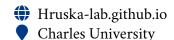
Eugen Hruška, Ph.D.



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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.

Thesis: NMR-spectroscopic Analysis of Interaction between Polycystin-2 and mDia1

Education

Ph.D., Physics, Rice University, USA
Thesis: Adaptive sampling of Conformational Dynamics

Bachelor, Biochemistry, University of Regensburg, Germany

Bachelor, Tech. Physics, Ilmenau University of Technology, Germany

Teaching

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
- 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
- Suwała, D., & **Hruska**, **E.** (2024). The wins and failures of current docking methods tested on the flexible active site of cytochromes p450. *Preprint*.

 Phttps://doi.org/10.26434/chemrxiv-2024-05299-v2
- 4 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
- **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
- **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
- 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
- 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
- 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.

Talks

- Docking predictivity determinants for the P450 flexible active site, International Conference on Cytochrome P450
- Exploration-exploitation tradeoff for protein conformations and dynamics, IMPACT CIIRC CTU
- 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
- Ground truth explainabilities for explainable artificial intelligence, ACS Fall
 - AutoSolvate: Open source high-throughput generation of explicitly solvated systems and microsolvated clusters, ACS Fall
- 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