



## Precise Determination of Energy Levels, Work Function and Explanation of Near-Ambient Superconductivity of Solids By Quantum Quantitative Model

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### ABSTRACT

The exact relation between the energy band structure of a solid and its crystalline structure is not known yet. In addition, the thought that the Brillouin zone contains all states or a number of states and these states varies from point to point, in a complicated manner, inside the zone needs to be reconsidered. Also, the explanation of the work function of a solid and considering it as a surface phenomenon and not a character of the solid still needs more clarification. Indeed, there is variety of physical phenomena that need explanation such as the electrical resistivity of materials. Therefore, the present work aims to find the exact relation between the crystal structure and its energy band structure and determine precisely the energy levels of the electrons in the solid by using a quantum quantitative model. Here we show that the quantum quantitative model based on the crystalline accommodation law can successfully get the exact relation between the crystalline structure of the solid and its energy band structure, and determine precisely the energy levels of each element. In addition, we could successfully get an acceptable physical explanation of the electrical resistivity of materials including superconductors. Moreover, it can predict exactly the values of the work functions of the elements, and determine precisely the crystal interaction energy and exchange interaction energy of the electrons inside the solid. The precise prediction of the work function of the elements is conclusive evidence of the validity of this model.

### Key Words:

Energy band structure, Energy levels, Exchange interaction energy, Work function, Crystalline Accommodation Law (CAL), Fermi Energy, Fermi sphere, Brillouin zone, Valence Electron Concentration VEC, Primitive Direct Cell, Superconductivity.

### 1. INTRODUCTION

The exact relation between the crystal structure and energy band structure of solids is not known yet. In addition, the thought that a Brillouin zone (BZ) contains all states or a number of states, and these states vary from point to point, in a complicated manner inside the zone needs to be reconsidered. Also, the explanation of the work function of a solid and considering it as a surface phenomenon and not a character of the solid still needs more clarification. Moreover, the precise determination of the exchange interaction energy of electrons inside the solid is still not available. Indeed, there is a variety of physical phenomena that need explanation such as the electrical resistivity of metals and the near-ambient

superconductivity. Of the four fundamental interactions in nature, the one dominant in crystals is the electromagnetic interaction. Three electromagnetic interactions exist in the crystal, the first is the ion-ion (i-i) interaction, the second is the electron-electron (e-e) interaction, and the third is the electron-ion (e-i) interaction. The ions or electrons do not affected by these interactions separately, but these interactions make a collective interaction, let us call it the crystal field or the crystal interaction. The ions and electrons in the crystal are affected by this crystal field, which forces them to a certain regular equilibrium distribution in space (crystal structure). The resulting crystal structure (real space) has periodic potential, which interacts with electrons inside the crystal, and allows them certain values of energy and prevents the other values (energy space). Therefore, for every crystal structure, there is an energy band structure related directly to it. Tarek El Ashram [1-3] succeeded in explaining the crystalline structure of materials using the crystalline accommodation law (CAL). This law was derived theoretically from the quantum conditions on the free electrons of Fermi gas inside the crystal and it was verified experimentally. CAL relates both the volume of Fermi sphere  $V_F$  and the volume  $V_B$  of BZ to the valence electron concentration (VEC) as the following:

$$\frac{V_F}{V_B} = n \frac{VEC}{2} \quad (1)$$

where  $n$  is the number of atoms per lattice point or primitive cell. Therefore, the present work aims to find the exact relation between the crystalline structure and its energy band structure and determine precisely the energy levels of the electrons in the solid by using a quantum quantitative model based on CAL (CALQQM).

## 2. COMPUTATIONAL METHODOLOGY

### *The Quantum Quantitative Model (CALQQM)*

The quantum quantitative model (CALQQM) is based on CAL with the following postulates:

#### *The postulates of CALQQ model*

1- For every primitive direct cell, there is always a primitive reciprocal cell in  $K$ -space, which is BZ. Therefore, the number of primitive cells per unit volume  $N_p$  will equal to the number of quantum states  $N_B$  per unit volume of direct space.

2- Each BZ accommodates only one quantum state and each state has two energy levels for two electrons with opposite spins.

3- The number of filled quantum states, is given by CAL in such a way;

$$N_F = \frac{n VEC}{2} = \frac{V_F}{V_B} \text{ this number will be a characteristic for each element or compound.}$$

4- The volume of Fermi sphere  $V_F$  represents the total volume of the filled quantum states for a given VEC per unit volume and can be determined from the following equation:

$$V_F = \frac{4}{3} \pi K_F^3 \quad (2)$$

where  $K_F$  is the Fermi electron wave vector and can be determined experimentally from Fermi energy as the following:

$$E_F = \frac{\hbar^2 K_F^2}{2m} \quad (3)$$

In addition,  $K_F$  can be calculated theoretically from VEC per unit volume as the following:

$$K_F = \left( \frac{3\pi^2 N}{V} \right)^{\frac{1}{3}} \quad (4)$$

where  $N/V$  is the number of valence electrons per unit volume (VEC per unit volume).

