

complete active space self-consistent field (CASSCF)

Computational scheme employed in *multiconfigurational SCF theory* especially suitable for studies of reactivity of *excited states*. The wavefunction is defined by selecting the set of active orbitals involved in the excitation or chemical reaction under investigation and is constructed as a linear expansion in the set of configuration functions that can be generated by occupying the active orbitals in all ways consistent with an overall spin and space symmetry (full *configuration interaction, CI*).

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