Journal of Natural Sciences Research
ISSN 2224-3186 (Paper) ISSN 2225-0921 (Online)
Vol.8, No.10, 2018

Compton Profile and Electron Momentum Density Study of (CdS)

Fareed Mohammed Fatimah Rashid* shahad Shaaban
School of Science, Tikrit University, Iraq

Abstract

The objective of this paper is to study theoretically the electron momentum density (EMD) of (CdS) using (FA, FE, RFA and superposition) models to the Compton profiles $J(P_Z)$ for Cd metal are calculated depending on several theoretical models by selecting different electronic arrangements ($4d^{10-x}$ $5s^{1+x}$) where (x=0.1,0.2,0.3,……,1) . The obtained theoretical Compton profile for (CdS) is found to be in good agreement with the recent experimental isotropic profile . Charge transfer for the compound has been estimated by ionic model for number of arrangement of (Cd^{+x})(S^{-x}). This model suggests a charge transfer of 0.8 electrons per Cd atom from 4d state to 3p state of S atom.

Keywords: EMD, CdS, Compton profile (CP), Renormalized Free Atom (RFA) model, Free Electron (FE) model, Superposition model, Ionic model, charge transfer.

1. Introduction

The inelastic scattering of electromagnetic radiation from electrons is define as a Compton scattering, is employed as a unique investigation to study the electron momentum density of the ground state (Cooper et al, 2004)

The Compton profile $J(P_Z)$ is given as

$$J(P_Z) = \iint \rho(p)\, dp_x dp_y \tag{1}$$

ρ(p) is electron momentum density in ground state and is determined as

$$\rho(P) = \frac{1}{(2\pi)^3} \sum_{occ} \left| \int \Psi(r) \exp(-ip.r)\, dr \right|^2 \tag{2}$$

where Ψ(r) is electronic wave function in the ground state the summation index is over all the occupied states .

The equ.(1) have been derived in the impulse approximation (IA)(Kaplan et al, 2003).

There is a big motivation for procedure of a Compton profile $J(P_Z)$ study of CdS with cubic zinc blende structures having a face centered cubic (Fcc) structure (Wright et al, 2004).

CdS have numerous subject of theoretical and experimental realization which include studies such as loss spectra , electron energy , photoemission studies , optical properties , band structure calculations , valence band of states densities (Filatova et al, 2004).

Cadmium sulfide looks like zinc sulfide and it's a immediate band gap semiconductor (gap = 2.42 ev) , CdS is an inrgorganic compound , a solid material yellow , easy insulation and purification (Lincot, 2006).

In this paper we reports the first theoretical Compton profile study of the compound. The polycrystalline sample are prefared because of the difficulty in getting the requested size (3mm thick and 15mm dia) single crystals from these materials also relative nature for bonding in this compound on Equal Valence Electron Density Scale. For the theoretical calculations attached to energy bands , momentum densities , Torino group (Saunders et al, 2003).

2. Theoretical method

2.1 Renormalized Free Atom model

Chodorow is The First to use this theoretical modal (Lide et al,1994) and then extend to (Cu) by Emsley (2001) this model simply considers that the atom is not free but confined to a specific cell in the solid. Calculation start from the free atom (FA) Hartree Fock wave (HF) function truncated them at wigner – seitz radius (R_0) and renormalized to a unity within this sphere to maintain the neutrality of the charge and that new wave function is used for further calculations is given as follows :

$$R_{nl}(r) = \begin{cases} N_{nl} R_{nl}^{atomic(r)} & r \leq R_0 \\ 0 & r > R_0 \end{cases} \tag{3}$$

Where $R_{nl}^{atomic(r)}$ is the wave function of the atomic radius with the quantum number (n,l).

(-s- electrons shell)

The momentum transformation of the Bloch function to the outermost "s" shell electrons is unhybridised of the cubic structure is given by

$$\Psi_k(p) = N\square(P-k, k_n)\, \Psi_k^c(p) \tag{4}$$

The Compton profile $J(P_Z)$ for (5s) calculation given by (Berggren et al, 1973):

$$J_{5s}(P_Z) = 4\pi \sum_{n=0}^{\infty} \left| \Psi_0^c(\vec{k}_n) \right|^2 G_n(P_Z) \tag{5}$$

For k_n=0

$$\Psi^{c}_{0}(0) = (2/\pi)^{1/2} \int_0^{r_0} d_r\, r^2\, \varnothing^{r}_{0}(r) \qquad (6)$$

For $k_n \neq 0$

$$\Psi^{c}_{0}(\vec{k}_n) = (2/\pi)^{1/2}\, k_n^{-1} \int_0^{r_0} d_r\, r \sin(k_n r)[\varnothing^{r}_{0}(r) - \varnothing^{r}_{0}(r_0)] \qquad (7)$$