5- The volume  $V_B$  of BZ is calculated from the following equation:

$$V_B = \frac{8\pi^3}{V_P} \quad (5)$$

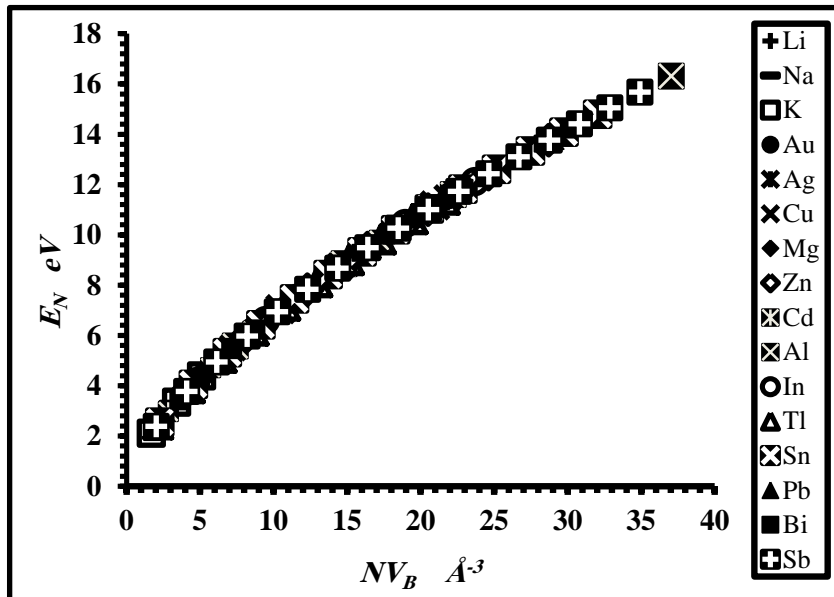
where  $V_P$  is the volume of the primitive direct cell, which can be determined experimentally from the XRD data shown in Table 1 [4]. The calculations were carried out on 16 metals of different valencies, which are: Li, Na, K, Au, Ag, Au with valency (+1), Mg, Zn, Cd with valency (+2), Al, In, Tl with valency (+3), Sn, Pb with valency (+4) and Bi, Sb with valency (+5).

**Table 1: XRD data of the studied elements.**

Element	card no	Cry. St.	$a$ (Å)	$b$ (Å)	$c$ (Å)
Li	89-3940	cub.	3.5092		
Na	89-4081	cub.	4.235		
K	89-4080	cub.	5.247		
Au	89-3697	cub.	4.0796		
Ag	89-3722	cub.	4.0855		
Cu	89-2838	cub.	3.615		
Mg	89-5003	hex.	3.208		5.209
Zn	87-0713	hex.	2.655		4.947
Cd	85-1328	hex.	2.9793		5.6181
Al	89-2837	cub.	4.05925		
In	85-1409	tetra.	3.251		4.945
Tl	89-4050	hex.	3.456		5.53
Sn	89-4898	tetra.	5.831		3.182
Pb	87-0663	cub.	4.93		
Bi	44-1246	rho.	4.547	4.7236	11.8616
Sb	85-1324	rho.	4.3007	4.5064	11.222

### 3. RESULTS AND DISCUSSION

#### 3.1 Band structure and Energy Level



**Fig. 1** The calculated energy levels  $E_N$  according to CALQQ model for 16 metals with different valencies.

Fig.1 shows the calculated energy levels for 16 pure metals with different valencies; +1, +2, +3, +4, +5. It is found that the energy levels depend on the product  $NV_B$  according to the following law, we shall call it Tarek's law;

$$E_N = T (NV_B)^{2/3} \quad (6)$$

where  $E_N$  in electron volt (eV) and  $V_B$  in  $\text{\AA}^3$  and  $N$  is the level number and takes the values;  $N = 0.5, 1, 1.5, 2, 2.5, \dots, V$ , where  $V$  is the label of the internal vacuum level  $E_V$ . The internal vacuum level  $E_V$  is defined as the highest energy level for electrons in the solid. If the electron in that level acquires more energy, it will leave the solid.  $T$  is a physical constant given by;  $T = 1.46622 \text{ eV} \cdot \text{\AA}^2$ , we shall call it Tarek's constant.  $E_F$  is obtained by substituting  $N = N_F$  in Tarek's law and  $N_F$  is obtained from CAL. Tarek's law relates the real space (crystal structure) with energy space (energy levels) and can be applied to any crystalline system. The most important parameter that determines the energy levels is the volume of primitive direct cell  $V_P$  that in turn determine the volume of quantum state  $V_B$ .

The energy levels diagrams are shown in Fig. 2. The first element, **Li** has only two levels  $E_F = 4.7 \text{ eV}$  and  $E_V = 7.46 \text{ eV}$  in one quantum state (the first BZ). **Na** has also two levels levels  $E_F = 3.22 \text{ eV}$  and  $E_V = 5.12 \text{ eV}$  in one quantum state (the first BZ). **K** has 3 levels;  $E_F = 2.1, E_1 = 3.33$  in the first BZ and  $E_V = 4.37 \text{ eV}$  in the second BZ. **Au** has also 3 levels;  $E_F = 5.52, E_1 = 8.75$  in the first BZ and  $E_V = 11.48 \text{ eV}$  in the second BZ. **Ag** has also 3 levels;  $E_F = 5.50, E_1 = 8.73$  in the first BZ and  $E_V = 11.45 \text{ eV}$  in the second BZ. **Cu** has only two levels  $E_F = 7.03 \text{ eV}$  and  $E_V = 11.16 \text{ eV}$  in the first BZ. **Mg** has 4 levels;  $E_F = 7.11$  in 2BZ,  $E_{2.5} = 8.25, E_3 = 9.3$  in 3BZ, and  $E_V = 11.48 \text{ eV}$  in 4BZ. **Zn** has 4 levels;  $E_F = 9.47$  in 2BZ,  $E_{2.5} = 11.0, E_3 = 12.4$  in 3BZ, and  $E_V = 13.75 \text{ eV}$  in 4BZ. **Cd** has 5 levels;  $E_F = 7.46$  in 2BZ,  $E_{2.5} = 8.65, E_3 = 9.77, E_{3.5} = 10.83$  in 3BZ, and  $E_V = 11.84 \text{ eV}$  in 4BZ. **Al** has 3 levels;  $E_F = 11.6, E_2 = 14.04$  in 2BZ,

