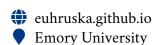
Eugen Hruska, Ph.D.



0000-0001-5679-8419MruskaEugen

in eugen-hruska✓ eugen.hruska@emory.edu

Research

2020 – present

■ Postdoctoral Fellow, Emory University

Investigated the molecule-solvent interface with high-throughput simulation and machine learning

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. Validated 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

Hruska, E., Gale, A., Huang, X., & Liu, F. (2022). Autosolvate: A toolkit for automating quantum chemistry design and discovery of solvated molecules. *submitted*.

https://doi.org/10.26434/chemrxiv-2022-px3r8

- 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
- 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
- **Hruska**, E. (2020). *Adaptive sampling of conformational dynamics* (Doctoral dissertation). Rice University. **6** 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
- 6 **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. https://doi.org/10.1063/1.5053582
- Palasubramanian, 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

- 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, Co-PI
- NSF proposal "Machine-learning & Intelligence Driven Adaptive Simulations", summited, SI
 - Summit DD Project CHM179, 13000 nodehours, accepted, PI
- 2019 Summit DD Project BIP191, 25000 nodehours, accepted

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

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, 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
 - Bronze medal, International Biology Olympiad, top high school biology competition
 - 2009 Ronze medal, International Young Physicists' Tournament

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 cybertools (HPC), bash, ŁTĘX

News | Blue waters Annual Report 2019