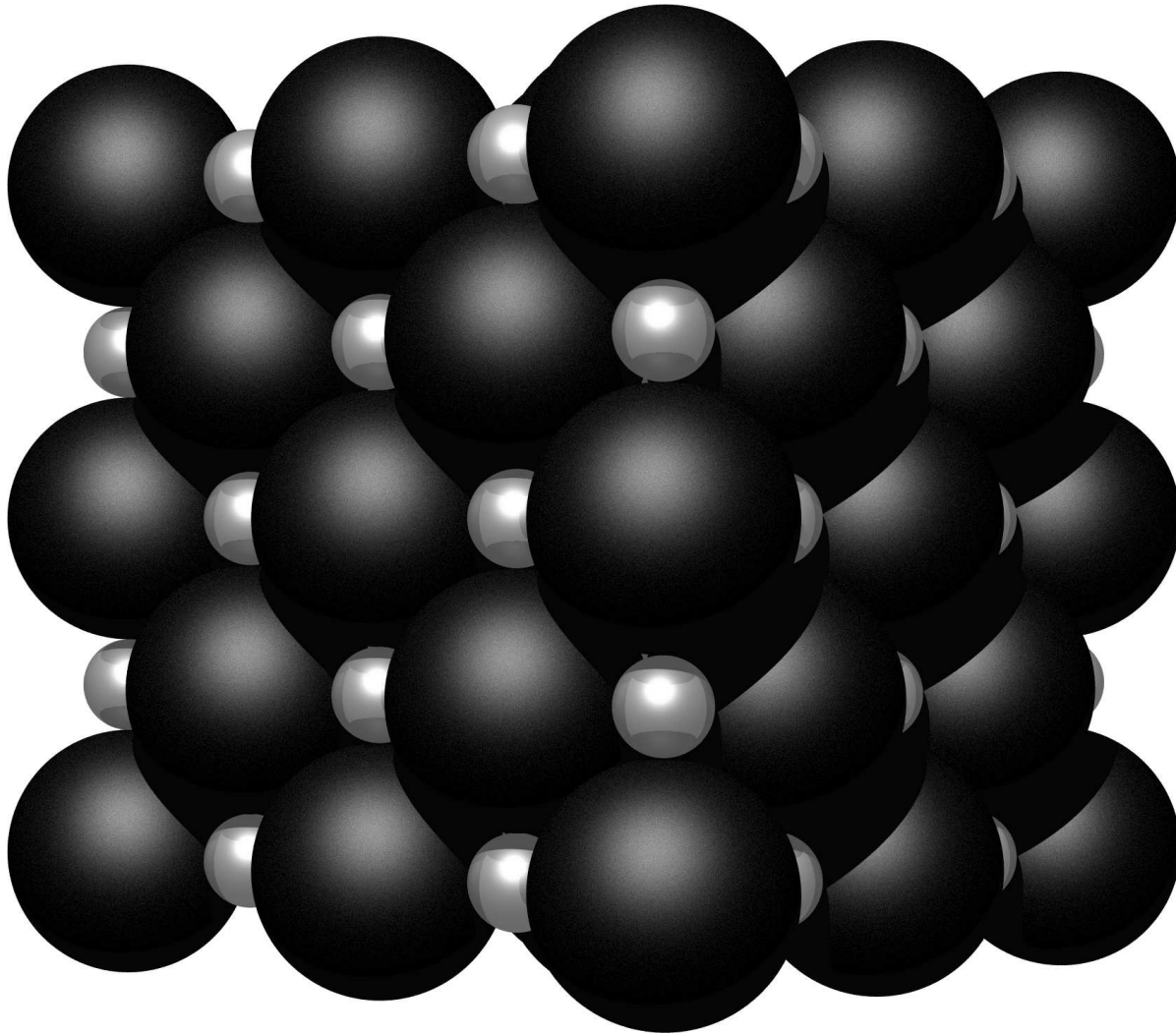Solids divide into 5 rough classes for purposes of studying cohesion
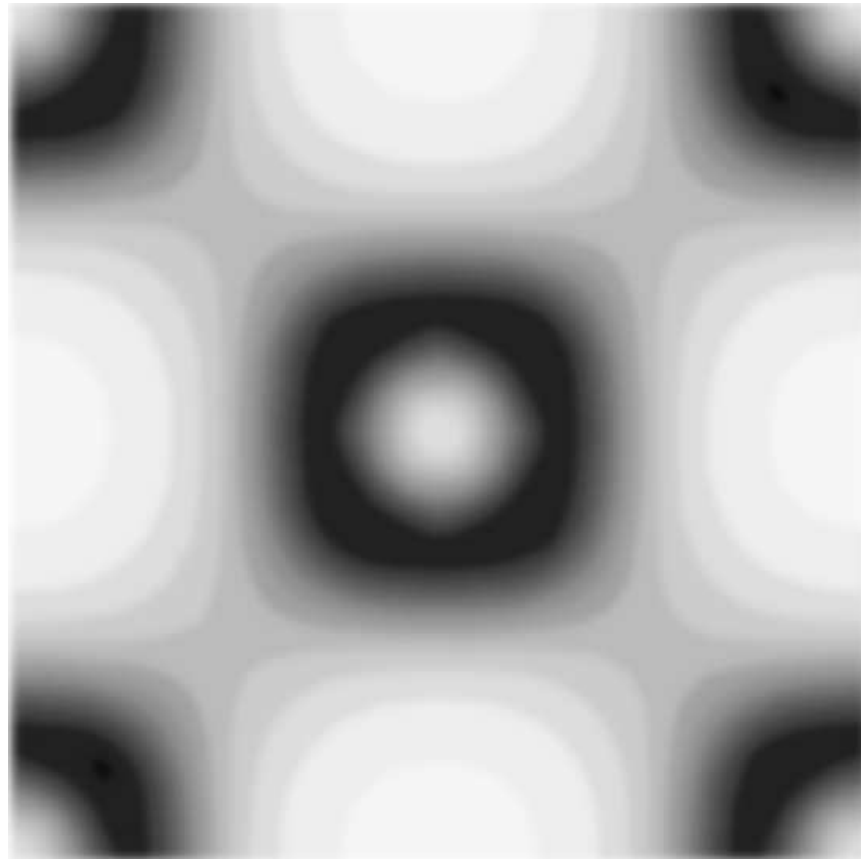
☞ Molecular