The $G_n(p_n)$ in the equ.(5) give as:

$$G_n(P_Z) = \frac{Nn}{4k_n}\{(P_F^2 - K_n^2)(K_n+P_F-P_Z) - \frac{1}{3}[(K_n+P_F)^3 - P_Z^3] + K_n[(K_n+P_F)^2 - P_Z^2]\} \quad (8)$$

N_n is the lattice reciprocal points number in the n^{th} cell in the reciprocal space the above model doesn't have as we mentioned before hybridization of (d) band is not valid for data on crystal sample, it does how ever give an chance to vary the band electron distribution in (s-d) shell to see the most favorite electron arrangement for a specific metal. For more details see Berggren (1972)

2.2 Free electron model

In the case of an the electron momentum density the equ. (1) reduces to the known form

$$J_{5S}(P_Z) = 2\pi \int_{P_Z}^{\infty} dp\, \rho(\vec{P})\, p \qquad (9)$$

If we consider the electrons of valence in a metal as a non interactive electron gas , the electron momentum density give as following

$$\rho(\vec{P}) = \text{constant} = \frac{n}{\frac{4}{3}\pi P_F^3} \qquad (10)$$

The (n) is free electrons number per site , P_F is the fermi momentum replacement ρ(p) from the equation (10) to the equation (9) give as

$$J_{5S}(P_Z) = \frac{3n}{4\pi P_F^3}(P_F^2 - P_Z^2) \qquad \text{for } P_Z \leq P_F \qquad (11)$$

Then the Compton profile of the free electron is invert parabola including interruptions of the first derive at ± P_F cooper (1985).

2.3 Superposition model

The Compton profile of a specific compound $J(P_Z)$ is computed by the formula (Manninen et al, 1981)

$$J^{x}_{s}(P_Z) = J^{Cd/+x}(P_Z) + J^{S/-x}(P_Z) \qquad (12)$$

$J^{Cd}(P_Z)$, $J^{S}(P_Z)$ are the theoretical Compton profiles of Cd and S metals respectively.

The Compton profile $J(P_Z)$ values of the formed metals Cd and S were taken from the available measurements.

For the reason of comparison we obtained the Compton profile by employing the free atom values, we also calculate theoretical Compton profiles for Cd and S.

3. Results and Discussion

For Cd metal

The theoretical values of Compton profile is shown in table (1), different configurations ($4d^{10}$-$5s^{1}$, $4d^{9.9}$-$5s^{1.1}$, $4d^{9.8}$-$5s^{1.2}$) are chosen by using renormalized free atom models, the best electron configuration was taking ($4d^{10}$-$5s^{1}$). This table also includs the theoretical results by using free electron and free atom models. All values are compared with available experimental data (Chu-Nan Chang et al, 1989), after being calculated all the theoretical values are normalized to an area of 19.19733 electrons being the number of electrons from 0 to 7 a.u. In the high momentum zone (p_z > 2 a.u.), all theoretical values are nearly equal, this is easily understand, because in this zone the contribution is due to core electrons are relatively agree with the experimental data. At the low momentum zone (p_z<0.4 a.u.) shows that the free atom model is higher and far from experiment, the free electron results are very close to the experimental while the RFA results are considerably flatter, all these values given in this table are plotted in Fig(1) which shows the comparison of the theoretical and experimental(Chu-Nan Chang et al, 1989) . When (p_z≤0.6), it is seen that the RFA values are lower than free electron results , but (0.7≤p_z≤2) a.u. the direction is reversed and the RFA values are higher than free electron results. To compare between free atom and free electron results, it seen that the free atom ($4d^{10}$-$5s^{2}$) results in low momentum are higher than the free electron ($4d^{9}$-$5s^{2}$) results but (0.4≤p_z≤0.7) a.u. the direction reversed and the free atom are lower than the free electron. Fig(2) shows the difference between theoretical and experimental profiles for (Cd). It is seen that in the low momentum ($J_{RFA}(p_z)$-$J_{exp.}(p_z)$) is larger than ($J_{FE}(p_z)$-$J_{exp.}(p_z)$), but ($J_{FA}(p_z)$-$J_{exp.}(p_z)$ and $J_{FE}(p_z)$-$J_{exp.}(p_z)$) have the same trend at p_z≥1 a.u. In the high momentum zone (p_z≥2a.u.). In order to compute the best electron arrangement, the total del square $\sum_0^{7a.u.} |\Delta J|^2$ was obtained for whole case. The values found were (0.2459275,2.222182) for (Free electron , RFA) configuration respectively. Therefore (free electron) seems the best configuration.

