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## Publications


1. 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

2. **Hruska**, **E.**, Gale, A., & Liu, F. (2021). Bridging the experiment-calculation divide: Machine learning corrections to redox potential calculations in implicit and explicit solvent models. *ChemRxiv*. https://doi.org/10.33774/chemrxiv-2021-mthjp

3. **Hruska**, **E.** (2020). *Adaptive sampling of conformational dynamics* (Doctoral dissertation). Rice University. https://scholarship.rice.edu/handle/1911/108744

4. **Hruska**, **E.**, Balasubramanian, V., Lee, H., Jha, S., & Clementi, C. (2020). Extensible and scalable adaptive sampling on supercomputers. *Journal of Chemical Theory and Computation*. https://pubs.acs.org/doi/10.1021/acs.jctc.0c00991

5. **Hruska**, **E.**, Abella, J. R., Nüske, F., Kavraki, L. E., & Clementi, C. (2018). Quantitative comparison of adaptive sampling methods for protein dynamics. *The Journal of Chemical Physics*, *149*(24), 244119. https://doi.org/10.1063/1.5053582

6. Balasubramanian, V., Bethune, I., Shkurti, A., Breitmoser, E., **Hruska**, **E.**, Clementi, C., Laughton, C., & Jha, S. Extasy: Scalable and flexible coupling of md simulations and advanced sampling techniques. In: *2016 ieee 12th international conference on e-science (e-science)*. IEEE. 2016, 361–370. https://ieeexplore.ieee.org/document/7870921