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Education

Ph.D.	University of Chemistry and Technology, Prague , Chemistry	Prague, Czech Republic
	Dissertation: <i>Computational Strategies for Nonadiabatic Molecular Dynamics</i> Supervisor: Prof. Petr Slavíček	2022 – 2026
M.Sc.	University of Chemistry and Technology, Prague , Physical Chemistry	Prague, Czech Republic
	Thesis: <i>Simulation and Data Analysis of Emission Lab Round Robin Tests</i> Supervisor: Dr. Pavel Kříž	2020 – 2022
B.Sc.	University of Chemistry and Technology, Prague , Chemical Engineering	Prague, Czech Republic
	Thesis: <i>Analysis of the Data from the Electron Microscope using Stochastic Model</i> Supervisor: Dr. Markéta Zikmundová	2017 – 2020

Experience

University of Chemistry and Technology, Prague , Research/Teaching Position	Prague, Czech Republic
- Performed nonadiabatic molecular dynamics using ABIN, Bagel, Molpro and ORCA. - Implemented custom software for quantum dynamics and electronic structure methods. - Taught undergraduate mathematics courses.	2022 – present 4 years
Christian-Albrechts University of Kiel , Research Internship	Kiel, Germany
- Implemented spin-diabatic surface hopping for spin-orbit transitions in Newton-X. - Performed CP2K solid-state pyrazine simulations under Prof. Anna Hehn. - Collaborated within the Group of Theoretical Spectroscopy and Heterogeneous Catalysis.	June 2026 – June 2026 1 month

Publications

Wavepacket Dynamics and Quantum Scattering in Spin-Orbit Induced Excitation	2026
T. Jíra, Å. Larson, L. Aissaoui, M. Buchowiecki 10.1103/mgff-cjs8 (Physical Review A)	
Critical Assessment of Curvature-Driven Surface Hopping Algorithms	2025
T. Jíra, J. Janoš, P. Slavíček 10.1021/acs.jctc.5c01176 (Journal of Chemical Theory and Computation)	
Sensitivity Analysis in <i>cis</i>-Stilbene Photodynamics	2024
T. Jíra, J. Janoš, P. Slavíček 10.1021/acs.jctc.4c01008 (Journal of Chemical Theory and Computation)	

Technical Skills

Programming Languages: C++, C, Zig, Python, Julia, Rust

Scientific Software: ORCA, Molpro, Gaussian, ABIN, Newton-X, CP2K, Libint2, LibXC, FFTW3, OpenBLAS

Systems & Environments: Arch Linux, HPC Clusters, LaTeX, Neovim

Languages: Czech (Native), English (Fluent)

Projects

Zinq

Open-source software for quantum dynamics and electronic structure methods.