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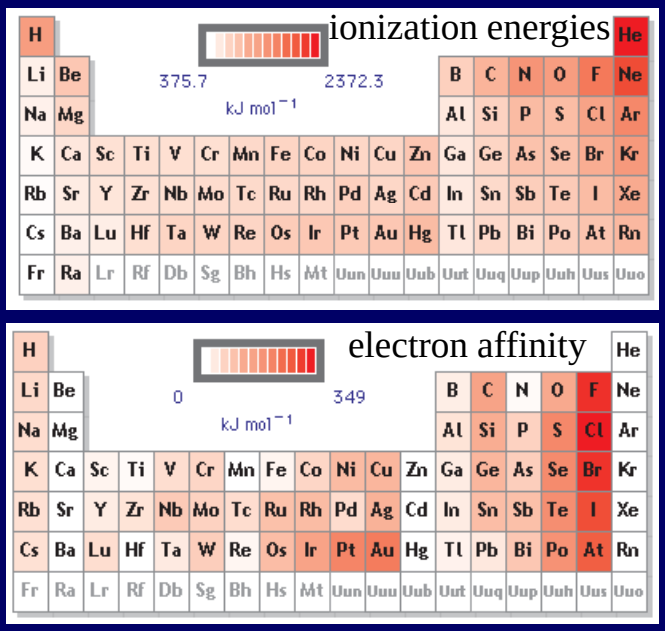
	Ne	Ar	Kr	Xe
c_o (theory)	3.13 Å	3.75 Å	3.99 Å	4.33 Å
c_o (exp.)	2.99 Å	3.71 Å	3.98 Å	4.34 Å
E^{coh} (theory)	27 meV	89 meV	120 mev	172 meV
E^{coh} (exp.)	20 meV	80 meV	110 mev	170 meV

Table 6.3: Equilibrium nearest neighbor distance c_o and cohesive energy E^{coh} of the noble gases, as resulting from experiment and the pair potential approximation discussed in the text (theory). The larger deviation of c_o for the lightest element Ne is due to zero-point vibrations, which are neglected in the theory [from Ashcroft and Mermin].



(96 kJ/mole = 1 eV). [From Webelements].

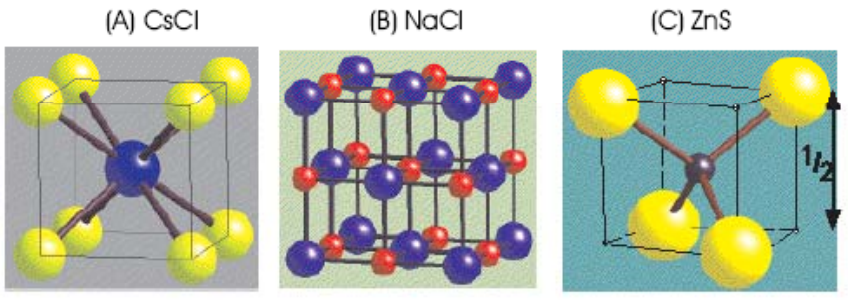
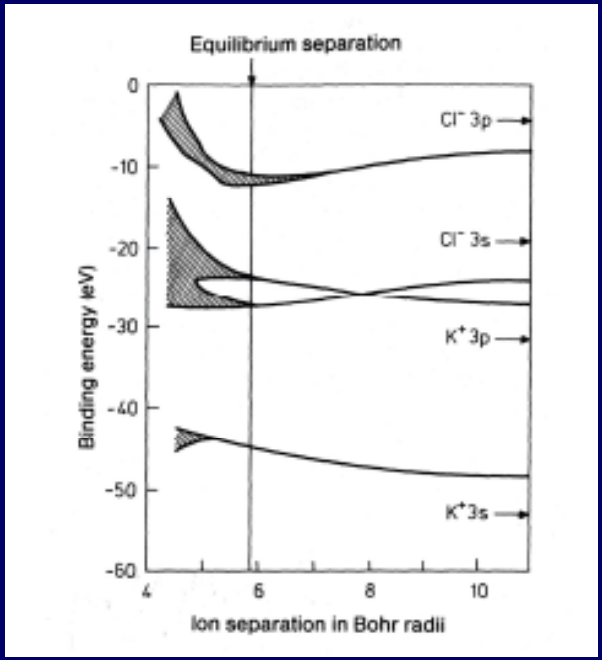


Figure 6.9: The two most common ionic crystal lattices: (A) Cesium chloride and (B) Sodium chloride; and (C)the less common zinc blende structure.


