

multiconfiguration SCF method

Also contains definition of: MCSCF method

Configuration-interaction method in which simultaneous optimization of both the shapes of molecular orbitals and contributions from different electronic configurations is carried out by using the variational method.

Note:

The MCSCF method with a large enough set of configurations allows a better estimation of the non-dynamic correlation energy than the conventional CIS, CID, and CISD methods.

Source:

PAC, 2007, 79, 293 (*Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006)*) on page 372