Eugen Hruška, Ph.D.

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Education/Research

2023 – · · · · **Academic Assistant (tenure track), Faculty of Pharmacy, Charles University, Czech Republic**
Quantitative prediction of drug metabolism with high-throughput simulation and explainable machine learning.

2020 – 2022 **Postdoctoral Fellow, Emory University, USA**
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).

2 **Hruska**, **Eugen**, Liang Zhao, and Fang Liu. "Ground truth explanation dataset for chemical property prediction on molecular graphs". In: *Preprint* (2022).

3 **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).

5 **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