

# Metallic Structure and Bonding

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**Abstract** This article briefly describes the current physical model of metallic structure and bonding. An alternative soft-sphere model of metal structure is introduced. Limitations of the current model are given and properties of metals which can be accounted for by the soft-sphere model are discussed. A simple soft-sphere formula, which calculated internuclear distances of Group 1 and Group 2 crystalline binary salts to a remarkable degree of accuracy, is applied to calculate metallic radii (equal to half the internuclear distances) of Group 1 and Group 2 metals precisely. A simple expression previously used to calculate lattice energies using the soft-sphere radii concept is used to calculate enthalpies of formation of Group 1 and Group 2 metal ions and results compare well with observed values. The work functions of Group 1 and Group 2 metals are shown to be inverse functions of the soft sphere ionic radii.

**Keywords:** metals, metallic bonding, metallic structure, band theory, metallic radii, enthalpy of formation, lattice energies, work function, free electron in metals, electron sea model, chemical bonding

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## 1. Introduction

Over 70% of all elements are metals. Although it is well known that most metals have hexagonal, cubic close packed or body centered cubic structures [1], metallic structure is not fully understood. Paul Drude [2], in 1900, was the first to propose the "free electron" model for electricity conduction in metals and metallic bonding. He suggested that in crystalline metals, positive ions were surrounded by an "electron gas". Estimates of the number of "free" electrons in a metal have also been described since the early twentieth century [3]. Band theory [4], which is based on quantum mechanics postulates the existence of energy bands in solids that influence the behavior of electrons. In his book, *The Nature of the Chemical Bond* [5], Pauling provided extensive details on the closest packing of spheres, metallic orbitals, metallic valencies, bond lengths, and bond numbers in metals. However, some common properties of metals (see below) were not discussed in his book nor were they accounted for in free electron/electron sea model of metallic structure and bonding.

### 1.1. The Current "Electron Sea" Model

Although band theory described the mechanism of electrical conduction correctly and is the accepted theoretical model for describing electrical conduction, it does not physically describe the structure of metals. It is still common to describe metallic structures and metallic bonding as "bonding which involves the delocalization of electrons throughout the metal solid" [6] or as "metal cations in a sea of electrons" [7]. It has been demonstrated

[8] that the current "free electron/electron sea" model used to describe metallic structure and properties is inadequate. This is not satisfactory for both researchers and students attempting to understand the physical structure and those properties and reactions of metals not included in the band theory.

## 2. The Soft-sphere Model

The soft-sphere model considers atoms and ions are compressible spheres. It was originally used to calculate internuclear distances of ionic compounds [9]. Values calculated when compared with experimental figures produced excellent agreement (with average difference between observed and calculated of less than 0.5%). We then extended the concept to metallic crystals. We consider that in a metal solid, the outermost electron(s) in each atom is/are not exactly "free" nor completely delocalized. The outermost electron(s) is/are separated/detached from the atom which forms a positive ion with one or more of the "detached" electron(s) behaving like negative ions. The detached outermost electron(s) can occupy certain equivalent positions that are at the midpoint between the nearest neighbors of the positive ions (similar to ionic crystals, where positive ions occupy positions between negative ions) but can move within these midpoint positions in a unit cell. For the remainder of this paper, these midpoint positions will be called "midpoint sites". Depending on the Group and metallic structure (hcp, ccp or bcc) the most likely number of outermost electrons detached from each individual metal atom range from one to a maximum of five. The soft-sphere ionic radii of Group 1 and Group 2 metals

(excluding beryllium) have already been determined very accurately [9] and in this work we use the elements of these 2 Groups to demonstrate the soft-sphere model of metallic structure and bonding.

Consider any crystal with a hexagonal (hcp) or cubic closed pack (ccp) structure of identical atoms, each atom has twelve co-ordination or twelve closest neighbors and in a body centered cubic each atom has eight closest neighbors. There are two atoms in each unit cell in a body centered cubic, six atoms in each unit in a hexagonal closed pack and four atoms per unit cell in a cubic closed packed or face centered cubic [10] crystal.

