

International Journal of Innovative Research in Science, Engineering and Technology

(A High Impact Factor, Monthly, Peer Reviewed Journal)

Visit: www.ijirset.com

Vol. 6, Issue 10, October 2017

Electronic Band Structure and Related Properties of Paramagnetic FCC Strontium

S. B. Madan

Associate Professor, Department of Physics, M. G. Science Institute, Ahmedabad. Gujarat, India

ABSTRACT: Self-consistent all electron, local density calculations are reported for fcc strontium using linear combination of Gaussian orbitals (LCGO) method. We obtain band structure, density of states, charge form factors and Compton profile. Results are compared with other calculations and with experiments wherever these exist.

KEYWORDS: Band structure, Density of states, Compton profile.

I. INTRODUCTION

The electronic structure of strontium is characterized largely from the plots of its first two bands on the line of its symmetry and their orientation with respect to Fermi energy E_F . In the earlier studies band structure of strontium was calculated as a function of pressure by several workers Vasvari et al[1] and as a function of atomic volume by Asano and Yamashita[2] where both these studies were based on arbitrarily varying the cell volume. Vasvari et al pointed out that the hybridization between the s, p and d states was making important contribution to the band structure near the Fermi level E_F . At a normal volume, the p like L'_2 level was situated somewhat below E_F and d-like W'_2 level above E_F therefore there was an electron like Fermi surface found around the L point and the hole-like Fermi surface around W point. With decrease in volume they found increase in the degree of hybridization as W'_2 went down relative to the L'_2 resulting into shrinkage of Fermi surface to very small area as L'_2 level reached above E_F and W'_2 below E_F . The band structure of fcc and bcc Sr were calculated by Asano and Yamashita[2] at normal volume V_0 and $0.8 V_0$ using non-relativistic KKR method. As the relative position of the d-bands depends rather sensitively on the choice of the crystal potential they adopted four different types of self-consistent potentials and from their calculations concluded that the approximate averaged Hartree-Fock potential was the best for the prediction of the metal semimetal transition as a function of the lattice constant. Their results were quantitatively the same as those of Vasvari et al[1]. The band structure determination for volume at known pressures was carried out using Slater's superior X α exchange method by Ashokamani and Kiyakutti[3]. They used Herman Skillman program[4] for finding free atom wave-functions and calculated band structure and Fermi surface topology at three different pressures 20, 30 and 35 Kbars using APW non-self-consistent method. Sigalas et al[5] calculated band structure and the total energy for 3d, 4d and 5d as well as alkaline earth metals using the semirelativistic fully self-consistent augmented-plane-wave (APW) method in the muffin-tin approximation without using the frozen potential procedure employed by Skriver[6]. The band structure calculations using self-consistent symmetrised relativistic APW (SPRAW) method was carried out by Kubo et al[7]. They used LDA to construct the exchange-correlation part of the one electron potential. The functional form of the exchange-correlation potential was assumed to be the free electron parametrisation of Gunnarson and Lundquist[8]. The starting charge density for the crystal was considered as the superposition of the self-consistent charge density for neutral atom Desclaux[9] in the configuration $5S^2$. The frozen core approximation was adopted and the lattice constant assigned was 11.50 au. They chose first ten high symmetry points in the irreducible Brillouin zone (IBZ). In the final stages self-consistency was achieved at 89k points in the IBZ.

In the present paper for the first time we study the band structure and some related properties of fcc strontium on the basis of self-consistent Gaussian orbitals method and local density approximation in density functional theory[10], which has been applied successfully to a number of metals[11,20]. In addition to this we use for the first time the exchange correlation potential due to Von Barth-Hedin(VBH)[21]. We have used here VBH potential with parameters given by [22].

