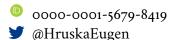
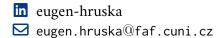
Eugen Hruška, Ph.D.







Education/Research

2023 - · · · Academic Assistant (tenure track), Faculty of Pharmacy, Charles University, Czechia

High-throughput simulation and explainable machine learning of drug-protein interactions.

High-throughput simulation of explicit solvation at DFT accuracy and explainable machine learning of chemical properties.

2014 – 2020 Ph.D., Physics, Rice University, USA

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).
- **Hruska**, **Eugen**, Liang Zhao, and Fang Liu. "Ground truth explanation dataset for chemical property prediction on molecular graphs". In: *Preprint* (2022).
- Hruska, Eugen et al. "AutoSolvate: A Toolkit for Automating Quantum Chemistry Design and Discovery of Solvated Molecules". In: *J. Chem. Phys.* (2022).
- **4 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).

Awards

2009: **Gold medal, International Physics Olympiad**, 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