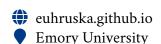
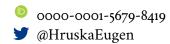
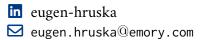
## Eugen Hruska, Ph.D.







## **Publications**

- 1 **Hruska**, **E.**, Gale, A., Huang, X., & Liu, F. (2022). Autosolvate: A toolkit for automating quantum chemistry design and discovery of solvated molecules. *submitted*.
- Hruska, E., Gale, A., & Liu, F. (2022). Bridging the experiment-calculation divide: Machine learning corrections to redox potential calculations in implicit and explicit solvent models. *J. Chem. Theory Comput.* https://doi.org/10.1021/acs.jctc.1c01040
- Gale, A., **Hruska**, E., & Liu, F. (2021). Quantum chemistry for molecules at extreme pressure on graphical processing units: Implementation of extreme-pressure polarizable continuum model. *J. Chem. Phys*, 154, 244103. https://doi.org/10.1063/5.0056480
- 4 **Hruska**, E. (2020). *Adaptive sampling of conformational dynamics* (Doctoral dissertation). Rice University. Https://scholarship.rice.edu/handle/1911/108744
- **Hruska**, E., Balasubramanian, V., Lee, H., Jha, S., & Clementi, C. (2020). Extensible and scalable adaptive sampling on supercomputers. *J. Chem. Theory Comput.*https://doi.org/10.1021/acs.jctc.0c00991
- **Hruska**, E., Abella, J. R., Nüske, F., Kavraki, L. E., & Clementi, C. (2018). Quantitative comparison of adaptive sampling methods for protein dynamics. *J. Chem. Phys.*, 149(24), 244119. https://doi.org/10.1063/1.5053582
- Balasubramanian, V., Bethune, I., Shkurti, A., Breitmoser, E., **Hruska**, **E.**, Clementi, C., Laughton, C., & Jha, S. (2016). Extasy: Scalable and flexible coupling of md simulations and advanced sampling techniques, 361–370.

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