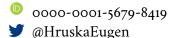
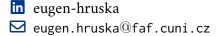
Eugen Hruška, Ph.D.







Research

2023 - · · · Academic Assistant (tenure track), Faculty of Pharmacy, Charles University, Czechia

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

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.

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**

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, Charles University

2021 CHEM531, sole instructor 1 lecture, Emory University

2020 Certificate in Teaching and Learning, Rice University

Teaching Assistant, Rice University
PHYS 101, 102, supervised experimental lab and evaluated students' progress.

Publications

- 1 Chen, X., Li, P., **Hruska**, E., & Liu, F. (2023). Δ -machine learning for quantum chemistry prediction of solution-phase molecular properties at the ground and excited states. *Physical Chemistry Chemical Physics*.
- Hruska, E., Gale, A., Huang, X., & Liu, F. (2022). AutoSolvate: A Toolkit for Automating Quantum Chemistry Design and Discovery of Solvated Molecules. *J. Chem. Phys.*, 156(12). https://doi.org/10.1063/5.0084833
- Hruska, E., Gale, A., & Liu, F. (2022). Bridging the experiment-calculation divide: Machine learning corrections to redox potential calculations in implicit and explicit solvent models. *J. Chem. Theory Comput.* & https://doi.org/10.1021/acs.jctc.1c01040
- **4 Hruska**, E., Zhao, L., & Liu, F. (2022). Ground truth explanation dataset for chemical property prediction on molecular graphs. *Preprint*. **⋄** https://doi.org/10.26434/chemrxiv-2022-96slg-v2
- Gale, A., **Hruska**, E., & Liu, F. (2021). Quantum chemistry for molecules at extreme pressure on graphical processing units: Implementation of extreme-pressure polarizable continuum model. *J. Chem. Phys*, 154, 244103. https://doi.org/10.1063/5.0056480
- **Hruska**, E. (2020). *Adaptive sampling of conformational dynamics* (Doctoral dissertation). Rice University. **6** https://scholarship.rice.edu/handle/1911/108744
- 7 **Hruska**, E., Balasubramanian, V., Lee, H., Jha, S., & Clementi, C. (2020). Extensible and scalable adaptive sampling on supercomputers. *J. Chem. Theory Comput.*§ https://doi.org/10.1021/acs.jctc.0c00991
- 8 **Hruska**, E., Abella, J. R., Nüske, F., Kavraki, L. E., & Clementi, C. (2018). Quantitative comparison of adaptive sampling methods for protein dynamics. *J. Chem. Phys.*, 149(24), 244119. https://doi.org/10.1063/1.5053582
- 9 Balasubramanian, V., Bethune, I., Shkurti, A., Breitmoser, E., **Hruska**, **E.**, Clementi, C., Laughton, C., & Jha, S. (2016). Extasy: Scalable and flexible coupling of md simulations and advanced sampling techniques, 361–370.
 - https://doi.org/10.1109/eScience.2016.7870921

Talks

- 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
- Deep learning of molecular dynamics representations, Emory Machine Learning in Chemistry Journal Club

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

Research grants/proposals

XSEDE Proposal, 9,888 GPU Bridges-2 SUs, accepted, Co-PI

NSF proposal "Machine-learning & Intelligence Driven Adaptive Simulations", submitted, SI

Summit DD Project CHM179, 13000 nodehours, accepted, PI

2019 Summit DD Project BIP191, 25000 nodehours, accepted

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

Awards

2012 Student award, German Physical Society

Scholarship, German Academic Scholarship Foundation, most prestigious scholarship in Germany

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

2007-2008 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

Other

Coding

Python (5+ years): pytorch (machine learning, GPUs), sklearn (machine learning), pyemma (markov state models), openmm (molecular dynamics), radical cybertools (HPC), TeraChem (DFT on GPU), bash, ŁTEX