THE IONIC BOND

Introduction

A good place to start the study of engineering materials is with the nature of the energies and forces involved in the bonding between atoms. When we do we find that there are four principle types of bonds: ionic, metallic, covalent and Van der Waals. While bonding in most materials involves a combination of types of bonds it is still convenient to think of materials in terms of their dominant type of bonding. These generalizations are very useful since many fundamental properties are directly related to the nature and strength of these bonds. For example, ceramics and glasses, whose bonding is primarily ionic but may also have covalent traits, tend to be brittle, chemically inert, poor electrical and thermal conductors and may be optically transparent while metals, due to their primarily metallic bonding, are ductile, shiny and electrically and thermally conductive. Certain covalently bonded materials are among the hardest (diamond) and have the highest melting points. The chemical bonds in the best known semiconductors, silicon and germanium, are almost purely covalent. Clearly when we know something about a material's bonding we are in a better position to predict and even control its structure and properties. Fortunately we can also make a number of generalizations regarding properties such as its melting point, stiffness and coefficient of thermal expansion even without having to consider the details of the band structure of inner and outer electron shells (the outer shells are most important in bonding and in the material's electrical properties). In fact, the methods of calculating these bonding energies and properties are, for the most part, quite simple.

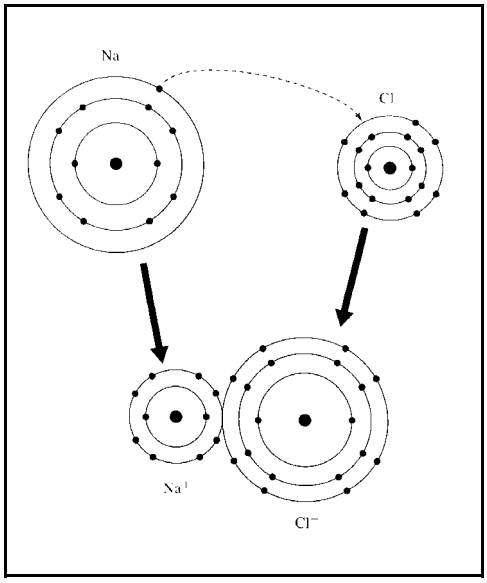

Figure 1. The formation of an ionic bond between a sodium and chlorine atom [1].

The chemical bond consists of two parts, an attractive component which acts over relatively large distances and a repulsive component which dominates at small interatomic spacings. For purely ionic bonds the energy of attraction is primarily due to the coulombic attraction between the outer shells of the oppositely charged ions. The equation for the lattice energy of an ionic compound is given by

$$E_a = \frac{Mz_1z_2q^2}{4\pi\epsilon_0 r} \qquad (1)$$

where M is the Madelung constant, r is the interatomic spacing, ϵ_0 is the permittivity in free space, q is the elementary charge and z_1 and z_2 are the valences of two ions. The energy of repulsion is due to the overlapping of the negatively charged electric fields of the inner shells and the positively charged nuclei. While the exact expression for this energy is difficult to derive a good approximation is given [2] by

