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Hückel molecular orbital (HMO) theory

The simplest molecular orbital theory of π-conjugated molecular systems. It uses the following approximations: π-electron approximation; LCAO representation of the π-molecular orbitals; neglect of electron-electron and nuclear-nuclear repulsions (in fact, the assumption that these cancel). The diagonal elements of the effective Hamiltonian, coulombic integrals, and the off-diagonal elements, resonance integrals, (accounted for only directly bonded atoms) are chosen as empirical parameters, all overlap integrals being neglected.

Source:
PAC, 1999, *71*, 1919 *(Glossary of terms used in theoretical organic chemistry)* on page 1944