At room temperature, all Group 1 metals have a bcc structure and each atom has one outermost electron. In the soft-sphere model of metallic structure and bonding, each atom has a single outermost electron which it loses to form a unipositive ( $1^+$ ) ion. Each positive ion has eight nearest identical neighbors of positive ions. Hence there are eight equivalent sites that are midpoint between the internuclear distance of a positive ion and its eight neighboring positive ions. The outermost electron which is detached from the atom can occupy and move around any one of these eight midpoint sites in a unit cell at any *one* time. Since there are two positive ions in each unit cell, there are only two detached electrons in each cell and, therefore, at any *one* time only two of the eight (or a quarter of) midpoint sites are occupied and the rest are vacant and under certain conditions can be occupied by other detached electrons moving in from other unit cells.

Group 2 metals present a slightly more complicated problem in that beryllium and magnesium have hcp structures at room temperature whereas both calcium and strontium possess the ccp structure and barium has a bcc structure respectively [11]. In any Group 2 metal crystal, each metal atom loses its two outermost electrons to form a dipositive ( $2^+$ ) ion. In a barium crystal (with a bcc structure), each dipositive ion has eight identical nearest neighbors of positive ions. Since there are two positive ions in each unit cell, there are four detached electrons in a cell. Hence, at any *one* time there are four electrons occupying the eight equivalent midpoint sites between the positive ions, which mean that only half of the eight sites are occupied. In calcium and strontium (with ccp structures), there are four positive ions and eight detached electrons (with each atom losing two electrons) occupying twenty four equivalent midpoint sites per unit cell. Thus, at any *one* time, only a third of the sites are occupied. Similarly for beryllium and magnesium (hcp), with two positive ions and four detached electrons per cell, at any *one* time only a third of the twelve sites are occupied.

The atomic/metallic radius of a metal atom (which is half the internuclear distance between the nearest neighbors) or distance between the centers of the positive ion and the detached outermost electron, just as in the case of an ionic crystal, can be calculated from the relationship [12]:

$$S(\text{calc})^k = [M]^k + [e]^k$$

S is the radius of the metal atom, [M] is the ionic radius of the positive ion, [e] is the "orbital radius" of the midpoint site containing the detached electron and the exponent  $k$  is defined previously.

## 2.1. Comparison between Calculated and Observed Radii of Group 1 and Group 2 Metals

Column B of Table 1 shows the soft-sphere ionic radii determined by previous work [9], the observed unit cell constants [13] quoted to appropriate number of decimal places (after taking account of the size of experimental uncertainties) are shown in columns C and D. Internuclear separations (between nearest neighbors) derived from unit cell constants of Group 1 and Group 2 metals are listed in Column E. The distances between the centers of the positive ions and spaces occupied by the detached electrons (or the metallic radii of the atoms) are given in Column F of the table. All figures are given in Angstrom ( $\text{\AA}$ ) units, where  $1 \text{ \AA}$  equals  $10^{-10}\text{m}$ . Since the soft-sphere radius of the beryllium ion has not been determined previously, for this work we have extrapolated from the known soft-sphere radii of Group 2 metals to obtain an estimate of  $0.75 \pm 0.04 \text{ \AA}$ .