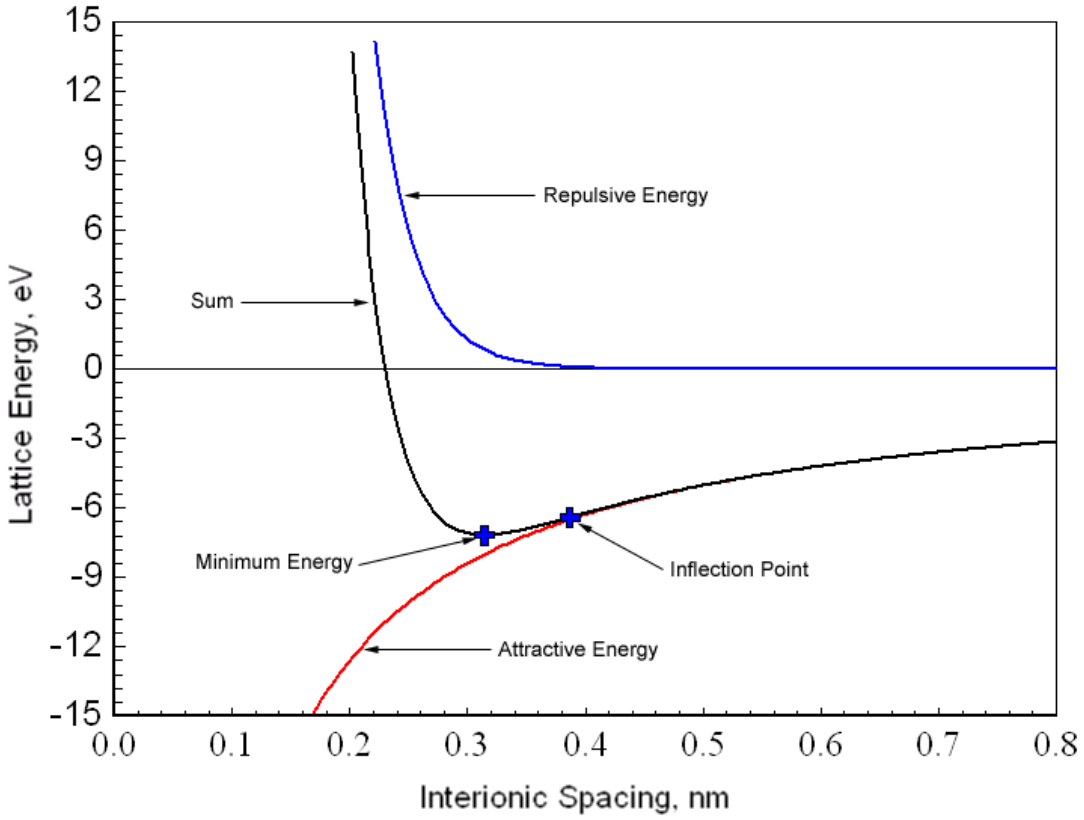

Figure 2 Calculated lattice energy for KCl.

$$E_r = b\lambda \exp\left(\frac{-r}{\rho}\right) \quad \textbf{(2)}$$

where b is the coordination number, λ is the repulsive energy coefficient and ρ is the repulsive range parameter. The total lattice energy is equal to the sum of the repulsive and attractive energies

$$E_{total} = E_a + E_r. \quad \textbf{(3)}$$

Figure 2 shows the individual and combined lattice energies as a function of interatomic spacing. Note that at large spacings there is still a small energy of attraction which increases ever more rapidly as the ions are brought closer together. On the other hand, the energy of repulsion is negligible at large spacings but when the ions are brought close enough together this term increases very quickly and soon dominates. Adding these two curves produces a minimum in the total lattice energy curve which defines both the equilibrium energy and interatomic spacing. This minimum is represented by the following equation:

$$E_0 = \frac{Mz_1z_2q^2}{4\pi\epsilon_0 r_0}\left(1-\frac{\rho}{r_0}\right) \quad \textbf{(4)}$$

where r_0 is the equilibrium spacing between nearest neighbor ions. A typical value for this equilibrium spacing is 0.3 nm and 6 eV is a typical value for this energy.

Mechanical (Elastic) Properties

The forces involved in the chemical bond are simply the first derivatives of bonding energies with respect to the interatomic spacing

$$F = \frac{dE}{dr} \approx \frac{\Delta E}{\Delta r} \quad \textbf{(5)}$$

By expressing chemical bonding in terms of forces we can better understand, and predict, certain mechanical properties, such as the elastic moduli, starting with the bulk modulus

$$K = \frac{1}{9r}\frac{1}{2}\frac{d^2E}{dr^2}_{r=r_0} = \frac{1}{9r}\frac{1}{2}\frac{dF}{dr}_{r=r_0} \approx \frac{1}{9r}\frac{1}{2}\frac{\Delta F}{\Delta r}_{r=r_0} . \quad \textbf{(6)}$$

The bulk modulus describes the elastic behavior of a material subjected to hydrostatic pressures and is related to the mechanical force required to change the volume per ion. It is also related to the material's shear modulus, its resistance to elastic deformation by shear forces, by the equation

$$G = \frac{3K(1-2\nu)}{2(1+2\nu)} \quad \textbf{(7)}$$

and to Young's modulus, the material's stiffness in uniaxial tension and compression, by

$$Y = \frac{3K(1+\nu)(1-2\nu)}{(1+2\nu)} \quad \textbf{(8)}$$

where ν is Poisson's ratio. The value of Poisson's ratio ranges from 0.1 for ceramics to 0.3 for metals.

