Chapter 33   ORBITALS, Part 4 and METALLIC BONDING

Our background is complete and we have covered a number of simpler cases. Having last left lithium, let's stroll across the Second Period. Things will get a bit more complicated as we go but the fundamentals are in place. We'll add a bit more to the story, too. We'll also finally get to metallic bonding.

33.1 More configurations

We will do nine Examples of configurations and bond orders, along with an occasional para/diamagnetism. Again, first find the total number of electrons and then plug this into the fill sequence. Here're the fill sequences again for the Second Period; keep them handy.

Fill sequence for Second Period diatomics

With mixing	$(\sigma_{2s})(\sigma_{2s}^*)(\pi_{2p})(\sigma_{2p})(\pi_{2p}^*)(\sigma_{2p}^*)$
Without mixing	$(\sigma_{2s})(\sigma_{2s}^*)(\sigma_{2p})(\pi_{2p})(\pi_{2p}^*)(\sigma_{2p}^*)$

We're not yet to the point where mixing matters. We will hit that in Example 3 below.

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Example 1. Be_2^+.

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▸ Find the total number of valence electrons: 3
▸ Enter into the MO fill sequence: $(\sigma_{2s})^2(\sigma_{2s}^*)^1$
▸ Bond order: 0.5

This thing can exist but it's got a weak bond since the bond order is only one-half. What about magnetic properties? The odd number of electrons tells us immediately that it is paramagnetic. How many electrons are unpaired? The σ_{2s} is filled, so those two electrons are spin-paired. Look for the partly filled portion, which is σ_{2s}^*.

$$\boxed{\uparrow}$$
$$\sigma_{2s}^*$$

Bingo: there's one unpaired electron.

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Example 2. Be_2.

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▸ Find the total number of valence electrons: 4
▸ Enter into the MO fill sequence: $(\sigma_{2s})^2(\sigma_{2s}^*)^2$
▸ Bond order: Zilch.

This is another dud, like He_2. All bonding electrons are offset by antibonding electrons. Notice that neutral Be_2 cannot exist but Be_2^+ can exist, although the bond order in the cation is only one-half.

Alright, we've run through the s-block. Now, we bop over to the p-block and continue through the Second Period. Notice that we have filled the $(\sigma_{2s})^2(\sigma_{2s}^*)^2$ levels with four electrons, so the next electron will go into σ_{2p} or π_{2p}, depending on whether there is significant mixing or not. Now we're stuck with this issue of mixing. As briefly noted in Section 32.3, it's a size thing: the diatomics of B, C and N follow the mixing sequence while the diatomics of O, F and Ne do not. Keep this in mind as we go: we start off with mixing but we switch at O_2.

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Example 3. B_2.

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▸ Find the total number of valence electrons: 6
▸ Enter into the MO fill sequence (with mixing): $(\sigma_{2s})^2(\sigma_{2s}^*)^2(\pi_{2p})^2$
▸ Bond order: 1

Diamagnetic or paramagnetic? There's an even number of electrons, so it could be either. Notice that π_{2p} is only partly filled; therefore, it will have unpaired electrons. Box it out.

$\boxed{\uparrow \mid \uparrow}$ It has two unpaired electrons.

π_{2p}

Notice that the electrons in the σ orbitals cancel each other for bonding; thus, σ bonding is cancelled. The bond order of one is due to π electrons only. This means that the single bond in B_2 is π type. This differs from our Valence Bond Approach and Lewis structures: for them, all single bonds were σ type.

OK, it's your turn.

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Example 4. C_2.

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▸ Find the total number of valence electrons: _____

▸ Enter into the MO fill sequence (with mixing):   _____

▸ Bond order: _____

▸ Diamagnetic or paramagnetic?   _____

Overall, the σ and σ* bonds cancel, but there are two π bonds.

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Example 5. C_2^{2-}.

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▸ Find the total number of valence electrons: 10
▸ Enter into the MO fill sequence (with mixing): $(\sigma_{2s})^2(\sigma_{2s}^*)^2(\pi_{2p})^4(\sigma_{2p})^2$
▸ Bond order: 3

It's diamagnetic: everything is exactly filled and every electron is spin-paired. The triple bond order is derived from two π bonds (within the $(\pi_{2p})^4$ portion) and one σ bond (the $(\sigma_{2p})^2$ portion). The $(\sigma_{2s}^*)^2$ portion cancels out $(\sigma_{2s})^2$.

