Towards a Database of Bond Orders: combining quantum chemistry and Machine learning

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Introduction to Bond Order(BO)

- BO is an entirely Quantun mechanical concept.
- Descriptor of nature and strength of a chemical bond.
- We will compute BO using the scheme proposed by Istvan Mayer[1] in a Hybrid Atomic Wannier Orbital(HAWO) basis.[2]

Aim: **To curate a bond order dataset from the GW100 test set and develop machine learning models to predict Mayer Bond Orders for unseen molecules**

[1]I,Mayer. (1983). “Charge, bond order and valence in the ab initio SCF theory.” *Chem. Phys. Letters*, 97(3), 270-274
[2]M,Hossain(2022) *et al*. “Hybrid Atomic Orbital Basis from First Principles: Bottom-Up Mapping of Self-Energy Correction to Large Covalent Systems.” *J. Phys. Chem. A,* 125(31).

Workflow

- GW100 test set
- Compute Mayer Bond Order
- Curate dataset
- Train our ML model
- Determine accuracy of the Model

Reference: Rupp, M. et al. (2012). “Fast and accurate modeling of molecular atomization energies with machine learning.” Physical Review Letters, 108(5), 058301.

Thank You!!!