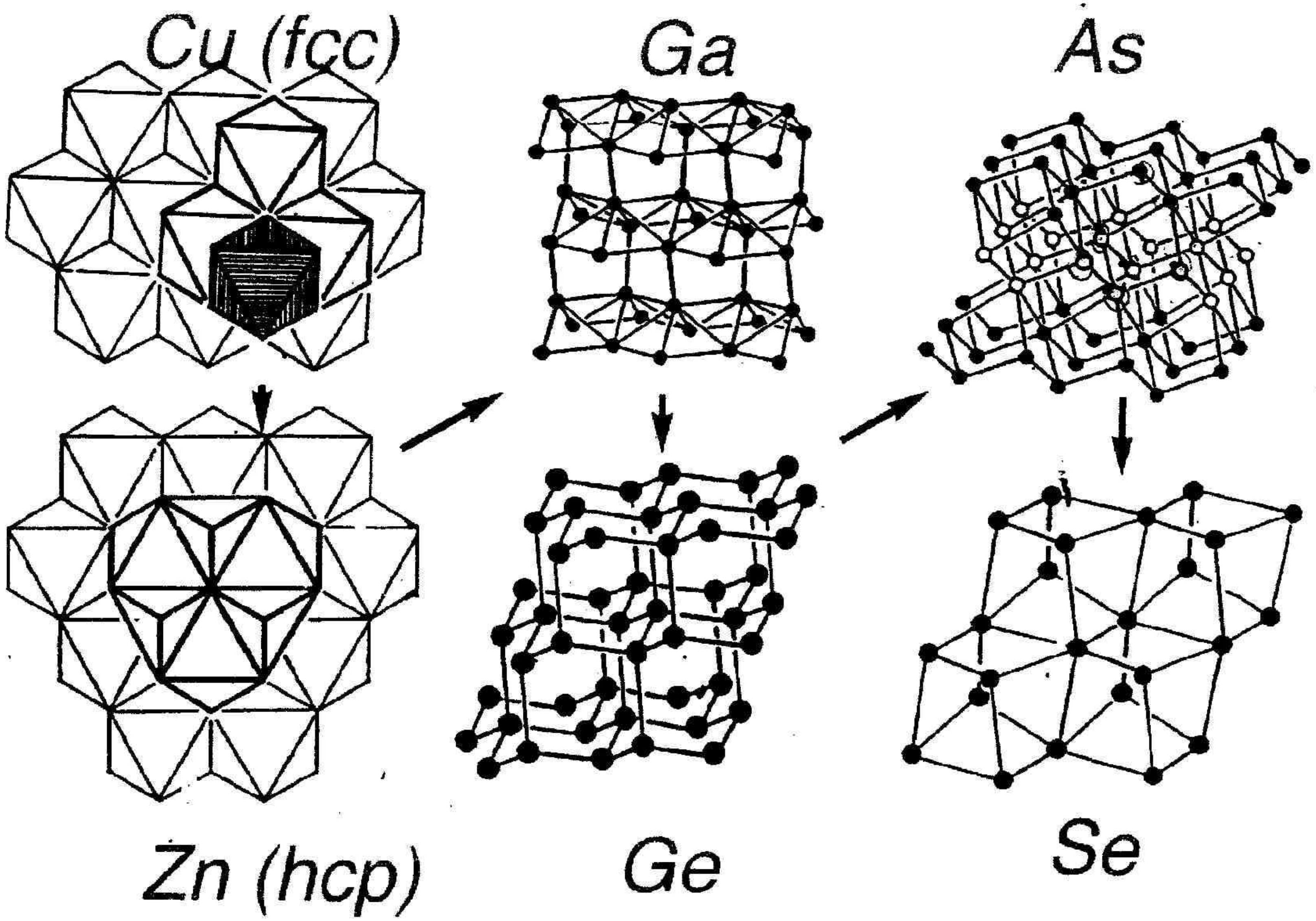
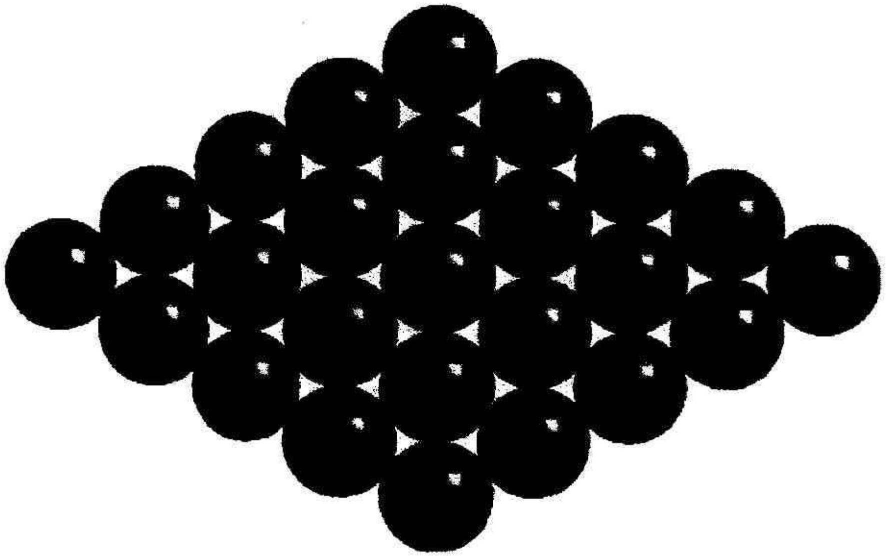
NON-METALS

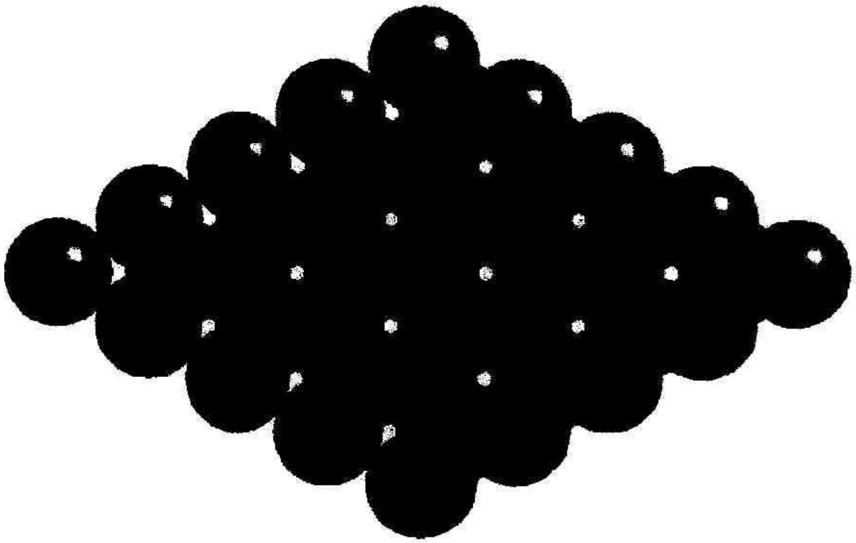
10	11	12	13/III	14/IV	15/V	16/VI	17/VII	18/VIII
								2 He 4.003
			5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
			13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
28 Ni 58.69	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	[redacted]	35 Br 79.90	36 Kr 83.80
46 Pd 106.4	47 Ag 107.9	48 Cd 112.4	49 In 114.8	50 Sn 118.7	51 Sb 121.8	52 Te 127.6	53 I 126.9	54 Xe 131.3
78 Pt 195.1	79 Au 197.0	80 Hg 200.6	81 Tl 204.4	82 Pb 207.2	83 Bi 209.0	84 Po 210.0	85 At 210.0	86 Rn 222.0

