

Electronically Excited and Open-Shell Species

- EOM-CC methods for excited (EE), ionized/electron-attached (IP/EA), and diradical states (SF, DIP, DEA): analytical gradients, properties, interface with PCM, Effective Fragment Potential Method and QM/MM;
- ADC family of methods (EE/SF/IP/EA) including ADC(2X) and ADC(3);
- RI-SOS-CIS(D): N⁴ excited state method;
- Restricted Active Space nSF methods for polyradicals and multiple bond breaking;
- Collinear and non-collinear SF-DFT for strongly correlated species;
- Analytical gradient and Hessian for TDDFT/TDA and full TDDFT;
- Non-adiabatic couplings within CIS, TD-DFT, and EOM-CC frameworks;
- Spin-orbit couplings within TDDFT, EOM-CC, and RAS-CI;
- Non-linear optical properties for EOM-CC and ADC (two-photon absorption, polarizabilities, RIXS);
- Wave-function analysis for EOM-CC, ADC, TDDFT, and CIS: Natural Orbitals, Natural Transition Orbitals, exciton descriptors, attachment-detachment densities, and more;
- Performance enhancements: RI/Cholesky, multi-core parallelization, single precision execution.

