










# Eugen Hruska, Ph.D.

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 Emory University




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## Research

- 2020 – present  **Postdoctoral Fellow, Emory University**  
Combining GPU-accelerated DFT and machine learning to investigate the drug-solvent interface.
- 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.



## 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




## Awards

- 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**




## Awards (continued)

- 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**




## 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



## Education

- 2014 – 2020  **Ph.D., Physics, Rice University**  
Thesis title: *Adaptive sampling of Conformational Dynamics*  
Advisor: *Cecilia Clementi*
- 2012 – 2014  **Bachelor, Biochemistry, University of Regensburg**
- 2012  **Bachelor, 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.

## Service

-  **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

## Service (continued)

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

## Other

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- Languages ■ English - fluent, German - native, Slovak - native
- Coding ■ Python (5+ years): pytorch (deep learning, GPUs), sklearn (machine learning), pyemma (markov state models), openmm (molecular dynamics), radical cyber-tools (HPC), bash,  $\LaTeX$
- News ■ Blue waters Annual Report 2019 [!\[\]\(0551a83d441798e532995956b603f604\_img.jpg\)](#)