Equilibrium separation
0
-10
-20
-30
-40
-50
-60
Binding energy (eV)
Cl⁻ 3p
Cl⁻ 3s
K⁺ 3p
K⁺ 3s
4
6
8
10
Ion separation in Bohr radii

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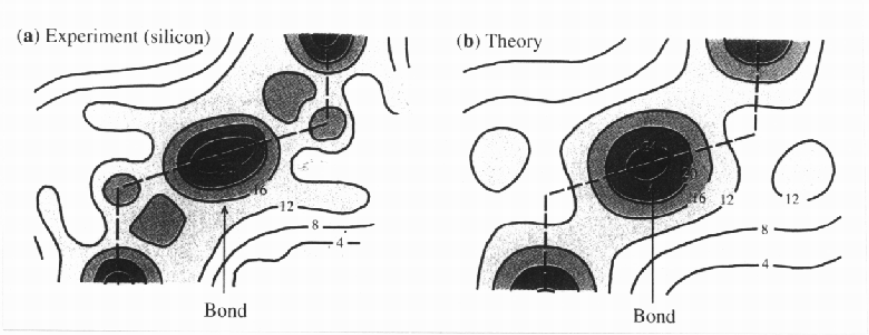
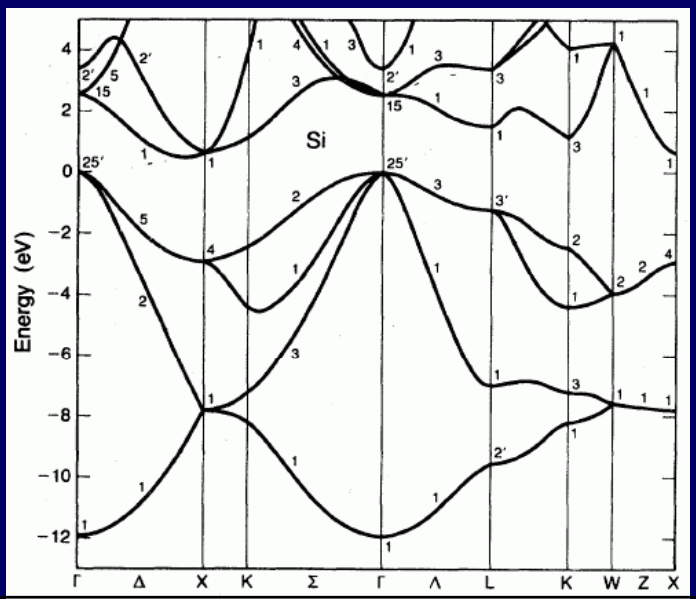
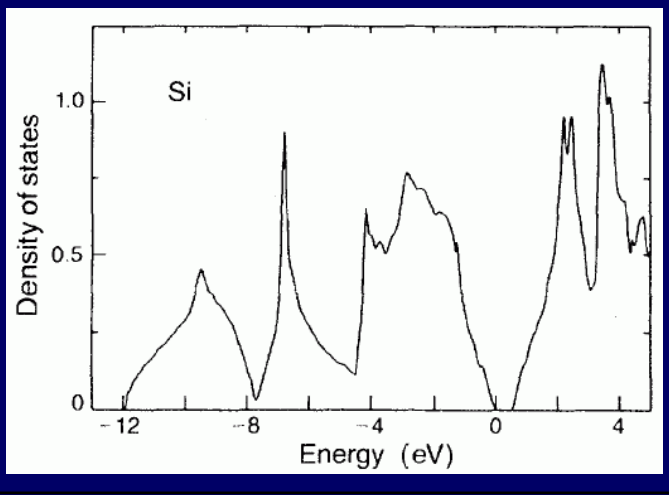