☞ Ionic

☞ Covalent

☞ Metallic

☞ Hydrogen bonded

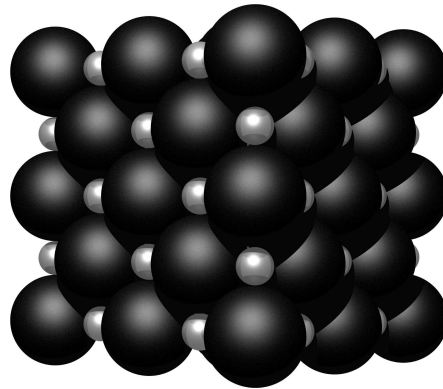Goal is to obtain conceptual and semi-quantitative estimates of cohesive energies, falling back upon elaborate calculations only as necessary.

Cohesive energy has nothing to do with the strength of solids. It allows one to decide what the ground state structure ought to be.
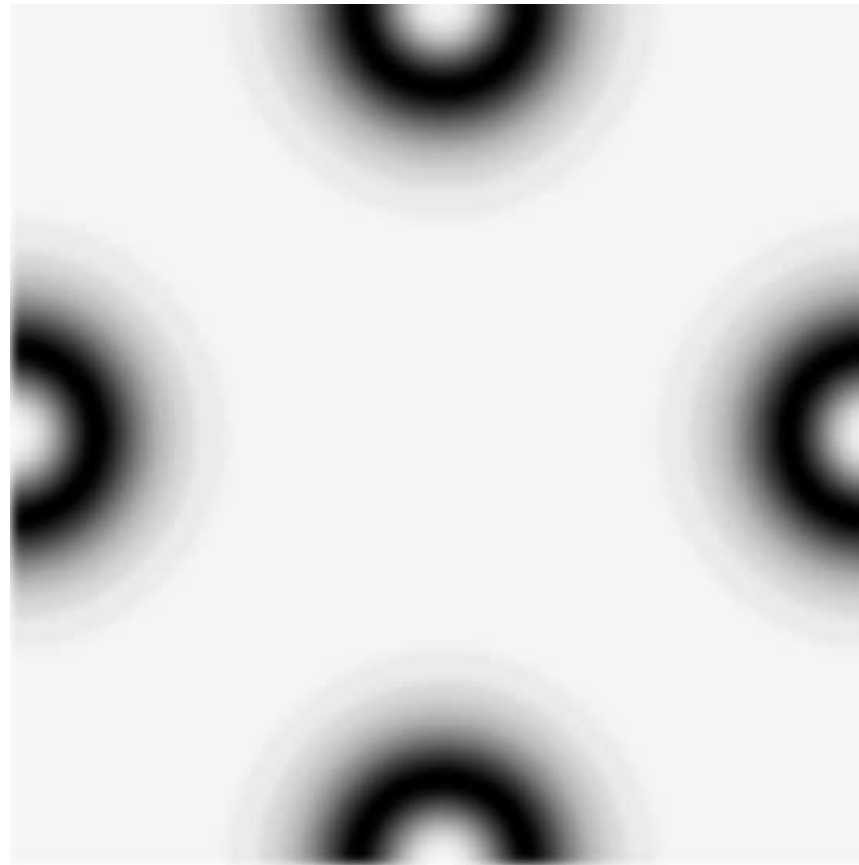
Semi-empirical procedure, assigning atoms a radius and modifying it slightly according to the number and type of neighbors

Radii of Atoms

El.	Z	M	I	R_1
Ac	3+	1.88		
Am	3+	1.81		
Ar	0		1.86	
Ag	1+	1.45	1.26	1.53
Al	3+	1.43	0.50	1.25
As	3−	1.39	2.22	1.21
Au	1+	1.44	1.37	1.52
Ba	2+	2.24	1.35	1.98
Be	2+	1.13	0.35	0.89
Bi	3−	1.70		1.52
B	3+	0.98	0.20	0.80
Br	1−		1.95	1.14
C	4+	0.92	0.15	0.77
	4−		2.60	
Ca	2+	1.97	0.99	1.74
Cd	2+	1.57	0.97	1.49
Ce	3+	1.83	1.01	1.65

