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## Publications

- 1 Chen, X., Li, P., **Hruska, E.**, & Liu, F. (2023).  $\Delta$ -machine learning for quantum chemistry prediction of solution-phase molecular properties at the ground and excited states. *Phys. Chem. Chem. Phys.*, 25(19), 13417–13428. <https://doi.org/10.1039/D3CP00506B>
- 2 **Hruska, E.**, Gale, A., Huang, X., & Liu, F. (2022). AutoSolvate : A Toolkit for Automating Quantum Chemistry Design and Discovery of Solvated Molecules. *J. Chem. Phys.*, 156(12). <https://doi.org/10.1063/5.0084833>
- 3 **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>
- 4 **Hruska, E.**, Zhao, L., & Liu, F. (2022). Ground truth explanation dataset for chemical property prediction on molecular graphs. *Preprint*. <https://doi.org/10.26434/chemrxiv-2022-96slq-v2>
- 5 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>
- 6 **Hruska, E.** (2020). *Adaptive sampling of conformational dynamics* [Doctoral dissertation, Rice University]. <https://scholarship.rice.edu/handle/1911/108744>
- 7 **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>
- 8 **Hruska, E.**, Abella, J. R., Nüske, F., Kavragi, 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>
- 9 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. <https://doi.org/10.1109/eScience.2016.7870921>

## Bookchapter

- 2022  Quantum Chemistry in the Age of Machine Learning, 1st Edition, Elsevier, Chapter 6: Machine learning: An overview, **Eugen Hruska**, Fang Liu, Editor: Pavlo Dral, ISBN: 9780323900492