METALS


Cu (fcc)
Ga
As
Zn (hcp)
Ge
Se



2–D closest packing

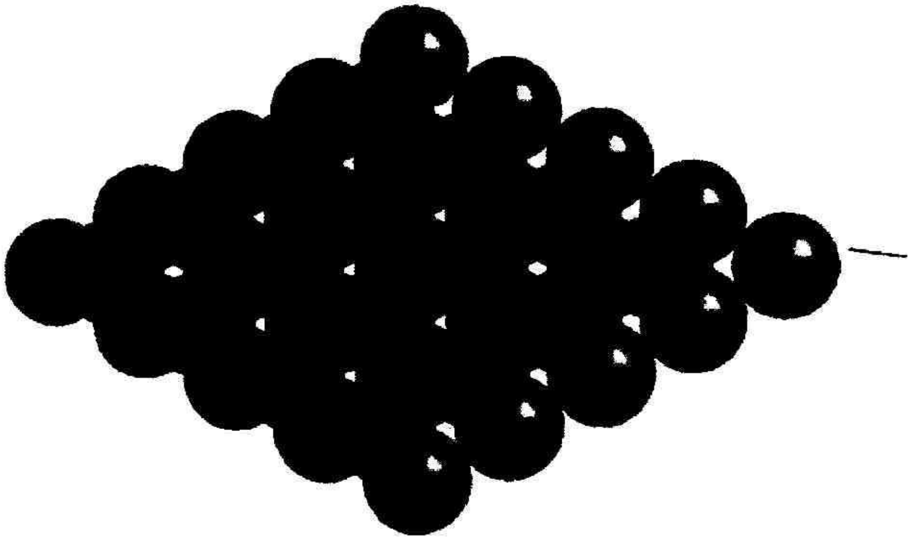


3–D closest packing

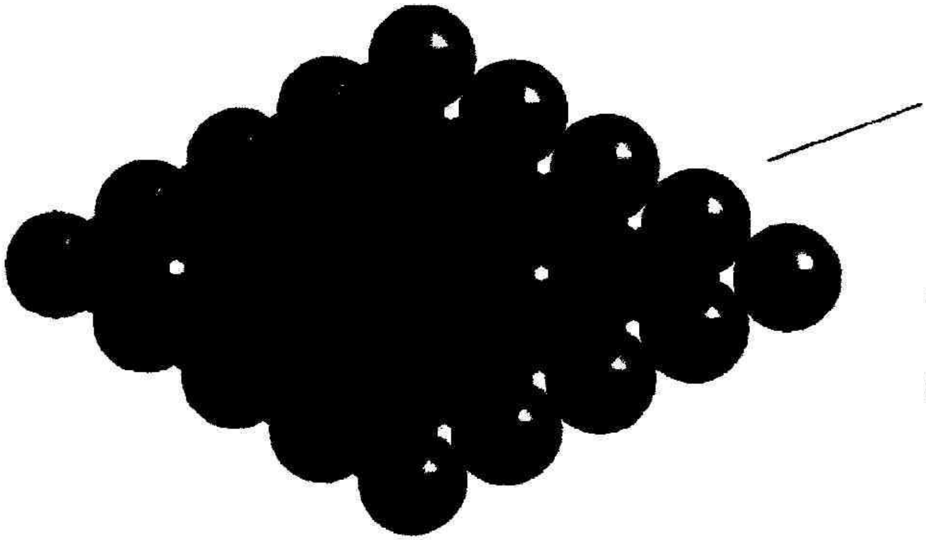
2nd layer sits in
dimples of first layer

3rd layer sits in dimples of 2nd layer

two possibilities for 3rd layer:

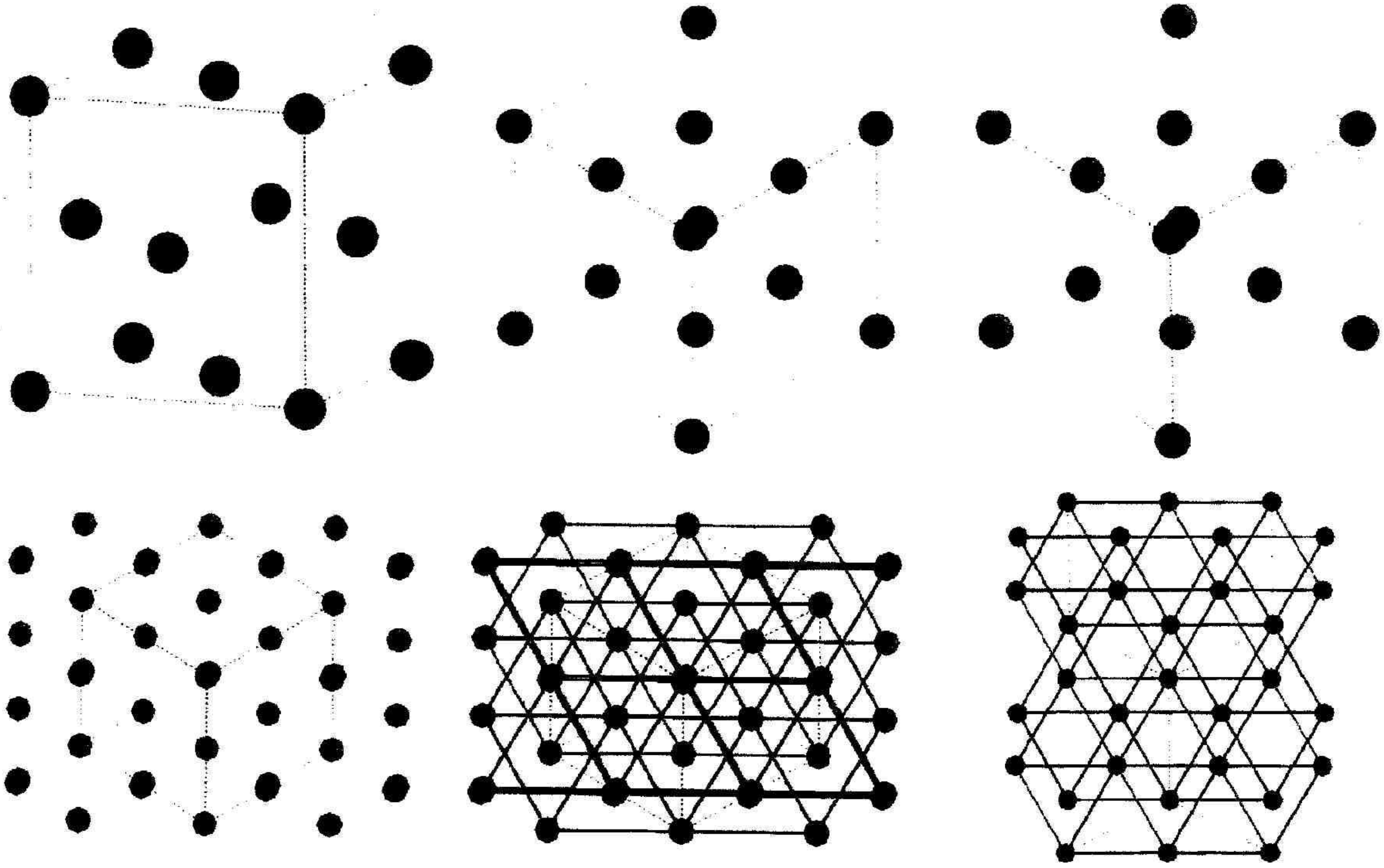


Directly above first layer: this is called hexagonal closest packed (hcp).



