Eugen Hruska, Ph.D.

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

Education/Research

2020 – · · · · **Postdoctoral Fellow, Emory University**
Investigated the molecule-solvent interface with high-throughput simulation and machine learning in Fang Liu's group.

2014 – 2020 **Ph.D., Physics, Rice University**
Thesis title: *Adaptive sampling of Conformational Dynamics* Advisor: *Cecilia Clementi*

Publications (selected)

1 **Hruska**, **Eugen**, Ariel Gale, and Fang Liu. "Bridging the Experiment-Calculation Divide: Machine Learning Corrections to Redox Potential Calculations in Implicit and Explicit Solvent Models". In: *J. Chem. Theory Comput.* (2022).

2 **Hruska**, **Eugen** et al. "AutoSolvate : A Toolkit for Automating Quantum Chemistry Design and Discovery of Solvated Molecules". In: *J. Chem. Phys.* (2022).

3 **Hruska**, **Eugen** et al. "Extensible and Scalable Adaptive Sampling on Supercomputers". In: *J. Chem. Theory Comput.* (2020).

4 **Hruska**, **Eugen** et al. "Quantitative comparison of adaptive sampling methods for protein dynamics". In: *J. Chem. Phys.* (2018).

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

Awards

2009: **Gold medal, International Physics Olympiad**, **top 50 in world**, 2011: Gold medal and Best Experiment, World Physics Olympiad, 2007-2008: **Gold medal**, International Junior Science Olympiad, 2012: Student award, German Physical Society, 2009: **Scholarship**, German Academic Scholarship Foundation