International Journal of Innovative Research in Science, Engineering and Technology

(A High Impact Factor, Monthly, Peer Reviewed Journal)

Visit: www.ijirset.com

Vol. 6, Issue 10, October 2017

Our computational procedures are briefly described in section II, the band structure in section III, the density of states in section IV, X-Ray form factors in section V, Compton profile in section VI, discussions and results in section VII and finally conclusion is summarized in section VIII.

II. COMPUTATIONAL METHOD

We have used the Linear combination of the Gaussian orbitals (LCGO) method as contained in the BNDPKG programs. The calculations are made based on the local density approximation to the density functional theory. This method does not require any shape approximations to charge densities or potentials. Details of method can be found in [10]. The Bloch wave functions needed in the self-consistent calculations were expanded in a set of independent Gaussian orbitals including in this case sixteen of s symmetry, twelve p, eight d and one f. We employed the basis set for Sr given by Poirier et al. [23] except that the most diffused s-orbital exponent was deleted, two p-orbital exponents [11] were added followed by a single f orbital of exponent 0.8 was added. The exchange correlation potential is treated in the manner described in [20]. Relativistic effects are not included. The Hamiltonian and overlap matrices considered in the computations are of dimension 99x99. The equilibrium lattice constant $a_0 = 10.88$ au of strontium at -0.41 Kbar of pressure was used from [24]. In the calculations the iterations leading to self-consistency were continued until the change in the leading Fourier coefficient of potential became 10^{-4} Ry or less. After establishing the self-consistency energy levels and wave functions were evaluated at 505 points in the irreducible wedge (1/48) of the Brillouin zone. The density of states was obtained by employing the linear analytic tetrahedron method.

III. BAND STRUCTURE

The calculated energy bands are displayed along certain symmetry directions in Fig.1. The selected energy separations are listed in Table 1 and the band structure has been computed using Gaussian orbital exponents listed in Table 2. In the fcc lattice Γ and X are convenient points to use for discussing s-d- and d- band band widths. However there can be minor difference between our band energy values compared with calculations of other authors on account of 1. Use of different exchange-correlation potentials and 2. Inclusion of relativistic effects.

IV. DENSITY OF STATES

The density of states is shown in Fig. 2. We find a value of the density of states at the Fermi energy $N(E_F) = 2.17$ at $^{-1}\text{Ry}^{-1}$. The peaks reported below E_F are at energy values -0.226 Ry, -0.204 Ry and -0.148 Ry where peak density of states values are 12.4475 at $^{-1}\text{Ry}^{-1}$, 15.688 at $^{-1}\text{Ry}^{-1}$ and 18.19 at $^{-1}\text{Ry}^{-1}$. However above Fermi energy the first peak is observed at energy -0.128 Ry and the DOS values being 43.798 at $^{-1}\text{Ry}^{-1}$ and the least possible density of states is obtained near Fermi energy value -0.142Ry which is 0.0087 at $^{-1}\text{Ry}^{-1}$.

V. X-RAY FORM FACTORS

The X-ray form factors are given by the expression below.

$$\rho(\vec{k}) = \int \rho(\vec{r}) (e^{i\vec{k}\vec{r}}) d^3r \quad (1)$$

Where the integration is over the whole crystal and is normalized so that $\rho(0) = n_e$ in which n_e is the number of electrons in the unit cell. The advantage of using LCGO method is that one can obtain $\rho(\vec{k})$ directly from the band structure calculations in terms of quantities called generalized overlap integrals [10] and without additional labour. We list our calculated X-ray form factors in Table 3. The form factors for the atom are calculated from our starting charge densities, while those for the solid are obtained self-consistently.

