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 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

fractional h-index 3 (OpenAlex), h-index 6 (WoS), citations 107 (WoS)

1. Chen, X., Sun, Y., **Hruska**, **E.**, Dixit, V., Yang, J., He, Y., Wang, Y., & Liu, F. (2024). Explainable machine learning identification of superconductivity from single-particle spectral functions. *Preprint*. https://arxiv.org/abs/2406.04445
2. 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
3. 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
4. **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
5. **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
6. **Hruska**, **E.**, & Liu, F. (2022). *Quantum chemistry in the age of machine learning, chapter 6: Machine learning: An overview*. Elsevier.
7. **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
8. 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
9. **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
10. **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
11. 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

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

Talks (continued)

- **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

2012

- **Student award, German Physical Society**

2011

- **Gold medal and Best Experiment, World Physics Olympiad**

2010

- **Bronze medal, International Biology Olympiad**

2009

- **Gold medal, International Physics Olympiad**

2009

- **Bronze medal, International Young Physicists' Tournament**

2007-2008

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

Other

Coding

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