# Intro to MO Theory

**Skills to Develop**

- Compare and contrast MO Theory and Valence Bond Theory

Molecular Orbital (MO) Theory is another theory to explain chemical bonding using orbitals. It was developed about the same time Valence Bond Theory was developed, primarily by Mulliken and Hund. (Mulliken was mentioned earlier because he proposed a definition of electronegativity, and Hund because of Hund's Rule.) It is a little harder to learn than Valence Bond Theory, but very useful.

Robert S. Mulliken, left, and Friedrich Hund, right.

Why do we need another theory after learning Valence Bond Theory? Although Valence Bond Theory works well to explain some properties of certain types of molecules, like shape and bond strengths in organic molecules, there are many situations when it doesn't work very well. For example, it isn't very good for predicting the magnetic properties of molecules. From Valence Bond Theory, you would not expect $O_2$ to have 2 unpaired electrons, but it does. It also isn't good for predicting the spectroscopic properties of molecules, including what color they are. For example, you can do Photoelectron Spectroscopy on molecules, in which you knock electrons off molecules using high-energy photons. By knowing the energy of the photons and the kinetic energy of the photoelectrons, you can find the binding energies of the electrons in the molecule. For water, you would expect from the Lewis structure that there are 2 different binding energies for valence electrons (because they are either lone pairs or bonding pairs) and another higher energy for the O 1s electrons. However, the data shows 4 different energies, meaning that the 4 electron pairs in the Lewis structure all have different energies. MO Theory can explain this. MO theory is also good for predicting how strong bonds are, for predicting stability of weird molecules (like $C_2$), and for describing bonding in molecules that have resonance structures.

## Contributors and Attributions

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