Quantum Approach To Solids

Introduction

We know that atoms and electrons obey the laws of physics,

- Electromagnetism
- Quantum Mechanics
- Classical Mechanics (incl. relativity)

Unfortunately in solids there are far too many atoms to analyse each one individually, so we generally observe *emergent phenomena* and create models based on our observations, rather than deriving everything from first principles.

A Couple of Crystal Structured Solids

Graphite and Diamond are two different ways of arranging the same element, Carbon. The reason there are two different materials is that different materials are formed under different conditions, for example, diamond is formed when carbon is put under a lot of pressure over a long time period.

Graphite is built up as hexagonal layers on top of each other, each carbon is connected in 3 bonds. In diamond each carbon atom is connected in 4 bonds, creating a "cube-like" arrangement. Here are graphics depicting graphite and diamond's layouts respectively,
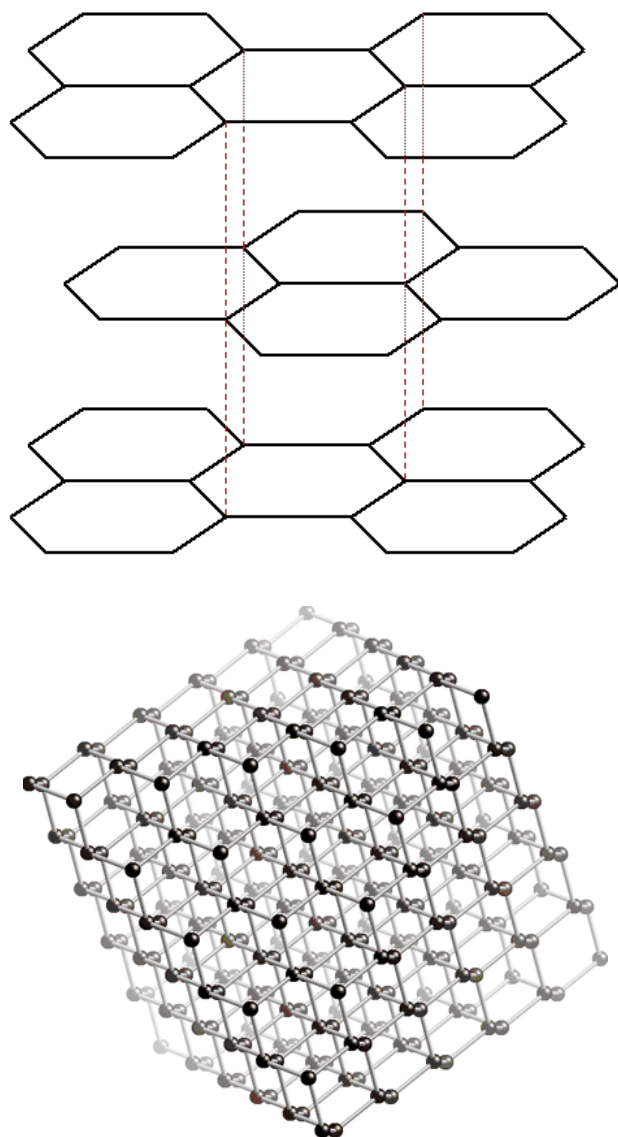
Electronic Configurations

Electrons fill up the orbitals around the nucleus, each shell (orbital) holding a fixed amount. Shells come in different "shapes" called orbitals, governed by the angular momenta of the electrons inhabiting the orbital, for this we give letters (s, p, d, e, f). Before the letter, we place a number to denote which type of that orbital it is. The last piece of this notation is that we use a superscript to show how many electrons are in that shell.

Here is an example of the element phosphorus in this notation,

$1\,s^2\ 2\,s^2\ 2\,p^6\ 3\,s^2\ 3\,p^3$
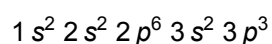
So, it has an inner s orbital with 2 electrons, another s orbital with 2 electrons, then a p orbital with 6 electrons and so on...

Bonding

Van der Waals force arises due to local electric dipoles forming between neighbouring electrons, this gives rise to weak electrostatic forces that obey LJ 6-12

There are three primary types of bonding,

- Covalent
- Metallic
- Ionic

There are also two secondary types of bonding,

- Van der Waals
- Hydrogen bonding