Bonding in solids

1/ Bohr model $E_n = \frac{-me^4}{8\epsilon_0 h^2 n^2} = \frac{-13.6\,eV}{n^2}$

$$r_n = \frac{n^2 h^2 \epsilon_0}{\pi m_e e^2} = n^2 a_0 \quad \text{where } a_0 = 0.53\,\mathring{A}$$

$E_2 = -3.39\,eV$
$r_2 = 2.1\,\mathring{A}$
$E_3 = -1.5\,eV$
$r_3 = 4.8\,\mathring{A}$

(−) indicates that these are bound states. That is, to unbind or free the e^- requires an input of 3.39eV.

$$\underbrace{-3.39\,eV + 3.39\,eV = 0}_{E \geq 0 \text{ free } e^-}$$

2/ (a) $\frac{k|q|^2}{r^2} = \frac{mv^2}{r} \rightarrow v = \sqrt{\frac{kq^2}{mr}}$

(b) $E = \frac{1}{2}mv^2 - k\frac{e^2}{r}$

* in potential, $q_1 = e$, $q_2 = -e$ so overall $U < 0$

* kinetic energies are always positive $K > 0$

$$= \frac{1}{2}m\frac{ke^2}{mr} - \frac{ke^2}{r}$$

$$E = -\frac{1}{2}\frac{ke^2}{r}$$

(c) $L = mvr = n\hbar$ now let $v = \sqrt{\frac{kq^2}{mr}}$

$$m\sqrt{\frac{kq^2}{mr}}\, r = n\hbar$$

$$\frac{m^{\cancel{2}} kq^2 r^{\cancel{2}}}{\cancel{m}\cancel{r}} = n^2\hbar^2 \longrightarrow r = \frac{n^2\hbar^2}{kq^2 m}$$

now $\hbar = \frac{h}{2\pi}$, $k = \frac{1}{4\pi\epsilon_0}$

$$r = \frac{n^2 h^2 \epsilon_0}{\pi m e^2}$$

2/(d) $E = -\frac{1}{2}\frac{ke^2}{r} = -\frac{1}{2}\frac{ke^2}{n^2 h^2 \epsilon_0}\pi m e^2$ where $k = \frac{1}{4\pi\epsilon_0}$

$$E = -\frac{me^4}{8\epsilon_0 h^2 n^2}$$

3/ refer to any Modern text for the Pauli exclusion principle

4/

	n	l	m		states
1s :	1	0	0	x2 for spin	2
2s :	2	0	0		2
2p :	2	1	-1		6
		1	0		
		1	1		
3s :	3	0	0		2
3p :	3	1	-1		6
		1	0		
		1	1		
4s	4	0	0		2
3d	3	2	-2		10
		2	-1		
		2	0		
		2	1		
		2	2		
4p	4	1	-1		6
		1	0		
		1	1		