De Broglie proposed that the same dualism of wave and corpuscle as is present in light may also occur in matter<sup>14</sup>, where the wavelength of a particle  $\lambda = h/mv$ ,  $h$  being Planck's constant,  $m$  is the mass of the particle and  $v$  it's velocity. For a particle moving in an orbit, it was also proposed that  $n\lambda = 2\pi r$ , where  $r$  is the radius of the orbit. For example, in a hydrogen atom with an electron orbital radius of  $0.529 \text{ \AA}$ ,  $\lambda$  is approximately  $3.3\text{\AA}$ . According to the de Broglie relationship the electron wave length is directly proportional to its speed and classical physics shows that the speed  $v$  is a function of the coulombic attraction and distance from the nucleus. By making appropriate estimates [15] of screening constants the coulombic attraction and hence approximate values of  $v$  can be obtained. Since the "detached" electrons in the mid-point sites are attracted equally by two positive ions and we assume that each one moves in orbital motion or radius  $r$  (equal to [e]) around the site. We have made an empirical assumption that (a)  $e$ , the "orbital radius" of the midpoint site containing the separated/detached electron and (b) the exponent  $k$ , are different for Group 1 and Group 2 metals because of the difference in charge on the positive ion, the value of  $k$  may also be influenced by the number of nearest neighbors. However, in order to limit the number of values of  $k$  in the calculations we have assumed  $k$  to be 1.5 for Group 1 and  $k$  equals 1.3 for Group 2. All Group 1 metals have one outermost electron and all have bcc structure, therefore we assume that the value of  $e$  for all five elements is the same. Based on the estimated value of  $v$ , we produced an approximate a value of 0.8 for  $e$ . For Group 2 metals, beryllium, magnesium, calcium and strontium have twelve co-ordination and we assume that  $e$  is approximately the same for all four elements and has the value of 0.565. Barium has eight co-ordination and the value of  $e$  is 0.23.

The observed metallic radii (or half the internuclear distance) of Group 1 and Group 2 metals are shown in Column B and the calculated radii in Column C of Table 2 respectively. As shown in Column D of the table, differences between the observed and calculated are in all cases less than  $0.01 \text{ \AA}$ . This is very good agreement since the experimental uncertainties of the appropriate cell constants can be as great as  $0.01 \text{ \AA}$  (as in the case of calcium).

**Table 1. Soft-sphere ionic radii and atomic/metallic radii of Group 1 and Group 2 metals**

Element	Soft-sphere radii(Å)	Cell constants		Internuclear separation Metallic radii	
		a	c	(Å)	(Å)
(A)	(B)	(C)	(D)	(E)	(F)
Li	1.094	3.509		3.039	1.520
Na	1.497	4.291		3.716	1.858
K	1.971	5.321		4.608	2.304
Rb	2.160	5.700		4.937	2.469
Cs	2.368	6.176		5.348	2.674
Be	0.750	2.286	3.584	2.256	1.128
Mg	1.282	3.209	5.211	3.203	1.602
Ca	1.657	5.580		3.946	1.973
Sr	1.861	6.086		4.303	2.152
Ba	2.084	5.023		4.350	2.175

**Table 2. Comparison of observed and soft-sphere atomic/metallic radii of Group 1 and Group 2 metals**

Element	Observed (Å)	Soft-sphere calculated (Å)	Obs - Calc (Å)
(A)	(B)	(C)	(D)
Li	1.520	1.512	0.008
Na	1.858	1.865	-0.007
K	2.304	2.298	0.006
Rb	2.469	2.474	-0.005
Cs	2.674	2.669	0.005
Be	1.128	1.124	0.004
Mg	1.602	1.610	-0.008
Ca	1.973	1.964	0.009
Sr	2.152	2.158	-0.006
Ba	2.175	2.175	0.000

## 2.2. Enthalpy of Formation of Group 1 (Monovalent) and Group 2 (Divalent) Positive Gaseous Metallic Ions

The lattice energy of a compound is the energy change when one mole of the compound at one atmospheric pressure is converted into gaseous positive and negative ions which are separated from each other at infinity. Lattice energies can be calculated using the Born-Haber

