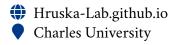
# Eugen Hruška, Ph.D.



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## **Employment/Research**

2023 - · · · ·	Academic Assistant (tenure track), Faculty of Pharmacy, Charles University, Czech Republic Quantitative prediction of drug metabolism with high-throughput simulation and explainable machine learning.
2020 - 2022	<b>Postdoctoral Fellow, Emory University, USA</b> High-throughput simulation of explicit solvation at DFT accuracy and explain- able 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	<b>Bachelor student, University of Regensburg, Germany</b> Localized interaction interface between proteins central to polycystic kidney disease.

#### Education

2014 – 2020	<b>Ph.D., Physics, Rice University, USA</b> Thesis title: <i>Adaptive sampling of Conformational Dynamics</i> Advisor: <i>Cecilia Clementi</i>
2011 – 2014	Bachelor, Biochemistry, University of Regensburg, Germany
2011 - 2012	Bachelor, Technical Physics, Ilmenau University of Technology, Ger-
	many
	Thesis title: NMR-spectroscopic Analysis of Interaction between Polycystin-2 and
	mDia1 Advisor: Hans R. Kalbitzer

#### Teaching

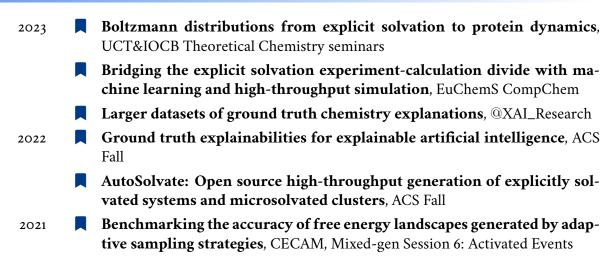
2023 - · · · ·	Applied Statistics, Applied Computer Technology, Physical Chemistry, Mathematics, Biophysics, Introduction to python for pharmacists, Ma- chine learning for pharmaceutical science, Charles University
2021	CHEM531 1 lecture, Emory University
2020	<b>Certificate in Teaching and Learning</b> , Rice University
2015 – 2016	<b>PHYS 101, 102</b> , Teaching Assistant, Rice University

#### **Publications**

- 1 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. Article A
- 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
- **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. I* https://doi.org/10.1021/acs.jctc.1c01040
- 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
- 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.
   https://doi.org/10.1109/eScience.2016.7870921

#### Talks



#### Talks (continued)

- **Reducing the error of redox potential calculations in implicit and explicit solvents with machine learning**, ACS Fall
- 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**

2024	IT4I, OPEN-30-9, Karolina 778 NH, awarded, PI
2023	IT4I, OPEN-27-38, Karolina 3500 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**

		<b>Coach for U.S. Physics Team</b> 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		
		<b>Mentor</b> 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 com-		
		petition, <b>top 50 in world</b>		

### Awards (continued)

2007-2008	Gold medal, International Junior Science Olympiad, top science competi- tion aged 15 and under
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, 些TEX