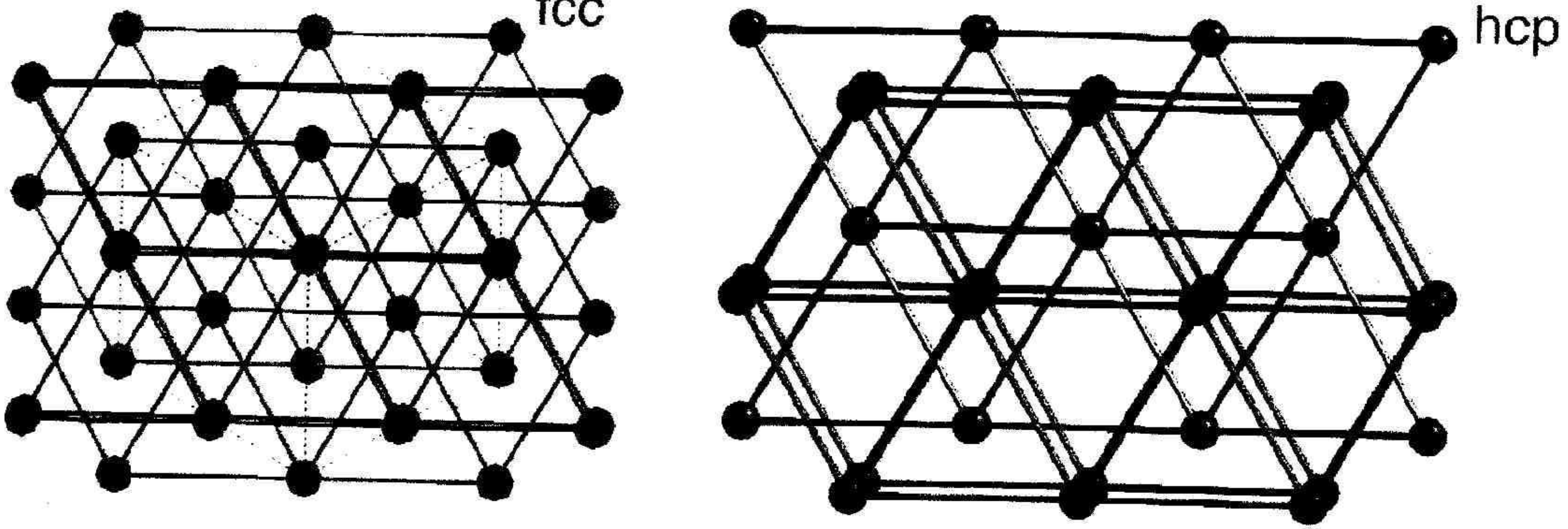
Directly above dimples of both 1st and 2nd layers: this is called face centered cubic (fcc).

fcc has a face centered cubic unit cell



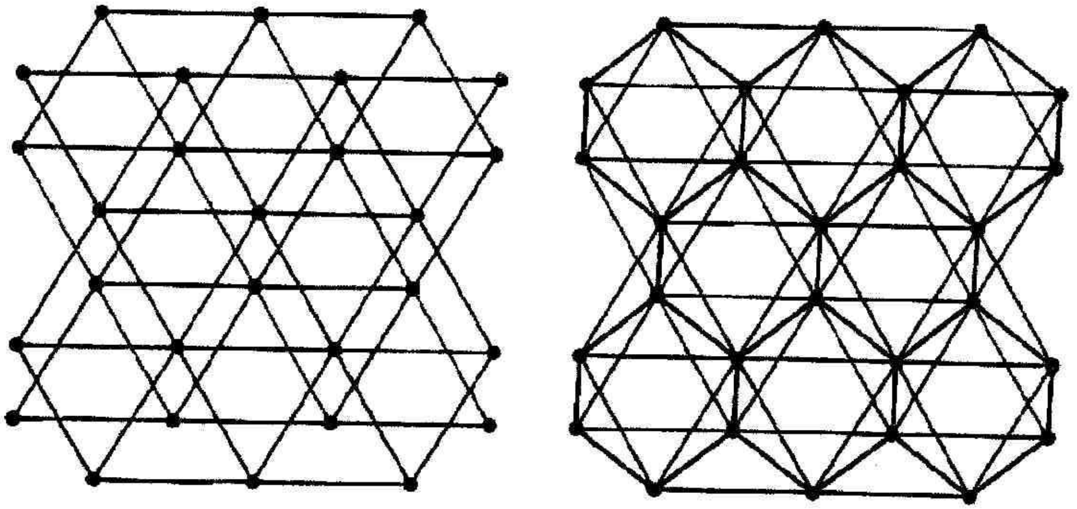
fcc: coordination number 12

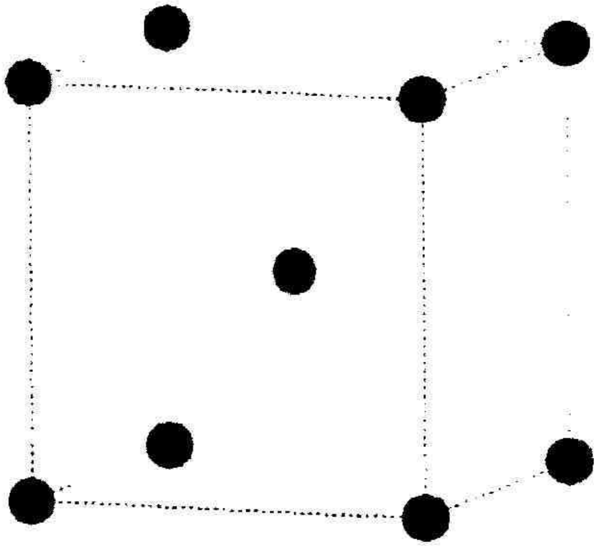
hexagonal closest packed (hcp) is a lot like fcc

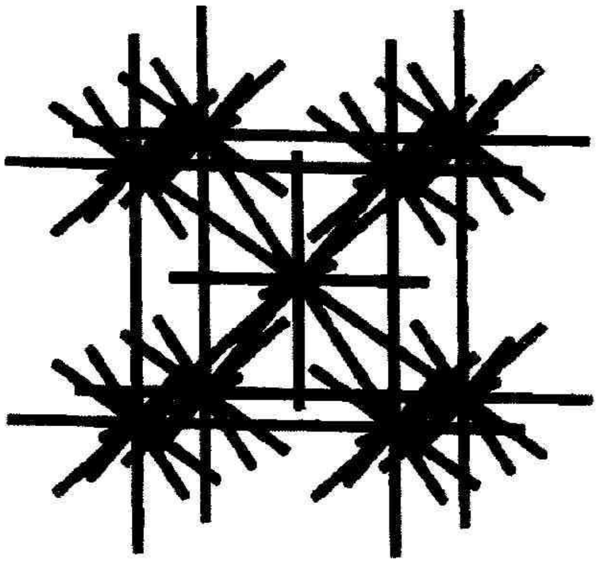


two layers of fcc and hcp look just the same.

the two layers form octahedral and tetrahedral voids.





