

spin-flip method

Quantum mechanical method for the calculation of open-shell excited states. The method accurately describes low-lying multi-configurational electronic states of diradicals and triradicals in an efficient and robust single-reference scheme. The target low-spin states (e.g., $S = 0$ or $S = 1/2$) are described as spin-flipping excitations ($S = -1$) from a well-behaved high-spin reference state (e.g., $S = 1$ or $S = 3/4$). By employing theoretical models of increasing complexity for the reference (e.g., SCF, MP2, CCSD), the accuracy in the target states' description can be systematically improved. The SF methods result in multistate single-step computational schemes, e.g., several low-lying states can be computed in a single calculation that includes both dynamical and non-dynamical correlation effects.

Source:

PAC, 2007, 79, 293 (*Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006)*) on page 427