International Journal of Innovative Research in Science, Engineering and Technology

(A High Impact Factor, Monthly, Peer Reviewed Journal)

Visit: www.ijirset.com

Vol. 6, Issue 10, October 2017

VI. COMPTON PROFILE

we report in this work a computation of the Compton profile and its anisotropy for alkaline earth metal strontium. Since core electrons do not differ appreciably in the solid form from those in the free atom, We have calculated total Compton profile of strontium considering core electron contribution of Hartree-Fock[25] and valence electron (5s) contribution as spherically averaged Compton profile of the valence electrons was computed using expression in [26].

$$J_{\vec{k}}(q) = \frac{\Omega}{2\pi^3} \int d^3p \rho(\vec{P}) \delta(q - p \cdot \hat{k}) \quad (2)$$

Where $\rho(\vec{P})$ is the momentum distribution function, \hat{k} is a unit vector along \vec{k} , Ω is the volume of the unit cell

$$q = \frac{\hbar\omega}{|\vec{k}|} - \frac{1}{2} |\vec{k}| \quad (3)$$

$\hbar\omega$ is the energy transferred to the electron after a Compton scattering event has occurred. The momentum density requires a summation over all occupied states at $T=0^0$ K, this can be written as (2).

$$\rho(\vec{P}) = \sum_{n, \vec{k}} \theta(E_F - E_n(\vec{k})) |\psi_n(k, \vec{P})|^2 \quad (4)$$

Where E_F is the Fermi energy, $E_n(\vec{k})$ is the energy of a state, θ is the unit step function and $\psi_n(k, \vec{P})$ is the momentum-space Bloch function which is related to the position-Space Bloch function by Fourier transformation. The directional profiles were calculated using 505 points in the $\frac{1}{48}$ th part of Brillouin zone. The Compton profiles $J_{\vec{k}}(q)$ along the [1 0 0], [1 1 0] and [1 1 1] directions together with the spherically averaged profile for each value of q ranging from 0 to 4.4 a.u. are given in Table 4. Differences of the Compton profile with respect to directions of the momentum transfer are shown in Fig.3 and the spherically averaged profile is plotted in Fig. 4. D G Pettifor[27] calculated the energy bands of the 4d transition metal series self-consistently within the atomic sphere approximation (ASA). The Maria A. Puerto et al.[28] performed first principles calculations to determine the structural and electronic properties of strontium in the crystallization phase Im-3m and Fm-3m within the formalism of the Density Functional Theory(DFT).

TABLE 1. Selected energy separations (in mRy) of fcc Sr bandstructure

Symmetry point	$\Gamma_1 - \Gamma_1$	$X_3 - \Gamma_1$	$X_3 - X_1$	$E_F - E(X_1)$	$E_F - E(\Gamma_1)$	$W_3 - W_2$
Method LCGO	443mRy	280mRy	69mRy	62mRy	274mRy	53mRy

International Journal of Innovative Research in Science, Engineering and Technology

(A High Impact Factor, Monthly, Peer Reviewed Journal)

Visit: www.ijirset.com

Vol. 6. Issue 10. October 2017

TABLE 2. Orbital exponents

1s	447503.770
2s	68033.846
3s	15907.645
4s	4680.1807
5s	1596.1083
6s	605.02676
7s	249.66549
8s	110.23712
9s	42.345809
10s	19.327492
11s	7.9437522
12s	3.9979269
13s	1.9333143
14s	0.71633472
15s	0.30581700
16s	0.054874829
1p	3942.2350
2p	935.36132
3p	303.60259
4p	115.89079
5p	48.560293
6p	21.499913
7p	8.946983
8p	3.8696502
9p	1.6177318
10p	0.64198255
11p	0.23849476
12p	0.0613097
1d	137.77423
2d	40.444277
3d	14.688086
4d	5.7521287
5d	2.3249548
6d	0.88911055
7d	0.305817085
8d	0.094379382
1f	0.8

TABLE 3. X-ray form factors of fcc Sr.

