons, Jülich, Germany, 2021 (Sep), virtual.
- Lorentz-CECAM workshop on 'Useful Quantum Computing for Quantum Chemistry', 2021 (Feb), virtual.
- Seminar of the Department of Physical and Theoretical Chemistry, University of Graz, Austria, 2019 (Oct).
- 7th 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.
- 4th Japan-Czech-Slovak (JCS) Symposium on Theoretical and Computational Chemistry 2011, Liblice, Czech Republic.

Pedagogical activity

- 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, P. Beran, M. Matoušek) and 1 MSc. (M. Matoušek, defended 2020) students at Charles University in Prague, Faculty of Mathematics and Physics.

Awards

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

International Collaborations

- Prof. Alán Aspuru-Guzik, University of Toronto, Canada: development of quantum algorithms for chemistry.
- Prof. Örs Legeza, Wigner Research Centre for Physics, Hungary: development of tensor network methods (MPS, TTNS) for application in chemistry.
- Prof. Jens Eisert, Freie Universität Berlin, Germany: fermionic mode transformations for tensor network states.
- Dr. Karol Kowalski, Pacific Northwest National Laboratory, USA: development of massively parallel QC-DMRG method.
- Prof. Katarzyna Pernal, Lodz University of Technology, Poland: development of DMRG-based adiabatic connection approaches.

Grant projects

- Grant agency of the Charles University, Project "Quantum chemistry on quantum computers" (2010-2012).
- Grant agency of the Czech Republic, Project "Massively parallel tensor network methods for strongly correlated quantum chemistry" (2018-2020).

Publications

- 35 peer-reviewed publications, 2 submitted, over 570 citations, h-index 13