cycle or from equations such as the Born-Landé/Born-Mayer equations or the improved Kapustinskii equation. The enthalpy of formation of a positive univalent Group 1 or divalent Group 2 metal ion is the energy change when one mole of the crystalline metal is converted into one mole of the gaseous positive metal ions separated from one (in the case of Group 1) and or two (in the case of Group 2) moles of electrons. In the case of a metal solid, the detached electron is treated as being equivalent to the "negative ion" bonded to positive ion. Under this assumption, the energy change when a crystalline metal is converted into one mole of the gaseous positive ions and the respective number of moles of "electrons" can then be regarded as equivalent to the lattice energy of an ionic crystal. The enthalpies of formation of gaseous metal atoms for Group 1 and Group 2 metals are shown in Column B of Table 3. The first and, for Group 2 only, second ionization energies of the metals are listed in Columns C and D respectively. Ionization energies are converted from eV (electron volts) to kJ/mole by the relationship of 1 eV = 96.49 kJ/mole. The enthalpies of formation of the appropriate gaseous ions are shown in Column E of the Table. All ionization energies, enthalpies of formation, work functions, bond dissociation energies and enthalpies of fusion that are utilized in this work are quoted from the *CRC Handbook of Chemistry and Physics* [16].

**Table 3. Enthalpies of formation of Group 1 and Group 2 metal ions**

Element	Enthalpies of formation of M(g)	Ionization energies		Enthalpies of formation M <sup>+</sup> (Group 1)/M <sup>2+</sup> (Group 2)
		1 <sup>st</sup>	2 <sup>nd</sup>	
(A)	(B) kJ/mole	(C) eV(kJ/mole)	(D)eV(kJ/mole)	(E)kJ/mole
Li	159.3	5.392(520.25)		679.6
Na	107.5	5.139(495.87)		603.4
K	89.0	4.341(418.83)		507.8
Rb	80.9	4.177(403.05)		484.0
Cs	76.5	3.894(375.72)		452.2
Be	324.0	9.323(899.55)	18.211(1757.19)	2980.7
Mg	147.1	7.646(737.78)	15.035(1450.75)	2335.6
Ca	177.8	6.113(589.86)	11.872(1145.50)	1913.2
Sr	164.4	5.695(549.50)	11.030(1064.29)	1778.2
Ba	180.0	5.212(502.87)	10.004(965.27)	1648.1

We have previously developed a simple expression to calculate lattice energies of Group 1 and Group 2 salts [9]. The results produced agreed well with lattice energies calculated from the Born-Haber cycle. We reproduce the expression here as follows:

$$(Lattice\ energy)\ E_L = R(H_o / M) \left( M^{k-1} \right) / \left( X^{k-1.3333} \right) \left( \frac{1}{2} \right)^{0.33333} (\Sigma Q_i^2)$$

where  $R$  is the Rydberg constant for infinite mass converted to kilo Joules per mole,  $H_o$  is the classical Bohr radius,  $M$  is the size of the cation,  $X$  is the size of the anion and  $Q_i$  is the charge on the ions. Hence, for sodium chloride  $\Sigma Q_i^2 = 1 + 1 = 2$  and for calcium chloride it is  $4 + 1 + 1 = 6$  etc.  $\Sigma Q_i^2$  is the sum of all the squares of the charges on the ions, since the higher the charge on the ions the more electrons need to be removed from the overlap region and the more energy is required to separate them.  $R$

is the amount of energy needed to remove an electron from a species the size of a hydrogen atom,  $(H_0/M)$  provides a ratio of the distance of the electron from the nucleus, since the greater the size the less is the energy needed to remove the electron.  $(M^{k-1})/(X^{k-1.3333})$  gives an approximation of the overlap, this is multiplied by a factor which is approximated to  $(\frac{1}{2})^{0.33333}$  because the electron is not removed to infinity away from both ions (but rather removed from the overlap region).