36 states → 36 electrons

$l: 0 \ldots n-1$ $\quad$ $m_l = -l \ldots +l$

5/ Na has 11 e^-

ground state e^- config $1s^2 2s^2 2p^6 3s^1$

6/ H → He ionization energy ↑

He → Li ↓

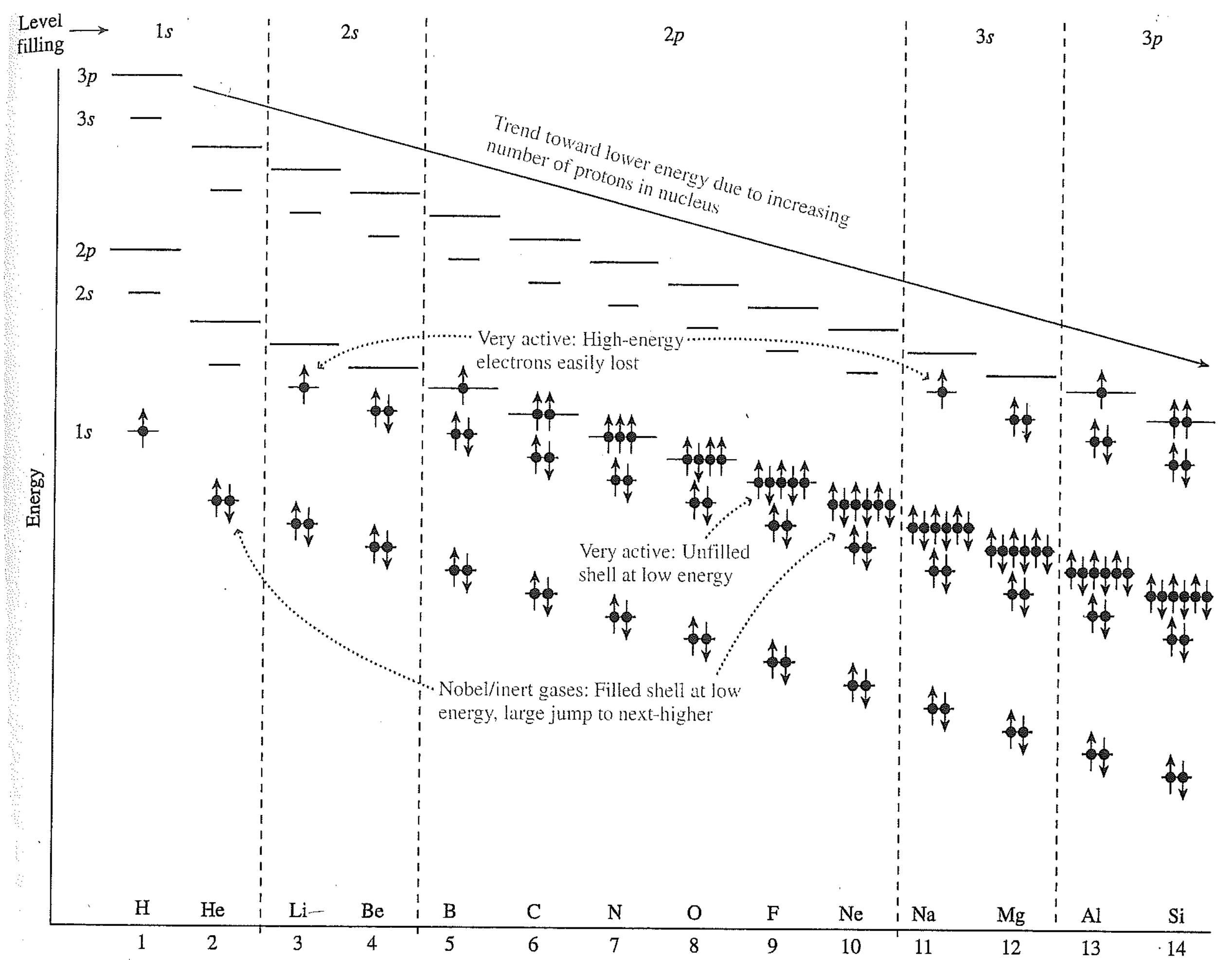
Li → Be ↑

Be → B ↓

B → C → N → O → F → Ne ↑

Ne → Na ↓

Harris, Mod. Phys 2nd ed.



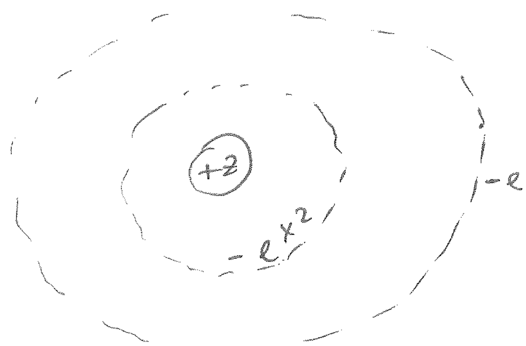
7/ (a) He : $Z = 2$ Li $Z = 3$. Assume e^- are in ground state $n = 1$

and $E = -13.6\ eV \frac{Z^2}{n^2}$

He: 54.4 eV

Li: 122 eV

(b) (c) Screening (or shielding) refers to the effect inner (or core) electrons have in lowering the attraction of the nucleus.



outer e^- sees smaller positive charge since there are inner e^- to "shield" the nucleus.

It's more effective in Li, since the outer most e^- in Li is at $n=2$, which is farther away from the nucleus than the inner $n=1$ electrons. (The n-value determines the radius $r_n = n^2 a_0$)

8/ see your text, the valence e^- take Part in bonding.

9/ (a) far right column. Highest ionization energies. Filled shell.

(b) far left (except Hydrogen). Relatively small ionizations. Barely populated outer shell.

(c) Column topped by Flourine. Large ionization energies. Almost filled.

10/ (a) for one Cl^- in a NaCl crystal $= 8.95\,eV$

If there are $6\cdot 10^{23}$ Cl^- ions

$$8.95\,eV \times (6\cdot 10^{23}) = 54\cdot 10^{23}\ eV$$

in Joules: $54\cdot 10^{23} \cdot 1.6\cdot 10^{-19}\,\frac{J}{eV} = 86\cdot 10^{4}\,J$

(b) the calc is exactly the same for Na^+. The lattice is cubic with Na^+ and Cl^- alternating positions.

