Eugen Hruška, Ph.D.

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Employment/Research

2023 – · · · · **Academic Assistant (tenure track), Faculty of Pharmacy, Charles University, Czech Republic**
Quantitative prediction of drug metabolism with high-throughput simulation and explainable machine learning.

2020 – 2022 **Postdoctoral Fellow, Emory University, USA**
High-throughput simulation of explicit solvation at DFT accuracy and explainable machine learning of chemical properties.

2014 – 2020 **Graduate Research Assistant, Rice University, USA**
Determined optimal adaptive sampling strategies for folding proteins and the upper limit for speed up with adaptive sampling. Developed a scalable and open-source adaptive sampling platform enabling deep learning. Showed adaptive seeding reaches accurate protein folding and protein dynamics.

2012 **Bachelor student, University of Regensburg, Germany**
Localized interaction interface between proteins central to polycystic kidney disease.

Talks

2024 **Exploration-exploitation tradeoff for protein conformations and dynamics**, IMPACT CIIRC CTU

2023 **Boltzmann distributions from explicit solvation to protein dynamics**, UCT&IOCB Theoretical Chemistry

Bridging the explicit solvation experiment-calculation divide with machine learning and high-throughput simulation, EuChemS CompChem

Larger datasets of ground truth chemistry explanations, @XAI_Research

2022 **Ground truth explainabilities for explainable artificial intelligence**, ACS Fall

AutoSolvate: Open source high-throughput generation of explicitly solvated systems and microsolvated clusters, ACS Fall

2021 **Benchmarking the accuracy of free energy landscapes generated by adaptive sampling strategies**, CECAM, Mixed-gen Session 6: Activated Events

Reducing the error of redox potential calculations in implicit and explicit solvents with machine learning, ACS Fall

Bookchapter

2022 Quantum Chemistry in the Age of Machine Learning, 1st Edition, Elsevier, Chapter 6: Machine learning: An overview, **Eugen Hruska**, Fang Liu, Editor: Pavlo Dral, ISBN: 9780323900492

Awards

2012 **Student award, German Physical Society**

High School

2009 **Gold medal, International Physics Olympiad**, top high school physics competition, **top 50 in world**

2011 **Gold medal and Best Experiment, World Physics Olympiad**

2007-2008 **Gold medal, International Junior Science Olympiad**, top science competition aged 15 and under

2010 **Bronze medal, International Biology Olympiad**, top high school biology competition

2009 **Bronze medal, International Young Physicists' Tournament**

Research grants

2024 Charles University starting grant PRIMUS24/MED/004 "Quantitative prediction of drug metabolism", awarded, PI

Computational grants

2024 IT4I, OPEN-30-9, Karolina 778 NH, awarded, PI

2023 IT4I, OPEN-27-38, Karolina 3500 NH, awarded, PI

2021 XSEDE, TG-CHE200099, Bridges2 GPU 9888 SUs, awarded, Co-PI

2020 Summit, CHM179, 13000 NH, awarded, PI

2019 Summit, BIP191, 25000 NH, awarded

Education

2014 – 2020 **Ph.D., Physics, Rice University, USA**
Thesis title: *Adaptive sampling of Conformational Dynamics*
Advisor: *Cecilia Clementi*

2011 – 2014 **Bachelor, Biochemistry, University of Regensburg, Germany**

2011 – 2012 **Bachelor, Technical Physics, Ilmenau University of Technology, Germany**
Thesis title: *NMR-spectroscopic Analysis of Interaction between Polycystin-2 and mDia1* Advisor: *Hans R. Kalbitzer*

Teaching

2023 – · · · · **Applied Statistics, Applied Computer Technology, Physical Chemistry, Mathematics, Biophysics, Introduction to python for pharmacists, Machine learning for pharmaceutical science**, Charles University

2021 **CHEM531** 1 lecture, Emory University

2020 **Certificate in Teaching and Learning**, Rice University

2015 – 2016 **PHYS 101, 102**, Teaching Assistant, Rice University

Other

Coding Python: pytorch (machine learning, GPUs), sklearn (machine learning), pyemma (markov state models), openmm (molecular dynamics), TeraChem (DFT on GPUs), bash, LaTeX