EE113FZ
Solid State Electronics
Lecture 4: Electron Shell Configuration

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What is to be Discussed Today?

- What is an electron shell?
- Electron shell configuration:
  - Shell identifiers;
  - Relative energy levels of shells and subshells;
  - How the shells and subshells fit together.
- How many electrons are there in a shell?
  - Principal quantum numbers and their effects;
  - Subshell configuration.

What We Know About Electrons in Atoms

- Electrons surround the nucleus in an atom;
- Electrons can only exist at particular energy levels due to quantisation;
- Electron orbitals have fairly defined shapes (Recall the wave equations from the previous lecture);
- The questions are:
  - How many electrons are there at each level and why?
  - What determines their orbital shape?

Electron Shell Configuration

- Electrons fill the shells following certain rules and these rules are defined by quantum mechanics:
  - Shell or principal quantum number (n): 1, 2, 3, 4, …
  - Angular momentum quantum number (ℓ): 0, 1, 2, …, (n-1)
  - Magnetic quantum number (m_l):
    $-\ell$, $(-\ell+1)$, $(-\ell+2)$, …, 0, …, $(\ell-2)$, $(\ell-1)$, ℓ
  - Spin quantum number (m_s): $\pm\frac{1}{2}$.

Can't remember? No problem.

The maximum number of electrons a shell with principal quantum number n can accommodate is $2n^2$.

Electron Shell Configuration

- The number of electrons that fit into each electron shell is given by

$$\text{No. of electrons} = 2n^2$$

  where n is the principal quantum number.
- So when $n = 1$, the max no. of electrons are $2(1)^2 = 2$.

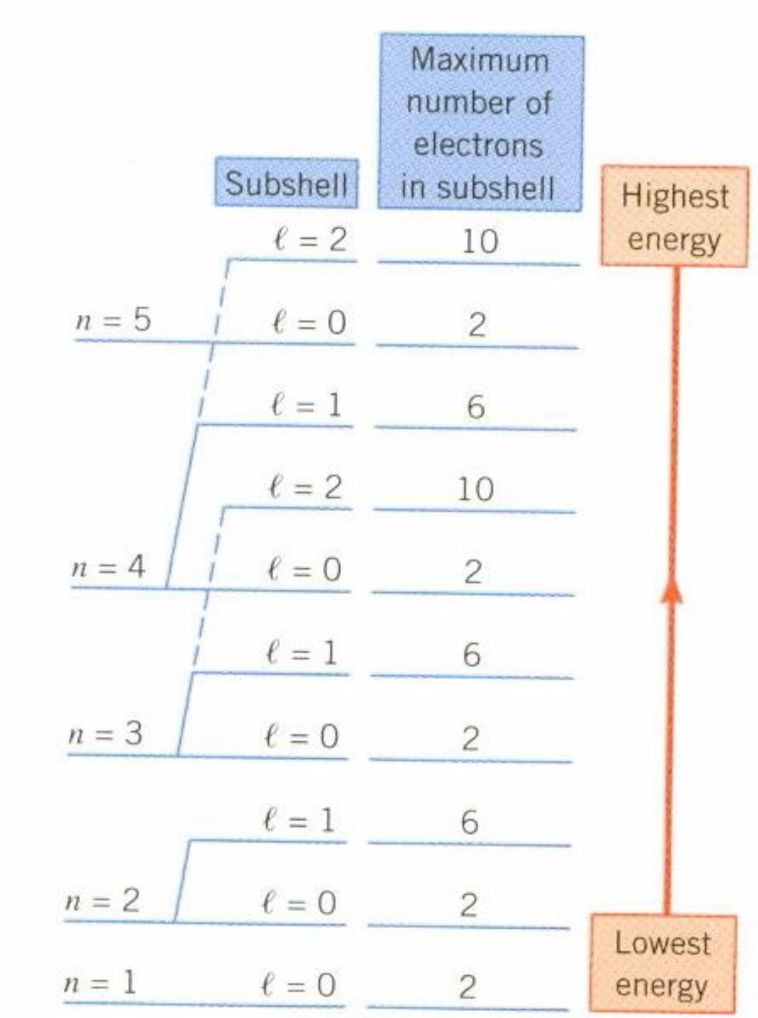
  If $n = 2$, then it's $2(2)^2 = 8$.

