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# localized molecular orbitals (LMO)

The molecular orbitals located on certain fragments of a molecular system and spatially separated from each other as much as possible. The LMOs are derived from the electron occupied canonical molecular orbitals by subjecting them to a unitary transformation determined by an appropriate physical criterion, *e.g.* by maximizing the sum of squares of the centroids of occupied MOs (the Foster–Boys procedure) or by minimizing the sum of the exchange (or Coulomb) repulsion integrals between the occupied MOs (the Edmiston–Ruedenberg procedure).

***Source:***
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1950

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