Thermal Properties

Calculations of bond energies and spacing and the corresponding experiments are often done for temperatures at absolute zero but they are also done for other temperatures. When we examine the results for the different temperatures we find that as the temperature increases the magnitude of the bond energy decreases and the equilibrium spacing between ions increases. This increase in spacing is what is commonly called thermal expansion and is one manifestation of the energy required to

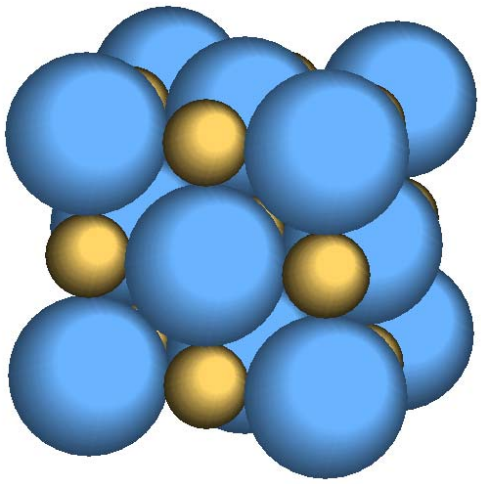

Figure 3. The NaCl-type structure is based on the fcc-unit cell with chlorine atoms at the lattice sites and sodium atoms at all octahedral sites. It could also be thought of as an fcc lattice with Na-Cl atoms pairs at each lattice site.

change the volume per atom. The decrease in the bond energy leads to an understanding of why materials become softer as they are heated. We also know from experience that if the temperature continues to increase the material will eventually reach a point where the bonds are so weak that atoms can easily move to other lattice sites, the crystalline structure may break down, and the material either melts or vaporizes. The amount of thermal energy required to melt the material is also shown in figure 2. Once we locate this point on the graph we should be able to estimate the melting point.

If the amount of thermal energy was greater than the lattice energy then the atoms in the structure would separate completely. Merely melting the material, however, would require considerably less thermal energy. The energy to cause melting is difficult to see in figure 2 but if we replot it as force versus distance then one will find a maximum slightly to the right of the equilibrium spacing. This is an interesting point whose interpretation strongly suggests the material is in a fluid state. At this point a significant restoring force exists (the force is quite high) so the material is not yet a gas. But if an applied force equal to the maximum is removed it is just as likely that the atom would return to its original position as it is to move further away. The material would be fluid.

The maximum on the *F*-*r* curve corresponds to the inflection point on the *E*-*r* curve. Once this energy E_1 has been found one can then estimate the melting point of the material. The energy required to raise the temperature of the material to its melting point is given by

$$\frac{\Delta E}{n} = c\Delta T \approx 3k_b\Delta T \qquad \textbf{(9)}$$

where c is the material's heat capacity, which can be approximated as $3k_B$ (k_B is Boltzmann's constant), and n is the number of lattice sites in the unit cell. The melting point can now be estimated using the following equation

$$T_{mp} \approx \frac{\Delta E}{n 3 k_B} + T_0 \qquad \textbf{(10)}$$

where T_0 is the temperature for which E_0 was calculated. Note that in this approximation the contribution of entropy has been ignored.

Objective

In this experiment the energies and forces involved in ionic bonding plus selected physical properties will be computed. The energy-spacing and force-spacing results will be graphed and the calculated properties will be compared to the values available in the literature. All calculations plus the graphing will be done using a spreadsheet. This spreadsheet program will be constructed using a logical, progressive approach which allows one to carefully examine each aspect of the program as it is being built. This spreadsheet will also be somewhat generalized, allowing one to calculate the bonding energies and forces for a number of ionic substances. Once this computer model has been built and validated against results listed in the tables at the end of this section the spreadsheet will be used to model the bonding and derive selected properties for other halite-type compounds.

Preparations

1. Go to the data books and look up the interatomic spacing, bonding energy, melting point, bulk modulus and Young's modulus for a number of inorganic compounds. Your objective here is to find the typical range of values for these properties.

2. Obtain the relevant data for the specific material for which you will be calculating the bonding energies.

3. Sketch the unit cell for this material. Label the positions of each ion and determine the spacing between neighboring anions and cations.

4. Decide on which units you will be using and obtain the necessary conversion factors.

5. Division by zero yields an indeterminate result and when using a computer program to divide by zero will produce divide-by-zero errors because the computer does not have enough information to be able to deal with an indeterminate result. Also, if you attempt to divide by a very small number you may get an overflow error because the resulting number is simply too large to be handled by the program. Both are likely to happen while constructing your spreadsheet. How do you plan to deal with these situations?

6. The numerical method you will be using to calculate the bonding energies and their derivatives involves an approximation of a curve with a series straight line segments. Comment on the errors you will be introducing into these calculations and how you plan to minimize their effects on your results.

7. Instead of approximating the heat capacity of your material as $3k_B$ you might want to look up the actual value and use it instead. You might also try looking up the equations for the Gibb's or Helmholtz free energies and calculate the free energy change associated with melting your material. It would be interesting to compare this to E_0 and to $E_0 - E_1$.

