

Density Functional Theory Features

- Over 200 density functionals including the Minnesota and B97 families;
- Analytic gradients and frequencies for LSDA, GGA, meta-GGA, hybrid, and rangeseparated hybrid functionals;
- Atom-atom empirical and non-local correlation treatment of dispersion;
- Analytic TD-DFT excitation energies, gradients, and frequencies for most functionals as well as spin-flip and reduced scaling variants;
- Analytic gradients and frequencies for TD-DFT and C-PCM for hybrid functionals;
- Double-hybrid functionals available with RI integrals to improve performance;
- Analytic frequencies for pure functionals with RI and analytic gradients for hybrids with RI;
- Industry-leading parallel performance in ERI and XC evaluation;
- GPU acceleration via BrianQC.

DFT Parallel Performance

