

frontier orbitals

Also contains definition of: LUMO

The *Highest-energy Occupied Molecular Orbital* (HOMO) (filled or partly filled) and *Lowest-energy Unoccupied Molecular Orbital* (LUMO) (completely or partly vacant) of a molecular entity. Examination of the mixing of frontier molecular orbitals of reacting molecular entities affords an approach to the interpretation of reaction behaviour; this constitutes a simplified perturbation molecular orbital theory of chemical behaviour.

See also: SOMO, subjacent orbital

Source:

PAC, 1994, 66, 1077 (*Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)*) on page 1116