8. Plot the bulk moduli and melting points against the bonding energies listed in table 2.

Procedure

Start these computations by defining all terms, parameters and constants that are used in these equations and make sure the units of measure for each are consistent. Next, define the parameters for the particular material whose bonding behavior is being modeled. Now it will be possible to compute the attractive, repulsive and total bond energies and then, taking the first derivative to be the central difference of these energy-distance data, one can compute the force-distance curves. When this is done one will be able to extract several physical properties, specifically:

Interatomic Spacing	Locating the minimum in the energy-distance data one can determine the interatomic (interionic) spacing.
Bond Strength	The minimum on the energy-distance curve gives the strength of the bonds in the lattice.
Elastic Moduli	The bulk modulus (compressibility) can be computed using equation 8. Provide your own estimate of Poisson's ratio and compute the tensile and shear moduli.
Melting point	Compute the energy required to reach melting point but not complete the melting process. Do this using a rough approximation of heat capacity.
Density	Calculate the density of your material from the mass and volume of a single unit cell.

After successfully completing these calculations for potassium chloride repeat them for other materials listed in table 2.

The remainder of this procedure will guide a person not experienced in modeling physical phenomena using spreadsheets through the process of building an organized, readable, reusable spreadsheet, one that can be used to model the bonding behavior of all of the ionic materials listed in table 2 and, with minor modifications, other ionic materials.

General Layout of the Spreadsheet

Put All Constants and Parameters in a Separate Block of Cells

As a general rule it is best to define all constants and parameters used by the equations in a separate block of cells. This makes it easier to debug the program, to change the units used and to experiment with the equations. It also makes constructing the spreadsheet simpler since it is easier to reference a particular cell than it is to memorize a parameter's value and enter it into each equation. Besides, later you may want to replace a particular parameter with an equation, for

instance, replacing a fixed value with an equation to this parameter a temperature-dependent variable.

Enter the Equations for Bond Energies and Forces in Columns
The main part of the spreadsheet will be a series of columns containing the values and equations for the interatomic spacing, the energy of attraction, the energy of repulsion and the total bonding energy. One could put all this into one large equation for the energy of the lattice but long equations are difficult to enter and even more difficult to debug. It is best to keep all equations to a reasonable length.

Define the Graphs
The graphs will be standard x-y graphs with interatomic spacing as the x axes and the bonding energies and forces plotted along the y axes. The line colors and styles and the legend will be used to identify the attractive, repulsive and total lattice energies and forces.

Construct the Spreadsheet

Enter the Header
Start by entering the basic details about this spreadsheet, such as the file name, title, owner, and the dates it was created and last revised, at the top. Next, enter a brief description of the purpose or function of this spreadsheet plus any literature citations that might be important. This header can be very useful when sharing the spreadsheet with others or when referring to it in the future.

Define the Physical Constants, Conversion Factors and Parameters for the Equations for Bonding Energies and Forces
Enter the values for every parameter used by all equations in cells just below the spreadsheet's header. Include their names and the units you are using. If the original units are not those you will be using in the equations then include a cell with the value of this parameter given in the correct units. Your equations will then reference these cells, saving you the trouble of including the units conversion factors in the equations.

Define the Parameters for the Material
Use a block of cells to define all details about the material that the bond energy and force equations will require. You might also want to include additional information such as the mineral name, lattice-type and references to your sources of information.

Define the Values for the Interatomic Spacing
The first column in your spreadsheet will contain the values for the interionic spacing which the equations for bond energy and force will use. The equation which generates these values will require only an initial value and an increment. Enter these two constants into the parameter section of your spreadsheet. Later you can adjust the value of the increment to change the range and resolution of interionic spacing and you can adjust the initial value to shift the curves to the left and right on the graphs and to fine tune the spreadsheet so that the best estimate of the energy minimum is obtained.

At the top of the first column you will reference the cell containing the initial value of the interionic spacing. In the next cell you will add the predefined increment to the value in the first cell. Finally, you will replicate this second cell, say 300 times, to generate a column containing all of the values

for the interionc spacing.

Calculate the Attractive, Repulsive and Total Lattice Energies and Forces
In the adjacent columns enter the equations for the attractive and repulsive energies. Enter them at the top of the columns and then replicate them so that these two columns are as long as the first column. Add these two columns together in column 4 to obtain the total lattice energy. Next, add three more columns containing the calculated coulombic, repulsive and total lattice forces. The equations for these columns will be simply the slopes (first derivative) of the corresponding bond energy values.

Create the Results Section
Construct a table-style summary of the reference and calculated properties. If this is done well it will make debugging, using and improving the accuracy of your spreadsheet much easier.