Unlike the diatomics in Examples 1 - 4, this diatomic is well available, most commonly in the ionic compound CaC_2 which is called "calcium carbide". The "carbide" name is not quite right but the name's been around so long that it has stuck. This compound finds numerous uses industrially; years ago, it was available in common stores. It reacts with water to form acetylene gas, C_2H_2, and it was used in gas lamps.

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Example 6. N_2.

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▸ Find the total number of valence electrons: 10
▸ Enter into the MO fill sequence (with mixing): $(\sigma_{2s})^2(\sigma_{2s}^*)^2(\pi_{2p})^4(\sigma_{2p})^2$
▸ Bond order: 3

It's diamagnetic: everything is exactly filled and all electrons are spin-paired. The triple bond order is derived from two π bonds (within the $(\pi_{2p})^4$ portion) and one σ bond (the $(\sigma_{2p})^2$ portion). Notice that these results are identical to the results for C_2^{2-}. That's because they are isoelectronic: both have the same number of electrons.

With N_2 we are now dealing with an actual elemental form which is very stable and in wide abundance. N_2 is extremely stable and very slow to react (at normal temperatures) because of its MO configuration with its triple bond. The very strong triple bond and the very slow reactivity account for why you breathe this element more than any other substance. Once formed, it hangs around a long time; thus, it has accumulated to massive amounts in the atmosphere over the eons. There are primarily only two things that react with N_2 in Nature. One is lightning, although being zapped by a lightning bolt is not exactly normal conditions. The other is the enzyme nitrogenase, which is found in numerous micro-critters throughout the biosphere. This enzyme is responsible for biological nitrogen fixation and it has the uncanny job of reacting with N_2 at normal biological conditions. (I mentioned biological nitrogen fixation way back in Chapter 2.) No one can yet explain how that enzyme works.

Speaking of breathing, let's go to our next diatomic molecule, O_2. Now there's a catch: beginning with O_2, we lose the mixing. We reverse the order for $...(\pi_{2p})(\sigma_{2p})...$ and we instead use $...(\sigma_{2p})(\pi_{2p})...$

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Example 7. O_2.

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‣ Find the total number of valence electrons: 12
‣ Enter into the MO fill sequence (<u>without</u> mixing): $(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2p})^2(\pi_{2p})^4(\pi_{2p}^*)^2$
‣ Bond order: 2

Diamagnetic or paramagnetic? π_{2p}^* is only partly filled, so it will have unpaired electrons and the molecule is paramagnetic. Let's see how many electrons are unpaired.

$$\boxed{\uparrow}\,\boxed{\uparrow}$$
π_{2p}^* There are two unpaired electrons.

Pause for a moment whilst I make four observations.

First observation: the loss of mixing for O_2 had no effect on the overall outcome. Both π_{2p} and σ_{2p} are full and there are electrons after them in the sequence (in π_{2p}^*). Quite frankly, it really didn't matter whether the sequence ran $...(\pi_{2p})^4(\sigma_{2p})^2...$ or whether it ran $...(\sigma_{2p})^2(\pi_{2p})^4...$ Either way, O_2 has a double bond and it has two unpaired electrons. This will be true for all remaining diatomics of the Second Period: either sequence gives the same outcome. Because of this, some instructors just use the sequence with mixing for everything as a simplification. It won't affect the bond order and it won't affect the magnetic properties.

Second observation: O_2 is paramagnetic with two unpaired electrons. Is this important? Yes. Let me repeat what I said in Section 24.3.

❝ There's also an extremely important difference in the way chemical units react, depending on whether they have all of their electrons paired or not. Perhaps the most obvious example is the very oxygen which you need to live. Normal O_2 in the air has two unpaired electrons in the molecule. You can make another form of O_2 with all of its electrons paired. These two react very differently. The version of O_2 with all electrons paired is even far more deadly than the normal O_2. That's Nature at work again. Subtle differences, dire consequences. ❞

Notice that there is another form of O_2 with all electrons paired. That corresponds to an excited state for O_2. Once again, our configurations here are for ground states. To get to an excited state, you must provide some energy in order to pay for the excitation.

Third observation: Molecular Orbital Approach correctly predicts the paramagnetism of O_2. The Lewis structure fails to predict this at all. I show the Lewis structure at left; it shows a double bond, which is in complete agreement with the MO Approach here, but the Lewis structure shows lone
$:\ddot{O} = \ddot{O}:$ pairs and it does not properly convey that there are two unpaired electrons. This is a shortcoming of the Lewis system. Our Valence Bond Approach likewise does not predict the paramagnetism of O_2 (although VBA can explain this at a higher level). Nevertheless, the paramagnetism of O_2 is fully predicted by MOA, even at our level of coverage.

