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Publications

fractional h-index 3 (OpenAlex), h-index 6 (WoS), citations 107 (WoS)

1. Chen, X., Sun, Y., **Hruska**, **E.**, Dixit, V., Yang, J., He, Y., Wang, Y., & Liu, F. (2024). Explainable machine learning identification of superconductivity from single-particle spectral functions. *Preprint*. https://arxiv.org/abs/2406.04445
2. Suwała, D., & **Hruska**, **E.** (2024). The wins and failures of current docking methods tested on the flexible active site of cytochromes p450. *Preprint*. https://doi.org/10.26434/chemrxiv-2024-05299
3. Chen, X., Li, P., **Hruska**, **E.**, & Liu, F. (2023). Δ-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
4. **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
5. **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
6. **Hruska**, **E.**, & Liu, F. (2022). *Quantum chemistry in the age of machine learning, chapter 6: Machine learning: An overview*. Elsevier.
7. **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
8. 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
9. **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
10. **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
11. 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