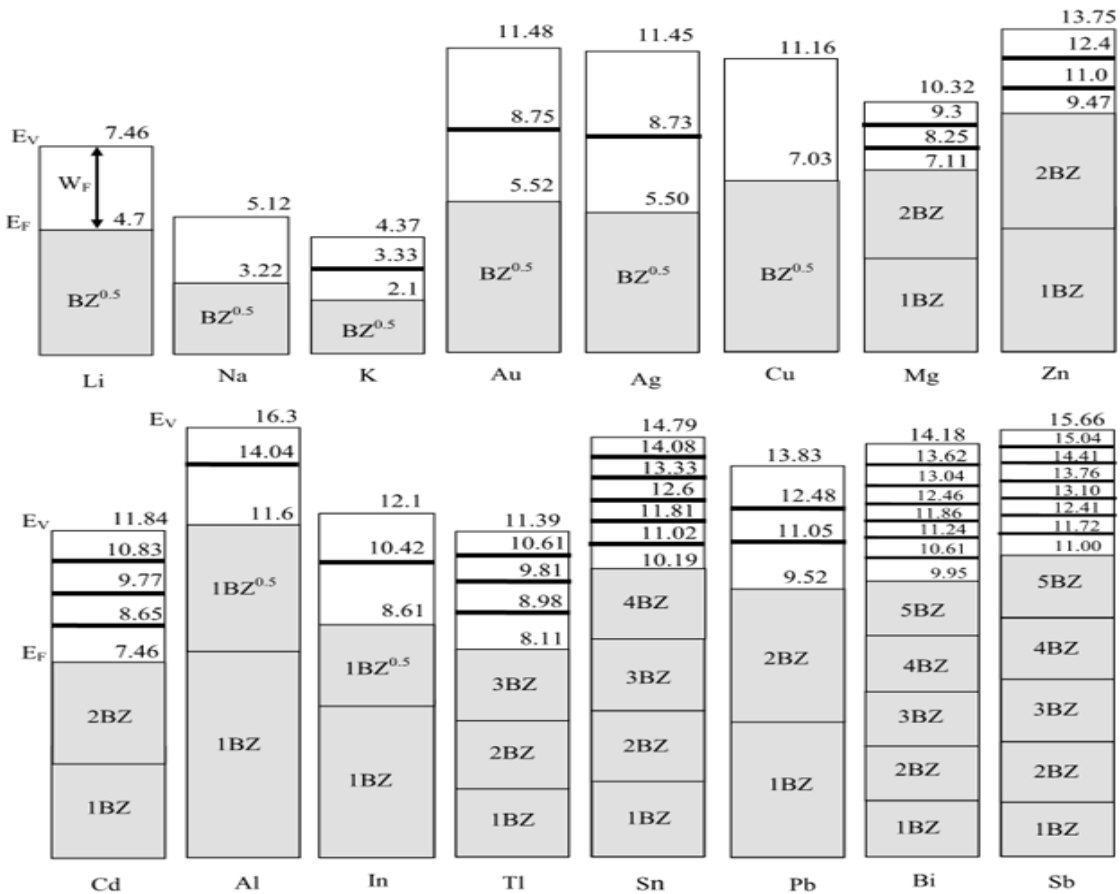


Fig. 2 The energy band units and energy levels of 16 metals with different valencies according to CALQQ model.

and  $E_V = 16.3 \text{ eV}$  in 3BZ. **In** has 3 levels;  $E_F = 8.61$ ,  $E_2 = 10.42$  in 2BZ, and  $E_V = 12.1 \text{ eV}$  in 3BZ. **Tl** has 5 levels;  $E_F = 8.10$  in 3BZ,  $E_{3.5} = 8.98$ ,  $E_4 = 9.81$  in 4BZ, and  $E_{4.5} = 10.61 \text{ eV}$ ,  $E_V = 11.39 \text{ eV}$  in 5BZ. **Sn** has 7 levels;  $E_F = 10.19$  in 4BZ,  $E_{4.5} = 11.02$ ,  $E_5 = 11.81$  in 5BZ, and  $E_{5.5} = 12.6 \text{ eV}$ ,  $E_6 = 13.33$  in 6BZ, and  $E_{6.5} = 14.08$ ,  $E_V = 14.79 \text{ eV}$  in 7BZ. **Pb** has 4 levels;  $E_F = 9.52$  in 2BZ,  $E_{2.5} = 11.05$ ,  $E_3 = 12.48$  in 3BZ, and  $E_V = 13.83 \text{ eV}$  in 4BZ. **Bi** has 8 levels;  $E_F = 9.95$  in 5BZ,  $E_{5.5} = 10.61$ ,  $E_6 = 11.24$  in 6BZ,  $E_{6.5} = 11.86$ ,  $E_7 = 12.46$  in 7BZ, and  $E_{7.5} = 13.04$ ,  $E_8 = 13.62$  in 8BZ, and  $E_V = 14.18 \text{ eV}$  in 9BZ. **Sb** has 8 levels;  $E_F = 11.0$  in 5BZ,  $E_{5.5} = 11.72$ ,  $E_6 = 12.41$  in 6BZ,  $E_{6.5} = 13.10$ ,  $E_7 = 13.76$  in 7BZ, and  $E_{7.5} = 14.41$ ,  $E_8 = 15.04$  in 8BZ, and  $E_V = 15.66 \text{ eV}$  in 9BZ.

