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Electronic Bonding of Atoms

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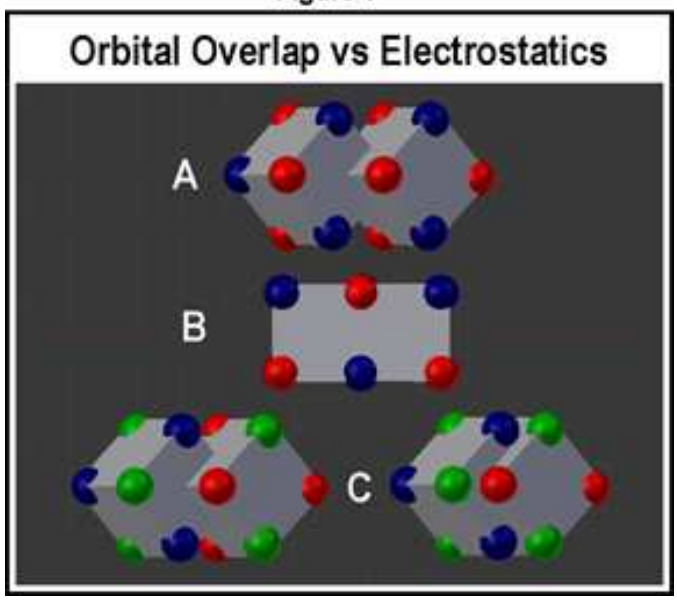
Bonded atoms make up our physical world. The principal parts that provide this composition are positive nuclei and negative electrons. While these may be just "waves" in a highly dimensional, mathematical universe, they are "solid" entities with mass that can be shot, herded, assembled, etc and make up what we view in our 3D world. "Bonding" occurs through electrostatic attractions; "de-bonding" through repelling. Simple bonding can occur through electrostatic interactions between an atom's nucleus and another atom's electrons with each atom's electrons beholden only to its own nucleus. More complex bonding requires that each atom's electrons coordinate with those of other atoms so that the electrons move between the atoms in concert. In this essay, I have outlined how these interactions are manifested according to the MCAS electronic model of atoms.[1]

In the MCAS electron model, the main orbitals involved in simple bond formation are 8-fold and point to cubic corner space. Bonding occurs when nuclei can approach one another on a line where there is an electron deficiency. The simple electrostatic meshing case is illustrated in figure 1, image A. The bond length and strength are determined by the attracting and repelling electrostatic forces. For orbital overlap to occur, the electron orbiting network of each must be synchronized. A simple case is illustrated in figure 1, image B. While it may be more aesthetically pleasing to some eyes, such a configuration may not necessarily produce an interaction with a lower energy state. The nuclei in images A and B are the same distance apart. The bond length in image B is set by the orbital overlap in addition to other electrostatics. The bond length for the simple electrostatic mesh (A) will be shortened when there are fewer negative non-bonding electrons (green colored orbitals in figure 1, image C) present to repel the bonding electrons (mid-nuclei red and blue orbitals).

Figure 1



[1] Williams, Joel M, http://www.wbabin.net/Science-Journals/Essays/View/4019 (in the General Science Journal)

The simple electrostatic bonding model is sufficient to indicate the bonding in the diatomic molecules of the elements carbon to neon (see figure 2). While current MO bonding gives the diatomic molecules different "bond orders" (single, double, triple), the MCAS electrostatic model has them all the same (single) in the ground state. For oxygen, this gives the "triplet" state (C2-C4) with two unpaired electrons. Elevating an electron in each produces the "singlet" state (C3-C3). The molecule in this elevated state is best represented by the orbital overlap model (figure 3) wherein 6 electrons occupy each of the orbital networks, indicated as blue and red.