**Table 4. Comparison of observed and calculated enthalpies of formation of  $M^+$ (Group 1)/ $M2^+$ (Group 2)**

	Observed kJ/mole	Soft-sphere calculated kJ/mole	Abs % difference
(A)	(B)	(C)	(D)
Li	679.6	683.6	0.6
Na	603.4	584.4	3.2
K	507.8	509.3	0.3
Rb	484.0	486.5	0.5
Cs	452.2	464.6	2.7
Be	2980.7	3108.2	4.3
Mg	2335.6	2135.7	8.5
Ca	1913.2	1784.6	6.7
Sr	1778.2	1645.3	7.5
Ba	1648.1	1569.2	4.8

We have applied the same expression used to calculate the lattice energy with only two very minor differences to calculate the enthalpies of formation of Group 1 and Group 2 metal ions.  $X$ , rather than being the size of an anion, is the “radius” of the space occupied by the electrons detached from the metal atom. In the expression,  $\Sigma Q_i^2$  is the sum of the squares of the charges on the positive ions and the detached outermost electron(s). For Group 1 metals,  $Q_i^2$  of the positive ion is one since each ion has a +1 charge. However,  $Q_i^2$  of the outermost electron is only 0.25 since at any *one* time only a quarter of the available midpoint sites are occupied. Hence,  $\Sigma Q_i^2$  is equal to 1 + 0.25 (1.25) for all the Group 1 metals. For elements of Group 2,  $Q_i^2$  for the positive ions in all cases is four (since they are all dipositive). However, there are two different values of  $\Sigma Q_i^2$ . For the first four elements, only a third of the sites are occupied by electrons. Hence,  $Q_i^2$  for the electrons is  $(1^2 + 1^2) \times 0.3333$  and  $\Sigma Q_i^2$  is approximately 4.7. As for barium, since half of the available midpoint sites are occupied at any *one* time,  $Q_i^2$  for the electrons is  $(1^2 + 1^2) \times 0.5$ . Hence  $\Sigma Q_i^2$  has a value of 4.0 plus 1.0 which equals 5.0. The soft-sphere calculated values are shown in Column C of Table 4. The conventionally produced results are shown in Column B and the absolute percentage differences are shown in Column D of the Table. Differences between observed and soft-sphere calculated are less than 10% for all cases.

### 3. Discussion

It is not exactly correct to consider that metals are malleable and ductile because of defects in the solid state. Non-metallic solids such as sulphur and phosphorus as well as ionic/covalent crystals contain solid state defects but are not malleable nor ductile. We believe that because not all available midpoint sites are occupied by electrons. When a metal is twisted or bent, electrons can move from one site to another within a unit cell, allowing the shape of

the metal to change without any bonds being broken. It has been shown that when sodium is under very high pressure the resistance of the metal increases drastically and acts more like an insulator [17] than a conductor of electricity. This behavior cannot be easily explained by the standard “electron sea” model. However, this can be accounted for by the soft-sphere model. When a metal is under high pressure, the shape and size of the unit cell changes. This reduces the volume of the sites occupied by the detached electrons and if the volume is reduced sufficiently the site can no longer be occupied. When the shape of the unit cell changes, the distance between some of the midpoint sites may increase to such an extent, the detached electrons occupying those sites may no longer be able to move from one site to another. Hence, if there are no vacant sites which can facilitate electron movement or if the electrons cannot move between sites in neighboring unit cells the metal becomes a virtual insulator.

Assuming that in a metal the positive ions are truly surrounded by “a sea of electrons”, it may be reasonable to assume that the work function of a metal is not a significant value since electrons from the “electron sea” can move freely to the surface of the metal. However, the work functions of some metals are much higher than some bond dissociation energies and ionization energies. For example, the work function of beryllium is 480.5 kJ/mole and the bond dissociation energy of the C-H bond is 338.4 kJ/mole, that of Cl-Cl is just 242.4 kJ/mole and that of Ca-Ca is only 16.5 kJ/mole and the first ionization energy of cesium is 3.8939 eV (equal to 375.6 kJ/mole) [16].