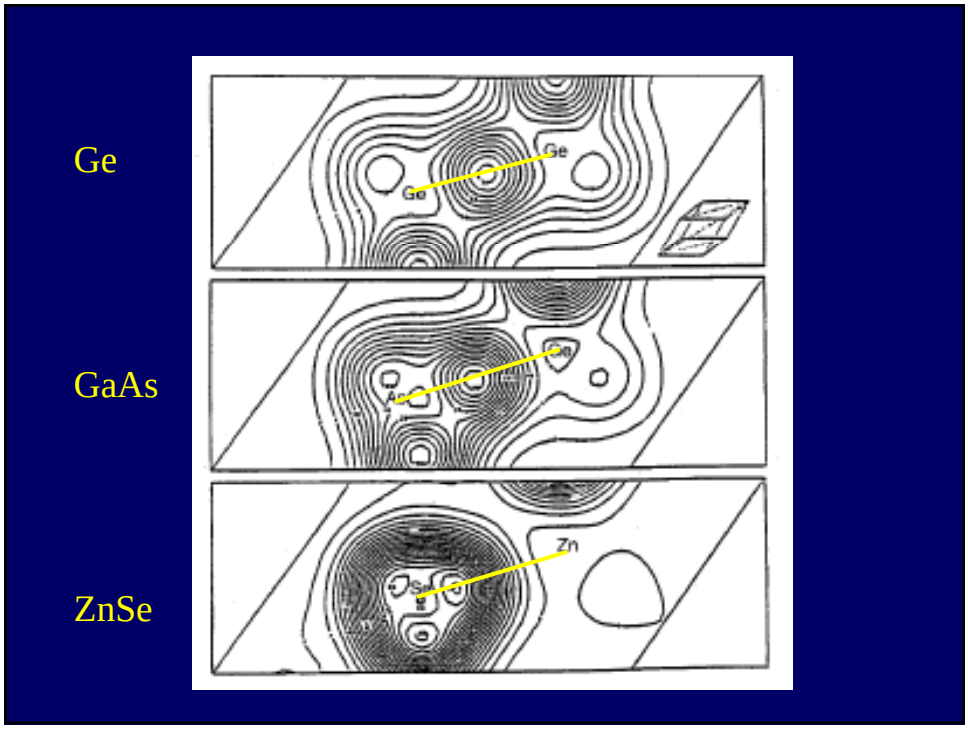
Si bandstructure

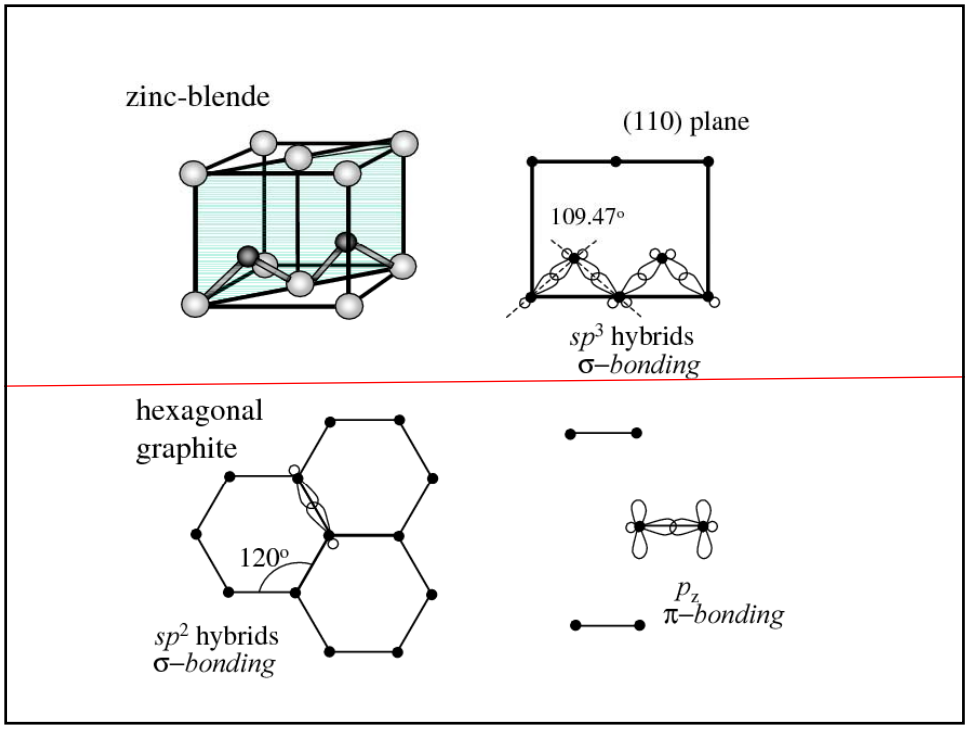


density of states

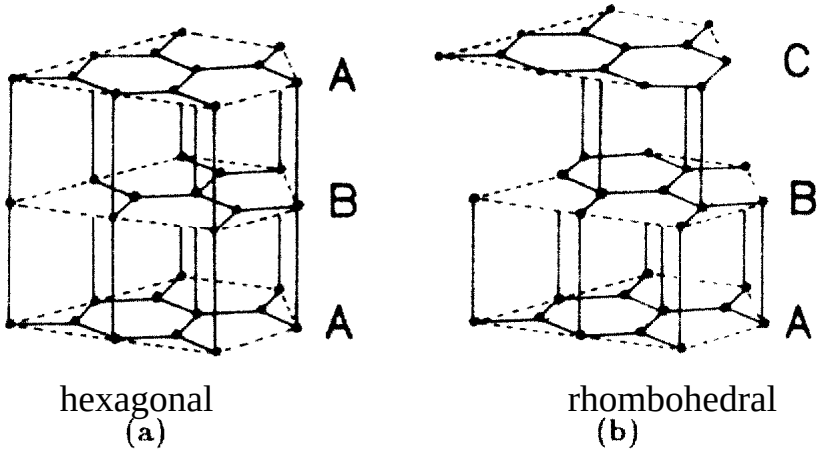


Element		a_o (Å)	E^{coh} (eV/atom)	B_o (Mbar)
C	theory	3,602	7,58	4,33
	exp.	3,567	7,37	4,43
	%diff.	<1%	3%	−2%
Si	theory	5,451	4,67	0,98