h	k	l	Atom
0	0	0	38.000014
1	1	1	32.077095
2	0	0	31.120823
2	2	0	27.957384
3	1	1	26.225140
2	2	2	25.712229
4	0	0	24.055004
3	3	1	23.024675
4	2	0	22.726522
4	2	2	21.644032
3	3	3	20.945015
5	1	1	20.952423
4	4	0	19.939478
5	3	1	19.404350
4	4	2	19.233379
6	0	0	19.237564
6	2	0	18.597151
5	3	3	18.150566
6	2	2	18.009218
4	4	4	17.463142
5	5	1	17.078379
7	1	1	17.079988
6	4	0	16.954416
6	4	2	16.474669
5	5	3	16.132084
7	3	1	16.132729
8	0	0	15.591804
7	3	3	15.283027
6	4	4	15.182247
8	2	0	15.182892
6	6	0	14.793619
8	2	2	14.793941
5	5	5	14.513821
7	5	1	14.513820
6	6	2	14.422379
8	4	0	14.068846
7	5	3	13.813517
9	1	1	13.813839
8	4	2	13.730768
6	6	4	13.407825

TABLE 4. Calculated Compton-profile

q	J[100](q)	J[110](q)	J[111](q)	J[av](q)
0.000	2.904654	3.219597	3.575970	3.221252
0.100	2.831392	3.163708	3.423896	3.135666
0.200	2.808828	2.955625	3.012161	2.928221
0.300	2.827738	2.566993	2.358806	2.587958
0.400	2.448374	2.213740	1.897783	2.199533
0.500	1.991514	1.857055	1.538617	1.813588
0.600	1.237022	1.294875	1.304502	1.280821
0.700	0.858153	0.724719	1.040363	0.844009
0.800	0.642234	0.508149	0.686044	0.592203
0.900	0.364117	0.431549	0.431525	0.412277
1.000	0.237210	0.377711	0.298794	0.317275
1.100	0.201647	0.307657	0.213260	0.253095
1.200	0.231416	0.216572	0.157886	0.205722
1.300	0.199888	0.142699	0.149368	0.160754
1.400	0.136833	0.093493	0.125071	0.113996
1.500	0.073167	0.065980	0.093883	0.075208
1.600	0.051281	0.061019	0.080745	0.063309
1.700	0.052166	0.062773	0.069508	0.061474
1.800	0.061263	0.062956	0.051413	0.059504
1.900	0.049596	0.051058	0.038605	0.047438
2.000	0.031297	0.035678	0.031160	0.033265
2.100	0.017328	0.025229	0.024489	0.022781
2.200	0.013499	0.018445	0.019165	0.017217
2.300	0.014797	0.013451	0.016727	0.014678
2.400	0.015973	0.011448	0.014470	0.013518
2.500	0.013823	0.011030	0.012155	0.012117
2.600	0.010852	0.011125	0.010825	0.010970
2.700	0.008569	0.010575	0.009844	0.009814
2.800	0.007641	0.009360	0.008911	0.008753
2.900	0.007339	0.008387	0.008028	0.007995
3.000	0.007648	0.007665	0.007556	0.007632
3.100	0.008033	0.006609	0.007225	0.007174
3.200	0.007344	0.005872	0.006553	0.006468
3.300	0.006185	0.005884	0.006256	0.006066
3.400	0.005396	0.006263	0.006167	0.005991
3.500	0.005295	0.006653	0.005602	0.005995
3.600	0.006091	0.006437	0.005325	0.006052
3.700	0.006494	0.005706	0.005321	0.005832
3.800	0.005358	0.004924	0.004935	0.005051
3.900	0.004261	0.003928	0.004547	0.004182
4.000	0.003857	0.003265	0.004566	0.003769
4.100	0.004562	0.003449	0.004391	0.004009
4.200	0.005205	0.004149	0.003899	0.004386
4.300	0.004958	0.004893	0.003896	0.004655
4.400	0.003578	0.004980	0.003861	0.004292

TABLE 5. Comparison of band values at some selected point of symmetry, Fermi energy E_F , and density of states. All energy values are in Ry and $N(E_F)$ in states/eV atom.