In the soft-sphere model, the separated/detached outermost electrons can only occupy midpoint sites between two positive ions inside a unit cell, which means that there is almost no outermost electron on the surface of the metal. Hence, energy has to be expended to draw those detached electrons onto the surface of the metal. The work function is an inverse function of the soft-sphere radius since the further the outermost electrons are from the nuclei of the positive metal ions the less energy is required to draw them to the surface. The work functions of the Group 1 and Group 2 metals can be approximated by the following simple expression:

$$W = C / [(R)^{1/2}]$$

$W$  is the work function,  $R$  is the soft-sphere ionic radius and the constant  $C$  is 3.08 for Group 1 and 3.85 for Group 2 metals. Column B of Table 5 lists the soft-sphere radii, Column C shows the work functions (in eV) calculated by the above formula, Column D shows the observed work functions in eV [16]. The absolute percentage differences are shown in Column E of Table 5. With the exception of beryllium (with a fairly big uncertainty in the size of the soft sphere radius), all values agree to better than 90%.

The detached electrons can move around different midpoint sites inside a unit cell. As discussed above, only some of those sites are occupied at any *one* time. Since all unit cells in a metal are identical and there are vacant sites which facilitate electron movement, a very small potential difference between the ends of a metal strip or wire can overcome the electrostatic attraction between the positive ions and detached electrons and generate an electron flow along the wire (i.e. an electric current). The attraction between the detached electrons and the positive ions in the

unit cell and the energy needed for the detached electrons to jump from one vacant midpoint site in a unit cell to another unit cell give rise to electrical resistance.

**Table 5. Observed and Soft-sphere calculated work functions of Group 1 and Group 2 metals**

Element	Soft-sphere Radii (Å)	Soft-sphere Calculated(eV)	Observed Work function (eV)	Abs % difference
(A)	(B)	(C)	(D)	(E)
Li	1.094	2.94	2.93	0.5
Na	1.497	2.52	2.36	6.7
K	1.971	2.19	2.29	4.2
Rb	2.160	2.10	2.26	7.3
Cs	2.368	2.00	1.95	2.6
Be	0.750	4.45	4.98	10.7
Mg	1.282	3.40	3.66	7.1
Ca	1.657	2.99	2.87	4.2
Sr	1.861	2.82	2.59	8.9
Ba	2.084	2.67	2.52	5.8

Metals are good conductors of heat and sound and the “free electron” model suggests that metals show high thermal conductivities due to the presence of the “electron gas”<sup>18</sup> in the metal and a similar explanation is also provided for the conductivity of sound in a metal. However, it has been calculated that the drift velocity of a “free” electron in copper is about 1mm/sec [19] whereas the speed of sound in a metal is of the order of thousands of meters per second. The thermal conductivity of a metal is a complex function of temperature and not directly proportional to temperature. For example, at 300° K, the thermal conductivity of silver is 4.29 W/cm K, whereas the thermal conductivity of diamond, which is a covalent solid without an “electron sea” has a thermal conductivity of over 8 W/cm K at this temperature [16]. A metal is a good conductor of heat and sound because of its density, regular packing and closeness of neighboring particles which allow heat and sound energy to pass quickly from one particle to another in all directions rather than the “electron sea”.

**Table 6. Enthalpies of fusion of Group 1 and Group 2 metals and some halides**

Element	metal	chloride	oxide	Nr of times difference between	
	kJ/mole	kJ/mole	kJ/mole	chloride/metal	oxide/metal
(A)	(B)	(C)	(D)	(E)	(F)
Li	3.00	19.80	35.60	6.6	11.9
Na	2.60	28.16	47.70	10.8	18.3
K	2.34	26.28	27.00	11.2	11.5
Rb	2.19	24.40	20.00	11.1	9.1
Cs	2.09	20.40	20.00	9.8	9.6
Be	7.90	8.66	86.00	1.1	10.9
Mg	8.48	43.10	77.00	5.1	9.1
Ca	8.54	28.05	80.00	3.3	9.4
Sr	7.43	16.22	81.00	2.2	10.9
Ba	7.12	15.85	46.00	2.2	6.5

