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). Δ-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
- **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

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

Talks (continued)

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**

Awards (continued)

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