Eugen Hruška, Ph.D.

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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 **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**

2009 **Scholarship, German Academic Scholarship Foundation**, most prestigious scholarship in Germany

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, Charles University**

2021 **CHEM531, sole instructor 1 lecture, Emory University**

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

Teaching (continued)

2015 – 2016 **Teaching Assistant, Rice University**
PHYS 101, 102, supervised experimental lab and evaluated students' progress.

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