# Atoms in general

- if we ignore $e^- - e^-$ interactions
  - then electrons each exist in a "hydrogenic" state $nlm$

$$a \to \frac{1}{Z} a \qquad E \to Z^2 E$$

(assuming nucleus is a point)

but only two electrons can have same values of $n, l, m$.

Electrons fill up hydrogenic "orbitals" ~~starting~~ from lowest energy up.

$n=1,\ l=0,\ m=0$

$n=2,\ l=0,\ m=0$

$n=2,\ l=1,\ m=-1, 0, +1$

$\vdots$

$\rho = \frac{r}{an}$

$r = an\rho$

$n$: shell

$l$: subshells

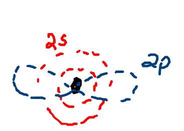
$(2l+1)\,2$ electrons in each subshell

$l=0$: s
$l=1$: p
$l=2$: d
3: f
4: g
$\vdots$

In hydrogen $E = -\frac{E_1}{n^2}$ no $l$ dependence.

in atoms, $E$ depends on $l$ too.


larger $l$, electron hangs out farther away




2p sees an effective nuclear charge smaller than $Ze$.

inner electrons <u>shield</u> the nucleus

result is a higher energy (less negative)

so larger $l$ $\longrightarrow$ larger energy
(b/c of $e^- - e^-$ interactions)

$n=2,\ l=1$
$n=3,\ l=0$ Na & Mg
$n=3,\ l=1$ Al – Ar
$n=4,\ l=0$
$n=3,\ l=2$ $\longleftarrow$ for $l=2$ shielding is so effective that it raises energy above next shell's s subshell

| Group→ ↓Period | 1 | 2 | | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 H | | | | | | | | | | | | | | | | | | 2 He |
| 2 | 3 Li | 4 Be | | | | | | | | | | | | 5 B | 6 C | 7 N | 8 O | 9 F | 10 Ne |
| 3 | 11 Na | 12 Mg | | | | | | | | | | | | 13 Al | 14 Si | 15 P | 16 S | 17 Cl | 18 Ar |
| 4 | 19 K | 20 Ca | | 21 Sc | 22 Ti | 23 V | 24 Cr | 25 Mn | 26 Fe | 27 Co | 28 Ni | 29 Cu | 30 Zn | 31 Ga | 32 Ge | 33 As | 34 Se | 35 Br | 36 Kr |
| 5 | 37 Rb | 38 Sr | | 39 Y | 40 Zr | 41 Nb | 42 Mo | 43 Tc | 44 Ru | 45 Rh | 46 Pd | 47 Ag | 48 Cd | 49 In | 50 Sn | 51 Sb | 52 Te | 53 I | 54 Xe |
| 6 | 55 Cs | 56 Ba | * | 71 Lu | 72 Hf | 73 Ta | 74 W | 75 Re | 76 Os | 77 Ir | 78 Pt | 79 Au | 80 Hg | 81 Tl | 82 Pb | 83 Bi | 84 Po | 85 At | 86 Rn |
| 7 | 87 Fr | 88 Ra | ** | 103 Lr | 104 Rf | 105 Db | 106 Sg | 107 Bh | 108 Hs | 109 Mt | 110 Ds | 111 Rg | 112 Cn | 113 Uut | 114 Fl | 115 Uup | 116 Lv | 117 Uus | 118 Uuo |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| * | 57 La | 58 Ce | 59 Pr | 60 Nd | 61 Pm | 62 Sm | 63 Eu | 64 Gd | 65 Tb | 66 Dy | 67 Ho | 68 Er | 69 Tm | 70 Yb |
| ** | 89 Ac | 90 Th | 91 Pa | 92 U | 93 Np | 94 Pu | 95 Am | 96 Cm | 97 Bk | 98 Cf | 99 Es | 100 Fm | 101 Md | 102 No |

2s
3s
4s
5s
6s
3d
4d
5d
4f
2p
3p
4p
5p
6p

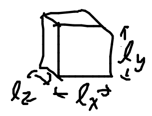
Solids (5.3)

Valence electrons (outermost) in a solid become "detached" from atoms & roam freely through material

i.e. valence electrons are affected by total potential inside solid from all atoms, not just one atom.

1) Free Electron Gas

- put electrons in a box




$V = 0$ inside

$V = \infty$ outside

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi(x,y,z)$$

$$\psi(x,y,z) = X(x)Y(y)Z(z)$$

$$-\frac{\hbar^2}{2m}X''(x) = E_x X(x) \qquad \text{etc.}$$

$$E = E_x + E_y + E_z$$

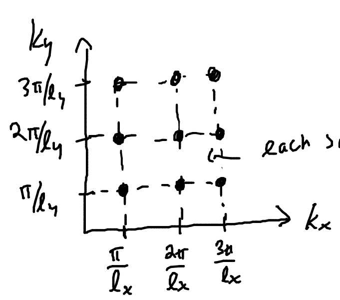
Let $k_x = \frac{\sqrt{2mE_x}}{\hbar}$ etc.

$$X(x) = A_x \sin k_x x \qquad k_x = \frac{n_x \pi}{l_x} \qquad n_x = 1,2,3,\ldots$$

$$E = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{l_x^2} + \frac{n_y^2}{l_y^2} + \frac{n_z^2}{l_z^2}\right) =$$

Define $\vec{k} = k_x\hat{x} + k_y\hat{y} + k_z\hat{z}$ $\qquad k_x = \frac{n_x\pi}{l_x}$

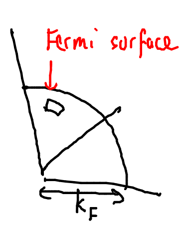
$$E = \frac{\hbar^2|k|^2}{2m}$$




each square has volume $\frac{\pi^3}{l_x l_y l_z} = \frac{\pi^3}{V}$

With $N$ electrons they fill up states 2 at a time from smallest energy upward

forms on $\frac{1}{8}$th sphere




volume of sphere is

$$\frac{1}{8}\left(\frac{4}{3}\pi k_F^3\right) = 2\,V_{\substack{\text{electron}\\ \text{state}}}\,\underbrace{N}_{\text{\# of electrons}}$$

$$2\frac{\pi^3}{V}N$$

$$k_F = \left(3\underbrace{\frac{N}{V}}_{\rho:\ \text{electron density}}\pi^2\right)^{1/3}$$

$$E_F = \frac{\hbar^2}{2m}k_F^2$$

Fermi energy
largest energy of an electron in a solid in its ground state