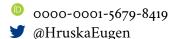
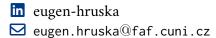
Eugen Hruška, Ph.D.







Research

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

High-throughput simulation and explainable machine learning of drug-protein interactions.

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.

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

Talks

- Boltzmann distributions from explicit solvation to protein dynamics, UCT&IOCB Theoretical Chemistry seminars
 - 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
 - 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
- Deep learning of molecular dynamics representations, Emory Machine Learning in Chemistry Journal Club

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
 - 2010 Ronze medal, International Biology Olympiad, top high school biology competition
 - 2009 Ronze medal, International Young Physicists' Tournament

Research grants

- PRIMUS24/MED/004 proposal "Quantitative prediction of drug metabolism", submitted, PI
- NSF proposal "Machine-learning & Intelligence Driven Adaptive Simulations", submitted, SI

Computational grants

- 2023 TT4I, OPEN-27-38, Karolina CPU 1000 NH, Karolina GPU 2500 NH, accepted, PI
- XSEDE, TG-CHE200099, Bridges2 GPU 9888 SUs, accepted, Co-PI
- Summit, CHM179, 13000 NH, accepted, PI
- 2019 Summit, BIP191, 25000 NH, accepted

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

Education (continued)

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

Applied Statistics, Applied Computer Technology, Physical Chemistry, Mathematics, Biophysics, Python, 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

Service

Coach for U.S. Physics Team

preparing top 20 US high school students representing USA in high school level international physics competition

■ Taste of Science organizing scientific outreach events for the general public

Mentor

preparing promising students for high school international science competitions

Other

Coding

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