From the energy band structure shown in Fig 2 it is found that there is no overlapping between the conduction band and the valence band. Therefore, the term overlapping is no longer true. Furthermore, the term semimetal for **Bi** and **Sb** also is no longer true, the only difference is that the valence band contains 5BZ. Moreover, it is found that the energy levels are discontinuous in agreement with the principles of quantum physics. Therefore, the main conclusion here is that the band energies are not continuous but are discontinuous and have certain values according to Tarek's law. The transition from a level to a higher level requires the absorption of energy difference between those levels. In addition, the transition from a level to a lower level requires the emission of energy difference between those levels. We will see in the next section that the work function is just the difference between the Fermi level and the internal vacuum level ( $E_V - E_F$ ).

### 3.2 Work Function

The work function  $W_F$  is defined, in this model, as the difference in energy between the internal vacuum level  $E_V$  and the Fermi level  $E_F$  and is given by;

$$W_F = E_V - E_F \quad (7)$$

When a photon of energy  $W_F$  incident on an electron with  $E_F$  the electron will rise to  $E_V$  and still belongs to the solid and cannot leave it unless the energy of the photon becomes greater than  $W_F$ . In this case the electron will leave the solid with kinetic energy given by,  $E_K = E_{in} - W_F$ , where  $E_{in}$  is the energy of the incident photon. Therefore, the work function is a character of the solid and not a surface phenomenon. Table 2 shows the calculated work functions  $W_F(\text{cal})$  and the observed  $W_F(\text{obs})$  [5-7]. It is clear that the values are very close with small difference that may be due to the experimental errors. Except for **Ag** a large deviation is found about 1.21 eV, **Ag** and **Au** have almost the same band structure and the deviation for **Au** is about 0.49 eV. It was found by [8] that the values of  $W_F$  for a thin film of polycrystalline **Au** varies from 4.4 to 5.4 eV depending on the surface cleanliness and ambient atmosphere. This means that the measured values tend to the calculated value 5.96 eV when good cleanliness of the surface and ultra high vacuum were taken into account. Therefore, the measurement of the work function of **Ag** should be repeated with high-cleaned surface and under ultra-high vacuum. This good agreement of the calculated and observed values of work functions of the elements is conclusive evidence of the validity of this model.

### 3.3 Band Unit, Space Unit and Total Energy

The band unit (**BU**) is defined as the band, which contains the allowed energy levels for the valence electrons inside the solid from the lowest level  $E_{0.5}$  to the highest level  $E_V$ , it includes both the valence states and the conduction states. **BU** repeats in energy space as the electrons move in periodic spatial space and represents the band structure of the solid and is given by;

$$BU = N_F BZ + N_C BZ \quad (8)$$

where  $N_F$  is the number of filled states in the valence band and  $N_C$  is the number of states in the conduction band. **BU** notation shown in Table 3 for 16 metals with different valencies. The number of **BU** per unit volume  $N_{BU}$  is given by;

$$N_{BU} = N_B/N_U \quad (9)$$

where  $N_U = N_F + N_C$  is the total states in **BU**, and  $N_B$  is the number of **BZ** per unit volume. For each quantum state in energy space, there is a primitive cell in the real space. Therefore, for each **BU** there is a real space unit (**SU**) in which the number of primitive direct cells equal to the number of states in **BU**. The total energy  $TE_N$  for a given level  $E_N$  is given by;

$$TE_N = N_{BU}E_N \quad (10)$$

where  $N_{BU}$  is the number of **BU** per unit volume which equal the number of electrons in each level.

From Table 3 and for **Cu**,  $N_U = 1$ ,  $N_B = 8.46 \times 10^{22} \text{ cm}^{-3}$  thus  $N_{BU} = 8.46 \times 10^{22} \text{ cm}^{-3}$ , The total energy for electrons with  $E_F$  is  $TE_F = N_{BU}E_F = 8.46 \times 10^{22} \times 7.03 = 59.47 \times 10^{22} \text{ eVcm}^{-3}$ . For **Bi**,  $N_U = 8.5$ ,  $N_B = 1.429 \times 10^{22} \text{ cm}^{-3}$  thus,  $N_{BU} = 1.68 \times 10^{21} \text{ cm}^{-3}$ . The total energy is  $TE_F = N_{BU}E_F = 1.68 \times 10^{21} \times 9.95 = 16.71 \times 10^{21} \text{ eVcm}^{-3}$ . Therefore, the energy of **Cu** in Fermi level is much greater than that of **Bi** however,  $E_F$  for **Bi** is greater than that of **Cu**.