El.	Z	M	I	R_1
Co	2−	1.25		
Cl	1−		1.81	0.99
Cr	3+	1.36		
Cs	1+	2.73	1.67	2.35
Cu	1+	1.28	0.96	1.35
Dy	3+	1.77		1.59
Er	3+	1.76		1.57
Eu	2+	2.04		1.85
F	1−		1.36	0.72
Fe	2−	1.27		
Ga	3+	1.41	0.62	1.27
Ge	4+	1.37	0.53	1.22
Ge	4−		2.72	
Gd	3+	1.80		1.61
H	1−	0.78	2.08	

El.	Z	M	I	R_1
He	0			
Hf	4+	1.58		
Hg	2+	1.57	1.10	1.49
Ho	3+	1.77		1.58
I	1−		2.16	1.33
In	3+	1.66	0.81	1.44
Ir	2−	1.36		
K	1+	2.38	1.33	2.03
Kr	0		2.00	
La	3+	1.88	1.15	1.69
Li	1+	1.56	0.68	1.23
Lu				1.56
Mg	2+	1.60	0.65	1.36

El.	Z	M	I	R_1	El.	Z	M	I	R_1	El.	Z	M	I	R_1
Mn	4+	1.30			Po	2−	1.76		1.53	Sn	4−		2.94	
Mo	2−	1.40			Pr	3+	1.83		1.65	Sr	2+	2.15	1.13	1.91
N	3−	0.88	1.71	0.74	Pt	2−	1.39			Ta	3−	1.47		
Na	1+	1.91	0.97	1.57	Pu	3−	1.58			Tb	3+	1.78		1.59
Nb	3−	1.47			Rb	1+	2.55	1.48	2.16	Te	2−	1.60	2.21	1.37
Nd	3+	1.83		1.64	Re	2−	1.38			Th	4+	1.80		
Ne	0		1.58		Rh	2−	1.35			Ti	4+	1.46	0.68	
Ni	2−	1.25			Ru	2−	1.34			Tl	3+	1.72	0.95	1.46
Np	2−	1.56			S	2−	1.27	1.84	1.04	Tm	3+	1.75		1.56
O	2−	0.89	1.40	0.74	Sb	3−	1.59	2.45	1.41	U	2−	1.56		
Os	2−	1.35			Sc	3+	1.64	0.81	1.44	V	3−	1.35		
P	3−	1.28	2.12	1.10	Se	2−	1.40	1.98	1.17	W	2−	1.41		
Pa	3−	1.63			Si	4+	1.32	0.41	1.17	Xe	0		2.17	
Pb	4+	1.75	0.84	1.43	Si	4−		2.71		Y	3+	1.80	0.93	1.62
Pd	2−	1.38			Sm	3+	1.80		1.66	Yb	2+	1.94		1.70
					Sn	4+	1.62	0.71	1.40	Zn	2+	1.39	0.74	1.31
										Zr	4+	1.60	0.80	

Ion Type		He	Ne	Ar	Kr	Xe
(inert core)				Cu^+	Ag^+	Au^+
Born exponent n	5	7	9		10	12

I is ionic radius: $R = I[z/6]^{1/(n-1)}$

R_1 is covalent radius: $R = R_1 - 0.13\ln[Z/z]$: for $Z < 0$, use $8 - |Z|$.

According to Wykoff, quartz in the β-cristobalite form is cubic ($a = 7.12$ Å) and has a basis with eight silicon atoms and sixteen oxygens, which in units of $a/8$ are at

Si:	(000)	(440)	(404)	(044)	(222)	(266)	(626)	(662)
O:	(111)	(551)	(515)	(155)	(177)	(537)	(573)	(133)
	(717)	(357)	(313)	(753)	(771)	(331)	(375)	(735)

The nearest-neighbor distance for this structure is 1.54 Å. The silicon has four neighboring oxygens, so $Z = z = 4$, while each oxygen has two neighboring silicons, and $Z = 6$, $z = 2$. According to table, the covalent radius of silicon is 1.17 Å, and that of oxygen is $0.74 - 0.14 = 0.60$ Å, which sum to 1.77 Å. The discrepancy is more than 10%; structure is wrong.

Energy produced by simple sums.

$$\mathcal{E} = \frac{1}{2} \sum_{ij} \phi(r_{ij}) \tag{L1}$$

Lennard–Jones potential

$$\phi(r) = -4\epsilon \left[\left(\frac{\sigma}{r}\right)^6 - \left(\frac{\sigma}{r}\right)^{12} \right]. \tag{L2}$$

Origin from dipole moments.

$$\phi(r) = [\vec{p}_1 \cdot \vec{p}_2 - 3(\vec{p}_1 \cdot \hat{r})(\vec{p}_2 \cdot \hat{r})]/r^3, \tag{L3}$$

Dipole moments induced by fluctuations

$$\phi \sim -\frac{\alpha_1 \alpha_2}{r^6}, \tag{L4}$$

Repulsive term of form r^{12} because...because...well, it has to be something!.

