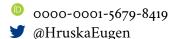
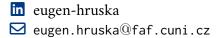
Eugen Hruška, Ph.D.







Employment/Research

Academic Assistant (tenure track), Faculty of Pharmacy, Charles University, Czech Republic

Quantitative prediction of drug metabolism with high-throughput simulation and explainable machine learning.

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.

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

Talks

- Exploration-exploitation tradeoff for protein conformations and dynamics, IMPACT CIIRC CTU
- 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
- Ground truth explainabilities for explainable artificial intelligence, ACS Fall
 - AutoSolvate: Open source high-throughput generation of explicitly solvated systems and microsolvated clusters, ACS Fall
- 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

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

- Gold medal, International Physics Olympiad, top high school physics competition, top 50 in world
- 2011 Gold medal and Best Experiment, World Physics Olympiad
- Gold medal, International Junior Science Olympiad, top science competition aged 15 and under
 - Bronze medal, International Biology Olympiad, top high school biology competition
 - 2009 Ronze medal, International Young Physicists' Tournament

Research grants

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

Computational grants

- IT4I, OPEN-30-9, Karolina 778 NH, awarded, PI
- 2023 TT4I, OPEN-27-38, Karolina 3500 NH, awarded, PI
- 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 Rachelor, Biochemistry, University of Regensburg, Germany

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, Ma-
	chine 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, LTEX