	exp.	5,429	4,63	0,99
	%diff.	<1%	1%	−1%
Ge	theory	5,655	4,02	0,73
	exp.	5,652	3,85	0,77
	%diff.	0,2%	4%	−5%

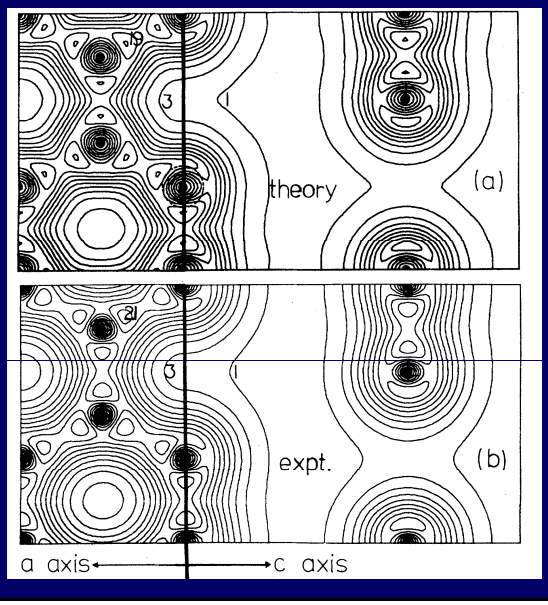

Ge
GaAs
ZnSe
Ge
Ge
Ga
As
Zn
Se


zinc-blende
(110) plane
109.47°
sp^3 hybrids
σ–*bonding*
hexagonal
graphite
120°
sp^2 hybrids
σ–*bonding*
p_z
π–*bonding*

