

more complex when discussing even comparatively simple polyatomic molecules, such as methane. MO diagrams can explain why some molecules exist and others do not. They can also predict bond strength, as well as the electronic transitions that can take place.

Qualitative MO theory was introduced in 1928, by Robert S. Mulliken and Friedrich Hund. A mathematical description was provided by contributions from Douglas Hartree in

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Molecular orbital diagram

BSc (H)

IIIrd part

A molecular orbital diagram or MO diagram, is a qualitative descriptive tool explaining chemical bonding in molecules in terms of Molecular orbital theory in general and the linear combination of atomic orbitals (LCAO) method in particular. A fundamental principle of these theories is that as atoms bond to form