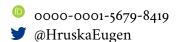
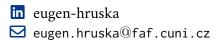
Eugen Hruška, Ph.D.







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*. **6** https://arxiv.org/abs/2406.04445
- 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
- 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*.
 6 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.*6 https://doi.org/10.1021/acs.jctc.0c00991
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