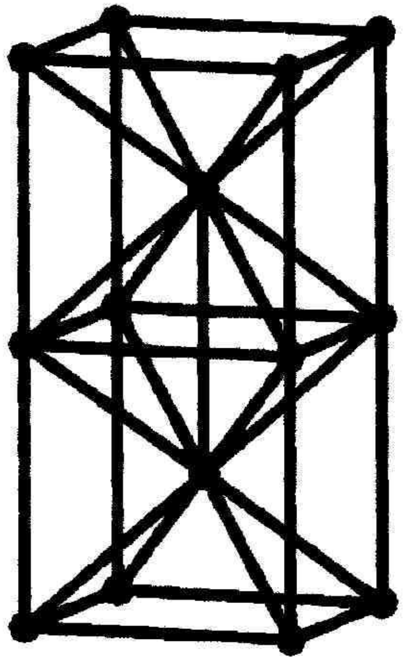


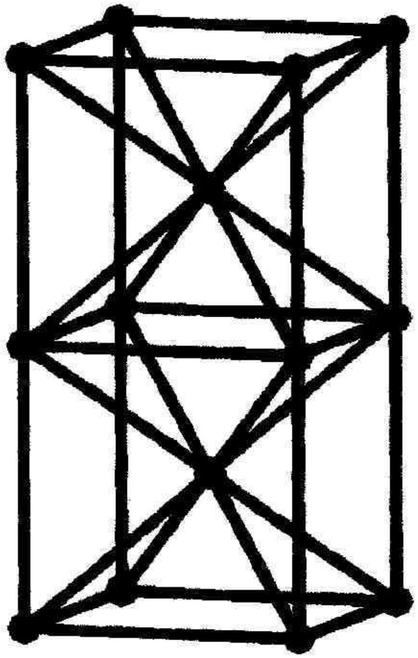
3rd common
metal
structure:

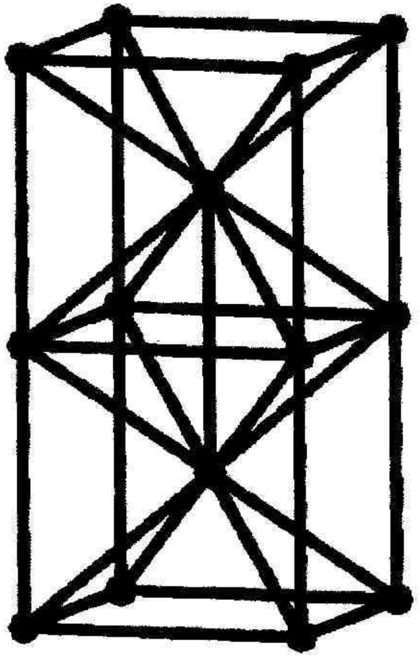
body
centered
cubic (bcc):

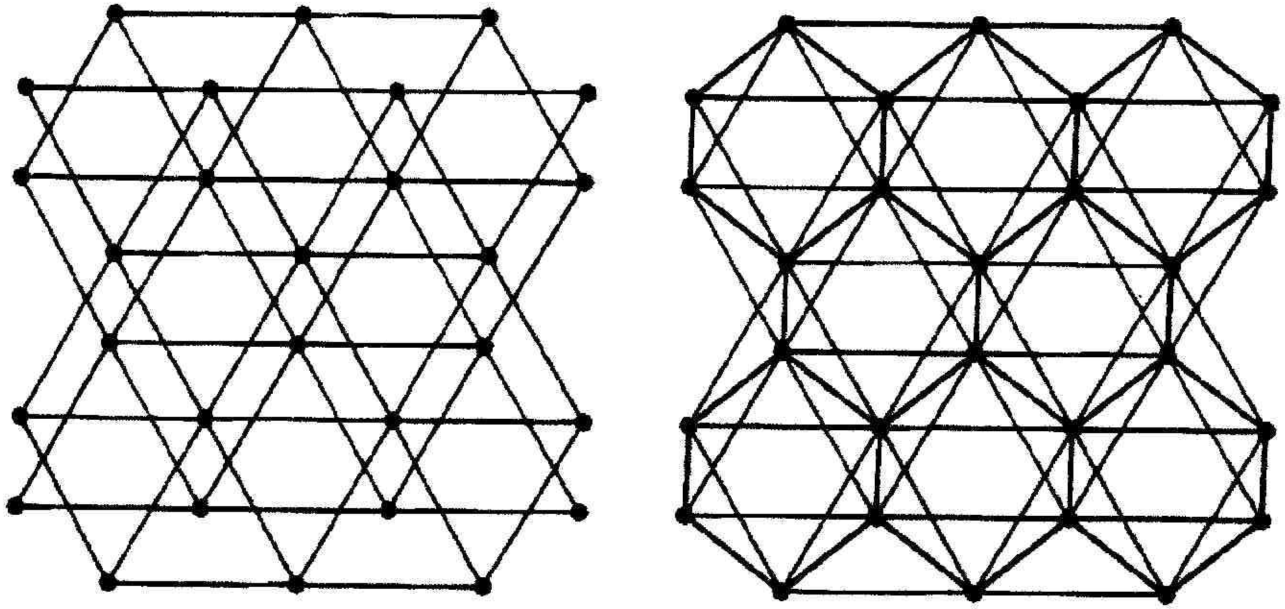
coord.
number = 14
(8+6)
a little less
closest
packed than
fcc or hcp

contains
distorted
tetrahedra
and
octahedra.

