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.

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*

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

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

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 cybertools (HPC), bash, LaTeX
- News: Blue waters Annual Report 2019

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**

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

2 **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

3 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

5 **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

7 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