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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*.

2 **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

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

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7 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