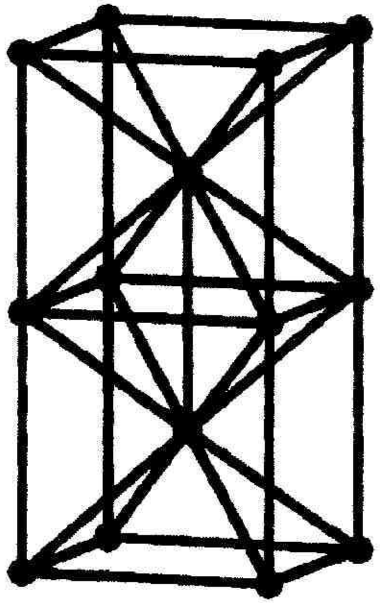






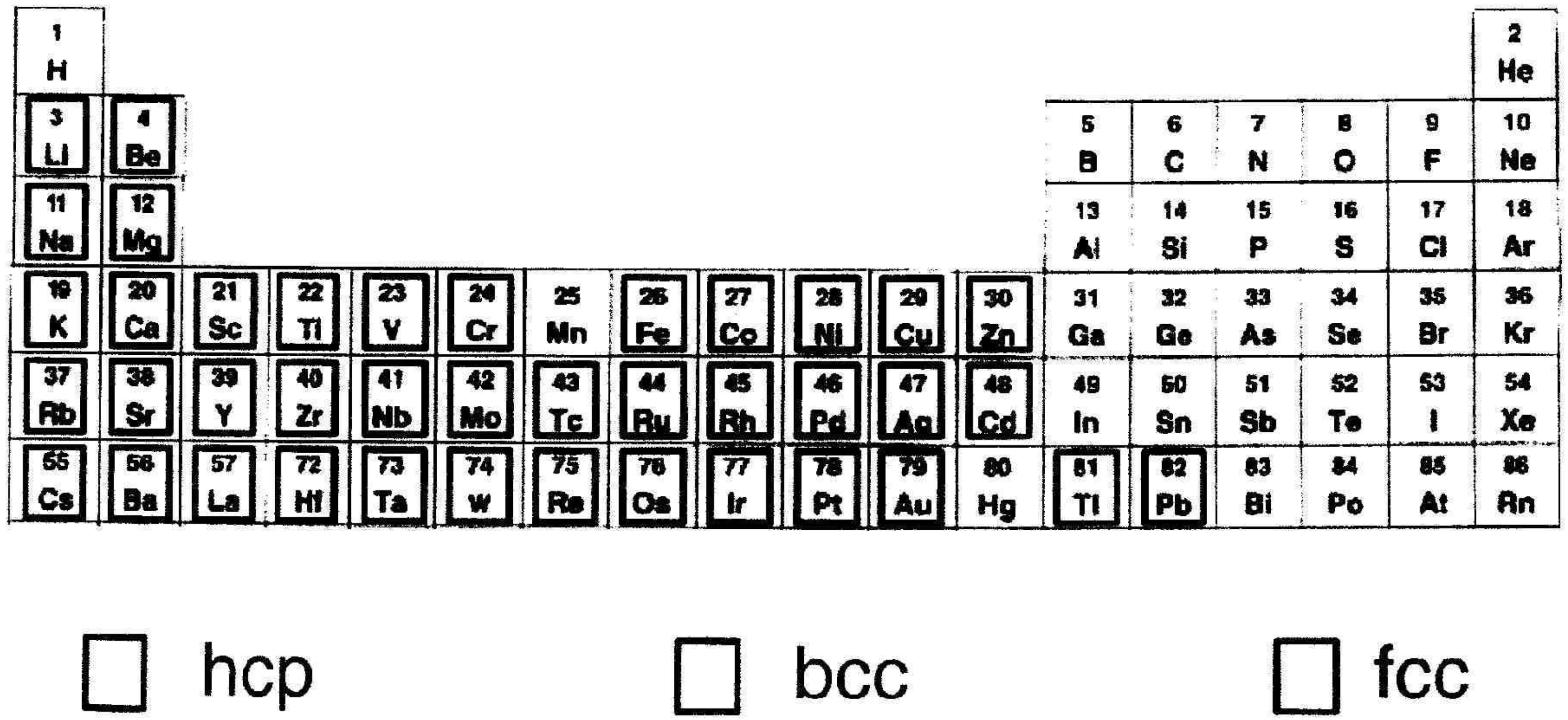


hcp and fcc



bcc

fcc, hcp and bcc for the main group and transition elements



1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
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
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
55 Cs	56 Ba	57 La	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

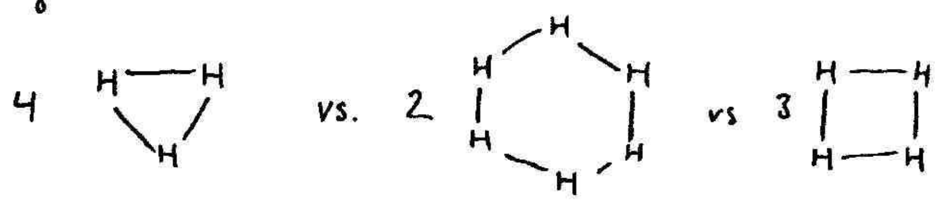
☐ hcp ☐ bcc ☐ fcc

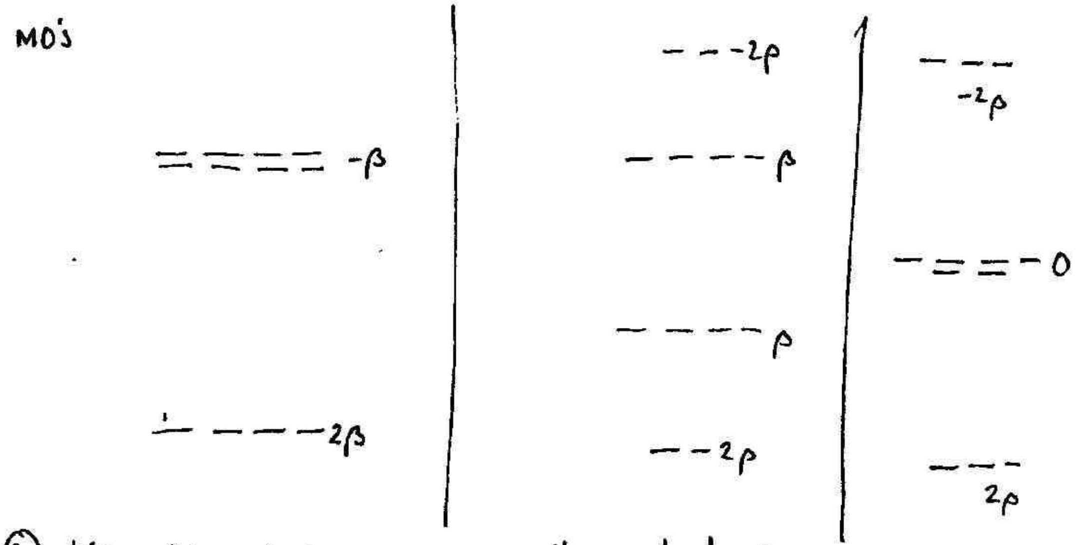
Stable structures at room temperature and pressure

42.10

Ⓐ Why are fcc, hcp & bcc stable for electron deficient systems?

Ⓑ We will not be able to calculate the MO diagrams for fcc & hcp in this class. Instead we will look at the simplest electronic system which capture some of the issues of electron deficiency:

