Eugen Hruska, Ph.D.

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Research

2020 – · · · · **Postdoctoral Fellow, Emory University**
Investigating the behavior of the molecule-solvent interface in Fang Liu's group.

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.

Publications

1 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

2 **Hruska, E.** (2020). *Adaptive sampling of conformational dynamics* (Doctoral dissertation). Rice University. https://scholarship.rice.edu/handle/1911/108744

3 **Hruska, E.**, Balasubramanian, V., Lee, H., Jha, S., & Clementi, C. (2020). Extensible and scalable adaptive sampling on supercomputers. *Journal of Chemical Theory and Computation*. https://pubs.acs.org/doi/10.1021/acs.jctc.0c00991

4 **Hruska, E.**, Abella, J. R., Nüske, F., Kavraki, L. E., & Clementi, C. (2018). Quantitative comparison of adaptive sampling methods for protein dynamics. *The Journal of Chemical Physics*, *149*(24), 244119. https://doi.org/10.1063/1.5053582

5 Balasubramanian, V., Bethune, I., Shkurti, A., Breitmoser, E., **Hruska, E.**, Clementi, C., Laughton, C., & Jha, S. Extasy: Scalable and flexible coupling of md simulations and advanced sampling techniques. In: *2016 ieee 12th international conference on e-science (e-science)*. IEEE. 2016, 361–370. https://ieeexplore.ieee.org/document/7870921

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, ENFL, oral

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**

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 700 lab, Supervised experimental lab and evaluated students' progress.

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): 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