









# Eugen Hruska, Ph.D.

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## 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

- 1 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.
- 2 **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).
- 3 **Hruska, Eugen** et al. "Extensible and Scalable Adaptive Sampling on Supercomputers". In: *Journal of Chemical Theory and Computation* (2020).
- 4 **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