Figure 2

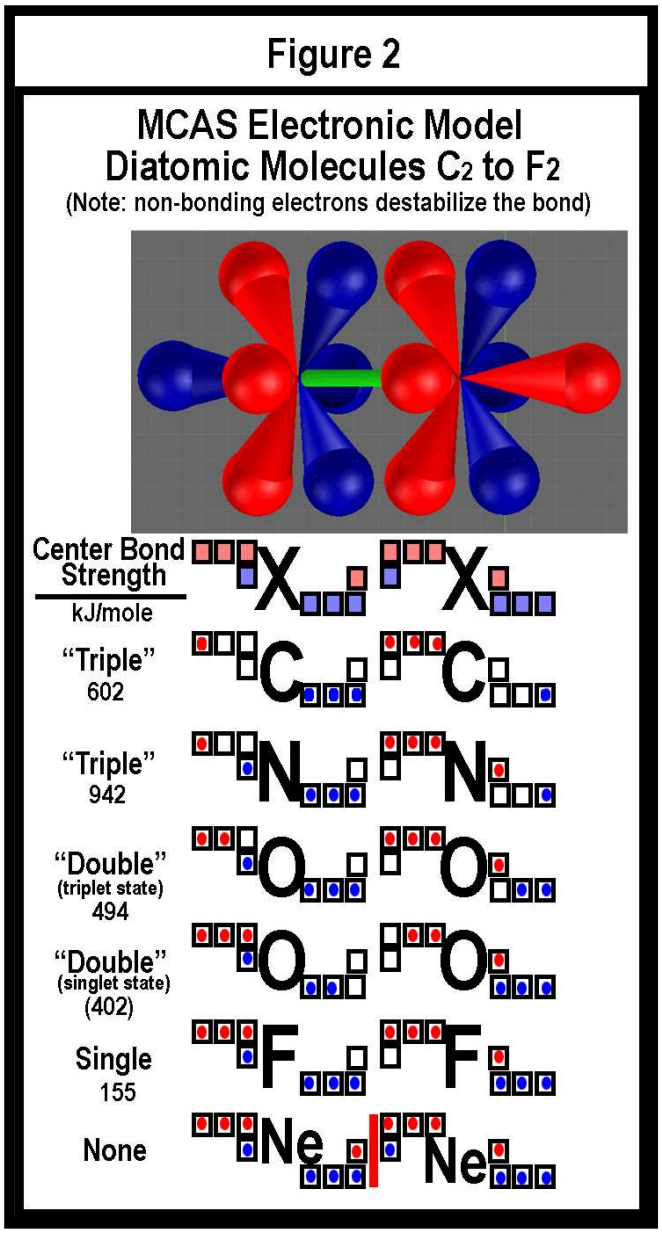
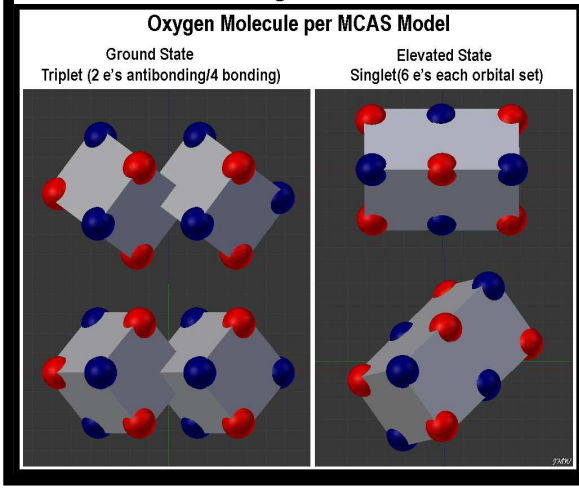


Figure 3



The two models indicate how the difference in the oxygen atom ground-state [C2-C4, 2-unpaired electrons] and elevated-state [C3-C3, no unpaired electrons] pairings give the observed experimental electron pairing in the diatomic molecule: again, 2 unpaired in the ground-state and no unpaired in the elevated state. This was a driving force for the current MO modeling to explain why the reverse was not the case as indicated by the octet and electron spin-pairing rules.

Allene (H_2CCCH_2) conforms to the orbital overlap model (see figure 4). The 4 hydrogen atoms (not shown) attach at the e-deficient terminal blue positions. As observed experimentally the end pairs are perpendicular to one another. Bonding to the center atom forces them to be "perpendicular". In the current MO model the orbitals have the center sp-hybridized with the unhybridized p-orbitals forming perpendicular pi-bonds. No such hybridizing is needed with the MCAS model, just orbital overlap.

This brings up an interesting question about the structure of carbon dioxide. The lowest energy of the oxygen molecule is the triplet state that has non-overlapped, electrostatic bonding. Does placing a carbon atom between them still follow the same form (figure 5, image A)? Or, do the three overlap in the style above for allene (figure 5, image B) in accord with the singlet form of O_2? Note that the "formal charges" on the two are -1+2-1 for A and 000 for B. What is the experimental evidence to favor B which is in conformity with the current MO, perpendicular double-bonded carbon?

