Metallic Bonding

Skills to Develop

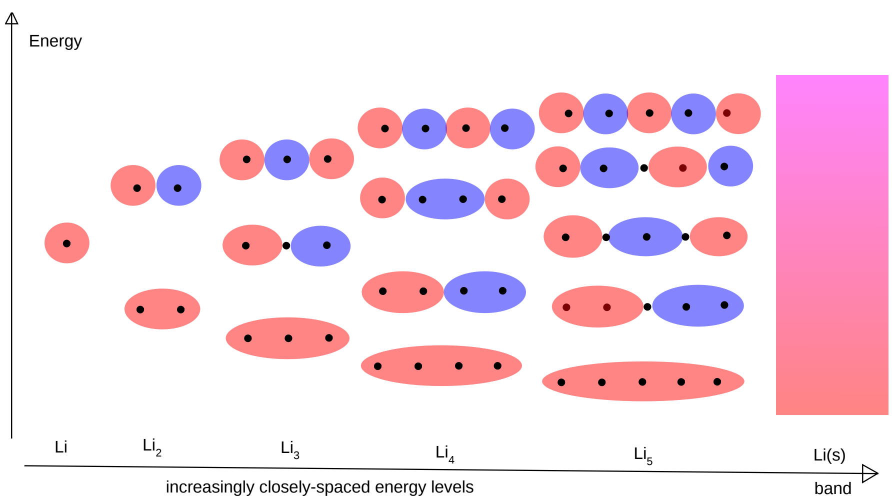
- Describe metallic bonding using MO theory

We previously discussed the "electron-sea model" of metallic bonding in the intro section and metal characteristics sections. This is a good time to review those sections, before we describe a better model. Why do we need a different model for metallic bonding than the electron-sea model? Although it explains some general properties of metals, like malleability and conductivity, it doesn't explain the relative properties of metals, like their hardness and melt points. These properties depend on how strong the bonding in the metals is. By the electron-sea model, we might think that more electrons makes the bonds stronger, so hardness and melt point would increase across the periodic table.

We can explain these properties using MO theory. In this case, we imagine combining many atomic orbitals (1 or more for each atom) to make and equal number of MOs that extend over the whole solid. Some MOs will have fewer nodes and be lower energy, while others will have more nodes and be higher energy. Each MO can hold no more than 2 electrons. Filling the lower energy MOs (bonding MOs) makes the bonds stronger, which is why alkali metals have low melt points and are soft (not many bonding MOs filled). Filling the higher energy MOs (antibonding MOs) makes the bonds weaker, which is why Cu, Ag, Au and Zn are soft and melt at low temperatures (Hg is a liquid at RT!).

When we have a really big number of MOs, some interesting things happen. One mole of Fe is about 7 mL or 7 cc (a pretty small amount). In each atom of Fe, we have 1 4s orbital, 5 3d orbitals, and 3 4p orbitals that can be involved in bonding. In a mole of Fe, we have 9 times Avogadro's number of AOs that can be involved in bonding. That's about 10^{24} AOs, which means the same number of MOs. There just isn't space to have much difference in energy between all those MOs. The MOs have to have energies not too different from the AOs (they are definitely higher and lower, but not by too much), so they are limited to a relatively narrow range of energies. This means that the energies form **bands** rather than separate energy levels.

We can start to see how this happens by imagining a line of Li atoms. As we increase the number of Li atoms, the orbitals get closer together. When the number of Li atoms reaches infinity, the MOs become infinitely close together.



Formation of a band in a chain of Li atoms: the MO energy levels become closer together as the number of MOs increases, until they are no longer separate.

Band theory explains the conductivity of metals: for electrons to move, electrons have to be able to change MOs without gaining much energy. If a band is partly-filled with electrons, they can easily change states because there are empty states almost the same energy as the full states. We can tell that the bands from s, p and d orbitals must overlap in metals, because the alkaline earth metals are conductors. If there were an energy gap between the s band and the p or d band, they would not conduct because the s band would be full.

Outside Links

- Clayton Spencer: Metals, Bonds, and Band Theory Part 1 (10 min)
- Clayton Spencer: Metals, Bonds, and Band Theory Part 2 (10 min)

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