

### **frontier orbitals**

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*.

1994, 66, 1116