Extended Solids and Ionic Bonding

Lecture 40

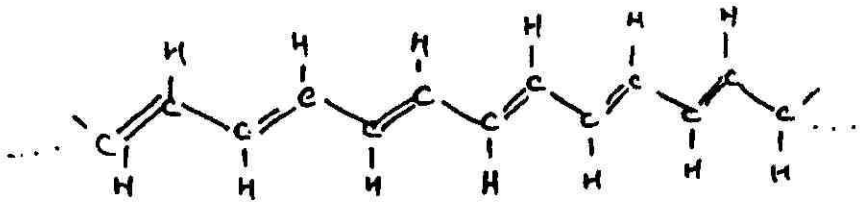
Bands and Localization.

① A lot of compounds are not normal molecules. The metals, plastics, glass (surrounding us) are all composed of large arrays of atoms all bonded to eachother. Our muscles, DNA bone and teeth (too) are all made of such large scale arrays.

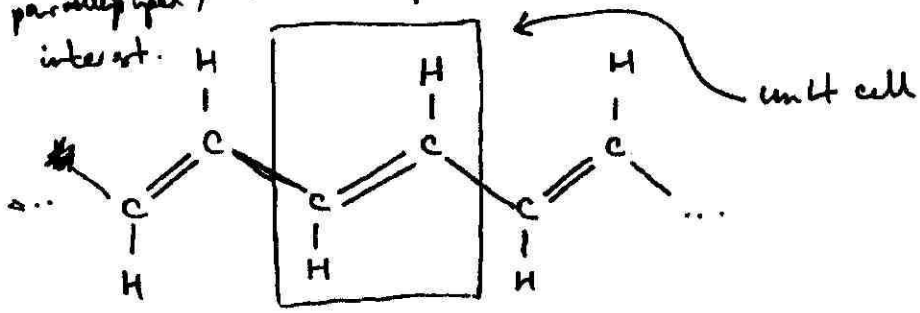
We call arrays which have 10^{15} or greater atoms all bonded into single units: extended solids. In these lectures we will look at the simplest of such extended solids, those with repeating units within them.

For example:

(polyacetylene)



② We note that our picture with dotted lines are a bit complicated. We therefore introduce the idea of the unit cell. The unit cell is a parallelogram (or in 3-D a parallelepiped) which repeats itself systematically in the extended solid of interest.



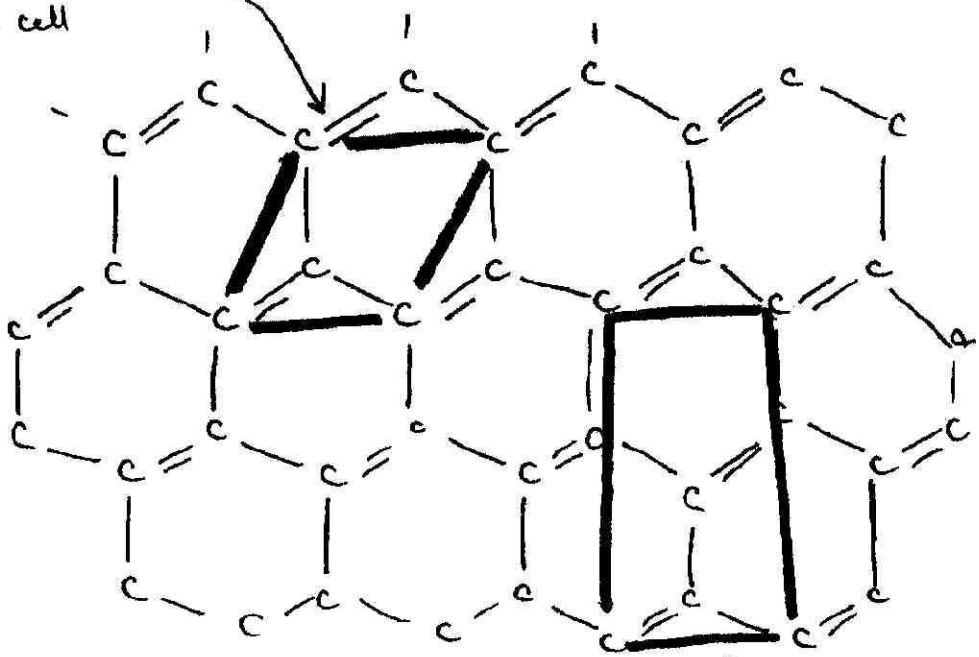
③ Extended solids for which there are unit cells are called crystals. It turns out most but not all extended solids can be viewed as crystals.

material	form
DNA	crystal or amorphous
muscle	crystal or amorphous
bone, teeth	crystal
metals	crystal
glass	amorphous
plastics	between amorphous, crystal

Those extended solids which do not have unit cells are called amorphous.

