

**complete active space self-consistent field second-order
perturbation theory (CASPT2)**

Theoretical scheme suitable for computations of accurate excitation energies and reaction barriers. In the first step, electron correlation is taken into account only to a certain extent by using a *CASSCF* formalism (the so called non-dynamic correlation), whereas the remaining electron correlation (the so called dynamic correlation) is included through the use of second-order perturbation theory.

2007, 79, 316