### 3.4 Crystal Interaction and Exchange Interaction Energy

Fig. 3 shows the variation of the crystal interaction energy  $\Delta E$  of the electrons inside the solid for 16 pure metals. The crystal interaction energy can be obtained from the width of the energy level  $\Delta E$  at the corresponding energy level. The maximum  $\Delta E$  in level  $E_{0.5}$  was found to be 7.03 eV for **Cu** and the minimum value was found to be 2.1 eV for **K**. It is found that the crystal interaction energy  $\Delta E$  (width of energy level) varies with energy according to the following equation:

$$\Delta E_N = \frac{0.5 E_N}{N} \quad (11)$$

From Tarek's law we get,

$$\Delta E_N = \frac{0.5 (NV_B)^{\frac{2}{3}}}{N} \quad (12)$$

where  $N$  is the level label which takes the values;  $N = 0.5, 1, 1.5, 2, \dots, V$ , where  $V$  is the label of the vacuum level  $E_V$ . The physical interpretation of  $\Delta E$  can be obtained from equation (12).  $\Delta E$  increases nonlinearly with the volume of **BZ** in **K**-space and since  $V_B$  is inversely proportional to the volume of primitive cell  $V_P$  in the real space.

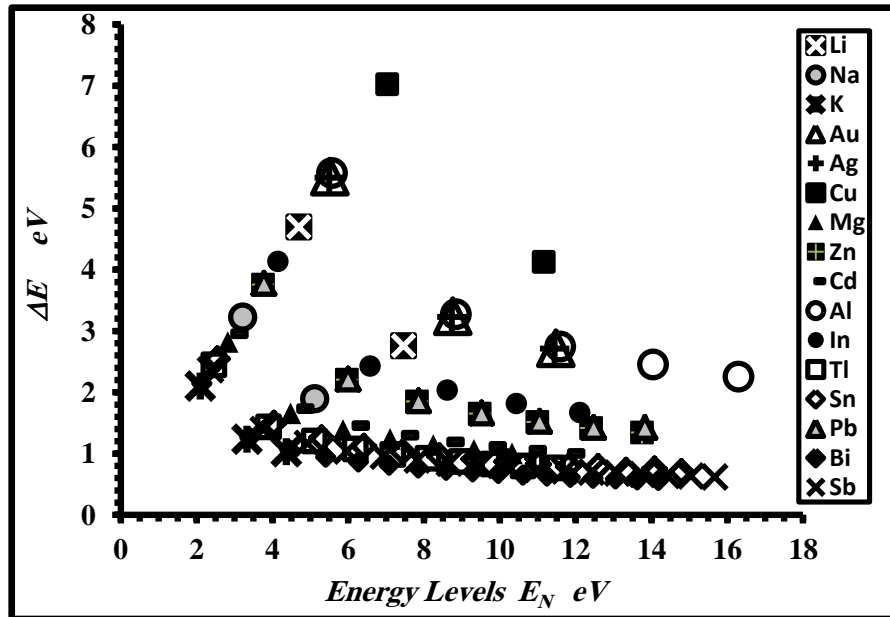
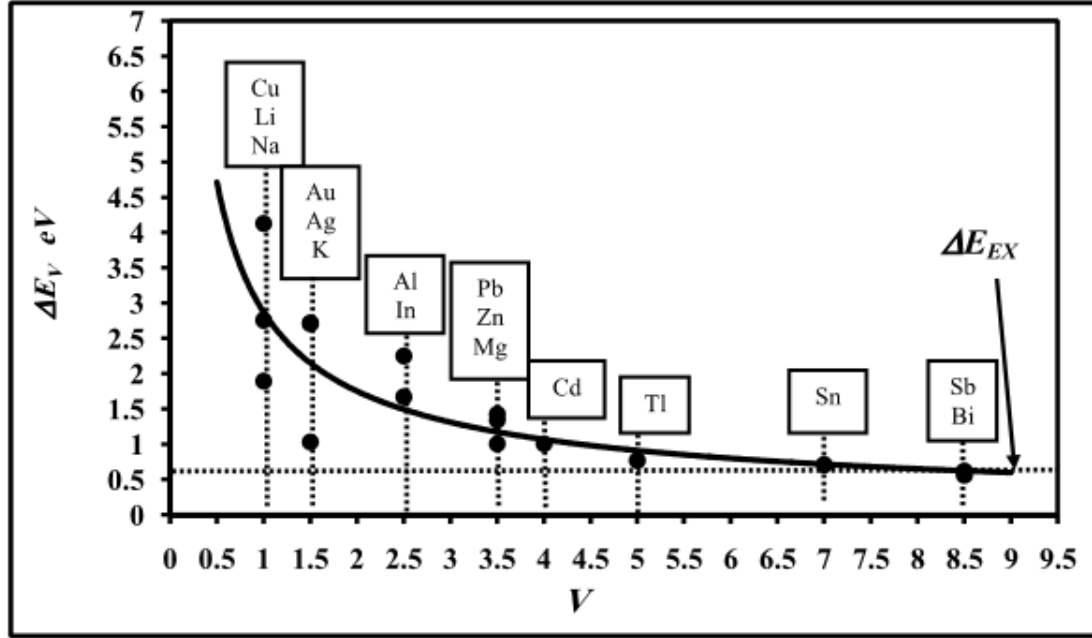


Fig. 3 The crystal interaction energy (energy level width)  $\Delta E$  for each energy level  $E_N$  for 16 metals with different valencies.

