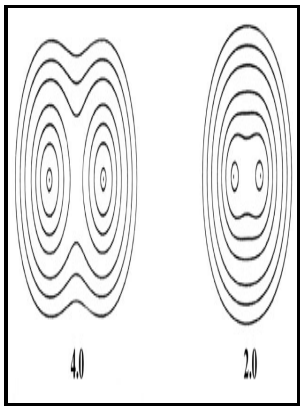
Electron densities in molecules and molecular orbitals

Academic Press - 10.8: Molecular Orbital Theory



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Tags: #Chapter #9, #Section #7

Chapter 9, Section 7

Bond Order in Molecular Orbital Theory In the Lewis electron structures, the number of electron pairs holding two atoms together was called the bond order. As a result, only the bonding σ orbital is occupied by electrons, giving a bond order of 1.

Molecular Orbitals

Chapter 9, Section 7 9.

Molecular Orbitals

The He 2 + ion has a total of three electrons. Molecular orbitals are associated with the entire molecule, however, not with a single atom. The generated DOSCAR file has 6 header lines and then 4500 lines containing the DOS and the integrated DOS as a function of the energy.

Electron Densities in Molecular and Molecular Orbitals

A bond order of 1 represents a single bond, a bond order of 2 represents a double bond, and a bond order of 3 represents a triple bond. Overlap of atomic orbital lobes with the same sign produces a bonding molecular orbital, regardless of whether it corresponds to the sum or the difference of the atomic orbitals.

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