Eugen Hruska, Ph.D.

euhruska.github.io 0000-0001-5679-8419 eugen-hruska
Emory University @HruskaEugen eugen.hruska@emory.com

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. https://doi.org/10.26434/chemrxiv.14538576.v2

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

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**

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