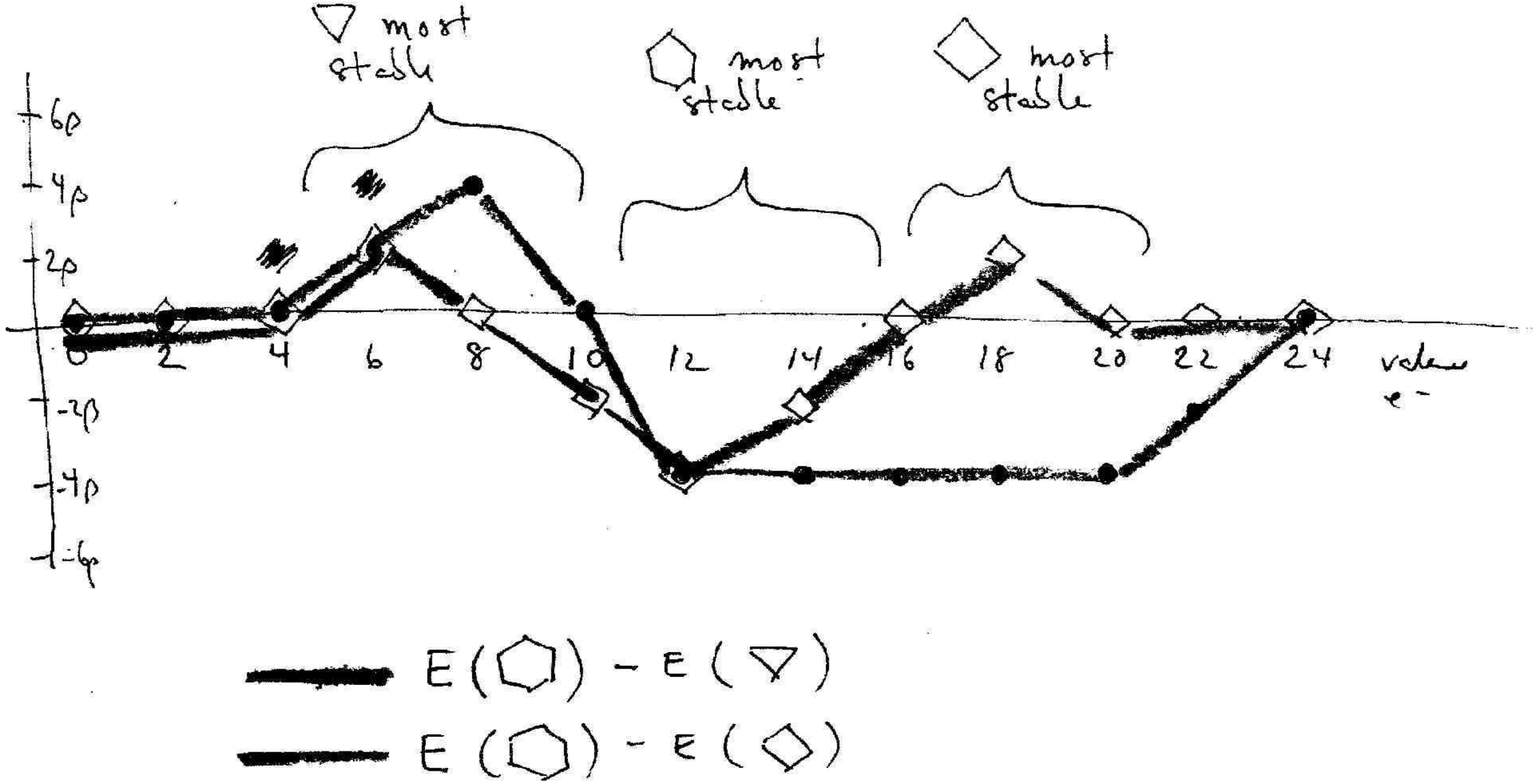




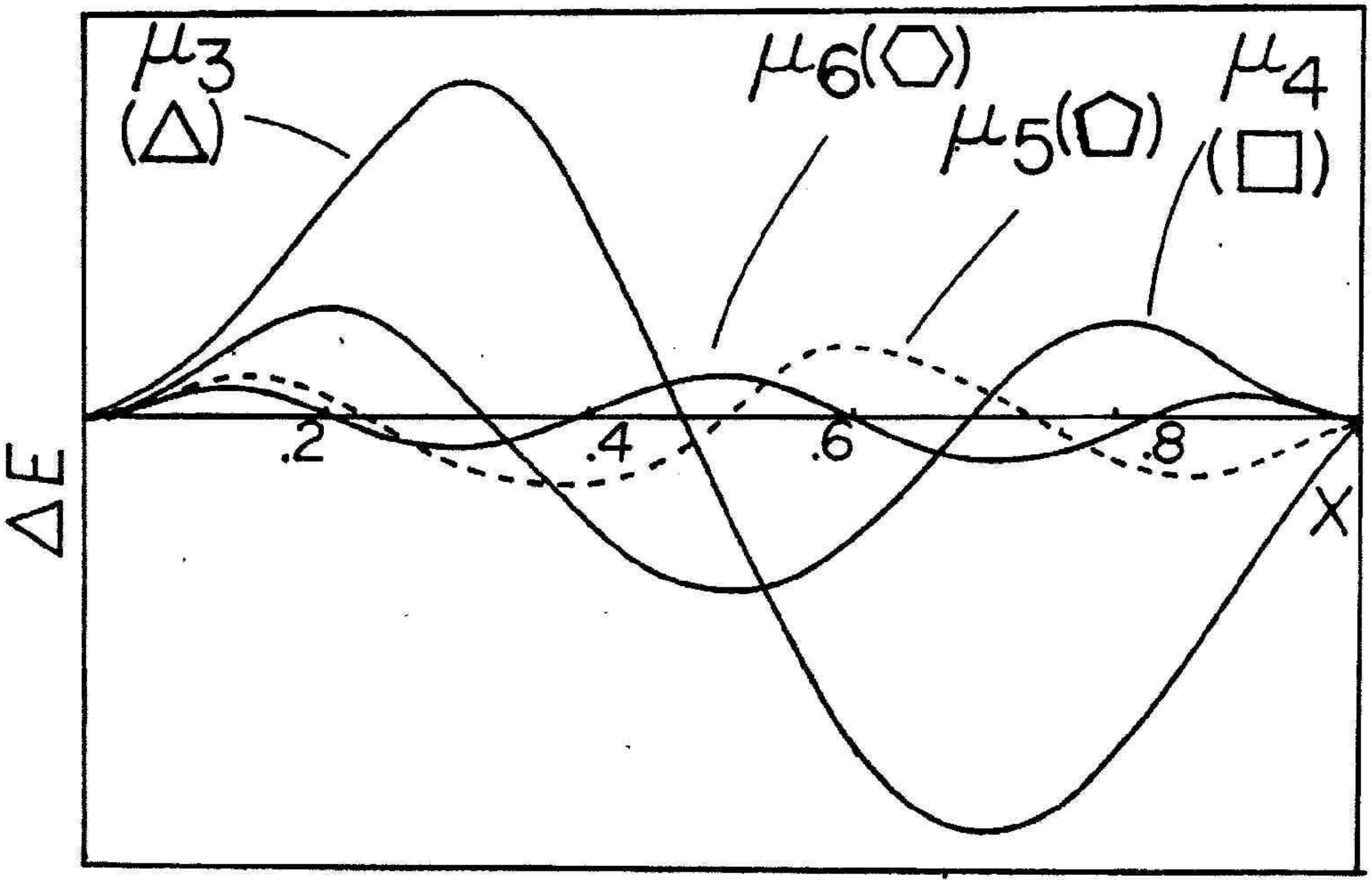
Ⓒ We can now compare the electronic energies for various numbers of valence e^-.

# valence e^-	3 ▽	2 ⬡	3 □
2	4β	4β	4β
4	8β	8β	8β
6	12β	10β	12β
8	16β	12β	12β
10	14β	14β	12β
12	12β	16β	12β
14	10β	14β	12β
16	8β	12β	12β
18	6β	10β	12β
20	4β	8β	8β
22	2β	4β	4β
24	0β	0β	0β

