

# Insights into basis-set convergence from diagrammatic decomposition

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We investigate the basis-set convergence of coupled cluster singles and doubles correlation energies. An analysis of different diagrammatic contributions in the amplitude equation shows that the second-order energy together with the particle-particle ladder term play a significant role for the energy convergence. Our findings are used to formulate an efficient basis-set extrapolation scheme that is applied to atoms, molecules, and solid-state systems.

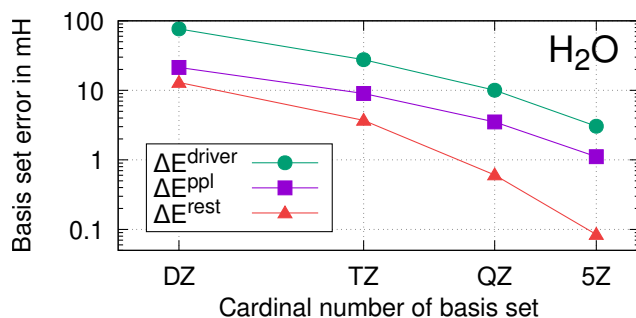


Figure 1: *Absolute basis set error of CCSD valence electron correlation energy contributions for  $\text{H}_2\text{O}$  using the aug-cc-PVXZ basis sets. The second-order energy ( $\Delta E^{\text{driver}}$ ) and the particle-particle ladder contribution ( $\Delta E^{\text{ppl}}$ ) show a different convergence compared to all other contributions ( $\Delta E^{\text{rest}}$ ). The reference energy is approximated using the aug-cc-PV6Z basis set.*

## References

1. Andreas Irmeler and Felix Hummel and Andreas Grüneis, arXiv:1903.05458 (2019)
2. Andreas Irmeler and Andreas Grüneis, arXiv:1903.05559 (2019)