





# Eugen Hruška, Ph.D.

 Hruska-Lab.github.io  
 Charles University




 0000-0001-5679-8419  
 @HruskaEugen

 eugen-hruska  
 eugen.hruska@faf.cuni.cz





## Research

- 2023 – ····  **Academic Assistant (tenure track), Faculty of Pharmacy, Charles University, Czechia**  
High-throughput simulation and explainable machine learning of drug-protein interactions.
- 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, Python, 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).  $\Delta$ -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>
- 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., Kaviraki, 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 | <ul style="list-style-type: none"><li>■ Boltzmann distributions from explicit solvation to protein dynamics, UCT&amp;IOCB Theoretical Chemistry seminars</li><li>■ Bridging the explicit solvation experiment-calculation divide with machine learning and high-throughput simulation, EuChemS CompChem</li><li>■ Larger datasets of ground truth chemistry explanations, @XAI_Research</li></ul> |
| 2022 | <ul style="list-style-type: none"><li>■ Ground truth explainabilities for explainable artificial intelligence, ACS Fall</li><li>■ AutoSolvate: Open source high-throughput generation of explicitly solvated systems and microsolvated clusters, ACS Fall</li></ul>   |
| 2021 | <ul style="list-style-type: none"><li>■ Benchmarking the accuracy of free energy landscapes generated by adaptive sampling strategies, CECAM, Mixed-gen Session 6: Activated Events</li><li>■ Reducing the error of redox potential calculations in implicit and explicit solvents with machine learning, ACS Fall</li></ul>  |


## Talks (continued)

---

- 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

---

- 2023  IT4I, OPEN-27-38, Karolina CPU 1000 NH, Karolina GPU 2500 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**
- 2007-2008  **Gold medal, International Junior Science Olympiad**, top science competition aged 15 and under


## Awards (continued)

---

- 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,  $\text{\LaTeX}$