④ Let's consider one of the simplest possible crystals, graphite.

2 C in unit cell
A primitive cell

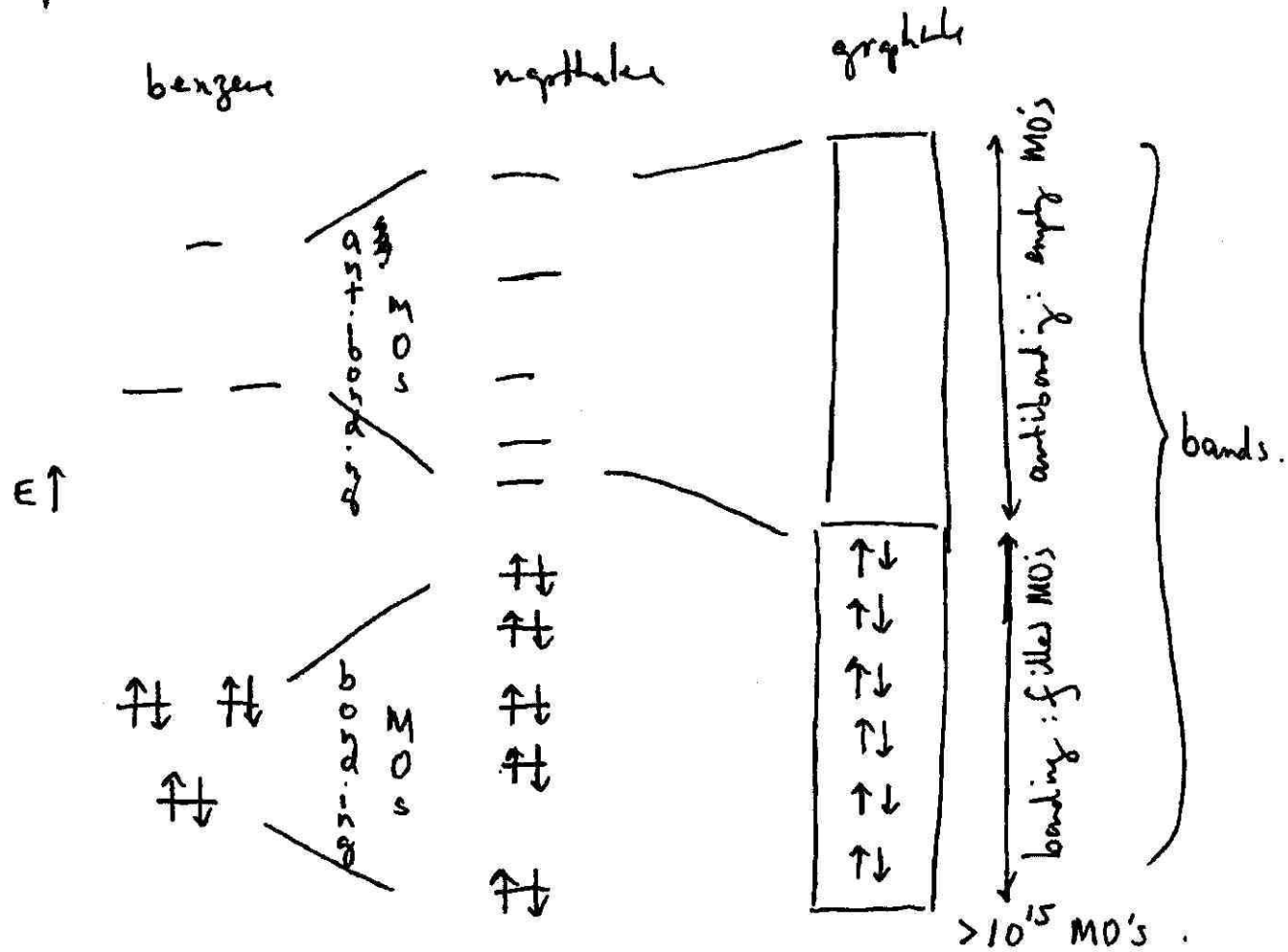


4 C in cell
Not the primitive cell!

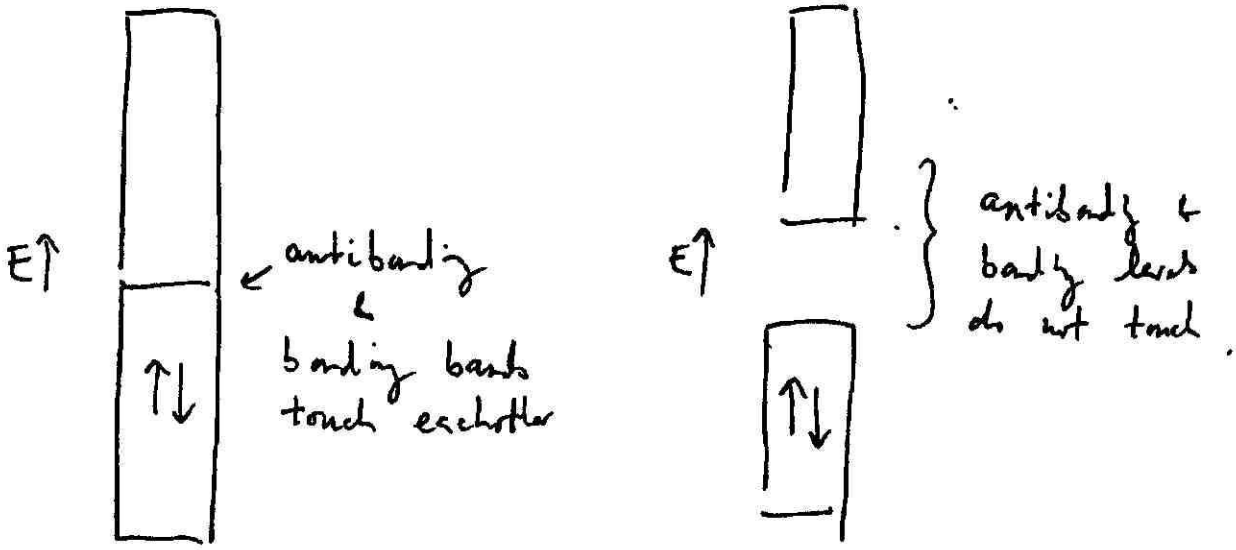
⑤ What does the MO of graphite look like?

That's a bit of a problem. By our rule 1 of MO diagrams the number of MOs = # AOs. Even in the small amount of graphite it takes to write a word there must be $>10^{15}$ atoms, & hence 10^{15} π AO's. That's a lot of MO's.

