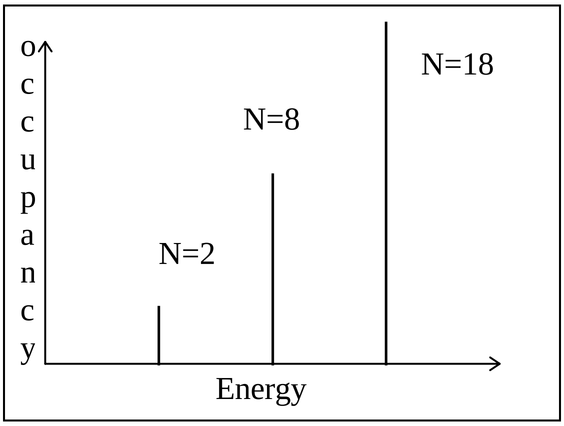
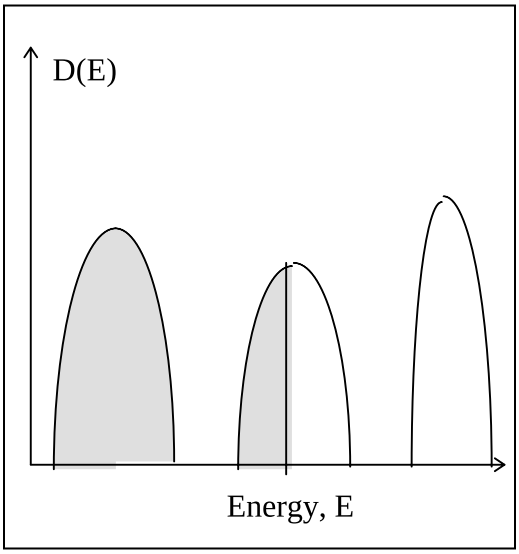
Electrons in condensed matter

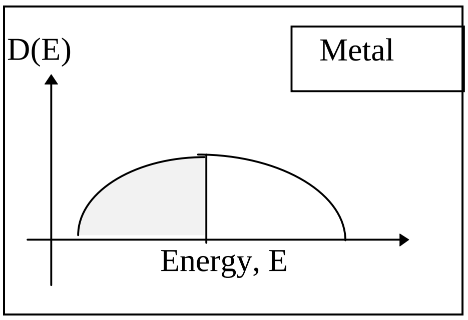
Introduction.



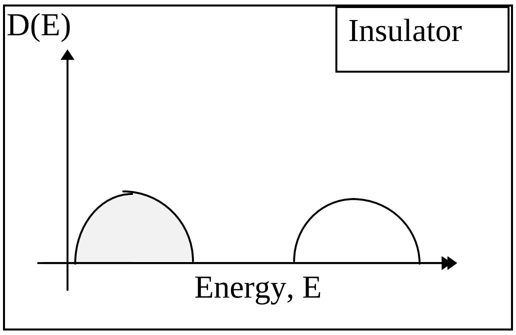
In atoms, electrons occupy discrete quantum states described by the quantum numbers n,l,m,m_s. These *electronic* states can be *degenerate*; states with up and down spin have the same energy in the absence of a magnetic field; in some cases angular momentum states have the same energy as well . The diagram on the left shows the occupancy of the states for a typical atom.

In materials, the electronic states of the atoms interact with each other to produce extended states spread throughout the crystal which are occupied by the electrons in the material. Since there are as many of these states as there were atomic states from the atoms that make up the crystal, there are very close together and the energy levels are almost continuous over much of the range. However, certain values of the energy are forbidden and we obtain bands of states with band gaps as with the lattice vibrations we considered before. A sketch is shown on the right. It is therefore convenient to use a *density of states* representation, where now the density of states *D(E)* is the number of electron states in the interval *E* and (*E+dE*). As with atoms, we fill the states in order of increasing energy, but obeying the exclusion principle. At zero temperature, we get (for metals) the position as shown in the shaded part of the diagram above. The energy of the highest filled state is called the *Fermi energy***.** The states of higher energy are the *empty states*