Fourth and final observation: I mentioned in Chapter 24 that bulk magnetic properties are a consequence of electron spin. You can see this in O_2 in its liquid phase, although you have to condense it below its boiling point of -183 °C (-297 °F) in order to get there. The liquid is attracted to a magnetic field and it can be held by a magnet. It's kind of weird seeing a liquid attracted to a magnet, and you need a strong magnet to do this, but it does work. This occurs due to the two unpaired electrons.

Let's continue. Your turn again.

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Example 8. O_2^{2-}. This is the peroxide ion.

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‣ Find the total number of valence electrons: _____

‣ Enter into the MO fill sequence: _____

▸ Bond order: _____

▸ Diamagnetic or paramagnetic? _____

By the way, peroxide is isoelectronic to F_2; if you do F_2, it has the same MO results as peroxide.

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Example 9. Ne_2.

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▸ Find the total number of valence electrons: _____

▸ Enter into the MO fill sequence: _____

▸ Bond order: _____

Go ahead and work it out. This molecule can't happen.

This concludes our primary Examples for doing MO approach. I hope you can see how all of this works. It's not too bad once you get the hang of the fill sequences. I will add a few further aspects before closing and moving on.

33.2 Further aspects

We did neutral O_2 and we did peroxide, O_2^{2-}. Peroxide is one diatomic ion for oxygen, but there are two others: O_2^- (called "superoxide") and a cation, O_2^+ (called "dioxygenyl"). The dioxygenyl cation is rare and there are not many compounds known with it. Superoxide is actually quite common, although unfortunately so: it is generated within your cells but it is very reactive and very harmful to biological tissue. This ion is part of the reason why normal O_2 can be toxic to you: reduction of O_2 by one electron generates this superoxide ion, and this reduction happens quite often inside cells. Once formed, superoxide then reacts with all sorts of stuff within your cells. This is a serious, potential problem for life forms which use or are exposed to O_2. Fortunately, Nature is aware of this, and Nature built into your cells certain enzymes which intercept much (although not all) superoxide ion before it can do real damage. The enzymes aren't perfect, however, and superoxide can still cause serious damage over a lifetime. There are also people whose enzymes do not work fully; this gives rise to serious and often fatal diseases.

The series O_2^+, O_2, O_2^- and O_2^{2-} provides an interesting comparison regarding antibonding electrons, magnetic properties, bond orders and bond lengths. All of these diatomics have the same configuration through $(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2p})^2(\pi_{2p})^4$, but then they have 1 - 4 electrons in (π_{2p}^*). Let's spell this out.

	Valence Electrons	Configuration	π_{2p}^*	Unpaired Electrons	Bond Order	Bond Length
O_2^+	11	$(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2p})^2(\pi_{2p})^4(\pi_{2p}^*)^1$	[↑][ ]	1	2.5	112 pm
O_2	12	$(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2p})^2(\pi_{2p})^4(\pi_{2p}^*)^2$	[↑][↑]	2	2	121 pm
O_2^-	13	$(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2p})^2(\pi_{2p})^4(\pi_{2p}^*)^3$	[↑][↑↓]	1	1.5	133 pm
O_2^{2-}	14	$(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2p})^2(\pi_{2p})^4(\pi_{2p}^*)^4$	[↑↓][↑↓]	0	1	149 pm

There are several noteworthy observations to make. Of the four, only peroxide is diamagnetic. Dioxygenyl and superoxide are paramagnetic with one unpaired electron, while O_2 has two. Check out the bond order effects. As we go down the series, another antibonding electron is added, so the bond order decreases. A lower bond order means a weaker bond and a longer bond, and the latter is evidenced by the bond lengths. See how all this ties together?

This ends the O_2 comparisons.

With all of our Examples so far, we have covered through the Second Period. Many of the same features carry into later Periods also; the valence atomic orbitals are then derived from higher n-shells. Mixing also happens for some diatomics of Third and lower Period elements but it is more complicated. Some fill sequences are affected but, in general, it doesn't influence bond order and it doesn't influence

magnetic properties. For example, P_2 has a triple bond and it is diamagnetic, just like N_2. (P_2 is not a common form; it is produced in the gas phase when elemental phosphorus is heated.) S_2 has a double bond and it has two unpaired electrons, just like O_2. (Again, S_2 is not common, but it is also obtained in the gas phase by heating the element.) The ion S_2^{2-} is well known in a number of ionic compounds; it has a single bond and it is diamagnetic, just like peroxide. All of the elemental halogens are diatomic molecules; they all have single bonds and they are all diamagnetic. Thus, it is reasonable to apply many aspects of the Second Period diatomics to later Periods as well, although some exceptions can happen. For example, Bi_2^{2-} has a double bond but it is diamagnetic instead of paramagnetic due to changes in the relative energies of the orbitals. Nevertheless, our coverage still applies in many cases even in lower Periods.