Annotate the Spreadsheet
Label each column, parameter, physical constant and result in the spreadsheet. Don't forget to include the units.

Construct the Graphs
Construct xy graphs for both the E-r and F-r results. In this spreadsheet column 1 contains the values for the x axis for both graphs, columns 2 through 4 contain the values for the first 3 series of the energy axis in the E-r graph and columns 5 through 6 contain the values for the data for the force axis on the F-r graph. Label the axes appropriately and include a legend. Insert the graph into the spreadsheet, above the columns and to the right of the parameters. Optionally, save these graphs as TIFF or JPEG files so that you can insert them into your report or you can copy them to the clipboard then paste them directly into your laboratory report.

Print the Spreadsheet
Print each graph separately and then print the top portion of the spreadsheet which includes the parameters, results, the first dozen or so values in the columns and possibly the inserted graphs. This can be placed in the appendix to show the reader how you set up and solved this problem using a spreadsheet.

Results
You might want to start with a brief description of the curves you calculated, noting the similarities and differences to those shown in figure 2 and the correspondence of key features in your E-r and F-r curves. Next, you will probably want to compare your results with those measured and calculated by others. In general, the differences between measured and calculated values of the bond energy are usually around 1 or 2%. Some of your results will be within these limits while others will not. Can you account for this and can you think of ways to improve on these results?

Discussion
The reader would probably like for you to start your discussion by confirming that your results are consistent with the description of ionic bonding given above. If everything looks OK up to this point you might want to comment on the possibility of using your spreadsheet to model the bonding and properties of the other materials listed in table 2. You might even want to take this to the next level and show that the equations you have used, the results of your calculations and the data in table

2 prove that there is a well-defined relationship between the nature of the chemical bond and certain physical properties. You might even think of other properties which one might be able to calculate using your spreadsheet. Finally, would it be possible to modify this spreadsheet to model other types of bonding?

Conclusions

If all has gone well your results will compare well with those measured and calculated by others. Looking back on this experiment you may also find that this exercise has provided you with both a valuable new set of skills which you can use to solve other engineering problems and also a good lesson on the fundamental aspects of chemical bonding which will help you understand something about the nature of all materials and the origins of many of their properties.

References and Additional Resources

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8. L.Pauling, The Nature of the Chemical Bond, 3rd edition, Cornell University Press, Ithaca, NY, pp. 505-510, (1960).

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10. ICDD Powder Diffraction Database, Sets 1-46, (1997).

Physical Constants

Avogadro's Number	N_A	6.022045×10^{23} mol^{-1}
Boltzmann's Constant	k_B	1.380662×10^{-23} J K^{-1}
Elementary Charge	q	$1.6021892 \times 10^{-19}$ C
Permittivity of Free Space	ϵ_0	$8.85418782 \times 10^{-12}$ C^2 N^{-1} m^{-2} or C^2 J^{-1} m^{-1}

Conversion Factors

1 eV	$1.6021917 \times 10^{-19}$ J
1 MPa	145 psi
1 calorie	4.184 J

Distance Between Any Two Points

The following equation gives the distance between point 1 and point 2 where their coordinates x,y,z are defined for any of the seven crystal systems where a, b and c and α, β and γ have their usual meanings.

$$d_{12}^2 = (x_1 - x_2)^2 a^2 + (y_1 - y_2)^2 b^2 + (z_1 - z_2)^2 c^2 + 2(x_1 - x_2)(y_1 - y_2) ab \cos\gamma + \quad \textbf{(11)}$$

$$2(y_1 - y_2)(z_1 - z_2) bc \cos\alpha + 2(z_1 - z_2)(x_1 - x_2) ca \cos\beta$$

Note that for orthogonal structures the cosine terms drop out.

Table 1. Crystallographic data for selected compounds [2,3,4,10]