Thermodynamic properties from

$$PV/k_BT = 1 - b_2/V \dots \tag{L5}$$

where

$$b_2 = \frac{1}{2} \int d\vec{r} \, [1 - e^{-\beta\phi(r)}]. \tag{L6}$$

Theory of solids obtained from measurements performed purely on gases.

Noble Gas	He	Ne	Ar	Kr	Xe
ϵ (eV)	$8.6 \cdot 10^{-4}$	0.0031	0.0104	0.0104	0.0200
σ (Å)	2.56	2.74	3.40	3.65	3.98

$$\mathcal{E}/N = \frac{1}{2} 4\epsilon \sum_{\vec{R} \neq 0} \left[\left(\frac{\sigma}{R}\right)^{12} - \left(\frac{\sigma}{R}\right)^6 \right]. \tag{L7}$$

$$\mathcal{E}/N \;=\; 2\epsilon \sum_{\vec{R}} (\frac{\sigma}{d})^{12}(\frac{d}{R})^{12} - (\frac{\sigma}{d})^{6}(\frac{d}{R})^{6} \tag{L8}$$

$$\equiv\; 2\epsilon[A_{12}(\frac{\sigma}{d})^{12} - A_6(\frac{\sigma}{d})^{6}] \text{ with } A_l \equiv \sum_{\vec{R}\neq 0} \left(\frac{d}{R}\right)^{l}. \tag{L9}$$

Lattice sums:

Crystal	fcc	bcc	hcp
A_6	14.4519	12.2519	14.4548
A_{12}	12.1319	9.1142	12.1353
$A_6^2/2A_{12}$	8.6078	8.2349	8.6088

Nearest–neighbor spacing in equilibrium:

$$d_0 = \sigma(\frac{2A_{12}}{A_6})^{1/6}, \tag{L10}$$

Cohesive energy:

$$\mathcal{E}/N = -\epsilon \frac{A_6^2}{2A_{12}}, \tag{L11}$$

Bulk modulus:

$$B = \mathcal{V} \frac{\partial^2 \mathcal{E}}{\partial \mathcal{V}^2}. \tag{L12}$$

$$B = \frac{4\epsilon}{\sigma^3} A_{12} \left(\frac{A_6}{A_{12}} \right)^{5/2}. \tag{L13}$$

Noble Gas	Ne	Ar	Kr	Xe
Experimental d_0 (Å)	3.13	3.75	3.99	4.33
d_0 from Eq. (L10) (Å)	2.99	3.71	3.98	4.34
Experimental $\mathcal{E}/N$ (eV/atom)	-0.02	-0.08	-0.11	-0.17
$\mathcal{E}/N$ from Eq. (L11)	-0.027	-0.089	-0.120	-0.172
Experimental B (dyne/cm^2)	$1.1 \cdot 10^{10}$	$2.7 \cdot 10^{10}$	$3.5 \cdot 10^{10}$	$3.6 \cdot 10^{10}$
B from Eq. (L13)	$1.81 \cdot 10^{10}$	$3.18 \cdot 10^{10}$	$3.46 \cdot 10^{10}$	$3.81 \cdot 10^{10}$

Atom	Electron affinity (eV)	Atom	First ionization potential (eV)
H	0.75	Li	5.32
F	3.40	Na	5.14
Cl	3.61	K	4.34
Br	3.36	Rb	4.18
I	3.06	Cs	3.90

Computing sums over particles interacting with $1/r$ potentials is very tricky because mathematically the sums can diverge or are ambiguous. Physically, ambiguities in the sums correspond to putting varying values of surface charge at outer surfaces of crystal, and the mathematical resolution corresponds to having no net surface charge.

$$\frac{e^2}{d} \sum_{\vec{R} \neq 0} \left[\frac{d}{R} - \frac{d}{|\vec{R} + \vec{d}|} \right] - \frac{e^2}{d} \equiv \frac{e^2}{d} [dS(0) - dS(\vec{d}) - 1], \tag{L14}$$

$$
\begin{aligned}
S(\vec{d}) &= \sum_{\vec{R} \neq \vec{0}} \frac{1}{|\vec{d} - \vec{R}|} = \int_0^\infty \frac{2\,d\rho}{\sqrt{\pi}} \sum_{\vec{R} \neq \vec{0}} e^{-\rho^2 |\vec{d} - \vec{R}|^2} \tag{L15} \\
&= \int_0^\infty \frac{2\,d\rho}{\sqrt{\pi}} \int \frac{d\vec{k}}{\rho^3 \sqrt{\pi}^3} \sum_{\vec{R} \neq \vec{0}} e^{-k^2/\rho^2 + 2i\vec{k}\cdot(\vec{d}-\vec{R})} \tag{L16} \\
&= \int_0^\infty \frac{2\,d\rho}{\sqrt{\pi}} \int \frac{d\vec{k}}{\rho^3 \sqrt{\pi}^3} \left[\left\{ \sum_{\vec{K}} \frac{(2\pi)^3}{\Omega} \delta(2\vec{k} - \vec{K}) \right\} - 1 \right] e^{-k^2/\rho^2 + 2i\vec{k}\cdot\vec{d}} \tag{L17}
\end{aligned}
$$