Figure 4

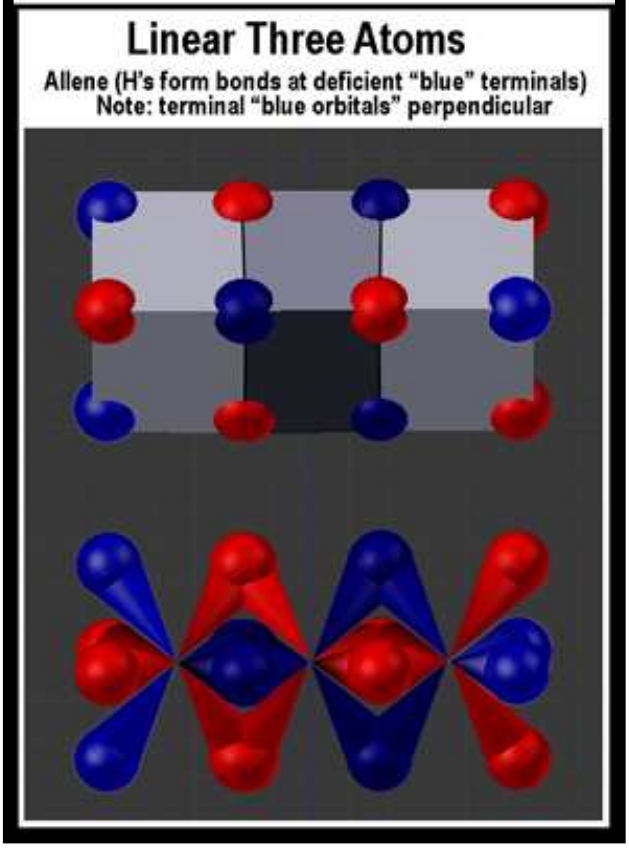
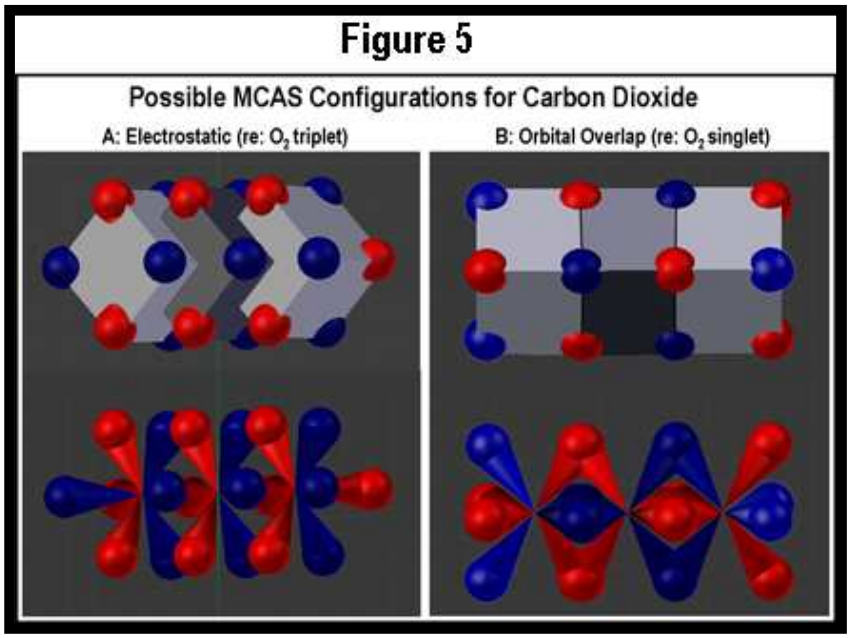
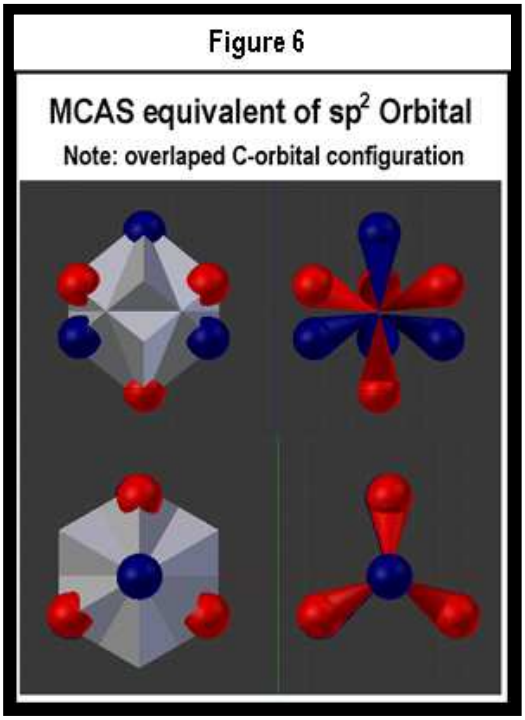


Figure 5



Resonance energy is the lowering of an electron's travel energy by removing some of the "reversals" that occur when an electron normally returns towards the nucleus that it just passed. Maximum resonance energy is obtained when the electron returns to its "starting" point WITHOUT reversing its direction; i.e., it completes a closed, albeit circuitous, loop. Aromaticity is the epitome of this behavior. The current MO methodology uses the sp2 hybrid to provide the mechanism. The MCAS rendition of this hybrid is shown in figure 6. Electrons in each C-orbital set enter or leave the atom in the same general direction, but divergently; i.e., the orbital sets are eclipsed instead of staggered. In accord with the general theory behind the MCAS model, electrons in the two orbital sets will be paired (moving opposite one another). An edge-edge distance is greater than a face-face distance.

