

the H_2 molecule. The H_2 molecule is a diatomic molecule, and its electronic structure is well described by the molecular orbital (MO) theory. The MO theory is a quantum mechanical theory that describes the electronic structure of molecules by combining the atomic orbitals (AOs) of the constituent atoms. In the case of H_2 , the two 1s AOs of the hydrogen atoms combine to form two molecular orbitals: a bonding σ_{1s} orbital and an antibonding σ_{1s}^* orbital. The bonding orbital is lower in energy than the atomic orbitals, and the antibonding orbital is higher in energy. The energy difference between the bonding and antibonding orbitals is the bond energy of the H_2 molecule. The MO theory also predicts the magnetic properties of the H_2 molecule. In the ground state, the two electrons in the H_2 molecule are paired in the bonding orbital, and the molecule is diamagnetic. In the excited state, the two electrons are unpaired in the bonding and antibonding orbitals, and the molecule is paramagnetic.

The MO theory is a powerful tool for understanding the electronic structure of molecules. It can be used to calculate the bond energy, bond length, and magnetic properties of molecules. It can also be used to predict the reactivity of molecules. The MO theory is a quantum mechanical theory, and it is based on the Schrödinger equation. The Schrödinger equation is a partial differential equation that describes the wave function of a system. The wave function is a mathematical function that describes the probability of finding a particle in a particular state. The Schrödinger equation is solved by finding the eigenvalues and eigenvectors of the Hamiltonian operator. The Hamiltonian operator is a mathematical operator that represents the total energy of a system. The eigenvalues are the energy levels of the system, and the eigenvectors are the wave functions of the system. The MO theory is a special case of the Schrödinger equation, and it is used to describe the electronic structure of molecules.

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