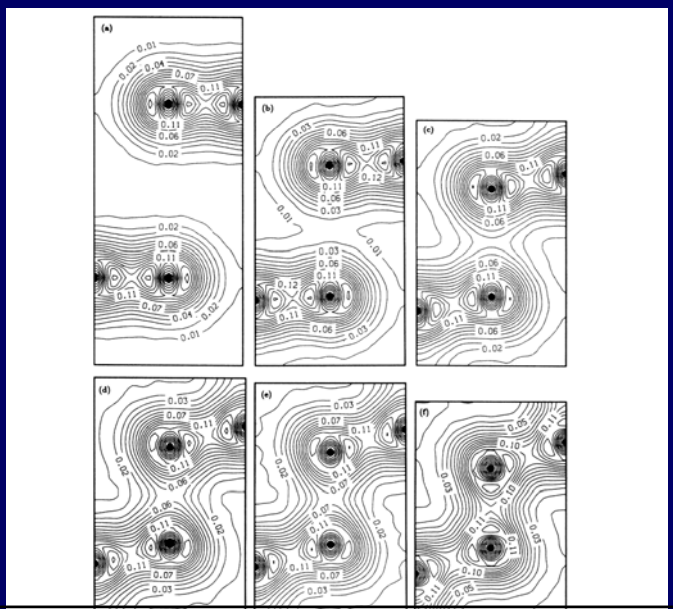
layered structures of graphite



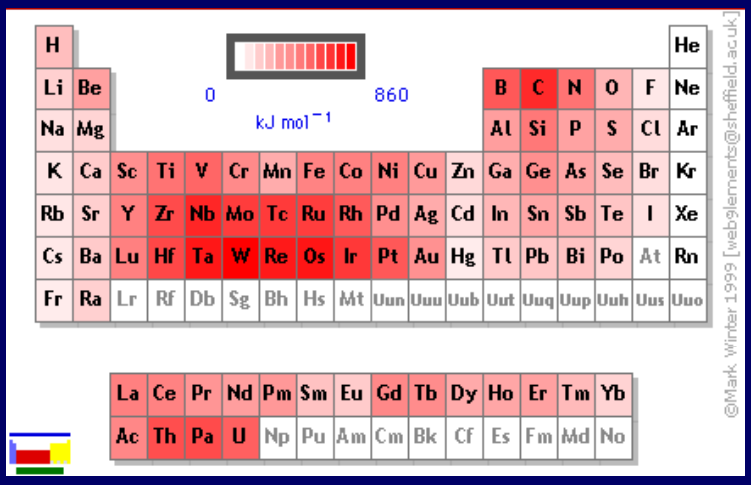
e-density graphite theory vs. experiment



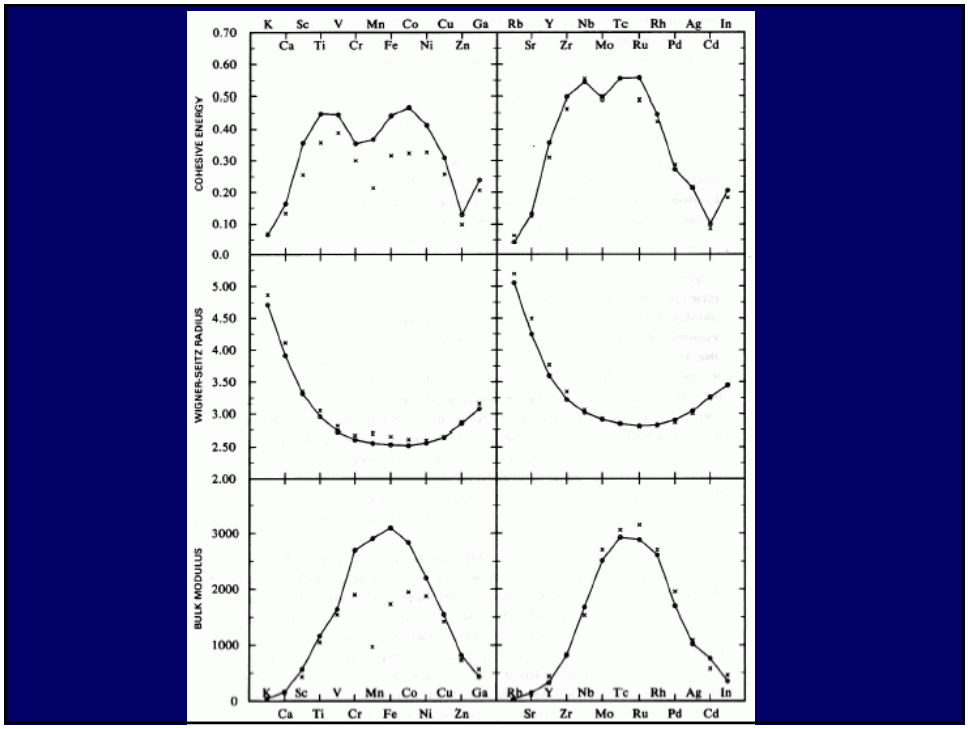
e-density graphite -- diamond phase transition



Cohesive energies



(96 kJ/mole = 1 eV). [From Webelements].


K Sc V Mn Co Cu Ga Rb Y Nb Tc Rh Ag In
Ca Ti Cr Fe Ni Zn Sr Zr Mo Ru Pd Cd
COHESIVE ENERGY
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.0
WIGNER-SEITZ RADIUS
5.00
4.50
4.00
3.50
3.00
2.50
2.00
BULK MODULUS
3000
2000
1000
0
K Sc V Mn Co Cu Ga Rb Y Nb Tc Rh Ag In
Ca Ti Cr Fe Ni Zn Sr Zr Mo Ru Pd Cd