









# Eugen Hruska, Ph.D.

 euhruska.github.io  
 Emory University




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 eugen-hruska

## Research

- 2020 – ····  **Postdoctoral Research Associate, Emory University**  
Investigating the behavior of the molecule-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](https://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, University of Regensburg**  
Thesis title: *NMR-spectroscopic Analysis of Interaction between Polycystin-2 and mDia1* Advisor: *Hans R. Kalbitzer*

## Research Publications






- 1 **Hruska, E.** (2020). *Adaptive sampling of conformational dynamics* (Doctoral dissertation). Rice University. <https://scholarship.rice.edu/handle/1911/108744>
- 2 **Hruska, E.**, Balasubramanian, V., Ossyra, J. R., Jha, S., & Clementi, C. (2019). Extensible and scalable adaptive sampling on supercomputers. *arXiv preprint arXiv:1907.06954*.  
<https://arxiv.org/abs/1907.06954v1>
- 3 **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>
- 4 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>

## Awards

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- 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**




## Teaching Experience

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- 2015     **Teaching Assistant, Rice University**  
PHYS 700 lab, Supervised experimental lab and evaluated students' progress.




## Service

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-  **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

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- 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,  $\text{\LaTeX}$ , ...
- News          Blue waters Annual Report 2019 