Second order Møller-Plesset (MP2) calculations for large molecules

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MP2 is the simplest configuration-based correlation method. It is preferable to DFT for dispersion forces, for hydrogen-bonded systems, and is useful for checking the reliability of DFT reaction barriers, and for extrapolating coupled cluster results to large basis sets. The following methods will be described:

- An efficient *canonical* MP2, based on a novel prescreening
- Parallel implementation on a Linux PC cluster
- Dual-basis MP2
- Full-accuracy local MP2
- Atomic orbital formulation of MP2 gradients

Examples include a study of π stacking between aromatic molecules, up to the circumcoronene dimer ($C_{108}H_{36}$), with basis sets over 2000 basis functions.