Jakub Martinka

Last update: December 23, 2025

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I am a PhD student interested in using machine learning to accelerate molecular simulations. I have broad experience with using both quantum chemistry and machine learning approaches. Python is my primary language, as I contribute to the open-source MLatom, but I contribute to Newton-X using C++.

Education

Ph.D. in **Modeling of chemical nanostructures and biostructures** 10/2022 – present
Thesis: Excited state molecular dynamics with non-adiabatic and spin-orbit effects assisted by machine learning
Faculty of Science, Charles University

MSc. in **Physical chemistry** *summa cum laude* 10/2020 – 9/2022
Thesis: Non-adiabatic molecular dynamics of photochemical processes accelerated by machine learning
Faculty of Science, Charles University

BSc. in **Biochemistry** 10/2017 – 9/2020
Thesis: Molecular modeling of the interaction between cytochrome P450s and their substrates/products
Faculty of Science, Charles University

Experience

Charles University, Faculty of Science, Department of Physical Chemistry 2024-5

– Teaching Quantum Chemistry course (covering DFT, HF, and post-HF methods, semiempirical, and machine learning approaches)). *Python, Psi4, PySCF, Gaussian, MLatom.*

J. Heyrovsky Institute of Physical Chemistry, CAS CR 12/2018 – present

– Worked at the department of Theoretical Chemistry. Contributed to Newton-X (C++), MLatom (Python). Experience with quantum chemistry packages: *Turbomole, Molpro, Molcas, Columbus, BAGEL, Molden.*

UniCredit Bank Czech Republic and Slovakia, a.s. 9/2020 – present

– Created, edited and maintained intranet pages. *PHP, JavaScript, HTML, CSS, SharePoint*

Summer schools, Workshops & Visits

Molecular Excited States Workshop 9 – 13/6/2025

– Got invited to workshop devoted to the theoretical modeling of the excited states of chemical molecules. My role is to present practical tutorials for machine learning applications in computational chemistry (Toruń, Poland).

Research visit (Xiamen University, China) 21/10 - 10/11/2024

– Completed a two-week stay with prof. Dral's research group, focusing on the application of ML in non-adiabatic molecular dynamics, including the implementation of the Fewest Switches Surface Hopping method in MLatom (Python).

Machine Learning for Chemistry Summer School 9/9 - 13/9/2024

– Attended a summer school organized by KIT covering: Molecular descriptors and ML based molecular property prediction, GNNs, MLPs, Molecular synthesis prediction, Self-driving labs. (Karlsruhe, Germany)

Research visit (Aix-Marseille Université, France) 22/1 - 27/1/2024

– Participated in a week-long stay with prof. Barbatti's research group, focusing on the application of ML techniques in non-adiabatic molecular dynamics - learning and sign correction of nonadiabatic couplings (Python).

Modern Wavefunction Based Methods in Electronic Structure Theory 27/8 - 2/9/2023

– Attended a summer school organized by Max-Planck-Institut für Kohlenforschung, focusing on the theory/implementation of quantum chemistry methods. (Pisa, Italy)

Autumn School of Quantum Chemistry 3 – 7/10/2020
– Participated in hands-on sessions and implemented quantum chemical methods - Hartree-Fock, Configuration Interaction, Møller–Plesset perturbation theory on top of Psi4 (in Python). (Prague, Czechia)

Swiss Equivariant Learning Workshop 11 – 14/7/2022
– Attended a summer school organized by EPFL covering: equivariant machine learning. (Lausanne, Switzerland)

Excited States and Nonadiabatic Dynamics CyberTraining Workshop 14 – 26/6/2021
– Completed a remote workshop orginised by State University of New York at Buffalo focusing on non-adiabatic molecular dynamics methods, concluding with a small project and its presentation. (remote due to COVID-19)

Conferences

3rd International Symposium on ML in QCh (Knoxville, TN USA) 5 – 7/10/2025
20th CESTC ACS best poster award (High Tatras, Slovakia) 8 – 11/9/2025
13th Triennial Congress of the WATOC (Oslo, Norway) 22 – 27/6/2025
11th Triennial Congress of the ISTCP (Qingdao, China) 13 – 18/10/2024
WTC Mariapfarr - Machine Learning for Chemistry (Bad Hofgastein, Austria) 27/2 – 1/3/2024
2nd International Symposium on ML in QCh (Uppsala, Sweden) 29/11 – 1/12/2023
17th International Congress of Quantum Chemistry (Bratislava, Slovakia) 26/6 – 1/7/2023
ICQC Satellite meeting on Strong Correlation in Molecules (Znojmo, Czechia) 20 – 23/6/2023

Talks & Popularization

Academix (essay on the Quantum Revolution) 2025
ChemQuest (evaluation of high-school student's project) 2024–5
Open science (leading a research intership for 8 high-school students) 2024–5
AI in context (talk covering applications of ML in Chemistry) 26/10/2023
Science fairs (presentation of group/department research) 2023–5
Ask a scientist (project focused on answering nonscientific questions) since 5/2023
Student conferences at J. H. Inst. (best talk awards) 2023–5
FameLab – Presentation & Masterclass training 30/9/2022 & 10 – 11/9/2022
Falling Walls Lab – Presentation 13/9/2022

Publications

[1] Martinka J., Martyka M., Pittner J. and Dral P. O., "Flexible Framework for Surface Hopping: From Hybrid Schemes for Machine Learning to Benchmarkable Nonadiabatic Dynamics" *submitted to JCTC* (2025).

[2] Martinka J., Zhang L., Hou Y.-F., Martyka M., Pittner J., Barbatti M. and Dral P. O., "A Descriptor Is All You Need: Accurate Machine Learning of Nonadiabatic Coupling Vectors", *Journal of Physical Chemistry Letters*, **16**, 11732–11744 (2025).

[3] Martinka J., Pederzoli M., Barbatti M., Dral P. O. and Pittner J., "A Simple Approach to Rotationally Invariant Machine Learning of a Vector Quantity", *Journal of Chemical Physics*, **161**, 174104 (2024).

Grants & Skills & Interests

Grants: GAUK 2024 (project 6224), POINT 2024, GAČR (project 23-06364S), AMULET project
Language: English **C1** German **A2** Japanese **A0** Czech (Native)
Computer: Python C/C++ UNIX/bash/vim HTML/CSS git/GitHub LaTeX
Interests: Science popularization, Programming, FOSS, Chess, Rock climbing, Football