$$= \int_0^\infty \frac{2\,d\rho}{\sqrt{\pi}} \left[\frac{\pi^3}{\rho^3 \sqrt{\pi}^3} \sum_{\vec{K}} \frac{1}{\Omega} e^{-K^2/4\rho^2 + i\vec{K}\cdot\vec{d}} - e^{-d^2\rho^2} \right] \tag{L18}$$

$$= \sum_{\vec{K}} \frac{4\pi}{\Omega K^2} e^{i\vec{K}\cdot\vec{d}} - \frac{1}{d}. \tag{L19}$$

$$S(\vec{d}) = \int_g^\infty \frac{2\,d\rho}{\sqrt{\pi}} \sum_{\vec{R}\neq\vec{0}} e^{-\rho^2(\vec{d}-\vec{R})^2}$$

$$+ \int_0^g \frac{2\,d\rho}{\sqrt{\pi}} \left[\frac{(\pi)^3}{\rho^3 \sqrt{\pi}^3} \sum_{\vec{K}\neq 0} \frac{1}{\Omega} e^{-K^2/4\rho^2 + i\vec{K}\cdot\vec{d}} - e^{-d^2\rho^2} \right] \tag{L20}$$

$$= \int_g^\infty \frac{2\,d\rho}{\sqrt{\pi}} \sum_{\vec{R}\neq 0} e^{-\rho^2(\vec{d}-\vec{R})^2} + \sum_{\vec{K}\neq 0} \frac{4\pi}{\Omega K^2} e^{-K^2/4g^2 + i\vec{K}\cdot\vec{d}} - \int_0^g \frac{2\,d\rho}{\sqrt{\pi}} e^{-\rho^2 d^2}.$$

$$\tag{L21}$$

$$dS(\vec{d}) - dS(0) + 1 \equiv \alpha \qquad \text{(L22)}$$

$$\frac{\mathcal{E}}{N_{\text{ion pairs}}} = -\alpha\frac{e^2}{d} = -\alpha\frac{14.4\,\text{eV}}{[d/\text{Å}]}, \qquad \text{(L23)}$$

α is the Madelung constant.

Structure	Madelung constant α
Cesium chloride	1.76268
Sodium chloride	1.74757
Wurtzite	1.638704
Zincblende	1.63806

Add repulsive term C/d^{12} because...because...well, it has to be something!.

$$\frac{\mathcal{E}}{N_{\text{ion pairs}}} = -\alpha\frac{e^2}{d} + \frac{C}{d^{12}}. \qquad \text{(L24)}$$

$$d_0 = \left[\frac{12C}{e^2\alpha}\right]^{1/11},$$ (L25)

$$\frac{\mathcal{E}}{N_{\text{ion pairs}}} = -\frac{11}{12}\alpha\frac{e^2}{d}.$$ (L26)

Compound	Experimental d_0 (Å)	Experimental $\mathcal{E}/N_{\text{ion pairs}}$ (eV)	Eq. (L26) $\mathcal{E}/N_{\text{ion pairs}}$ (eV)
LiF	2.01	10.83	11.45
LiCl	2.57	8.85	8.98
LiBr	2.75	8.51	8.39
LiI	3.01	7.92	7.66
NaCl	2.82	8.18	8.18
NaF	2.32	9.62	9.96
NaBr	2.99	7.81	7.72
NaI	3.24	7.32	7.13
KF	2.67	8.55	8.63
KCl	3.15	7.42	7.33
KBr	3.30	7.16	6.99
KI	3.53	6.74	6.53
RbF	2.83	8.18	8.16
RbCl	3.29	7.17	7.01
RbBr	3.44	6.90	6.70
RbI	3.67	6.52	6.28
AgCl	2.77	9.53	8.32
AgBr	2.89	9.40	7.99

$$\mathcal{E}_{\text{el}} \equiv \quad - \quad \int d\vec{r}\, n(\vec{r}) \sum_{\vec{R}} \frac{e^2}{|\vec{r} - \vec{R}|} + \frac{e^2}{2} \sum_{\vec{R} \neq \vec{R}'} \frac{1}{|\vec{R} - \vec{R}'|}$$
$$+ \frac{1}{2} \quad \int d\vec{r}_2 d\vec{r}_1 \frac{e^2 n(\vec{r}_1) n(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|}. \tag{L27}$$

$$\frac{\mathcal{E}_{\text{el}}}{N} = -\frac{\alpha}{2}\frac{e^2}{r_s}, \tag{L28}$$

$$r_s = [\frac{3}{4\pi}\frac{\mathcal{V}}{N}]^{1/3} \tag{L29}$$

Madelung constants for metals

bcc	fcc	hcp	sc	Diamond
1.791 86	1.791 75	1.791 68	1.760 12	1.670 85

$$\frac{\mathcal{E}_{\text{kin}}}{N} = \frac{3}{5}\frac{\hbar^2 k_F^2}{2m} = \frac{3}{5}\frac{\hbar^2}{2m}(\frac{9\pi}{4})^{2/3}\frac{1}{r_s^2} \tag{L30}$$

$$\frac{\mathcal{E}_{\text{ex}}}{N} = -\frac{3}{4\pi}e^2 k_F = -\frac{3}{4\pi}e^2 \left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_s}. \tag{L31}$$

$$\frac{\mathcal{E}}{N} = \left[-\frac{24.35}{(r_s/a_0)} + \frac{30.1}{(r_s/a_0)^2} - \frac{12.5}{(r_s/a_0)}\right] \text{eV/atom}. \tag{L32}$$

