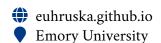
Eugen Hruska, Ph.D.



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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.

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

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 &

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

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	Bronze medal, International Biology Olympiad, top high school biology com-
	petition
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*.

 ### 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
- **4 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
- 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