

Eugen Hruška, Ph.D.

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Researcher ID: AAY-5878-2020

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). 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>
- 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 approaches 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**