- Each shell also has a letter associated with it.

Electron Shell Configuration

Shell Number (Principal Quantum Number, *n*)	Shell Letter	Electron Capacity
1	K	2
2	L	8
3	M	18
4	N	32
5	O	50
6	P	72

How the Electron Shells Are Related?



- As *n* increases, more electron's can be accommodated in a shell;
- This also means that the number of subshells increases as does the total energy in the system.

Electron Shell Configuration

- There are rules about how the various quantum numbers (n, l, m_l and m_s) can combine;
- The principal quantum number, n, can never be zero. Allowed integer values are 1, 2, 3, etc;
- The angular momentum quantum number, l, can be any integer between zero (0) and (n-1);
- The magnetic quantum number, m_l, can be any integer between $-l$ and $+l$.

Subshell Configuration

- What happens when the effect of the angular momentum quantum number, *l*, is included?
- Effectively the inclusion of, *l*, gives extra shapes to orbitals that electrons can take;
- These subshells (collections of orbitals) also have letters associated with them;
- Each subshell can have different orbitals defined by the magnetic quantum number, m_l;
- Each orbital can only have 2 electrons (with different spin quantum numbers, m_s) ;
- Subshells first fill singly and then double up, according to the Pauli exclusion principle.

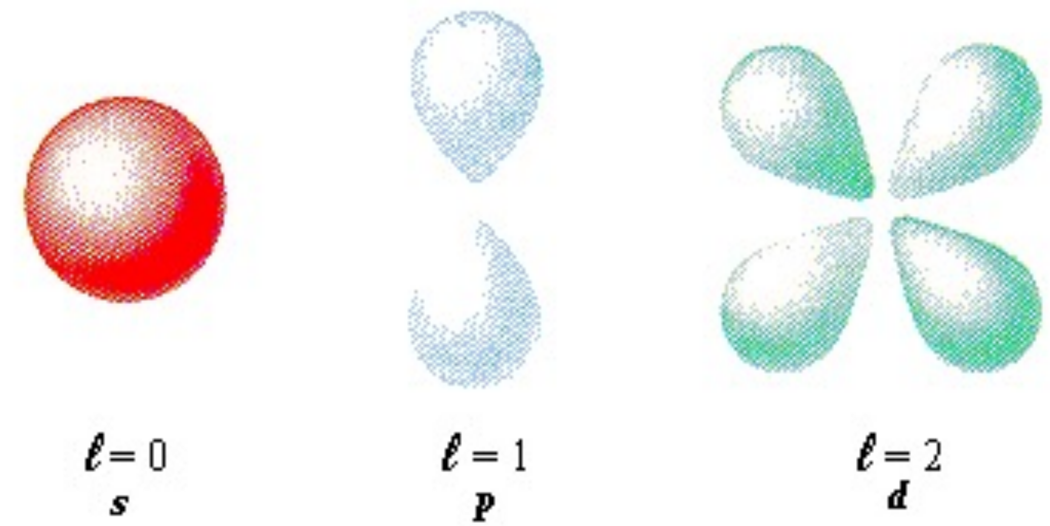
Shells, Subshells, and Orbitals

- We have used terms “shells”, “subshells”, and “orbitals” in our discussion. Let’s make a clear distinction between them;
- Shells are collections of subshells with the same principal quantum number, *n*;
- Subshells are collections of orbitals with the same principal quantum number, *n*, and the same angular momentum quantum number, *l*.

Subshell Shapes

- The angular momentum quantum number, *l*, describes the shape of the subshell;
- These are spherical (*l* = 0), polar (*l* = 1), cloverleaf (*l* = 2).

This is not strictly true but we do not want to bog ourselves down here.

