





Eugen Hruška, Ph.D.

 Hruska-Lab.github.io
 Charles University








 0000-0001-5679-8419
 @HruskaEugen

 eugen-hruska
 eugen.hruska@faf.cuni.cz


Research

- 2023 –  **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.
- 2012  **Bachelor student, University of Regensburg, Germany**
Localized interaction interface between proteins central to polycystic kidney disease.

Talks

- 2023  **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
- 2020  **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





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/proposals

- 2021  XSEDE Proposal, 9,888 GPU Bridges-2 SUs, accepted, Co-PI
- 2020  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

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, 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, \LaTeX