










# Eugen Hruska, Ph.D.

 euhruska.github.io  
 Emory University




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## Research

- 2020 – . . . . .  **Postdoctoral Fellow, Emory University**  
Combining GPU-accelerated DFT and machine learning to investigate drug-solvent interfaces.
- 2014 – 2020  **Graduate Research Assistant, Rice University**  
Determined optimal adaptive sampling strategies for folding proteins and the upper limit for speed up with adaptive sampling. Developed open-source package ExTASY, a scalable and open-source adaptive sampling platform enabling deep learning: [github.com/ClementiGroup/ExTASY](https://github.com/ClementiGroup/ExTASY). Showed adaptive sampling reaches accurate protein folding and protein dynamics.
- 2012  **Bachelor student, University of Regensburg**  
Localized interaction interface between proteins central to polycystic kidney disease with NMR.


## Education

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

## Teaching Experience




- 2015  **Teaching Assistant, Rice University**  
PHYS 101, 102 lab, Supervised experimental lab and evaluated students' progress.
- 2020  **Certificate in Teaching and Learning, Rice University**  
11 credit course.
- 2021  **Guestlecture, CHEM531, Emory University**  
Prepared and taught full lecture.

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

- 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
- 2020  **Deep learning of molecular dynamics representations**, Emory Machine Learning in Chemistry Journal Club

## Bookchapter

- 2022  Quantum Chemistry in the Age of Machine Learning, Chapter 6: Machine learning: An overview, **Eugen Hruska**, Fang Liu, accepted

## Proposals

- 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
- **Tutor**  
for international science competitions, preparing promising students

## 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), pyemma (markov state models), openmm (molecular dynamics), radical cybertools (HPC), bash,  $\LaTeX$