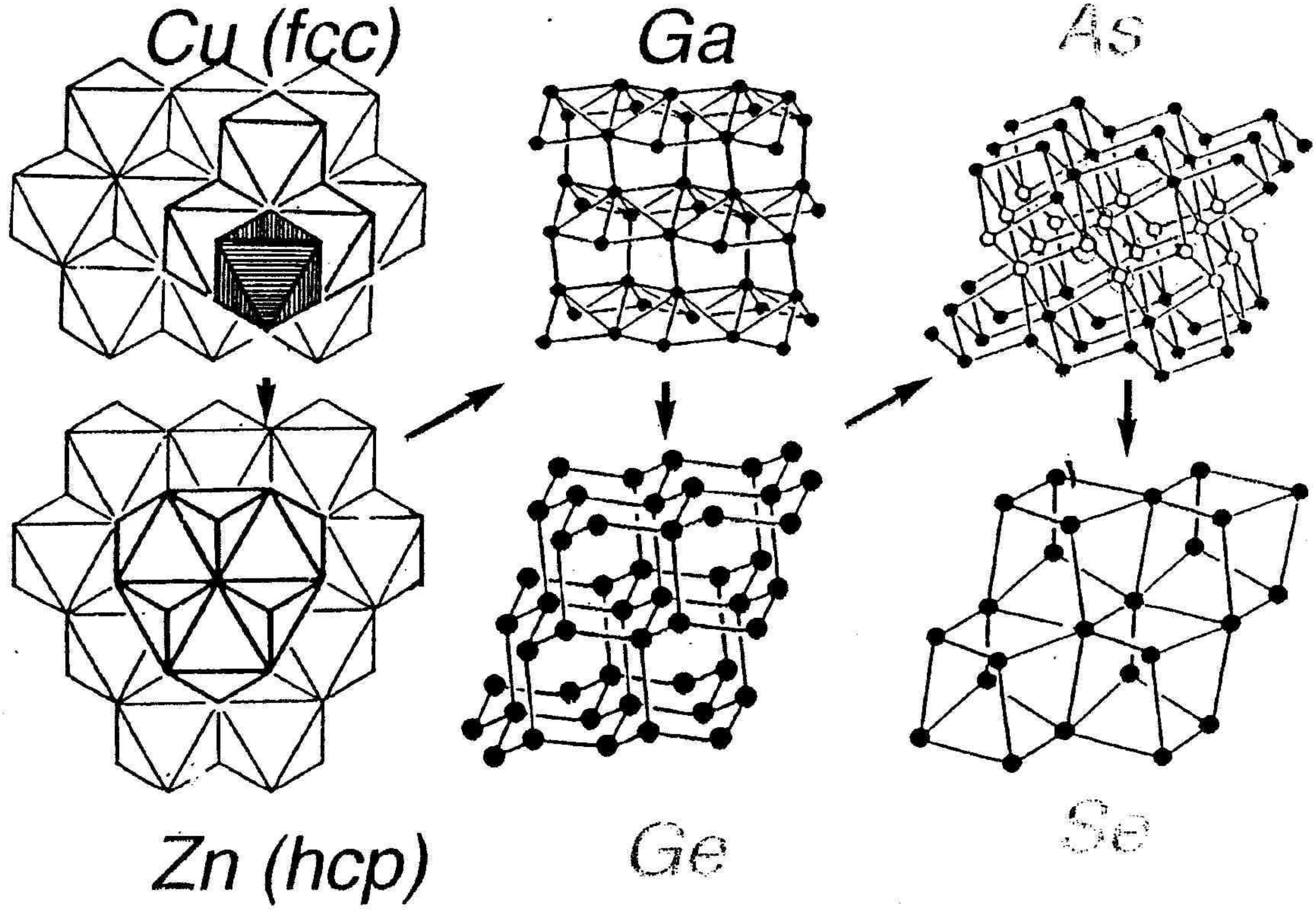
Note triangle are most stable below half-filled
band (8 - 10 e^-), ⬡ " " " at " "
" (10 - 16 e^-) & square are most stable near
3/4 filled band (18 e^-).


▽ most stable
⬡ most stable
◇ most stable
+6β
+4β
+2β
-2β
-4β
-6β
0
2
4
6
8
10
12
14
16
18
20
22
24
valence e⁻
E(⬡) - E(▽)
E(⬡) - E(◇)