OK, all of our Examples so far have covered homonuclear cases. I said in the very beginning of Chapter 32 that I would mention heteronuclear cases. Here's the mention.

Some heteronuclear diatomics can be accommodated by our coverage here but others have different fill sequences. I'll mention the NO^+ cation as an example of one which does follow our coverage. Here, you do it. It takes the fill sequence with mixing. Just do everything the same way.

▸ Find the total number of valence electrons: _____

▸ Enter into the MO fill sequence (with mixing):   _____

▸ Bond order: _____

▸ Diamagnetic or paramagnetic?   _____

Care to check your answers? Your answers are in Examples 5 and 6. The results are the same for NO^+ as they are for C_2^{2-} and for N_2.

OK, let's do a bit with delocalization, just to show how Molecular Orbital Approach handles this. Recall (Section 27.1) that a localized bond involves sharing electrons between two atoms and over one bond connection. Delocalization involves sharing over three or more atoms and over two or more connections. I'll show two examples of this: one with σ delocalization and one with π delocalization.

For the first, let's shoot for something of astronomical importance: H_3^+.

What is H_3^+? Well, it's not exactly an Earthly ion but it is a heavenly ion. It's in outer space and, on the grand scale of the cosmos, it's the most abundant polyatomic ion in the universe. That's not a bad distinction, is it? Its shape and its bonding are a bit different from what we have covered so far. The ion forms an equilateral triangle as shown at left. The Lewis structure and VBA description are a bit beyond what we've covered. MOA, however, handles this fairly easily. That's because there are only two electrons in this ion and we only have $1s$ orbitals to work with, as shown at right. I am dropping the cation charge sign at this point because I want to bring in orbital amplitude sign, as shown at lower left.

That combination is the most favored interaction. All three orbitals overlap with the same amplitude sign; this additive combination gives us one molecular orbital which now extends over all three atoms and over all three connections. That's the delocalization aspect. This gives the bonding MO as shown at right; it is a σ_{1s} type and it holds the two electrons. Two more MOs are also formed from other amplitude sign combinations, but they are empty and we don't have to worry about them. That's the bonding for H_3^+. The bond order is a measly 1/3 which is OK in the extreme, frigid cold of much of space but it wouldn't last at normal conditions.
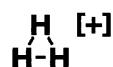
Let's turn to π delocalization. I'll use nitrite ion, NO_2^-, since this is the example which was used to first introduce delocalization back in Chapter 27. The Lewis structures are repeated at left. Let me repeat a point which I made back then.
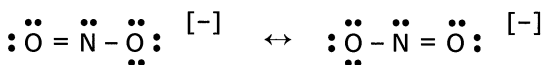
❝ Whenever you can draw different Lewis structures for the same polyatomic unit, this indicates that one or more bonds (and, perhaps, lone pairs) is delocalized. For nitrite, there are a total of three bond pairs in the ion. Two of these bond pairs are localized... The third bond pair is delocalized over both NO connections. ❞

Later, I made a point about the lone pairs in nitrite.

❝ One lone pair is actually delocalized while the others are not. In the resonance structures as drawn..., the LP on the bottom is delocalized over the two terminal oxygens. **❞**

Let's now put these aspects into the framework of the Molecular Orbital Approach. I won't do the whole bonding picture; I just want to cover the delocalized π bond and lone pair.
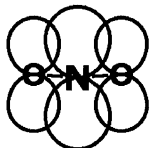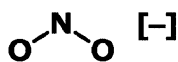
We start with the bent shape of nitrite, shown at left. To get a better view of the orbitals involved, I'm going to flip this on its edge, giving the picture below at right. In this drawing, the central N is forward and drawn slightly larger. To simplify things, I will again leave out the charge sign.

