Eugen Hruška, Ph.D.

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Employment/Research

2023 – · · · · **Academic Assistant (tenure track), Faculty of Pharmacy, Charles University, Czech Republic**
Quantitative prediction of drug metabolism with high-throughput simulation and explainable machine learning.

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, Introduction to python for pharmacists, Machine learning for pharmaceutical science**, 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

Talks (continued)

- **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

2024 - PRIMUS24/MED/004 startup grant "Quantitative prediction of drug metabolism", awarded, PI

Computational grants

2024 - IT4I, OPEN-30-9, Karolina 778 NH, awarded, PI

2023 - IT4I, OPEN-27-38, Karolina 3500 NH, awarded, PI

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

2020 - Summit, CHM179, 13000 NH, awarded, PI

2019 - Summit, BIP191, 25000 NH, awarded

Public Outreach

- **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