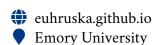
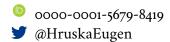
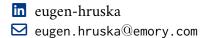
Eugen Hruska, Ph.D.







Research

2020 - · · · ·

Postdoctoral Fellow, Emory University

Investigating the behavior of the molecule-solvent interface in Fang Liu's group.

2014 - 2020

▶ Ph.D., Physics, Rice University

Thesis title: Adaptive sampling of Conformational Dynamics Advisor: Cecilia Clementi

Publications selected

- Gale, Ariel, **Eugen Hruska**, and Fang Liu. "Quantum Chemistry for Molecules at Extreme Pressure on Graphical Processing Units: Implementation of Extreme Pressure Polarizable Continuum Model". In: *J. Chem. Phys* 154 (2021), p. 244103.
- 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: *ChemRxiv* (2021).
- Hruska, Eugen et al. "Extensible and Scalable Adaptive Sampling on Supercomputers". In: *Journal of Chemical Theory and Computation* (2020).
- **Hruska**, **Eugen** et al. "Quantitative comparison of adaptive sampling methods for protein dynamics". In: *The Journal of Chemical Physics* 149.24 (2018), p. 244119.

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**, rank **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