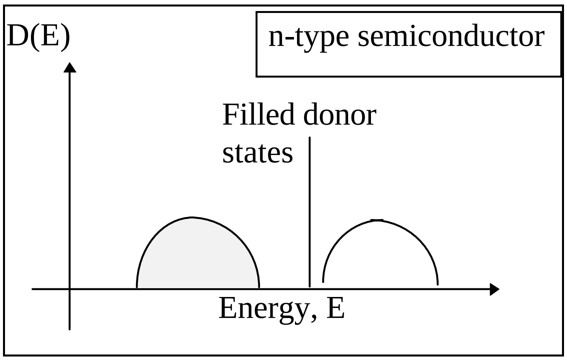


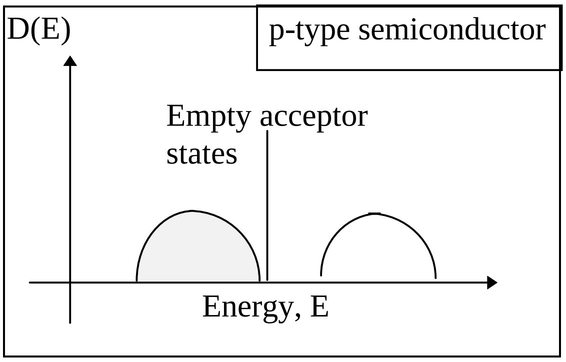


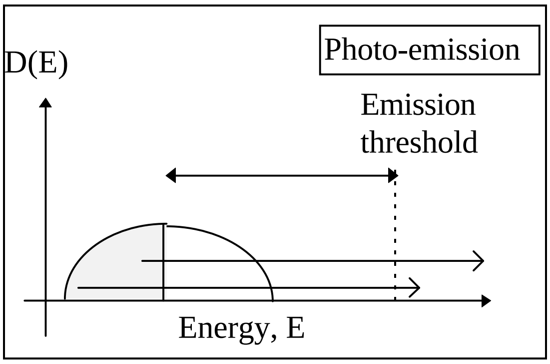
Effects of the band structure:
Electrical: The electrons in their lowest energy configuration have zero net velocity and no current flows (we will prove this later.) If a potential is applied across a material, some electrons can gain energy; they can only do this if there is a higher energy state for them to occupy at that energy. If the Fermi energy is within a band, finding these states is no problem, the material easily conducts current and we have a *metal*. If the Fermi energy is at the top of a band and there is a large gap (greater than about 3eV) between that and the



next one then we have an *insulator*. The filled band(s) are called valence band(s) and the empty bands conduction band(s). If the gap is smaller, thermal excitation will produce a small number of electrons in the conduction band of lowest energy. We have an *intrinsic semiconductor*; a temperature-dependent conductivity. It is also possible to produce temperature-dependent electrical conductivity by *doping* a semiconductor with suitable impurities - giving an *extrinsic semiconductor*. These impurities produce *localised* states in the band gap which can accept electrons from or donate electrons to the bands. If the result is an extra empty state close to the valence band (within a few tenths of an electron volt), then electrons from the valence band can be excited into this state leaving an unfilled band that can now conduct - we have an *p-type semiconductor*. If the result is an extra filled state close to the conduction band, an electron can be excited into the conduction band which can then conduct; we have an *n-type semiconductor*.

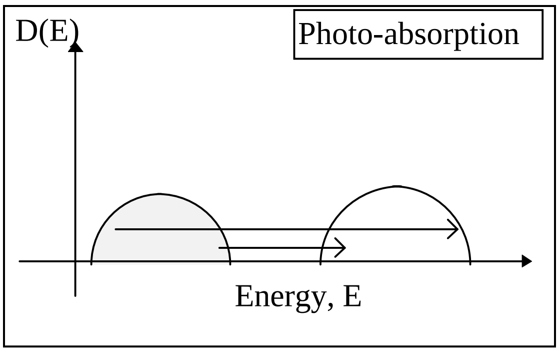






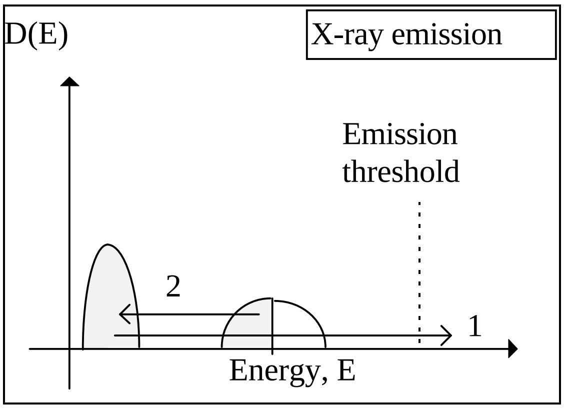
Optical: Photons can be absorbed by electrons (thus raising their energy by $\hbar\omega$ - the photo-electric effect). Two main effects occur:

Photoemission: If the photon energy is greater than the *work function* (the energy needed to ionise electrons at the Fermi energy - the double headed arrow in the diagram on the left) the electron absorbing the energy escapes from the material. If all the photons have the same energy, the distribution of energies of the electrons is characteristic of the structure of the bands. Single arrows on the left show the ejection of electrons.



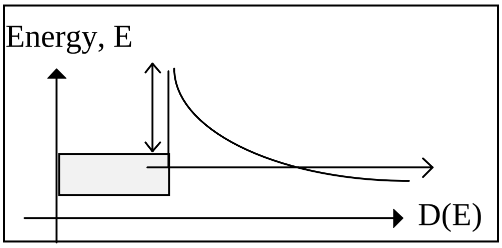
Photoabsorption: the electrons remain in the material. If the radiation has a wide range of frequencies; the spectrum of those absorbed gives information on the band structure. In *metals*, photons of any energy

can be absorbed - they are therefore opaque at all frequencies. In *insulators*, photons with energy less than the band gap are not absorbed. 3eV corresponds to a wavelength of about 900nm (in the visible). Insulators are often transparent, sometimes coloured depending on the size of the gap. *Semi-conductors* tend to be opaque in the visible region.
Photoconductivity. If photons of sufficient energy are shone onto an insulator or semi-conductor, they excite electrons from the valence to the conduction band and produce electrical conductivity.

