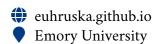
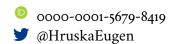
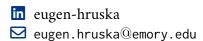
Eugen Hruska, Ph.D.







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- 1 **Hruska**, E., Gale, A., Huang, X., & Liu, F. (2022). Autosolvate: A toolkit for automating quantum chemistry design and discovery of solvated molecules. *submitted*.

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- 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. **6** 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
- 6 **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
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 - ♦ https://doi.org/10.1109/eScience.2016.7870921