Valence bond (VB) theory assumes that all bonds are localized bonds formed between two atoms by the donation of an electron from each atom. This is actually an invalid assumption because many atoms bond using delocalized electrons. In molecular oxygen VB theory predict that there are no unpaired electrons. VB theory does a good job of qualitatively describing the shapes of covalent compounds. While Molecular Orbital (MO) theory is good for understanding bonding in general. It is more difficult to learn, but predicts the actual properties of molecules better than VB theory. MO theory actually predicts electron transitions because of the differences in the energy levels of orbitals in the molecule. MO theory has been more correct in numerous instances and for this reason it is preferred.

Valence Bond theory describes covalent bond formation as well as the electronic structure of molecules. The theory assumes that electrons occupy atomic orbitals of individual atoms within a molecule, and that the electrons of one atom are attracted to the nucleus of another atom. This attraction increases as the atoms approach one another until the atoms reach a minimum distance where the electron density begins to cause repulsion between the two atoms. This electron density at the minimum distance between the two atoms is where the lowest potential energy is acquired, and it can be considered to be what holds the two atoms together in a chemical bond.