# Eugen Hruška, Ph.D.

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## Employment/Research

2023 – · · · · **Assistant professor, Faculty of Pharmacy, Charles University, Czech Republic**
Quantitative prediction of drug interactions 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 software enabling deep learning.

## Education

2014 – 2020 **Ph.D., Physics, Rice University, USA**
Thesis: *Adaptive sampling of Conformational Dynamics*

2011 – 2014 **Bachelor, Biochemistry, University of Regensburg, Germany**

2011 – 2012 **Bachelor, Tech. Physics, Ilmenau University of Technology, Germany**
Thesis: *NMR-spectroscopic Analysis of Interaction between Polycystin-2 and mDia1*

## Teaching

2023 – · · · · **Applied Statistics, Applied Computer Technology, Physical Chemistry, Mathematics, Introduction to python for pharmacists, Machine learning for pharmaceutical science, Atomistic Simulation**, Charles University

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

2015 – 2016 **PHYS 101, 102**, Teaching Assistant, Rice University

# Publications

h-index: 6 (OpenAlex), citations excluding self: 142 (Scopus)

1. Chen, X., Sun, Y., **Hruska**, **E.**, Dixit, V., Yang, J., He, Y., Wang, Y., & Liu, F. (2025). Detecting thermodynamic phase transition via explainable machine learning of photoemission spectroscopy. *Newton*, *1*(3). https://doi.org/10.1016/j.newton.2025.100066

2. Grenda, P., Ogos, M., & **Hruska**, **E.** (2025). Automated structural refinement of docked complexes in cytochrome p450 using molecular dynamics. *Preprint*. https://doi.org/10.26434/chemrxiv-2025-mvv4k-v3

3. Suwała, D., & **Hruska**, **E.** (2024). The wins and failures of current docking methods tested on the flexible active site of cytochromes p450. *Preprint*. https://doi.org/10.26434/chemrxiv-2024-05299-v2

4. 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

5. **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

6. **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

7. **Hruska**, **E.**, & Liu, F. (2022). *Quantum chemistry in the age of machine learning, chapter 6: Machine learning: An overview*. Elsevier.

8. **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

9. 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

10. **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

11. **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

12. 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

2025 **Docking predictivity determinants for the P450 flexible active site**, International Conference on Cytochrome P450

2024 **Exploration-exploitation tradeoff for protein conformations and dynamics**, IMPACT CIIRC CTU

2023 **Boltzmann distributions from explicit solvation to protein dynamics**, UCT&IOCB Theoretical Chemistry

**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

## Research grants

2024 - 2027 Charles University starting grant PRIMUS24/MED/004 "Quantitative prediction of drug metabolism", PI

2024 - 2029 Charles University grant, UNCE/24/MED/008, "ADVanced models, Experimental apporaches and bioinformatics in pharmacological ReSEsearch (ADVERSE)", member of team

## Computational grants

2023 – · · · · IT4I, OPEN-30-9, FTA-23-21, OPEN-27-38, Karolina, PI

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

2019, 2020 Summit, BIP191 (25000 NH), CHM179 (13000 NH, PI)

## Awards

### High School

2009 **Gold medal, International Physics Olympiad**

2007-2008 **Gold medal, International Junior Science Olympiad**