Symmetry Point	Γ_1	X_1	X_3	L_1	L_2'	W_2'	W_3	W_3	K_1	K_3	E_F	$N(E_F)$
Moruzzi et al.	0.038	0.236	0.321	0.229	0.330	0.290	0.364	0.364	0.280	0.326	0.302	0.31
Present work	0.033	0.244	0.313	0.219	0.333	0.302	0.356	0.356	0.244	0.313	0.307	0.16

International Journal of Innovative Research in Science, Engineering and Technology

(A High Impact Factor, Monthly, Peer Reviewed Journal)

Visit: www.ijirset.com

Vol. 6, Issue 10, October 2017

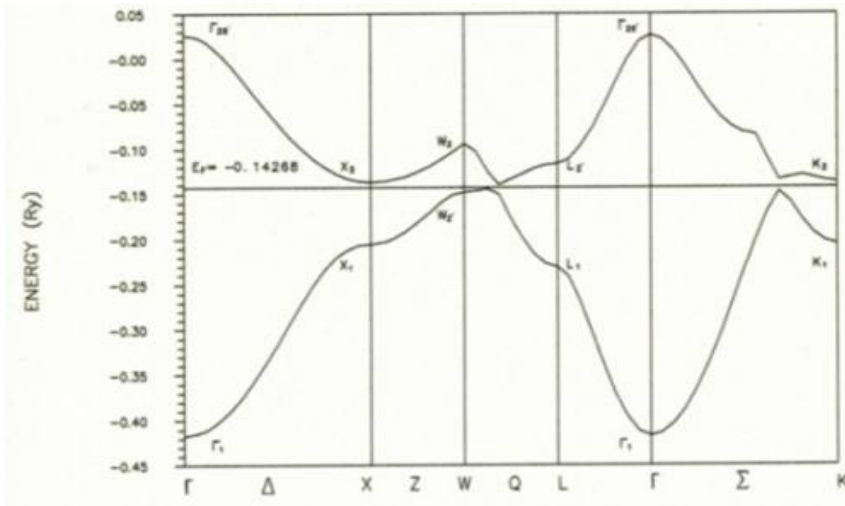


Fig. 1. Band structure of fcc Sr in paramagnetic phase

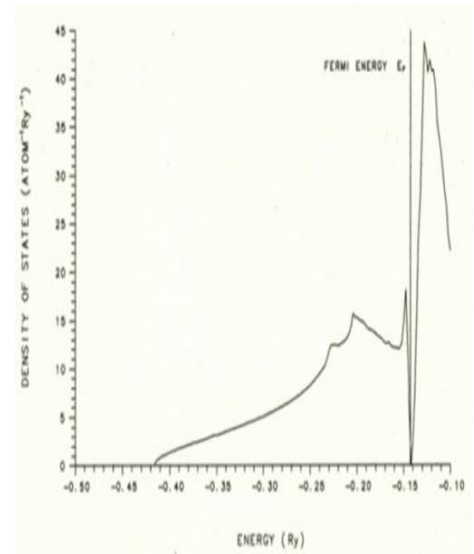


Fig. 2. Density of states in fcc Sr

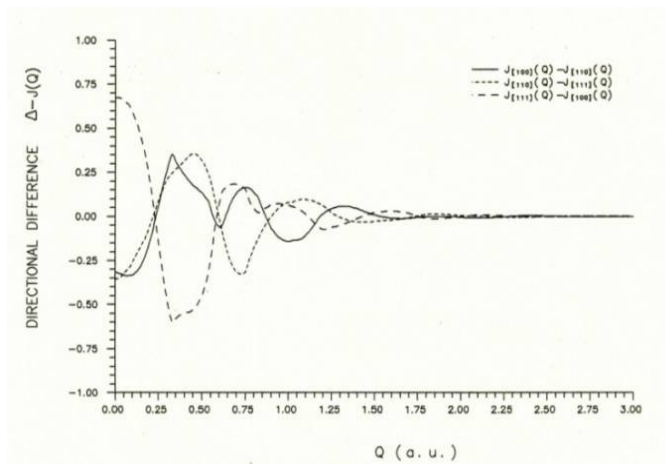


Fig. 3. Anisotropy (compton profile)