$$86\cdot 10^{4}\,J\ ,\quad 54\cdot 10^{23}\,eV$$

(c) (d) one mole $= \dfrac{54\cdot 10^{23}\,eV + 54\cdot 10^{23}\,eV}{2} = 54\cdot 10^{23}\,eV$

in Joule... $860\ kJ$

11/ (a)

$$U(r) = -\int_{\infty}^{r}\left(-\frac{A a_0^2}{r^2} + \frac{B a_0^{10}}{r^{10}}\right)dr$$

$$= -\left[-\frac{A a_0^2\,(r)^{-1}}{-1} + \frac{B a_0^{10}\,r^{-9}}{-9}\right]_{\infty}^{r}$$

$$= \frac{-A a_0^2}{r} + \frac{B a_0^{10}}{9 r^9} - [0]$$

$$U(r) = \frac{-A a_0^2}{r} + \frac{B a_0^{10}}{9 r^9}$$

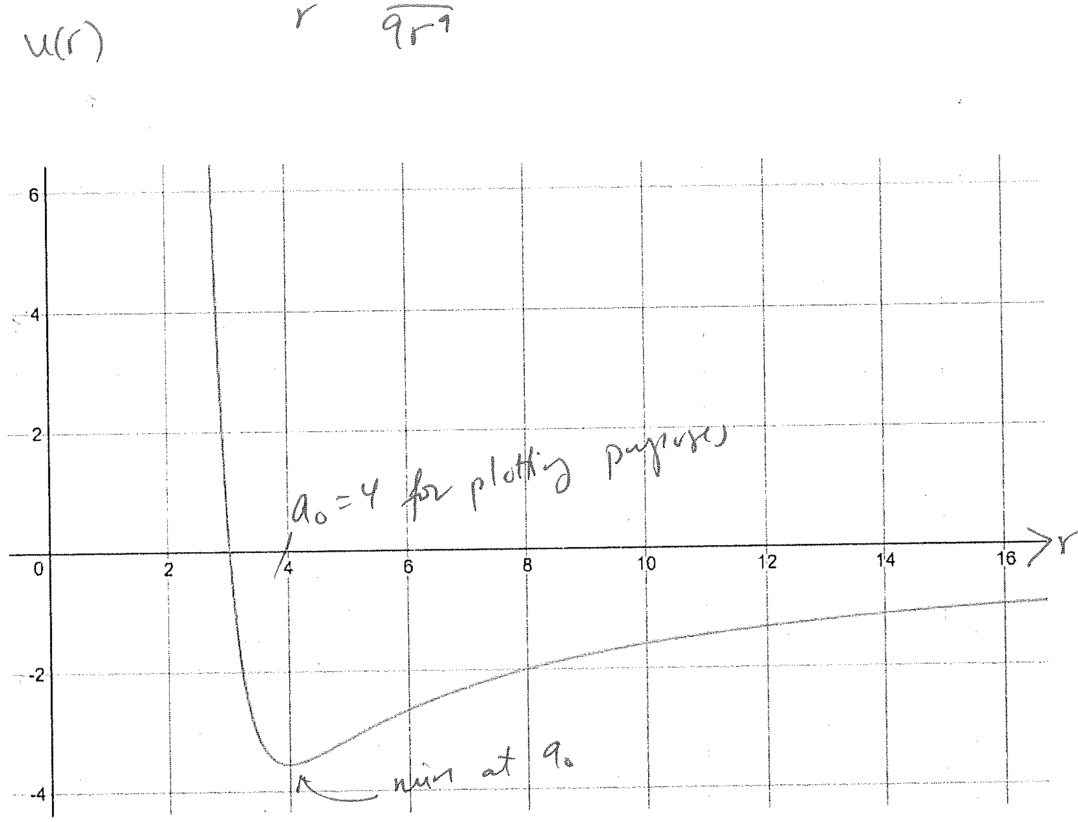
11/ (b) at equlbm, $F=0$

$$F(r=a_0) = 0 = -\frac{Aa_0^2}{a_0^2} + \frac{Ba_0^{10}}{a_0^{10}} = 0$$

$$-A + B = 0$$

$$\therefore A = B$$

(c) $$u(r) = -\frac{a_0^2}{r} + \frac{a_0^{10}}{9r^9}$$



12/ (a) $F_{coulomb} \propto \frac{1}{r^2}$ $F_{rep} \propto \frac{1}{r^{10}}$

$$\frac{F(2a_0)}{F(a_0)} = \frac{1}{4a_0^2}\,a_0^2 = \frac{1}{4}$$

$$\frac{F(2a_0)}{F(a_0)} = \frac{1}{2^{10}a_0^{10}}\,a_0^{10} = \frac{1}{1024}$$

r^{-2} drops to 25%

r^{-10} drops to 0.1%

r^{-10} drops much faster

(b) The energy is

$$E(r) = -\frac{Aa_0^2}{r} + \frac{Aa_0^{10}}{9r^9}$$

attraction Coulomb

repulsion.

for $r = a_0$ $$E(a_0) = -\frac{Aa_0^2}{a_0} + \frac{Aa_0^{10}}{9a_0^9}$$

$$= -Aa_0 + \frac{Aa_0}{9}$$

attraction, Coulomb

repulsion.

about $\frac{1}{9} \simeq 11\%$ decrease in energy

13/ H_2 covalent

LiF ionic

KF ionic

N_2 covalent

CH_4 covalent

CO_2 covalent

H_2O covalent

$NaCl$ ionic

Na_2S ionic

14/ optional/e.c.

See your text for more detail.

The conduction e^- act as the "glue" between ions. Ions are attracted to the free, conduction e^-.