Get general (wrong) prediction

$$\frac{r_s}{a_0} = 1.6, \tag{L33}$$

Metals

Element	Z	n (10^{22} cm^{-3})	k_F (10^8 cm^{-1})	$\mathcal{E}_F$ (eV)	T_F (10^4 K)	v_F (10^8 cm s^{-1})	r_s/a_0
Li	1	4.60	1.11	4.68	5.43	1.28	3.27
Na	1	2.54	0.91	3.15	3.66	1.05	3.99
K	1	1.32	0.73	2.04	2.37	0.85	4.95
Rb	1	1.08	0.68	1.78	2.06	0.79	5.30
Cs	1	0.85	0.63	1.52	1.76	0.73	5.75
Cu	1	8.49	1.36	7.04	8.17	1.57	2.67
Ag	1	5.86	1.20	5.50	6.38	1.39	3.02
Au	1	5.90	1.20	5.53	6.42	1.39	3.01
Be	2	24.72	1.94	14.36	16.67	2.25	1.87
Mg	2	8.62	1.37	7.11	8.26	1.58	2.65
Ca	2	4.66	1.11	4.72	5.48	1.29	3.26
Sr	2	3.49	1.01	3.89	4.52	1.17	3.59
Ba	2	3.15	0.98	3.64	4.22	1.13	3.71
Zn	2	13.13	1.57	9.42	10.93	1.82	2.31
Cd	2	9.26	1.40	7.47	8.66	1.62	2.59
Hg	2	16.22	1.69	10.84	12.59	1.95	2.15
Al	3	18.07	1.75	11.66	13.53	2.02	2.07
Ga	3	15.31	1.65	10.44	12.11	1.92	2.19
In	3	11.50	1.50	8.62	10.01	1.74	2.41
Sn	4	14.83	1.64	10.22	11.86	1.89	2.22
Pb	4	13.19	1.57	9.45	10.97	1.82	2.30
Sb	5	16.54	1.70	10.99	12.75	1.97	2.14
Bi	5	14.04	1.61	9.85	11.43	1.86	2.26
Mn	4	32.61	2.13	17.28	20.05	2.46	1.70
Fe	2	16.90	1.71	11.15	12.94	1.98	2.12
Co	2	18.18	1.75	11.70	13.58	2.03	2.07
Ni	2	18.26	1.76	11.74	13.62	2.03	2.07

$$U(r) = \begin{cases} 0 & \text{for } r < R_c \\ -Ze^2/r & \text{for } r > R_c. \end{cases} \tag{L34}$$

$$\frac{\mathcal{E}_{ps}}{N} = \int_0^{R_c} d\vec{r} \frac{N}{\mathcal{V}} \frac{e^2}{r} = \frac{N}{\mathcal{V}} 2\pi e^2 R_c^2 \tag{L35}$$

$$= \frac{3}{4\pi r_s^3} 2\pi e^2 R_c^2 = 41 \frac{a_0 R_c^2}{r_s^3} \text{eV/atom} \tag{L36}$$

$$\Rightarrow \frac{\mathcal{E}}{N} = \left[-\frac{24.35}{(r_s/a_0)} + \frac{30.1}{(r_s/a_0)^2} - \frac{12.5}{(r_s/a_0)} + 41 \frac{a_0 R_c^2}{r_s^3} \right] \text{eV/atom}. \tag{L37}$$

$$r_s/a_0 = \sqrt{11.9[R_c/\text{Å}]^2 + .667} + 0.817. \tag{L38}$$

| Element	R_c (Å)	r_s/a_0, measured	r_s/a_0, Eq. (L38)
Li	0.92	3.27	4.09
Na	0.96	3.99	4.23
K	1.20	4.95	5.04
Rb	1.38	5.30	5.65
Cs	1.55	5.75	6.23

Calculated radii r_s are all about 10% too large because electronic structure has not been computed in accurate way.

Perfectly periodic one–dimensional chain of ions is always unstable against small displacements of ions caused by interaction with electrons.