Substance	Mineral Name	Crystal Lattice	Lattice Constants, nm	Madelung Constant	Density, Mg/m^3	PDF File Number
KBr	-	FCC (NaCl-type)	a=0.660050	1.747565	2.749	36-1471
KCl	Sylvite	FCC (NaCl-type)	a=0.629170	1.747565	1.988	41-1476
KF	Carobbiite	FCC (NaCl-type)	a=0.534758	1.747565	2.523	36-1458
KI	-	FCC (NaCl-type)	a=0.706550	1.747565	3.126	04-0471
LiBr	-	FCC (NaCl-type)	a=0.550130	1.747565	3.465	06-0319
LiCl	-	FCC (NaCl-type)	a=0.513960	1.747565	2.074	04-0664
LiF	Griceite	FCC (NaCl-type)	a=0.402700	1.747565	2.638	04-0857
LiI	-	FCC (NaCl-type)	a=0.600000	1.747565	4.116	01-0592
NaBr	-	FCC (NaCl-type)	a=0.597353	1.747565	3.206	36-1456
NaCl	Halite	FCC (NaCl-type)	a=0.564020	1.747565	2.163	05-0628
NaF	Villiaumite	FCC (NaCl-type)	a=0.463329	1.747565	2.804	36-1455
NaI	-	FCC (NaCl-type)	a=0.647300	1.747565	3.671	06-0302
RbBr	-	FCC (NaCl-type)	a=0.688900	1.747565	3.360	08-0480
RbCl	-	FCC (NaCl-type)	a=0.658100	1.747565	2.818	06-0289
RbF	-	FCC (NaCl-type)	a=0.565160	1.747565	3.844	22-0886
RbI	-	FCC (NaCl-type)	a=0.734200	1.747565	3.564	06-0218
TiO_2	Rutile	Tetragonal	a=0.45933, c=0.29592	2.248037	4.250	21-1276
TiO_2	Anatase	Tetragonal	a=0.37852, c=0.95139	2.400000	3.893	21-1272
ZnS	Sphalrelite (Zinc Blend)	FCC	a=0.54060	1.638060	4.097	05-0566
ZnS	Wurtzite	Hexagonal	a=0.382098, c=0.62573	1.641320	4.090	36-1450
SiO_2	β-Quartz	Hexagonal	a=0.511, c=0.537	4.1719	2.539	47-1144
CsCl	-	Cubic	a=0.41230	1.762670	3.989	05-0607
MgF_2	Sellaite	Tetragonal	a=0.46200, c=0.30509	2.3810	3.177	41-1443
MgO	Periclase	NaCl-type	a=0.42112	1.747565	3.585	45-0946
ZnO	Zincite	Hexagonal	a=0.324982, c=0.520661	1.4985	5.675	36-1451
CdI_2	-	Hexagonal	a=0.42481, c=1.37265	2.355	5.669	33-0239
Cu_2O	Cuprite	Cubic	a=0.42696	2.221240	6.106	05-0667
Al_2O_3	Corundum	Rhombohedral	a=0.47587, c=1.29929	4.171900	3.987	46-1212
CaF_2	Fluorite	Cubic	a=0.546305	2.3650	3.181	35-0816

Table 2. Selected room temperature properties of materials having the NaCl-type structure [2,3,6].

Substance	Interionic Spacing nm	Repulsive Energy Parameter eV	Repulsive Range Parameter nm	Measured Lattice Energy eV	Calculated Lattice Energy eV	Gibb's Free Energy kJ/mol	Melting Point K	Bulk Modulus GPa	Poisson's Ratio	Shear Modulus GPa	Young's Modulus GPa
KBr	0.3298	2392.6	0.0336	-6.886	-6.908	-380.8	1007	15.1	0.254	8.9	22.2
KCl	0.314655	2132.5	0.0326	-7.190	-7.008	–409.2	1043	17.4	0.249	10.5	26.2
KF	0.2674	1362.7	0.0298	-8.230	-8.200	-537.8	1131	31.1	0.260	17.8	44.9
KI	0.3533	2964.7	0.0348	-6.500	-6.266	-324.9	954	11.7	0.251	7.0	17.5
LiBr	0.2751	614.8	0.0340	-8.230	-7.849	–342.0	823	25.7	0.248	15.6	38.9
LiCl	0.2570	509.7	0.0330	-8.621	-8.365	-384.4	878	31.8	0.238	20.2	50.0
LiF	0.2014	307.9	0.0291	-10.507	-10.503	-587.7	1118	66.6	0.198	50.5	120.9
LiI	0.3000	623.1	0.0366	-7.706	-7.203	-270.2	722	17.1	0.200	10.99	26.38
NaBr	0.2989	1383.5	0.0328	-7.528	-7.337	-348.9	1020	19.9	0.250	11.9	29.8
NaCl	0.282010	1092.3	0.0321	-7.918	-7.745	-384.2	1074	23.9	0.249	14.4	36.0
NaF	0.231710	666.8	0.0290	-9.297	-9.332	-543.5	1266	48.1	0.231	31.6	77.7
NaI	0.3237	1643.6	0.0345	-7.077	-6.791	-286.1	934	16.1	0.274	8.6	21.9
RbBr	0.3445	3151.9	0.0338	-6.617	-6.431	-381.8	966	13.8	0.268	7.6	19.2
RbCl	0.3291	3318.4	0.0323	-6.908	-6.739	-407.8	991	16.2	0.268	8.9	22.6
RbF	0.2815	1851.6	0.0301	-7.866	-7.823	-	1068	27.3	0.276	14.4	36.9
RbI	0.3671	4150.6	0.0348	-6.283	-6.054	-328.9	920	10.8	0.262	6.1	15.5
MgO	0.2110	-	-	-	-42.405	-569.4	2852	153.3	0.172	128.6	301.5
CaO	0.2100	-	-	-	-37.437	-604.0	2614	-	-	-	-