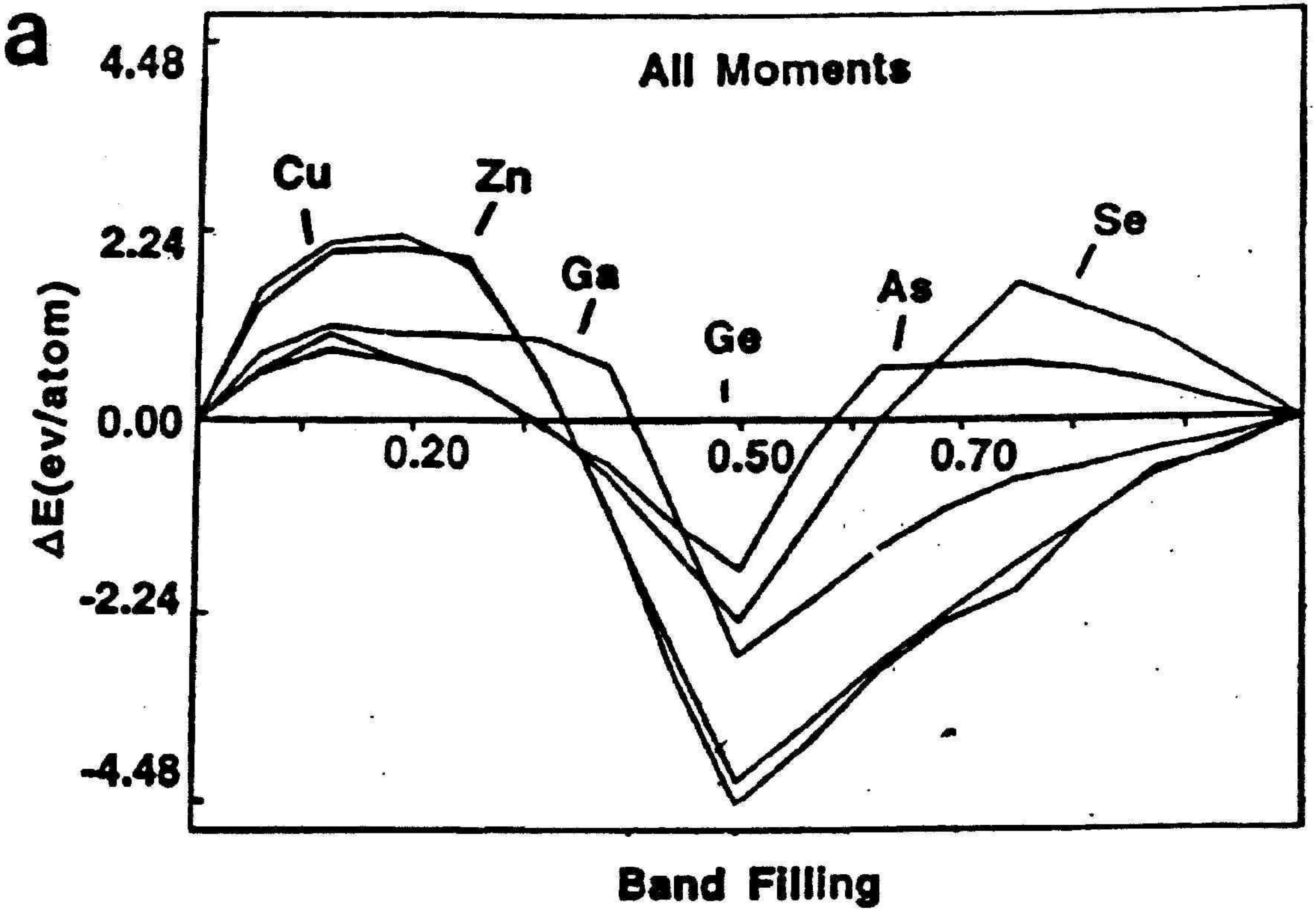
42.13



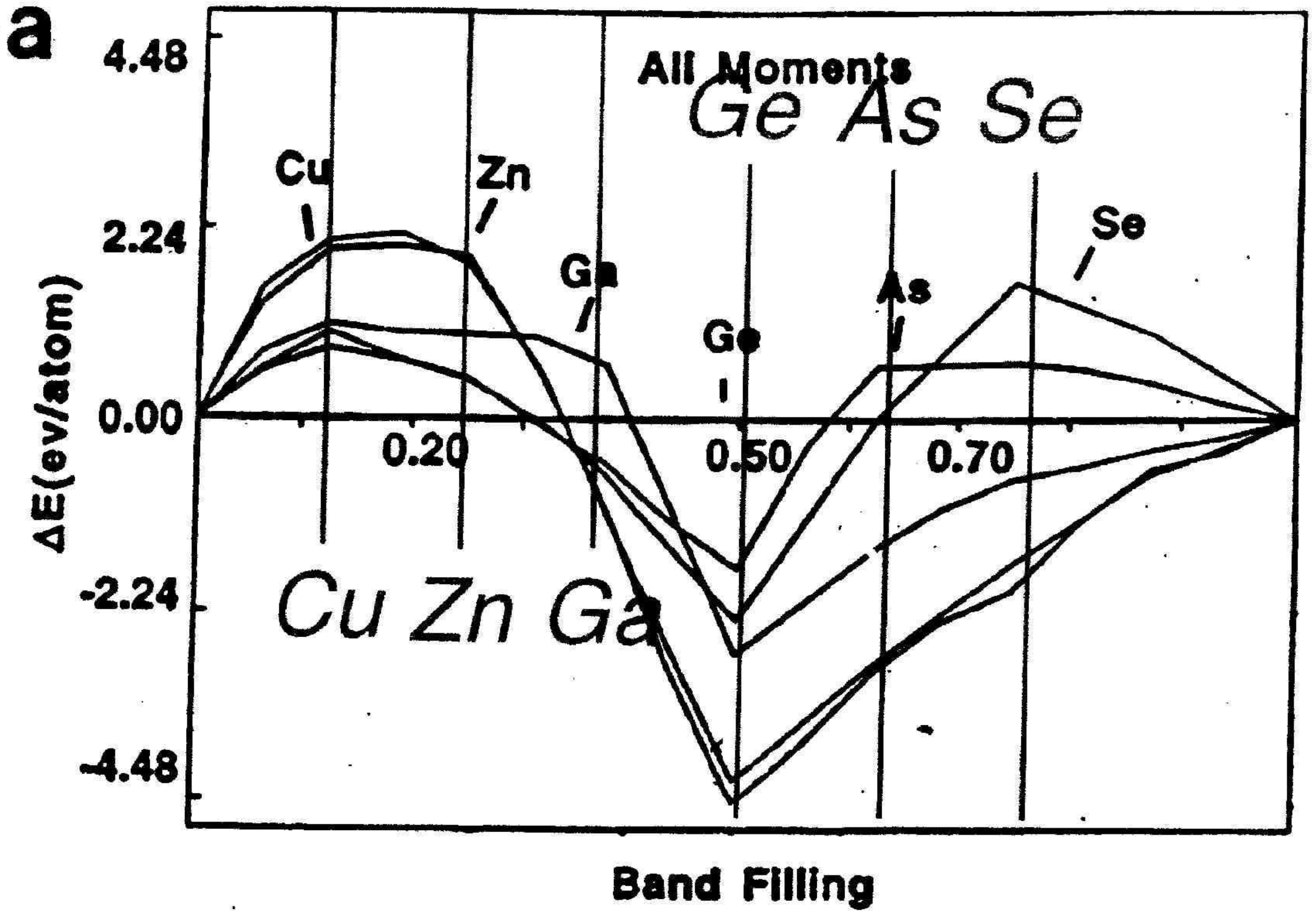
42.14



42.15

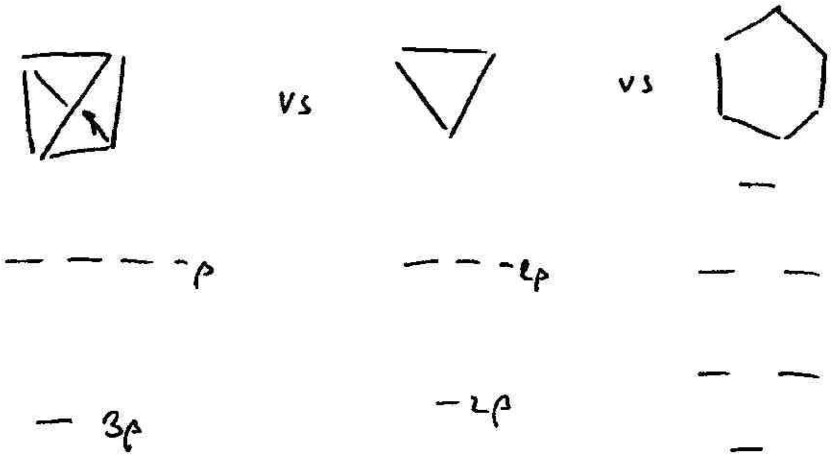

a
All Moments
Cu
Zn
Ga
Ge
As
Se
ΔE(ev/atom)
4.48
2.24
0.00
-2.24
-4.48
0.20
0.50
0.70
Band Filling

42.16

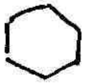
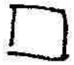

a
All Moments
Ge As Se
Cu
Zn
Ga
Ge
As
Se
Cu Zn Ga
4.48
2.24
0.00
-2.24
-4.48
ΔE(ev/atom)
0.20
0.50
0.70
Band Filling

42.17

Summary:

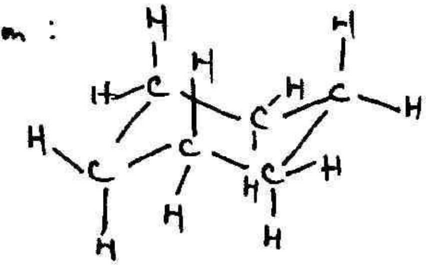


1/4 bonding state	1/3 bonding states	1/2 bonding states?

bcc	Ga	diamond	α-Bi
fcc	B	α-Bi	α-Se
hcp			Po
			
very e^- deficient band	somewhat e^- deficient band	1/2 filled band	e^- rich

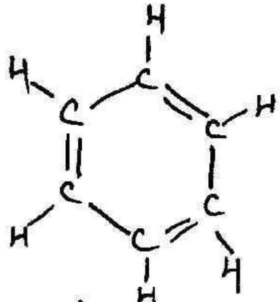
The preference of electron deficient elements to adopt ▽ structure & half-filled band elements to adopt ⬡ structure can be seen in these main group-hydrogen compounds & ions.

Compare the 2 most stable ring systems of carbon:



cyclohexane

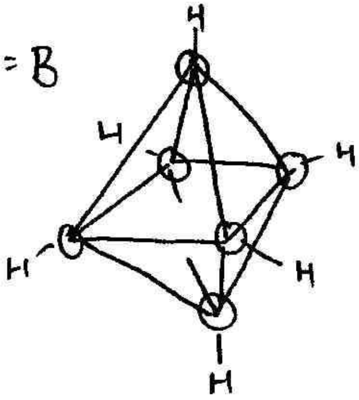
&



benzene

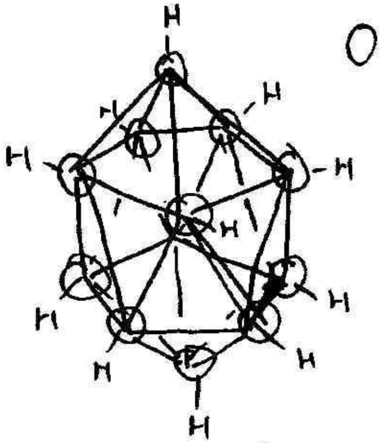
and boron:

O = B



$B_6H_6^{2-}$

O = B



$B_{12}H_{12}^{2-}$