We need the $2p$ AO on each atom which is perpendicular to the plane of the three atoms. I show these three orbitals at left. Notice that these $2p$ AOs are interacting in side-to-side p-to-p fashion, so the molecular orbitals from this interaction will be π-type. Since three AOs are interacting, then three MOs will result. I show the most favored interaction at right, with the amplitude signs. This interaction gives one π_{2p} bonding MO and it holds two electrons. This one MO will span all three atoms; thus, it is a delocalized π_{2p} orbital. In addition, there are two other MOs to consider which have other combinations of the amplitude signs. One of these is a nonbonding MO which also holds two electrons; a nonbonding MO has no significant effect on bonding even though it has electrons. It acts as a lone pair but, now in this case, it's delocalized. The final orbital is a delocalized π_{2p}^{*} antibonding orbital but this one has no electrons; since it has no electrons, then it has no effect whatsoever.
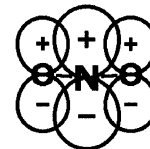
These two examples show how delocalization can be described in MOA. Compared to Lewis and VBA, MOA avoids the notion of separate resonance structures which tend to complicate things. So why bother with resonance structures? Well, formulating delocalized orbitals with MOA can get very complicated very quickly, whereas resonance stays more simplistic. It's just like I've been saying all along. They're tools. Lewis. VBA. MOA. They're all tools. Sometimes one works better than the others.

This concludes our introduction to delocalization within the Molecular Orbital Approach. Delocalization can extend over more than just three atoms: it can extend over six atoms or ten atoms or seventeen atoms or whatever. Delocalization can occur for σ and for π, for bonding, for nonbonding and for antibonding orbitals. This is the lead into our next discussion: metallic bonding.

33.3 Bands and conductors

Metallic bonding is our third major type of chemical bonding to be covered. We've done lots of stuff with ionic bonding and we've done lots of stuff with covalent bonding. Now, metallic bonding. Why now? Why here? In order to explain metallic bonding, we needed two things: Molecular Orbital Approach and delocalized orbitals.

Metallic bonding is an extreme of covalent bonding. It is extreme in the sense of delocalization. And I do mean EXTREME DELOCALIZATION. Metals are three-dimensional network solids: zillions of atoms, bonded together, in three dimensions. The orbitals are delocalized over zillions and zillions of atoms; not just three, not just six, not just ten or seventeen or whatever. Zillions. And it's not just two electrons in one orbital which are involved. It's <u>zillions of electrons in zillions of orbitals</u>, <u>delocalized over zillions of atoms</u>. This extreme delocalization is what makes metallic bonding. It's what makes a metal a metal. It's what allows metals to conduct electricity.

The main approach to understanding metallic bonding is called Band Theory, which is an extension of the Molecular Orbital Approach. In order to reach Band Theory from our MOA coverage, let me make a few additional, brief points. We have seen with MOA that a number of atomic orbitals interact to form the same number of molecular orbitals. We have also seen that, although some MOs may have the same energy (such as the two in π_{2p} or in π_{2p}^{*}), in most cases there is a significant energy gap between the various levels of orbitals. The specific pattern of energy levels gives rise to the MO configurations for the ground state. Transitions to excited states are possible, but this can be expensive; many of these transitions cost a considerable amount of energy, much like transitions which we had covered in Chapters 20 and 21.

Now let's take this to the extreme.

Consider a zillion metal atoms bonding in a three-dimensional network. (For just one millimole of a metal, this number is 6.022×10^{20} atoms!) Depending on which metal we are dealing with, each atom

may have nine orbitals (one *s*, three *p* and five *d* orbitals) available for bonding. Each atom may also contribute one or several or many valence electrons for this bonding. For one zillion atoms all bonded together, we may have nine zillion molecular orbitals. Some will have the same energy. On the other hand, many will have energies which are extremely close to the energies of other orbitals simply because there are so many. In essence, the result is a spread of zillions of MO energy levels within some upper and lower limit. This is what I've tried to show at right. (OK, there aren't zillions of lines drawn, but there're enough to get the general idea.) Each line represents one energy level, but there could be many separate orbitals within each level. This gives rise to the term "band", whence the term "Band Theory". A band is a spread of zillions of orbitals of very close energies, and for which the overall energies are contained within some specific range. Between successive levels, the energy separation is extremely small. The key result of this is that the orbital energies are now so closely spaced that the price of excitation is extremely small. In fact, normal temperature can provide enough thermal energy to pay for some excitations. Let's see how that works and see some of the consequences.