File: Ionic Bonding-2.xls
Owner: Mike Meier
Created: June 19, 1997
Revised: January 11, 2003
Description: Calculation of ionic bonding energies, forces and related properties for materials with the NaCl-type structure.

Conversion Factors

From	To	Value	Units
Joules	eV	6.242E+18	eV/J
Coulombs	eV s	6.242E+18	eV s/C
GPa	ksi	145	ksi/GPa
Calories	Joules	4.184	J/cal

Physical Constants

Avogadro's Number:	6.022E+23	per mole		
Boltzmann's Constant:	1.381E-23	J/K	8.618E-05	eV/K
Proton Charge:	1.602E-19	C		
Velocity of Light:	2.998E+08	m/s		
Permittivity:	8.854E-12	C2/Nm2		

Enviromental Parameters

Temperature:	298	K
Pressure:	1	atmospheres

Material

Substance:	KCl			
Mineral Name:	Sylvite			
Melting Point:	1043	K		
Density:	1.988	Mg/cm3		
Crystal Lattice:	NaCl type			
Lattice Constants:	0.629170	0.629170	0.629170	a,b,c in nm
Lattice Angles:	90.000	90.000	90.000	degrees
Equivalent Sites:	4			
Coordination Number:	6			
Reference Ion:	0	0	0	u,v,w
Nearest Ion:	0	0	0.5	u,v,w
	Type	Number	Valence	At.Wt.
Cation:	K+	4	1	39.0983
Anion:	Cl-	4	-1	35.453

Interionic Spacing (independent variable)

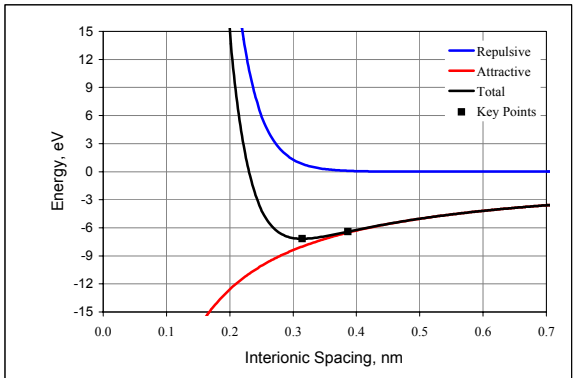
Initial Value:	0.061895	nm
Increment:	0.002500	nm

