Eugen Hruska, Ph.D.

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Research

2020 – · · · · **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. 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

2021 Quantum Chemistry in the Age of Machine Learning, Chapter 6: Machine learning: An overview, **Eugen Hruska**, Fang Liu, submitted

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, rank **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

2020 NSF proposal "Machine-learning & Intelligence Driven Adaptive Simulations", SI, submitted

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)

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

Other

Languages	English - fluent, German - native, Slovak - native
Coding	Python (5+ years): tensorflow, pytorch (deep learning, GPUs), sklearn (machine learning), pyemma (markov state models), openmm (molecular dynamics), radical cybertools (HPC), bash, LaTeX
News	Blue waters Annual Report 2019