Displacement of ion at location n is Δ_n.

$$\tfrac{1}{2}aY\Delta_n^2. \tag{L39}$$

$$\Delta_n = \Delta_G \cos Gna. \tag{L40}$$

$2\pi/G$

a
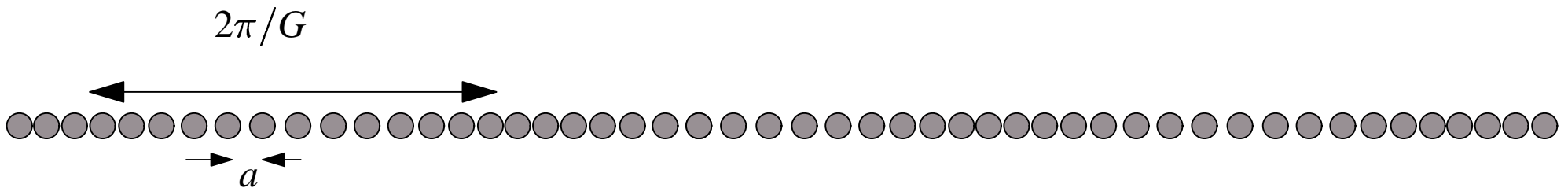
$$U \cos Gx = (\Delta_G u_0/a) \cos Gx. \tag{L41}$$

$$\mathcal{E} = \tfrac{1}{2}(\mathcal{E}_k^0 + \mathcal{E}_{k-G}^0) \pm \sqrt{(\mathcal{E}_k^0 - \mathcal{E}_{k-G}^0)^2/4 + |U|^2}. \tag{L42}$$
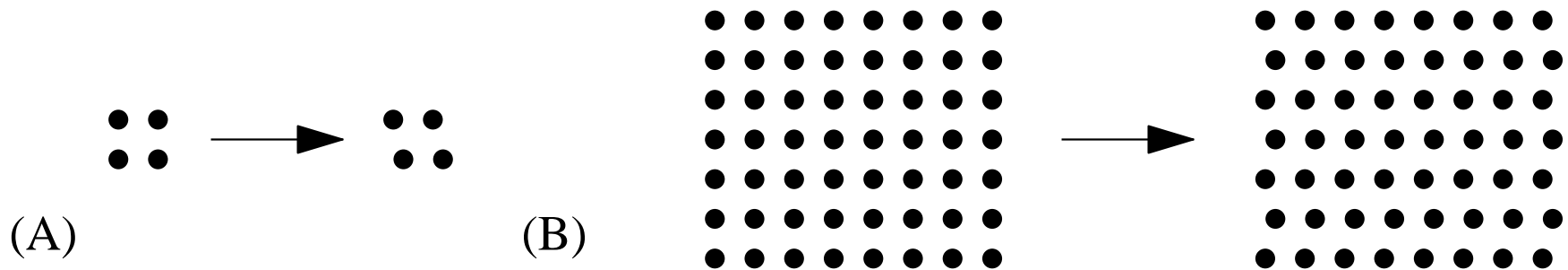
$$L \int_{-k_F}^{k_F} \frac{dk}{\pi} \left\{ \tfrac{1}{2}(\mathcal{E}_{k-G}^0 - \mathcal{E}_k^0) - \sqrt{(\mathcal{E}_{k-G}^0 - \mathcal{E}_k^0)^2/4 + |U|^2} \right\} \tag{L43}$$

$$= L \int_{-k_F}^{k_F} \frac{dk}{\pi} \left\{ \frac{\hbar^2}{4m}([k-2k_F]^2 - k^2) \right.$$

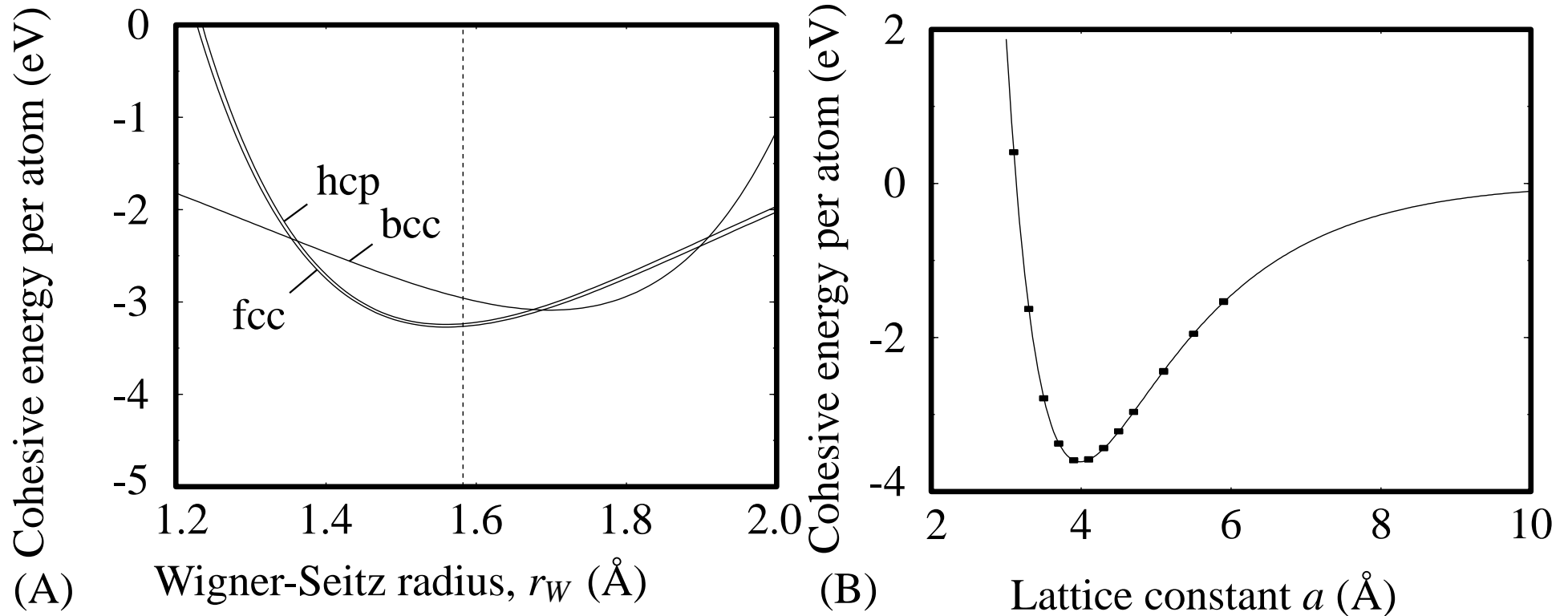$$\left. - \sqrt{(\frac{\hbar^2}{4m}([k-2k_F]^2 - k^2))^2 + |U^2|} \right\} \tag{L44}$$

