







# Eugen Hruška, Ph.D.

 HruskaLab.github.io  
 Charles University




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## 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

- 2021  **CHEM531, sole instructor 1 lecture, Emory University**
- 2020  **Certificate in Teaching and Learning, Rice University**
- 2015 – 2016  **Teaching Assistant, Rice University**  
PHYS 101, 102, supervised experimental lab and evaluated students' progress.







## Publications

- 1 **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>

- 2 **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>
- 3 **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>
- 4 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>
- 5 **Hruska, E.** (2020). *Adaptive sampling of conformational dynamics* (Doctoral dissertation). Rice University. <https://scholarship.rice.edu/handle/1911/108744>
- 6 **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>
- 7 **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>
- 8 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

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| 2023 |  <b>Larger datasets of ground truth chemistry explanations</b> , @XAI_Research   |
| 2022 |  <b>Ground truth explainabilities for explainable artificial intelligence</b> , ACS Fall   |
|      |  <b>AutoSolvate: Open source high-throughput generation of explicitly solvated systems and microsolvated clusters</b> , ACS Fall                     |
| 2021 |  <b>Benchmarking the accuracy of free energy landscapes generated by adaptive sampling strategies</b> , CECAM, Mixed-gen Session 6: Activated Events |
|      |  <b>Reducing the error of redox potential calculations in implicit and explicit solvents with machine learning</b> , ACS Fall                        |
| 2020 |  <b>Deep learning of molecular dynamics representations</b> , Emory Machine Learning in Chemistry Journal Club                                       |





## Bookchapter

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| 2022 |  Quantum Chemistry in the Age of Machine Learning, 1st Edition, Elsevier, Chapter 6: Machine learning: An overview, <b>Eugen Hruska</b> , Fang Liu, Editor: Pavlo Dral, ISBN: 9780323900492 |
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## Research grants/proposals

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- 2021     XSEDE Proposal, 9,888 GPU Bridges-2 SUs, accepted, Co-PI
- 2020     NSF proposal "Machine-learning & Intelligence Driven Adaptive Simulations", submitted, SI
-  Summit DD Project CHM179, 13000 nodehours, accepted, PI
- 2019     Summit DD Project BIP191, 25000 nodehours, accepted


## Service

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-  **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

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- 2012     **Student award, German Physical Society**
- 2009     **Scholarship, German Academic Scholarship Foundation**, most prestigious scholarship in Germany

## 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
- 2010     **Bronze medal, International Biology Olympiad**, top high school biology competition
- 2009     **Bronze medal, International Young Physicists' Tournament**

## Other

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- Coding     Python (5+ years): pytorch (deep learning, GPUs), sklearn (machine learning), pymma (markov state models), openmm (molecular dynamics), radical cyber-tools (HPC), TeraChem (DFT on GPU), bash,  $\text{\LaTeX}$