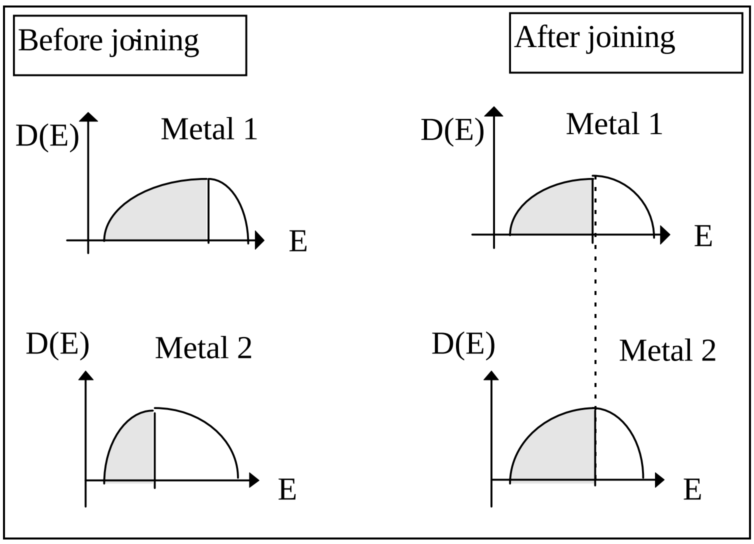


Miscellaneous
X-ray emission (Auger spectroscopy): If a material is bombarded by high-energy electrons, they will knock electrons out of the material, some of them in low energy states (arrow 1). Electrons in high-energy states will then fall into these states (arrow 2), emitting X-rays. The distribution of the X-ray energies is characteristic of the band structure of the material.

Thermionic emission. This is similar to photo-emission. If the work function is small enough, the energy to eject electrons from the material can be provided by heat.

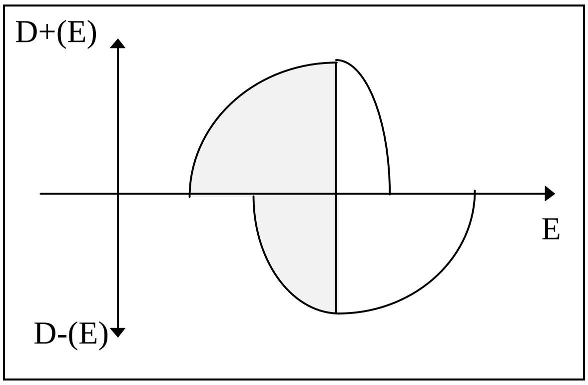


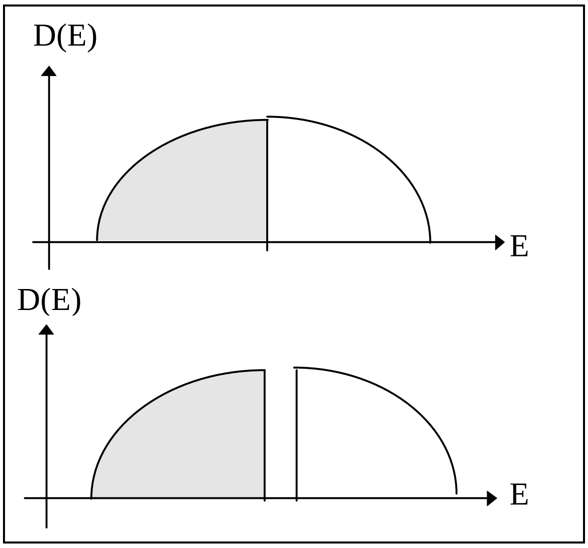
Field emission. If a metal is subjected to a strong enough potential difference (so that the energy of the escaped electron is lower than at the Fermi level, the electrons in the band can tunnel through the barrier represented by the work function (double-headed arrow in the diagram).



Contact potentials. If two metals with different work functions are joined, then electrons flow to the one with the higher work function (i.e. the one with electron states available at lower energy) as shown on the left. Since the nuclei (and any electrons tightly attached to the nuclei) cannot move, this produces a local dipole and a potential difference.

Ferromagnetism If the bands of the spin up and spin down electrons do not have the same energies, then one spin band is preferentially occupied. This gives macroscopic regions of net spin leading to magnetisation. We shall discuss the phenomenon of magnetism in solids in much more detail later on.





Superconductivity. A gap, caused by electron-lattice interactions, appears at the Fermi level. States below the gap are highly correlated (Cooper pairs) and the existence of the gap means that they cannot be scattered. The energy gap is of the order of kT_C where T_C is the *critical temperature*. Below this temperature, the material is a superconductor; above it the material is (usually) a normal metal. We give a brief introduction to superconductivity at the end of the course.