$$= \frac{2L}{\pi} k_F \left\{ 2\mathcal{E}_{k_F}^0 - \sqrt{|U|^2/4 + (2\mathcal{E}_{k_F}^0)^2} - \frac{|U|^2}{8\mathcal{E}_{k_F}^0} \sinh^{-1}(4\mathcal{E}_{k_F}^0/|U|) \right\}. \tag{L45}$$

$$\frac{L}{4} \Delta_G^2 Y. \tag{L46}$$

$$\Delta_{2k_F} = \frac{8a\mathcal{E}_{k_F}^0}{|u_0|} \exp \left\{ \frac{-\pi\mathcal{E}_{k_F}^0 a^2 Y/k_F}{|u_0|^2} \right\}. \tag{L47}$$

(A) (B)

H_2O

(A) Cohesive energy per atom (eV) vs Wigner-Seitz radius, r_W (Å), showing hcp, bcc, and fcc curves.

(B) Cohesive energy per atom (eV) vs Lattice constant a (Å).

Results of computing cohesive energies with full–fledged band structure codes takes a universal form. It's not quite clear why! The energies of almost all solids with respect to uniform contraction and compression take a universal form described by just a few constants.

$$\frac{4\pi}{3} r_W^3 = \frac{\mathcal{V}}{N}. \tag{L48}$$

$$a_* = \eta \left(\frac{r_W}{r_{W0}} - 1 \right), \tag{L49}$$

$$\mathcal{E}(r_W) = \mathcal{E}_0 e^{-a_*} \left(-1 - a_* - 0.05 a_*^3 \right). \tag{L50}$$

Cohesive Energy from Band Calculations

El.	r_{W0} (Å)	η	$\mathcal{E}_0$ (eV)	El.	r_{W0} (Å)	η	$\mathcal{E}_0$ (eV)	El.	r_{W0} (Å)	η	$\mathcal{E}_0$ (eV)
Ag	1.60	5.94	2.96	Fe	1.41	5.16	4.29	Pt	1.53	6.47	5.85
Al	1.58	4.71	3.34	Gd	1.99	4.27	4.14	Rb	2.75	4.18	0.86
Au	1.59	6.75	3.78	Ge	1.76	5.05	3.87	Re	1.52	6.15	8.10
Ba	2.46	4.41	1.86	Hf	1.74	4.66	6.35	Ru	1.48	6.04	6.62
Be	1.25	4.01	3.33	In	1.84	5.11	2.60	Si	1.68	4.88	4.64
Ca	2.18	4.52	1.83	Ir	1.50	6.52	6.93	Ta	1.62	4.92	8.09
Cd	1.73	8.08	1.16	K	2.57	3.94	0.94	Th	1.99	4.12	5.93
Ce	2.02	3.11	4.77	Li	1.72	3.10	1.65	Ti	1.62	4.76	4.86
Co	1.39	5.31	4.39	Mg	1.77	5.60	1.53	Tl	1.90	5.74	1.87
Cr	1.42	5.59	4.10	Mo	1.55	5.85	6.81	V	1.49	4.81	5.30
Cs	2.98	4.17	0.83	Na	2.08	3.70	1.13	W	1.56	5.69	8.66
Cu	1.41	5.30	3.50	Nb	1.63	4.84	7.47	Y	1.99	4.23	4.39
Dy	1.96	4.85	3.10	Ni	1.38	5.11	4.44	Yb	1.99	3.94	1.60
Er	1.94	4.94	3.30	Pb	1.93	6.37	2.04	Zn	1.54	7.16	1.35
Eu	2.27	4.75	1.80	Pd	1.52	6.41	3.94	Zr	1.77	4.48	6.32

$$\mathcal{E} = \langle \Psi | \hat{\mathcal{H}}(\vec{R}_1 \ldots \vec{R}_N) | \Psi \rangle \tag{L51}$$

$$\vec{F}_l = -\frac{\partial \mathcal{E}}{\partial \vec{R}_l}. \tag{L52}$$

$\vec{R}_1$

θ

$\vec{R}_2$

$\vec{R}_3$