Figure 6



The basic bonding modes in the MCAS methodology have now been described. They are summarized in figure 7.

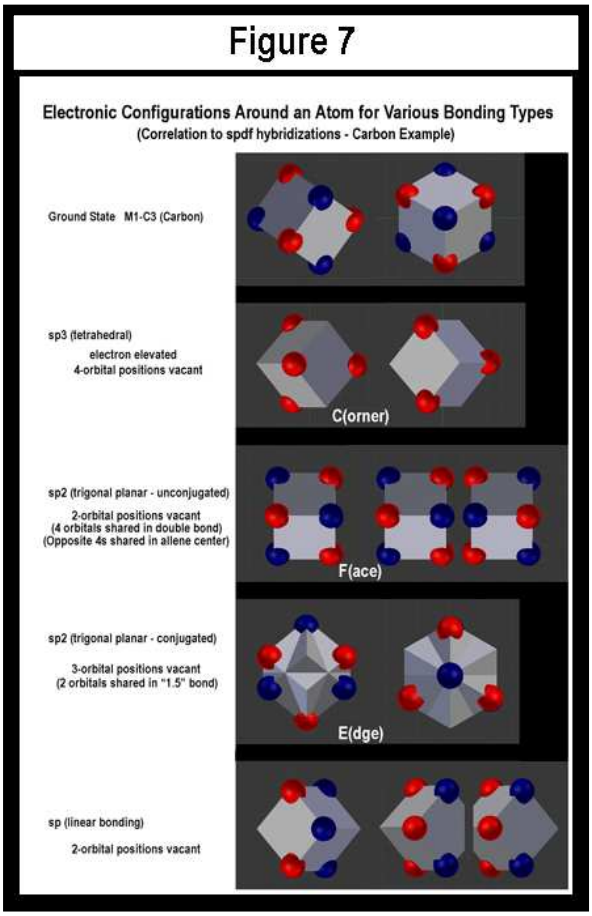
1. C(orner) bond mode – "single" bond
   Meshing occurs electrostatically without orbital overlap.

2. Orbital overlap bond modes – "multiple" bond

   - F(ace) - non-conjugated double
   - E(dge) – conjugated

3. The triple-bond of the current MO methodology is just a special case of the C(orner) mode where the "triple" bond between two carbon atoms, i.e., results from only a single electron in each of the anti-bonding orbital sets and thus destabilizes the bond much less. See C_2 in figure 2.

Figure 7



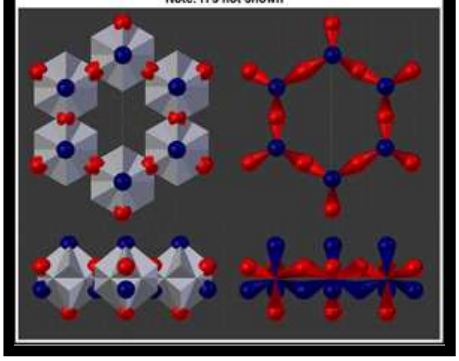
Several examples of **E**(dge) bonding will now be given.

The most widely recognized molecule with this type bonding is benzene. The 6-membered carbon ring is shown without the hydrogen atoms, but with and without the reference objects in figure 8. Note the two (red and blue) orbital groups. Also note that the electron orbitals between nuclei are not on a direct line between the nuclei, but are above and below the "bond-line". As the electrons are paired in opposing motion, the electrons in the two circuitous rings travel in opposite directions as required for pairing.

Figure 8

MCAS Model of Benzene

Note: H's not shown

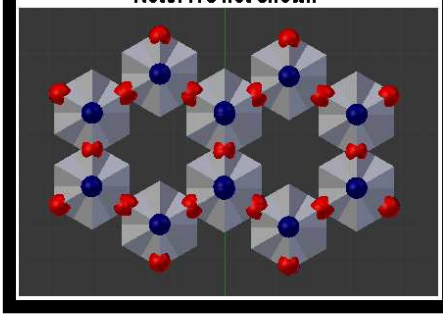


The 10-carbon atoms of naphthalene are joined in the two rings structure shown in figure 9 without the hydrogen atoms.

Figure 9

MCAS Model of Naphthalene

Note: H's not shown



The MCAS bonding in the carbonate ion is shown in figure 10. The oxygen atoms are -1 each (6 unshared nodes and 2 shared nodes) with the central carbon +1 (6 shared nodes).

Figure 10

MCAS Model for $CO3^{=}$