⑥ Yes, we know how to calculate these 10^{15} MO's. But, no, we will not study this in this course. Instead we will just make a few hopefully fairly simple observations. Let's just look at the π-MO's. Consider benzene → naphthalene → graphite.



⑦ In extended solids the MO's become bands. We can imagine 2 possibilities.



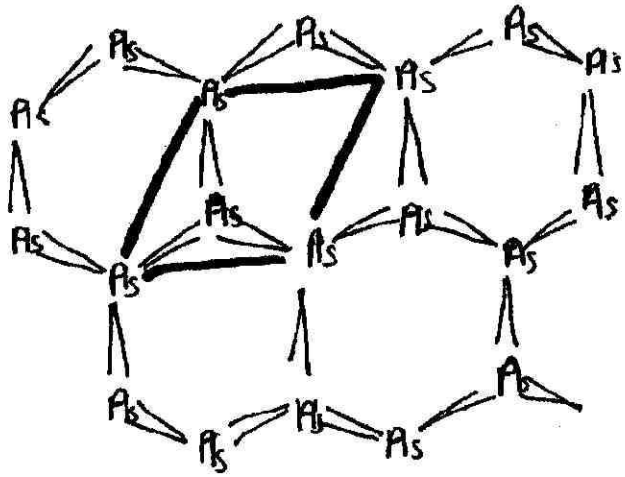
Ⓐ Metals Ⓑ Insulators

Ⓐ Metals : Colour varies from black (graphite) to red (copper) or yellow (gold). Most are silver colored.

