# 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.

## 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

## Publications

1 Chen, X., Li, P., **Hruska**, **E.**, & Liu, F. (2023). $\Delta$-machine learning for quantum chemistry prediction of solution-phase molecular properties at the ground and excited states. *Phys. Chem. Chem. Phys.*, *25*(19), 13417–13428. https://doi.org/10.1039/D3CP00506B

2 **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

3 **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-2022-96slq-v2

5 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

6 **Hruska**, **E.** (2020). *Adaptive sampling of conformational dynamics* [Doctoral dissertation, Rice University]. 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

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

## Research grants

2023 PRIMUS24/MED/004 proposal "Quantitative prediction of drug metabolism", submitted, PI

2020 NSF proposal "Machine-learning & Intelligence Driven Adaptive Simulations", submitted, SI

## Computational grants

2023 IT4I, OPEN-27-38, Karolina CPU 1000 NH, Karolina GPU 2500 NH, accepted, PI

2021 XSEDE, TG-CHE200099, Bridges2 GPU 9888 SUs, accepted, Co-PI

2020 Summit, CHM179, 13000 NH, accepted, PI

2019 Summit, BIP191, 25000 NH, 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**

### 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**

## Other

Coding

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