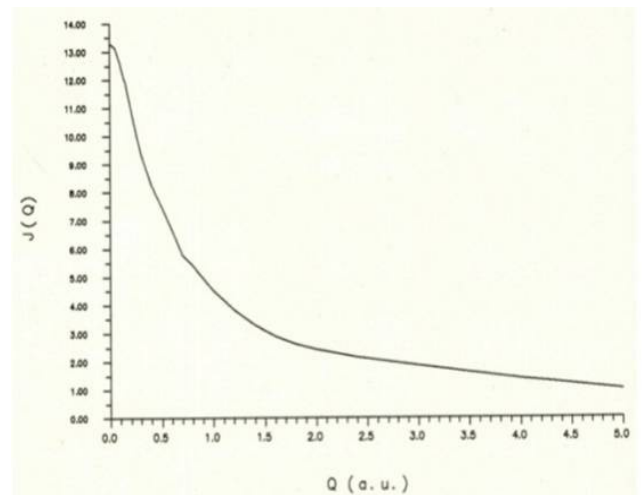


Fig. 4. Total compton profile

VII. RESULT AND DISCUSSIONS

The band structure of fcc strontium is shown in Fig.1 along the principal symmetry axis in the Brillouin zone. The density of states $N(E)$ corresponding to these band structures are shown in Fig.2. As seen in Fig.1 the purely p-like L_2' state is well above Fermi level E_F (about 26mRy.) and a d like W_2' is located well below the Fermi level E_F (about 5 mRy.) hence as in the case of Kubo et al.[7] since p-like L_2' state does not go below Fermi level E_F it does not give rise to electron like Fermi surface around L point and as d-like W_2' state does not go above Fermi level E_F it does not give rise to hole-like Fermi surface around W point. Moreover we find in the present calculation from Fig. 2. E_F situated just at the valley of $N(E)$ curve which exhibits semi-metal property of Sr. Our results at V_0 show that W_2' state is located below E_F and L_2' is located above E_F while that in L_2' level is situated below E_F and W_2' level as above E_F but in the

International Journal of Innovative Research in Science, Engineering and Technology

(A High Impact Factor, Monthly, Peer Reviewed Journal)

Visit: www.ijirset.com

Vol. 6, Issue 10, October 2017

case of Kubo et al.[7] at their V_0 have got both E_F and L_2' located below Fermi level E_F because of the SPRAW method along with inclusion of relativistic effects mainly due to spin orbit interactions. This small discrepancy is attributable to the exclusion of relativistic effects in our present case as well as in [10]. However our present calculations of band structure and density of states compare well for all the values of bands at different symmetry points relative to muffin tin zero and also compare well for $N(E)$, E_F and $N(E_F)$ with Moruzzi, Janak and Williams[24] in their calculated electronic properties for fcc Sr as shown in the Table 5.

VIII. CONCLUSION

We have presented band structure, density of states, X ray form factors and Compton profile using Linear combination of Gaussian orbitals successfully. The comparison of band energy values as well as E_F and $N(E_F)$ compare well with the values calculated by Moruzzi, Janak and Williams[24] in the muffin-tin approximation by Korringa-Kohn-Rostoker (KKR) method. Though we have not considered any relativistic effect we conclude that LCGO method is very efficient for finding out band structure and related properties of an element like Sr.

ACKNOWLEDGEMENT

I am thankful to Professor V. B. Gohel: Head, P.G.Department of Physics, Electronics & Space Science, School of Sciences, Gujarat University, Ahmedabad-9, India and Professor A. R. Jani: Head, P.G. Department of Physics, S. P. University, Vallabh Vidyanagar 388120, India for providing me great assistance in the computation of the BNDPKG FORTRAN programs for calculating the band structure.