Thus, the small volume of primitive cell (real space) leads to greater interaction energy. Therefore, the maximum value for **Cu** is due to the minimum volume of its primitive direct cell, which is  $11.81 \text{ \AA}^3$ . **K** has the largest primitive direct cell,  $72.22 \text{ \AA}^3$  so that it has the minimum interaction energy. Also it is found for **Tl**, **Sn**, **Bi** and **Sb** at the vacuum level  $E_V$ , that  $\Delta E$  converges to  $0.56 \text{ eV}$  (see Fig. 4).



**Fig. 4** The relation between the crystal interaction energy (level width)  $\Delta E$  and the internal vacuum level energy.

The exchange interaction is electromagnetic interaction between two electrons (e-e interaction) in the free state when approaching each other. It includes both the Coulomb interaction and the spin interaction and these interactions cannot be separated. Free state means that the two electrons are far away from the crystal field. Fig. 4 shows the relation between internal vacuum level width  $\Delta E_V$  and the level label. It is clear that  $\Delta E_V$  decreases by increasing  $V$  until it converges to  $0.56 \text{ eV}$  for **Sb** and **Bi**, which have the highest vacuum level. For the next hypothetical level ( $E_{V+0.5}$ ) that will be far away from the crystal field,  $\Delta E_{EX}$  was found to be  $0.5 \text{ eV}$  which is the exchange interaction energy of the electrons in the free state.

#### 4.1 Metals

From Ohm's law the resistivity is given by;

$$\rho = \frac{\varepsilon}{nev} \quad (13)$$

where  $\varepsilon$  is the applied electric field,  $e$  is the electron charge. In this model,  $n$  will equal to  $N_{BU}$  the number of electrons per unit volume with  $E_F$ , and  $v$  is the incremental velocity of the electrons imparted by the applied electric field.  $v$  is given by:  $v = (\hbar \Delta K_F / 2\pi m)$ , because only the electrons with  $E_F$  which can be accelerated. Where  $\Delta K_F$  is the change in the Fermi wave vector,  $\hbar$  is Planck's constant. Therefore, we can re-write equation (13) as:

$$\rho = \frac{2\pi m \varepsilon}{e \hbar N_{BU} \Delta K_F} \quad (14)$$

The parameters that depend on the nature of material in equation (14) are  $N_{BU}$  and  $\Delta K_F$ .

Therefore, the resistivity is inversely proportional to the product  $N_{BU} \Delta K_F$ . Fig. 5 shows the relation between  $\rho$  and  $N_{BU} \Delta K_F$ . It is clear that the experimental data agree very well with the calculated product  $N_{BU} \Delta K_F$ . The small discrepancy may be due to the experimental errors and structural state of the samples

during measurements. The data for the electrical resistivity was taken from [9] and is shown in Table 4. The change in the Fermi wave vector was calculated from the following equation;

$$\Delta K_F = 0.3622 \frac{(N_F V_B)^{\frac{1}{3}}}{\sqrt{N_F}} \quad (15)$$

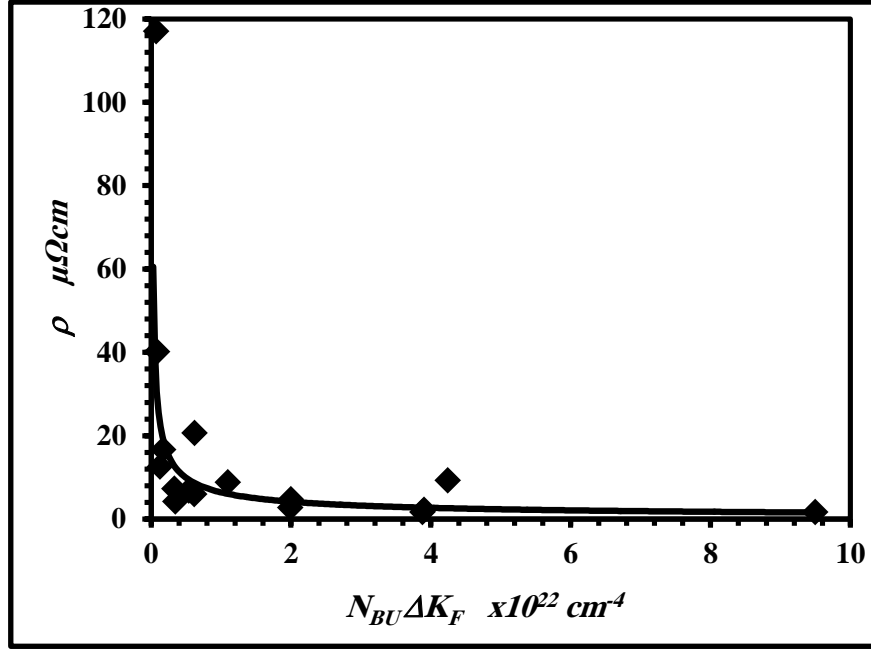


Fig. 5 :The dependence of resistivity on the change of Fermi wave vector and the number of electrons in Fermi level.

#### 4.2 Semiconductors

Semiconductors, as a crystalline materials, have energy band structure similar to that of metals, the only difference is that there no free electrons in semiconductors. However, if the temperature is raised and some electrons become free, the applied electric field will cause these electrons to drift in the reverse direction. Thus, the resistivity of semiconductor is high because  $N_{BU}$ , in this case, is small. Therefore, the resistivity of semiconductor is temperature dependent, since  $N_{BU}$  increases with increasing temperature.

