Jakub Martinka

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🌐 Personal web page

Last updat: September 6, 2024

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
Charles University, Faculty of Science

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

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

EXPERIENCE

Theoretical and computer chemistry course   2/2024 – present
– Teaching hands-on practicals.   *Python, Gaussian, Newton-X*

UniCredit Bank Czech Republic and Slovakia, a.s.   9/2020 – present
– Created and edited intranet pages.   *HTML, CSS, SharePoint*

Československá obchodní banka   7/2022 – 11/2022
– Worked with content of internet banking and edited JavaScript of PDF forms.   *JavaScript, SharePoint*

J. Heyrovsky Institute of Physical Chemistry, CAS CR   12/2018 – present
– Worked at the department of Theoretical Chemistry.   *Turbomole, Molpro, Newton-X, MLatom*

Private lessons, Top Learning s.r.o.   9/2015 – present
– Tutored in Math, Physics, and Chemistry.

Charles University, Faculty of Science, Department of Biochemistry   11/2020 – 5/2021
– Created 3D models of organelles and proteins for a new textbook.   *Blender, VMD*

SUMMER SCHOOLS & WORKSHOPS

Research visit   22/1 - 27/1/2024
– A week-long stay with Mario Barbatti's research group, focusing on the application of machine learning techniques in nonadiabatic molecular dynamics. (Aix-Marseille Université, France)

Modern Wavefunction Based Methods in Electronic Structure Theory   27/8 - 2/9/2023
– Attended a summer school organized by Max-Planck-Institut für Kohlenforschung. (University of Pisa, Italy)

Autumn School of Quantum Chemistry   3 – 7/10/2020
– Participated in hands-on sessions and implemented quantum chemical methods. (HF, CI, MP2, ML) in Python (Czech Republic)

Swiss Equivariant Learning Workshop   11 – 14/7/2022
– Attended presentations and hands-on sessions on various machine learning techniques. (EPFL, Lausanne, Switzerland)

Science Popularization Workshop 2022
– Participated in a workshop on the popularization of science organized by the J. Heyrovsky Institute of Physical Chemistry with communication experts from the Czech Academy of Sciences. (Czech Republic)

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

CONFERENCES & PRESENTATIONS

WTC Mariapfarr - Machine Learning for Chemistry 27/2 - 1/3/2024
– Attended lectures and presented a poster. (Graz University of Technology, Austria)

The International Symposium on Machine Learning in Quantum Chemistry 29/11 - 1/12/2023
– Attended lectures and presented a poster. (Uppsala University, Sweden)

17th International Congress of Quantum Chemistry 26/6 - 1/7/2023
– Attended lectures and presented a poster. (Bratislava, Slovakia)

ICQC Satellite meeting on Strong Correlation in Molecules 20 - 23/6/2023
– Attended lectures and presented a poster. (Znojmo, Czech Republic)

POPULARIZATION

ChemQuest 20/4/2024
– I evaluated the participants of the ChemQuest competition as a member of the evaluation committee.

Open science 2024
– Initiated an internship opportunity for high school students within the Open science project.

AI in context 26/10/2023
– Delivered a popularization talk discussing the utilization of machine learning techniques in quantum chemistry.

Science fair 8 - 10/6/2023
– Presented the ongoing science at the J. Heyrovsky Institute of Physical Chemistry during the Science fair event.

Ask a scientist since 5/2023
– A Czech project whose purpose is to scientifically answer any questions. Actively engaged in the project, conducting reviews, and writing answers.

Student conference at J. Heyrovsky Institute of Physical Chemistry 24/5/2023
– Presented my PhD research focusing on machine learning in nonadiabatic molecular dynamics.

FameLab – **Presentation** & **Masterclass training** 30/9/2022 & 10 – 11/9/2022
– Chosen among 11 finalists for the national round, participated in presentation training. Topic: Quantum Chemistry in the Age of Machine Learning.

Falling Walls Lab – **Presentation** 13/9/2022
– Chosen among 14 finalists for the national round. Topic: Breaking the Wall of Excited States Dynamics.

SKILLS & INTERESTS

Grants: GAUK 2024 (project 6224)

Language: English **C1**   German **A2**

Computer: C/C++   Python   bash/perl   HTML/CSS   MATLAB   LaTeX   git/GitHub

Interests: Popularization of science, History of physics, Travelling, Chess, Rock climbing, Football