zillions AOs ⇸ ⇸ ⇸ zillions MOs

(At 0 K)

these levels
are empty

◄◄◄

electrons fill
these levels
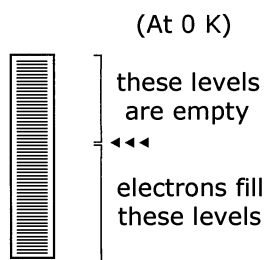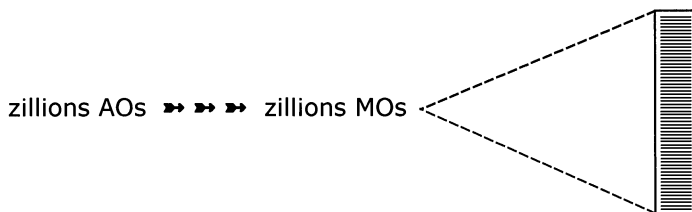
We start with everything in the ground state by removing all thermal energy. This means that we start at zero kelvin. Depending on the metal and on how many zillions of electrons are available, these electrons would fill the energy levels to some point in the band, an example of which is shown at left. The uppermost level of electrons at zero kelvin is called the Fermi level, shown by ◄◄◄ in the diagram at left.

Now, if we warm things up to ordinary temperatures, electrons in orbitals near the Fermi level can get excited into higher levels just by the thermal energy which is available. There are now electrons free to roam the orbitals just above the Fermi level, and that opens some spaces in the orbitals just below the Fermi level. Given the room to roam, and the fact that roaming involves delocalization over zillions of atoms, then it is very easy to actually move electrons around; this leads to electrical conductivity.

Although we can get some excitations with just thermal energy, you can still do excitations using photons. In fact, this gives metals their luster. Here's how that works. There are many levels at higher energies which have slightly different energies relative to each other; thus, you can get some transition with just about any energy and therefore involving just about any visible photon. For this reason, the metal absorbs virtually all wavelengths of visible light. Furthermore, relaxation occurs immediately after the excitation, and a photon of the same wavelength (and energy) is emitted. In essence, many of the photons that went in come back out as other photons, and that accounts for the reflectivity and luster. Most metals absorb and emit all visible photons pretty much the same, regardless of photon wavelength (color). Some metals, however, absorb and emit certain wavelengths better than others; as such, these metals also have a color, such as gold or copper.

As you can see, Band Theory accounts for numerous metallic properties. It also accounts for why metals tend to be strong and why metals are malleable. The strength is due to the three-dimensional network of chemical bonds. Malleability is a result of the extreme delocalization. Deforming a metal can change its physical shape and it can move the atoms around a bit, but the MOs are still there and they are still delocalized. Yes, metals can crack under repeated stress, but they can withstand such deformation better than can a typical ionic solid or a typical covalent network solid. But not all metals are strong solids, and there will be variations depending on specific cases. Some metals can be squeezed and deformed with your fingers. (Your fingers better be in gloves to do this since the soft metals are very reactive, including toward moisture). And then there's mercury which is a liquid at room temperature, but even the liquid metals still have metallic bonding and still conduct electricity.

This ends our discussion of metallic bonding. This ends our discussion of chemical bonding in general. In fact, this ends many things polyatomic, at least on the molecular scale. It is now time to weigh in on an even bigger scale.

Prepare to change the focus.

Problems

1. True or false.

   a. The σ_{2p} orbital is higher in energy than the σ^*_{2p} orbital.

   b. Antibonding electrons reduce the bond order.

   c. C_2 has a triple bond.

   d. All electrons in N_2 are spin paired.

   e. O_2^+ has three unpaired electrons.

   f. F_2 has a double bond.

   g. Every stable diatomic unit has more bonding electrons than antibonding electrons.

2. Give the configuration of each of the following. For each, what is the bond order? Is it diamagnetic or paramagnetic? How many unpaired electrons are there?

   a. C_2 b. O_2 c. N_2^- d. F_2^+

3. What is the bond order for each of the following configurations? How many unpaired electrons are in each?

   a. $(\sigma_{2s})^2(\sigma^*_{2s})^2(\pi_{2p})^3$

   b. $(\sigma_{2s})^2(\sigma^*_{2s})^2(\sigma_{2p})^2(\pi_{2p})^4(\pi^*_{2p})^4(\sigma^*_{2p})^1$

   c. $(\sigma_{2s})^2(\sigma^*_{2s})^2(\pi_{2p})^4(\sigma_{2p})^2$

   d. $(\sigma_{2s})^2(\sigma^*_{2s})^2(\sigma_{2p})^2(\pi_{2p})^4(\pi^*_{2p})^1$