#### 4.3 Insulators

The situation of insulators is similar to that of semiconductors, however in this case the thermal agitation cannot break the bonds. So  $N_{BU} = 0$  and hence the resistivity becomes infinite according to equation (14). Doping insulators by metallic elements can cause insulators to conduct electricity because in this case the dopant element provides free electrons that will make the conduction.

#### 4.4 Superconductors

Superconductivity is a temperature dependent phenomenon in which the resistivity of a metal becomes zero at very low temperature. From equation (14)  $\Delta K_F$  is the temperature dependence term in this case because the temperature decreases and hence  $N_{BU}$  is constant. From equation (15)  $\Delta K_F$  depends on  $V_B$  which in turn depends on  $V_P$ . Therefore,  $\rho = 0$  when  $V_B$  becomes infinite and  $V_B$  becomes infinite when  $V_P$  tends to zero and this cannot be happen but rather it decreases by increasing the temperature or by compression. So that  $V_B$  increases until at a certain critical temperature  $T_C$  there is a critical volume of primitive cell in real space  $V_{PC}$  at which the electrons are forced, due to cell contraction, to form cooper pairs (bosons) as suggested by BCS theory. In this case, there is no any restriction (such as Pauli



Exclusion Principle) on the motion of bosons,  $V_B$  becomes infinite, and hence the resistivity will be zero. Therefore, we can design a superconductor at room temperature if we make  $V_P$  as small as possible. This predicted behavior is observed recently [10], which confirm the validity of this model.

## 5. CONCLUSIONS

By using CALQQM, the energy levels of 16 metals with different valencies are determined precisely in agreement with the experimental data. It is found that the energy levels are discontinuous in agreement with the principles of quantum physics. The essential conclusion is that for every crystalline structure there is an energy band structure related directly to it by Tarek's law, which gives the allowed energy levels in the solid. CALQQM could successfully explain and predicted the work functions of the elements and proved that it is a characteristic of the solid and not a surface phenomenon. Moreover, the most important conclusion we got is that the explanation of near ambient superconductivity. In addition, we could successfully get an acceptable physical explanation of the electrical resistivity of metals, semiconductors, and insulators.

**Table 2: The calculated work function according to CALQQM and the observed for 16 metals with different valencies.**

<i>Metal</i>	<i>System S.G.</i>	<i>VEC per atom</i>	<i>n</i>	<i>N<sub>f</sub></i>	<i>V<sub>P</sub> Å<sup>3</sup></i>	<i>V<sub>B</sub> Å<sup>3</sup></i>	<i>V<sub>F</sub> Å<sup>3</sup></i>	<i>E<sub>F</sub> eV</i>	<i>E<sub>V</sub> eV</i>	<i>W<sub>F</sub> (cal) eV</i>	<i>W<sub>F</sub> (obs) eV</i>
Li	Cubic Im $\bar{3}$ m	1	1	0.5	21.60	11.48	5.73	4.69	7.46	2.67	2.93
Na	Cubic Im $\bar{3}$ m	1	1	0.5	37.97	6.53	3.26	3.22	5.12	1.9	2.36
K	Cubic Im $\bar{3}$ m	1	1	0.5	72.22	3.43	1.71	2.10	4.37	2.27	2.29
Au	Cubic Fm $\bar{3}$ m	1	1	0.5	16.97	14.61	7.30	5.52	11.48	5.96	5.47
Ag	Cubic Fm $\bar{3}$ m	1	1	0.5	17.04	14.55	7.27	5.50	11.45	5.95	4.64
Cu	Cubic Fm $\bar{3}$ m	1	1	0.5	11.81	21.00	10.49	7.03	11.15	4.12	4.48
Mg	Hex. P6 <sub>3</sub> /m mc	2	2	2	46.42	5.34	10.67	7.10	10.32	3.22	3.66
Zn	Hex. P6 <sub>3</sub> /m mc	2	2	2	30.19	8.21	16.30	9.47	13.75	4.28	4.9
Cd	Hex. P6 <sub>3</sub> /m mc	2	2	2	43.13	5.74	11.48	7.46	11.47	4.01	4.08
Al	Cubic Fm $\bar{3}$ m	3	1	1.5	16.72	14.83	22.24	11.59	16.3	4.71	4.26
In	Tetr. I4 <sub>1</sub> /amd	3	1	1.5	26.13	9.49	14.23	8.61	12.1	3.49	4.09
Tl	Hex. P6 <sub>3</sub> /m mc	3	2	3	57.20	4.33	13.00	8.10	11.39	3.29	3.84
Sn	Tetr. I4 <sub>1</sub> /amd	4	2	4	54.09	4.58	18.34	10.19	14.79	4.6	4.42
Pb	Cubic Fm $\bar{3}$ m	4	1	2	29.95	8.28	16.56	9.52	13.83	4.31	4.25
Bi	Rho. R $\bar{3}$ m	5	2	5	69.97	3.54	17.51	9.95	14.18	4.23	4.34
Sb	Rho. R $\bar{3}$ m	5	2	5	60.35	4.11	20.69	11.0	15.66	4.66	4.7

**Table 3: The band unit includes valence and conduction bands for 16 metals with different valencies according to CALQQM model.**

