










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.


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.**, Gale, A., & Liu, F. (2021). Bridging the experiment-calculation divide: Machine learning corrections to redox potential calculations in implicit and explicit solvent models. *ChemRxiv*. <https://doi.org/10.33774/chemrxiv-2021-mthjp>
- 3 **Hruska, E.** (2020). *Adaptive sampling of conformational dynamics* (Doctoral dissertation). Rice University. <https://scholarship.rice.edu/handle/1911/108744>
- 4 **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>
- 5 **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>
- 6 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
- 2020  **Deep learning of molecular dynamics representations**, Emory Machine Learning in Chemistry Journal Club






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.
- 2021  **guestlecture, CHEM531, Emory University**
Prepared and taught interactive 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): 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 