

multireference configuration interaction

Acronym: MRCI

Configuration-interaction method in which the configurations are built by excitation out of a wavefunction obtained by using, e.g., the multiconfiguration SCF method.

Note:

One of the methods to account for dynamic correlation.

Source:

PAC, 2007, 79, 293 (*Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006)*) on page 373