REFERENCES

- [1] Vasvari B, Animalu A C E & Heine V. Phys.Rev.(USA) 154(1967)535
- [2] Asano S. and Yamashita J. J Phys Soc. Jpn(Japan), 35(1973) 767
- [3] R. Ashokamani and K Iyakutti Ind. Jnl of Pure and Applied Physics 22,1984 572
- [4] Herman F & Skillman S, Atomic Structure Calculations, Prentice Hall New Jersey 1963
- [5] M. Sigalas, D. A. Papaconstantopoulos and N.C. Bacalis
- [6] H.L. Skriver , Phys. Rev. B 31, 1909(1984)
- [7] Y Kubo J. Phys F(GB) vol (17), no. 2 p 383-96 1987
- [8] Gunarsson O and Lundqvist B I 1976 Phys. Rev. B 13 4274-98
- [9] Desclaux J P 1975 Comput. Phys. Commun. 9 31-45
- [10] C. S. Wang and J. Callaway, Comput. Phys. Commun. 14, 327 (1978)
- [11] G. S. Tripathi, N. E. Brener and J. Callaway, Phys. Rev. B 38 10454(1988)
- [12] A. R. Jani, N. E. Brener and J. Callaway, Phys. Rev. B 38 9425 (1988)
- [13] A. R. Jani, G.S. Tripathi, N. E. Brener and J. Callaway, Phys. Rev. B 40 1593 (1989)
- [14] D. Bagayoko and J. Callaway, Phys. Rev. B 28 5419 (1983)
- [15] J. Callaway, Xianwu Zou and D. Bagayoko Phys. Rev. B 27 631(1983)
- [16] D. Bagayoko, A. Zielger and J. Callaway, Phys. Rev. B 27 7046 (1983)
- [17] J.Callaway and C. S. Wang and Phys. Rev. B 16, 2095 (1977)
- [18] C. S. Wang and J.Callaway Phys. Rev. B 15, 298 (1977)
- [19] D. G. Laurent, C. S. Wang and J.Callaway, Phys. Rev. B 17, 455 (1978)
- [20] P. Blaha and J.Callaway Phys. Rev. B 12, 7664 (1985)
- [21] U. Von Barth and L. Hedim, J. Phys. C. 5, 1629 (1972)
- [22] A.K.Rajgopal, S.P. Singhal and J. Kimball (Unpublished) as quoted by A. K. Rajgopal, Advances in Chemistry and Physics. Edited by G. I. Prigogine and S.A. Rice(Wiley, New York, 1979, Vol. 41, P. 59
- [23] R. Poirier, R. Kari and I. G. Csizmadia, Physical Science Data Vol. P34. Handbook of the Gaussian Basis Set(Elsevier, New York, 1985), P. 632
- [24] V. L. Moruzzi, J. F. Janak and A.R. Williams, Calculated Electronic Properties of Metals (Pergamon, New York, 1978) P 112
- [25] F. Biggs, L. B. Mendelsohn and J. B. Mann, At. Data Nucl. Data Tables 16, 201(1975)
- [26] J. Rath, C. S. Wang , R. A. Tawil and J. Callaway, Phys. Rev. B 8. 5139 (1973)
- [27] D G Pettifor,Journal of Physics F:Metal Physics, Volume 7, Number 4 1971-1988 Journal of Physics F:Metal Physics,doi:10.1088/issn.03054608,Print ISSN:0305-4608
- [28] Maria A. Puerto, Gabriel A. Fonseca, Wilmer Y. Cordoba, William O. Sosa, Jose Otalora, Jairo A. Rodriguez Advances in Ciencias Inqenieria 2012;3(4)117-123 ISSN:0718-8706(Print) Publisher: Executive Business School Country of publisher:Chile