<i>Metal</i>	<i>System S.G.</i>	<i>VEC per atom</i>	$N_F$	$N_C$	$N_U$	<i>Band unit notaion</i>
Li	Cubic $Im\bar{3}m$	1	0.5	0.5	1	$BZ^{0.5} + BZ^{0.5}$
Na	Cubic $Im\bar{3}m$	1	0.5	0.5	1	$BZ^{0.5} + BZ^{0.5}$
K	Cubic $Im\bar{3}m$	1	0.5	1	1.5	$BZ^{0.5} + BZ$
Au	Cubic $Fm\bar{3}m$	1	0.5	1	1.5	$BZ^{0.5} + BZ$
Ag	Cubic $Fm\bar{3}m$	1	0.5	1	1.5	$BZ^{0.5} + BZ$
Cu	Cubic $Fm\bar{3}m$	1	0.5	0.5	1	$BZ^{0.5} + BZ^{0.5}$
Mg	Hex. $P6_3/m$ mc	2	2	1.5	3.5	$2BZ + 1BZ^{0.5}$
Zn	Hex. $P6_3/m$ mc	2	2	1.5	3.5	$2BZ + 1BZ^{0.5}$
Cd	Hex. $P6_3/m$ mc	2	2	2	4	$2BZ + 2BZ$
Al	Cubic $Fm\bar{3}m$	3	1.5	1	2.5	$1BZ^{0.5} + BZ$
In	Tetr. $I4_1/amd$	3	1.5	1	2.5	$1BZ^{0.5} + BZ$
Tl	Hex. $P6_3/m$ mc	3	3	2	4	$3BZ + 2BZ$
Sn	Tetr. $I4_1/amd$	4	4	3	7	$4BZ + 3BZ$
Pb	Cubic $Fm\bar{3}m$	4	2	1.5	3.5	$2B + 1BZ^{0.5}$
Bi	Rho. $R\bar{3}m$	5	5	3.5	8.5	$5BZ + 3BZ^{0.5}$
Sb	Rho. $R\bar{3}m$	5	5	3.5	8.5	$5BZ + 3BZ^{0.5}$

**Table 4: The crystal interaction energy  $\Delta E$  (level width) in different energy levels for 16 metals with different valencies and the electrical resistivity explanation.**

Metal	System S.G.	VEC per atom	n	$V_P \text{ \AA}^3$	$V_B \text{ \AA}^3$	F	$\Delta E_F \text{ eV}$	V	$\Delta E_V \text{ eV}$	$N_{BU} \times 10^{22} \text{ cm}^{-3}$	$N_{BU} \Delta K_F \times 10^{22} \text{ cm}^{-4}$	$\rho \text{ } \mu\Omega\text{cm}$
Li	Cubic $\text{Im}\bar{3}\text{m}$	1	1	21.60	11.48	0.5	4.7	1	2.76	4.62	4.24	9.29
Na	Cubic $\text{Im}\bar{3}\text{m}$	1	1	37.97	6.53	0.5	3.22	1	1.9	2.63	2.00	4.7
K	Cubic $\text{Im}\bar{3}\text{m}$	1	1	72.22	3.43	0.5	2.10	1.5	1.03	0.88	0.54	6.8
Au	Cubic $\text{Fm}\bar{3}\text{m}$	1	1	16.97	14.61	0.5	5.52	1.5	2.72	3.92	3.90	2.2
Ag	Cubic $\text{Fm}\bar{3}\text{m}$	1	1	17.04	14.55	0.5	5.50	1.5	2.71	3.91	3.88	1.63
Cu	Cubic $\text{Fm}\bar{3}\text{m}$	1	1	11.81	21.00	0.5	7.03	1	4.13	8.46	9.49	1.69
Mg	Hex. $\text{P6}_3/\text{m mc}$	2	2	46.42	5.34	2	1.24	3.5	1.0	0.61	0.34	4.2
Zn	Hex. $\text{P6}_3/\text{m mc}$	2	2	30.19	8.21	2	1.65	3.5	1.34	0.94	0.61	5.96
Cd	Hex. $\text{P6}_3/\text{m mc}$	2	2	43.13	5.74	2	1.30	4	1.00	0.57	0.33	7.3
Al	Cubic $\text{Fm}\bar{3}\text{m}$	3	1	16.72	14.83	1.5	2.74	2.5	2.25	2.39	1.99	2.76
In	Tetr. $\text{I4}_1/\text{amd}$	3	1	26.13	9.49	1.5	2.04	2.5	1.67	1.53	1.09	8.8
Tl	Hex. $\text{P6}_3/\text{m mc}$	3	2	57.20	4.33	3	0.92	5	0.77	0.34	0.17	16.6
Sn	Tetr. $\text{I4}_1/\text{amd}$	4	2	54.09	4.58	4	0.86	7	0.71	0.26	0.12	12.6
Pb	Cubic $\text{Fm}\bar{3}\text{m}$	4	1	29.95	8.28	2	1.66	3.5	1.42	0.95	0.62	20.6
Bi	Rho. $\text{R}\bar{3}\text{m}$	5	2	69.97	3.54	5	0.67	8.5	0.56	0.16	0.07	117
Sb	Rho. $\text{R}\bar{3}\text{m}$	5	2	60.35	4.11	5	0.74	8.5	0.62	0.19	0.08	40.1

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