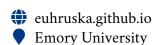
# Eugen Hruska, Ph.D.



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#### Research

2020 - · · · Postdoctoral Fellow, Emory University

Combining GPU-accelerated DFT and machine learning to investigate the drugsolvent interface.

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.

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

2012 – 2014 **Bachelor, Biochemistry, University of Regensburg** 

Bachelor, Physics, Ilmenau University of Technology

Thesis title: NMR-spectroscopic Analysis of Interaction between Polycystin-2 and mDia1 Advisor: Hans R. Kalbitzer

**Talks** 

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

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

# **Bookchapter**

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

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

# **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.

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

Tutor

for international science competitions, preparing promising students

#### **Other**

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, LTEX

News | Blue waters Annual Report 2019 **6** 

## **Awards**

2012 Student award, German Physical Society

**Scholarship, German Academic Scholarship Foundation**, most prestigious scholarship in Germany

## **High School**

Gold medal, International Physics Olympiad, top high school physics competition, rank top 50 in world

# **Awards (continued)**

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	<b>Bronze medal, International Biology Olympiad</b> , top high school biology competition
2009	Bronze medal, International Young Physicists' Tournament

#### **Publications**

- 1 **Hruska**, **E.**, Gale, A., Huang, X., & Liu, F. (2022). Autosolvate: A toolkit for automating quantum chemistry design and discovery of solvated molecules. *submitted*.
- 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.* \$\sigma\$ https://doi.org/10.1021/acs.jctc.1c01040
- 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
- **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
- **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. Ahttps://doi.org/10.1063/1.5053582
- 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