When a metal wire with an electric current flowing through it is placed in a transverse magnetic field, a potential difference is developed across the wire at right angles to both the field and the length of the wire. This is known as the Hall effect [20]. It happens because the magnetic field at right angles to the length of the wire creates a force acting on each electron and since, within every unit cell, there are many vacant sites between the positive ions for the electrons to occupy, detached

electrons can move across at right angles to the length of the wire and congregate into more sites on one side of the wire than the other, thus developing a potential difference across the cross section of the wire and at right angles to the field and length of the wire.

Enthalpies of fusion of most halides, oxides and other binary compounds can be many times higher than that of the metals. For example, Column B of Table 6 lists the enthalpies of fusion of Group 1 and Group 2 metals, Columns C and D show the enthalpies of the chlorides and oxides of those metals respectively. The number of times that the enthalpies of the chlorides and oxides are greater than that of the metals (enthalpy of chloride/oxide divided by enthalpy of respective metal) are listed in Columns E and F respectively. These figures clearly show that, with the exception of beryllium, the enthalpies of fusion of the chlorides and oxides are at least twice or up to eighteen times the enthalpy of the respective metals. This cannot be easily accounted for by the standard electron sea model even if it is assumed that the bond formed between the metal and chlorine/oxygen is much stronger than the bonding in the metal itself. However, as we have already shown above, in every unit cell in a metal crystal, each positive ion is surrounded by only two (in Group 1) or four (in Group 2) detached electrons in the midpoint sites between the positive ions. In a halide or oxide crystal every positive ion/negative ion (depending on the structure of the crystal) is always surrounded by more than four times oppositely charged ions. So for example, in sodium chloride each sodium ion is surrounded by six chloride ions and vice versa. This means that, for every mole of metal, fewer bonds are made when a metal solidifies, but many more bonds are made when a metal halide or oxide solidifies. Beryllium chloride is an exception because its structure is different from other chlorides and oxides (beryllium chloride possesses a chain structure [21], whereas most other halides and oxides of Groups 1 and 2 metals have typical crystal formations such as the sodium chloride, wurtzite, rutile or fluorite structures).

It has been suggested by some authors that the number of free (or loosely attached) electrons in a metal lies in the range of 1 to 3.5 per atom [22]. Calculations have also shown that only a very small percentage of electrons in a metal are “free” [23]. This can easily be accounted for by the soft-sphere model. There are only a limited number of sites that the “free” electrons can occupy. For example, in a body centered cubic structure, there are only eight available midpoint sites for the detached electrons and since there are two atoms per unit cell the maximum number of electrons that can be detached from each atom is four. Hence, it is not surprising that the number of “free” electrons per atom is limited to a very low number. Our proposed model of metal structure and bonding is a realistic “physical” description of metallic structure and complementary to band theory rather than an alternative it. The model has now been extended to include transition metals [24].

## 4. Conclusion

In contrast to the popular “electron sea” model, we are able to show that, for Group 1 and Group 2 metals, the

atomic/metallic radii and enthalpy of formation of the positive ions calculated with the soft-sphere model and soft-sphere radii give very good agreement with experimental values. We also showed that the work functions of Group 1 and Group 2 metals are inverse functions of the soft-sphere radii. Additionally, the soft-sphere model can (in a qualitatively manner) account for the differences between the enthalpies of fusion of metals and their halides and oxides. The changes in resistance of a metal under pressure can also be interpreted by the soft-sphere model. There is strong evidence that the soft-sphere model is a more realistic representation of the structure and bonding of metals than the “electron sea” model. The soft-sphere model should be introduced to students and researchers as an alternative to the “free electron/electron sea” model.

## Statement of Competing Interests

There are not competing interests involved in this work.

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