







Eugen Hruska, Ph.D.

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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. 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*
- 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.

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)

📖 Tutor

for international science competitions, preparing promising students

Other

Coding



Python (5+ years): pytorch (deep learning, GPUs), sklearn (machine learning), pyemma (markov state models), openmm (molecular dynamics), radical cybertools (HPC), bash, L^AT_EX