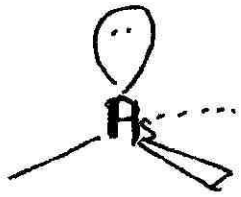
Ⓑ Insulators. Colours vary from black to all the other possible colours. Often clear.

⑧ For the remainder of this lecture we will think about case Ⓑ : Insulators. It turns out for almost all good insulators one can draw simple picture of their electronic configuration.

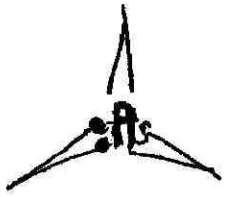
Example : Arsenic



Each As has one lone pair & three bonds.



side-view



top-view.

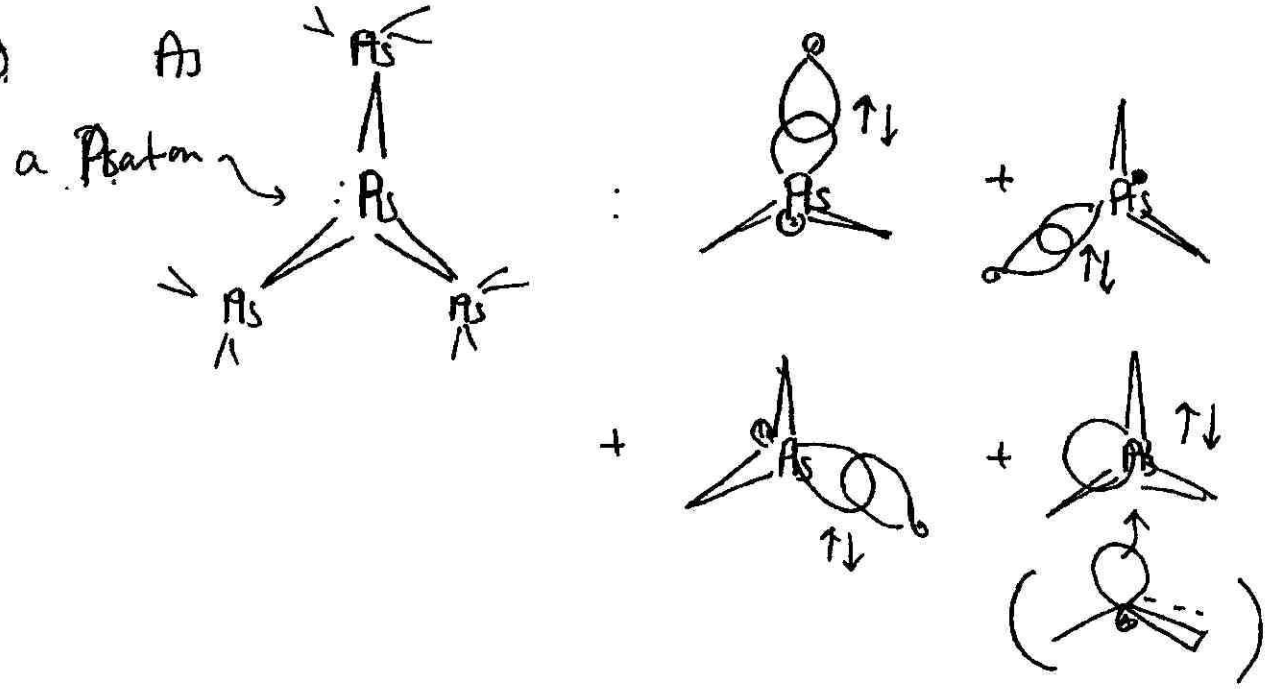
We can associate a pair of electrons with each bond & with the lone pair represented as ⁚.

⑨ Why is it possible for us to associate one pair of $\bar{e}$ with each bond? What does this have to do with MO theory?

⑭ For all molecules it is always possible (to my knowledge) to combine the MO's to make the Lewis picture.

We will use this fact for extended solids, where we do not know how to make the MO diagram.

⑮ As



⑯ We will use this understanding to study the structure of As, Sb, Bi and Se, Te & Po in the next lecture.