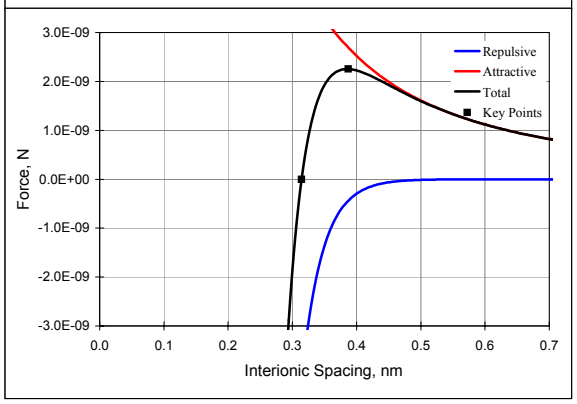
Repulsive Energy

Energy Parameter:	2132.5	eV
Range Parameter:	0.032600	nm

Coulombic Attraction

Madelung Constant:	1.747565





Results

Property	Reference	Calculated	Units	Calculated	Units	Difference	Note
Cell Containing E min:	-						Uses the Quattro Pro @MinLookup function on column D
Cell Containing F max:	-						Uses the Quattro Pro @MaxLookup function on column G
Equilibrium Spacing:	0.314585	0.314395	nm	3.14395	Angstroms	-0.06%	Ionic spacing at the minimum for column D
Lattice Constant, a:	0.629170	0.628790	nm	6.28790	Angstroms	-0.06%	For this structure, a=2r0
Energy Minimum:	-7.190	-7.176	eV	-692.3	kJ/mole	-0.20%	Minimum, column D
Total Lattice Energy:	-7.190	-7.175	eV	-692.2	kJ/mole	-0.21%	Equation 4
Force at Emin:	n/a	#VALUE!	N	-	-	-	Minimum, column G, absolute value
dF/dr at F=0:	n/a	99.299	N/m	-	-	-	dF/dr at E min
Bulk Modulus:	17.40	17.55	GPa	2.54	1e6 psi	0.84%	Equation 6
Poisson's Ratio:	0.249	0.215	-	-	-	-	t the correct value for the shear modulus.)
Shear Modulus:	10.50	10.49	GPa	1.52	1e6 psi	-0.08%	Equation 7
Young's Modulus:	26.20	25.49	GPa	3.70	1e6 psi	-2.70%	Equation 8
Maximum Force:	n/a	2.252E-09	N	-	-	-	Maximum, column G
Energy at F max:	n/a	-6.415	eV	-	-	-	Energy at maximum for column G
delta E:	n/a	0.760	eV	73.4	kJ/mole	-	
Melting Point:	1043.0	1033.4	K	760.4	C	-0.92%	Equation 10
Mass:	n/a	4.952E-22	grams/u.cell	-	-	-	
Density:	1.988	1.992	g/cm3	-	-	0.19%	

Ionic Spacing nm	Repulsive Energy eV	Attractive Energy eV	Total Energy eV	Repulsive Force Newtons	Attractive Force Newtons	Total Force Newtons	dF/dr N/m	Energy Data Symbols	Energy Data Lables	Force Data Symbols	Force Data Lables
0.061895	1916.374	-40.660	1875.714								
0.064395	1774.906	-39.082	1735.825	-8.731E-06	9.738E-08	-8.634E-06					
0.066895	1643.882	-37.621	1606.261	-8.086E-06	9.022E-08	-7.996E-06	2.456E+05				
0.069395	1522.530	-36.266	1486.264	-7.490E-06	8.383E-08	-7.406E-06	2.275E+05				
0.071895	1410.136	-35.005	1375.132	-6.937E-06	7.810E-08	-6.859E-06	2.108E+05				
0.074395	1306.039	-33.828	1272.211	-6.425E-06	7.293E-08	-6.352E-06	1.953E+05				
0.076895	1209.627	-32.729	1176.899	-5.950E-06	6.826E-08	-5.882E-06	1.809E+05				
0.079395	1120.332	-31.698	1088.634	-5.511E-06	6.402E-08	-5.447E-06	1.676E+05				
0.081895	1037.629	-30.730	1006.898	-5.104E-06	6.017E-08	-5.044E-06	1.553E+05				
0.084395	961.030	-29.820	931.210	-4.727E-06	5.666E-08	-4.671E-06	1.438E+05				
0.086895	890.087	-28.962	861.125	-4.378E-06	5.344E-08	-4.325E-06	1.332E+05				
0.089395	824.380	-28.152	796.228	-4.055E-06	5.049E-08	-4.005E-06	1.234E+05				
0.091895	763.524	-27.386	736.138	-3.756E-06	4.778E-08	-3.708E-06	1.143E+05				
0.094395	707.160	-26.661	680.499	-3.479E-06	4.528E-08	-3.433E-06	1.058E+05				
0.096895	654.958	-25.973	628.984	-3.222E-06	4.297E-08	-3.179E-06	9.804E+04				
0.099395	606.608	-25.320	581.289	-2.984E-06	4.084E-08	-2.943E-06	9.080E+04				
0.101895	561.828	-24.699	537.130	-2.764E-06	3.886E-08	-2.725E-06	8.410E+04				
0.104395	520.354	-24.107	496.247	-2.560E-06	3.702E-08	-2.523E-06	7.788E+04				
0.106895	481.941	-23.543	458.398	-2.371E-06	3.530E-08	-2.335E-06	7.213E+04				
0.109395	446.364	-23.005	423.359	-2.196E-06	3.371E-08	-2.162E-06	6.680E+04				
0.111895	413.413	-22.491	390.922	-2.034E-06	3.222E-08	-2.001E-06	6.187E+04				
0.114395	382.895	-22.000	360.895	-1.884E-06	3.082E-08	-1.853E-06	5.729E+04				
0.116895	354.629	-21.529	333.100	-1.744E-06	2.952E-08	-1.715E-06	5.306E+04				
0.119395	328.451	-21.078	307.372	-1.616E-06	2.830E-08	-1.587E-06	4.913E+04				
0.121895	304.204	-20.646	283.558	-1.496E-06	2.715E-08	-1.469E-06	4.550E+04				