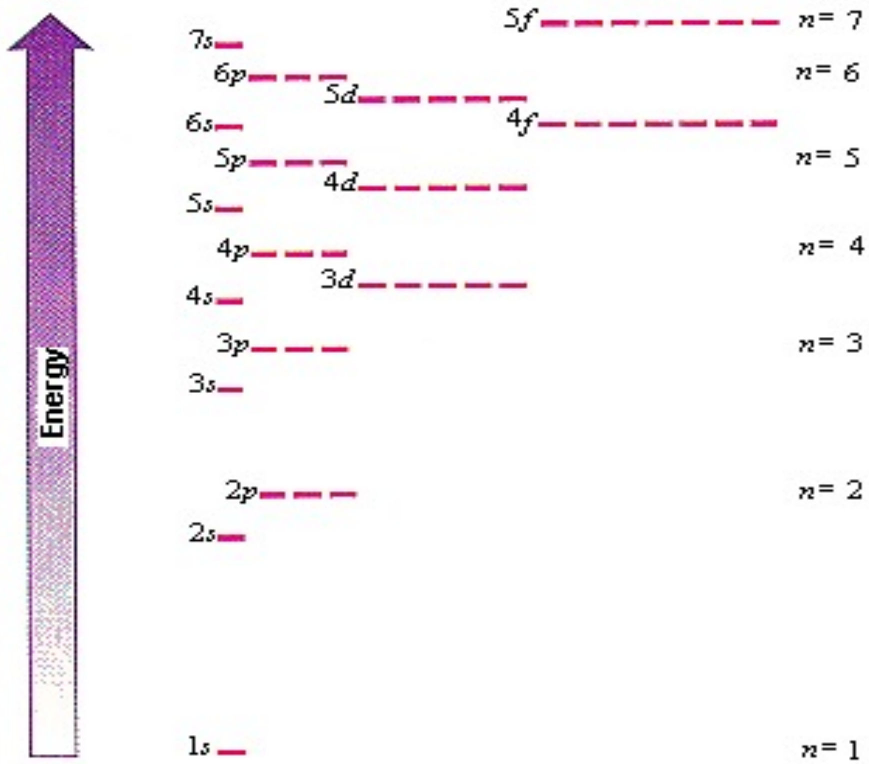


http://chemed.chem.purdue.edu/genchem/topicreview/bp/ch6/quantum.html

How do All the Orbitals Fit Together?

- n gives the shell and hence the number of electrons in that shell;
- Then l gives the subshell. Subshells also have their labels:
  - $l = 0$, subshell is called *s*,
  - $l = 1$, subshell is *p*,
  - $l = 2$, subshell is called *d*,
  - $l = 3$, subshell is called *f*.
- Each subshell can have a few orbitals with different m_l's (One may understand m_l as defining the orientation of the orbitals; but strictly speaking, shapes and orientations are correlated).

Electron Subshell Configuration



- You may have noticed that the 3*d* subshell has a higher energy level than the 4*s* subshell. Yes, it is indeed true. Energies of electrons are not only decided by their principal quantum numbers.

http://chemed.chem.purdue.edu/genchem/topicreview/bp/ch6/quantum.html

Electron Shell Configuration

Shell name	Subshell name	Subshell max electrons	Shell max electrons
K	1s	2	**2**
L	2s	2	2 + 6 = **8**
	2p	6	
M	3s	2	2 + 6 + 10 = **18**
	3p	6	
	3d	10	
N	4s	2	2 + 6 + + 10 + 14 = **32**
	4p	6	
	4d	10	
	4f	14	

- Each subshell has a letter;
- Each subshell has at least an orbital where electrons can be located;
- Each orbital has a shape, such that orbitals don't interfere with each other.

Electron Subshell Total Electron Calculation

- Each subshell can hold $(4l + 2)$ total electrons;
- Recall when $n = 1$, shell is *K* and l can only be 0. So subshell is *s.* Therefore, the total number of electrons is:

  $((4*0) + 2) = 0 + 2 = 2$;
- Recall when $n = 2$, shell is L and l can be 0 or 1, so subshell is *s* and *p.* Therefore, the total number of electrons is:

  $((4*0)+2)$[*s* subshell] $+((4*1)+2)$[*p* subshell] $= 2 + 6 = 8$.

Satisfy yourselves that this is correct for all shell numbers.

Applications of the Theory

- We can do calculations for
  - The energy levels of electrons;
  - Size of the radius of the orbitals;
  - The electron shell configuration;
  - The number of electrons in each shell, subshell, and orbital (2);
  - The amount of energy gained or lost when an electron moves from one orbital to another;
  - The effect of that movement.