

as linear combinations of atomic orbitals (LCAO).

These approximations are now made by applying the density functional theory (DFT) or Hartree-Fock (HF) models to the Schrödinger equation.

The other foundational theory of quantum chemistry is the valence bond theory.

Molecular orbital theory was developed in the 1930s after valence bond theory had been established (1927), primarily through the efforts of Friedrich Hund, Robert Mulliken, John C. Slater, and John Lennard-Jones. MO theory was originally called the Hund-Mulliken theory. According to physicist and physical chemist Erich Huckel, the first quantitative use of molecular orbital theory was the 1929 paper of Lennard-Jones.

26/5
page-1

Chemical bonding

rose April 21
(11)

Molecular orbital theory (MO) In chemistry, Molecular orbital theory is a method for describing the electronic structure of molecules using quantum mechanics. Electrons are not assigned to individual bonds between atoms, but are treated as moving under the influence of the nuclei in the whole molecule. The spatial and energetic properties of electrons are described by quantum mechanics as molecular orbitals. A molecular orbital contains two or more atoms in a molecule and contains valence electrons between atoms. Molecular orbital theory, which was proposed in the early 20th century, revolutionized the study of bonding by approximating the states of bonded electrons - the molecular orbitals -