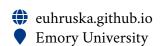
# Eugen Hruska, Ph.D.



0000-0001-5679-8419@HruskaEugen

in eugen-hruska☑ 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)**

- 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).
- **Hruska**, **Eugen** et al. "AutoSolvate : A Toolkit for Automating Quantum Chemistry Design and Discovery of Solvated Molecules". In: *J. Chem. Phys.* (2022).
- **Hruska**, **Eugen** et al. "Extensible and Scalable Adaptive Sampling on Supercomputers". In: *J. Chem. Theory Comput.* (2020).
- **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