Superposition model of CdS

To calculate the Compton profile $J(P_Z)$ for cadmium sulfide (CdS) we used superposition model , depending on the calculated values of (Cd) element that are obtained by using (RFA, FE and FA) models given in table (1). Theoretical Compton profile values for the sulfur element of electronic arrangement ($3s^1\ 3p^5$) are taken directly from tables of (Biggs et al, 1975). All theoretical as well as experimental values of CdS compound are normalized to an area under curve (26.64467) electrons of free atom. Table (2) includes three theoretical results of $J(P_Z)$ for (free atom , free electron & RFA) computed by superposition model by using equation (12) we now compare the different theoretical and experimental profiles in the high momentum zone ($P_Z > 1.0$ a.u.) it is apparent that theoretical values are close to experimental values. As for the low momentum zone $P_Z = (0\text{-}0.3$ a.u.) it is apparent that the free atom model and free electron model shows disagreement, on the whole the values are considerably flatter but RFA values are close to the experiment. In fig (3) we plot this comparison, when $P_Z < 0.4$ a.u. it is seen that the RFA values are lower than (free electron , free atom) results but at ($0.6 \le P_Z \le 1.2$) the trend is reversed and RFA values are higher than free electron and free atom. For comparison between free atom and free electron it appears that in low momentum region free atom higher than those results of the free electron but between P_Z = (0.3a.u. and 0.8a.u.) the trend reversed and the values of the free electron are larger than the values of free atom. At $P_Z > 1.2$ a.u. all values be nearly similar. In the fig (4) we plot the difference between the theoretical and the experimental values for Compton profile of (CdS). in the low momentum region ($J_{FA}(p_z) - J_{exp.}(p_z)$) is large than ($J_{FE}(p_z) - J_{exp.}(p_z)$) and ($J_{RFA}(p_z) - J_{exp.}(p_z)$) but are almost the same at $P_Z > 1$a.u. also in the high momentum region ($P_Z > 4$), the differences are almost same. In order to determine the best electron configuration the total square deflection $\sum_0^{7a.u.} | \Delta J |^2$ was obtained and gives the values (12.41766,1.737822,0.05552225) for FA, FE and RFA respectively hence (RFA) gives a better results.

Charge transfer

To determine charge transfer of CdS compound experimental Compton profile of Cd (Chu-Nan Chang et al, 1989) was used to obtain the valence electron profile. We considered charge transfer from Cd to S by ionic arrangement (Cd^{+x})(S^{-x}) ($0 \le x \le 1$) and x is charge transfer. Here, the transfer 0.8 electrons from the valence 4d state of Cd atom to the 3p state of S atom. To evaluate the contribution for valence Compton profile for Cd we have subtracted the corresponded inner core contribution from the experimental Compton profile of the Cd metal and then the profile was divided by the number of valence electron. This contribution was added as discussed above that is:

$$J(P_Z)\text{exp.}\{1s^2.....4d^{10}\} - J(P_Z)\text{core}\ \{1s^2.....4p^6\} = J(P_Z)\text{valence} \qquad (13)$$

$$J(P_Z)\text{for one valence electron} = J(P_Z)\text{valence}/10 \qquad (14)$$

Table (1) : gives the theoretical results Compton profiles of (Cd) with available experimental measurements (Chu-Nan Chang et al, 1989). All the values have been normalized to an area of (19.19733) electrons.

P_Z (a.u.)	$J(P_Z)$			Exp. (Chu-Nan Chang et al, 1989)
	Free atom $4d^{10}\ 5s^2$)(	Free electron $4d^9\ 5s^2$)(	Core+RFA ($4d^{10}\ 5s^1$)	
0	9.04	7.500	6.803	7.433±0.07
0.1	8.8	7.475	6.794	7.40
0.2	8.2	7.394	6.753	7.301
0.3	7.49	7.266	6.686	7.146
0.4	6.88	7.085	6.613	6.924
0.5	6.45	6.836	6.503	6.672
0.6	6.18	6.535	6.342	6.391
0.7	5.99	6.175	6.235	6.106
0.8	5.84	5.739	6.117	5.831
1	5.54	5.502	5.820	5.380
1.2	5.18	5.146	5.426	5.007
1.4	4.76	4.731	4.960	4.610
1.6	4.31	4.302	4.478	4.186
1.8	3.87	3.877	4.006	3.738
2	3.46	3.479	3.575	3.350
3	2.08	2.119	2.156	2.188±0.03
4	1.52	1.571	1.577	1.624
5	1.22	1.268	1.257	1.299
6	0.991	1.031	1.016	0.989±0.02
7	0.8	0.832	0.821	0.703

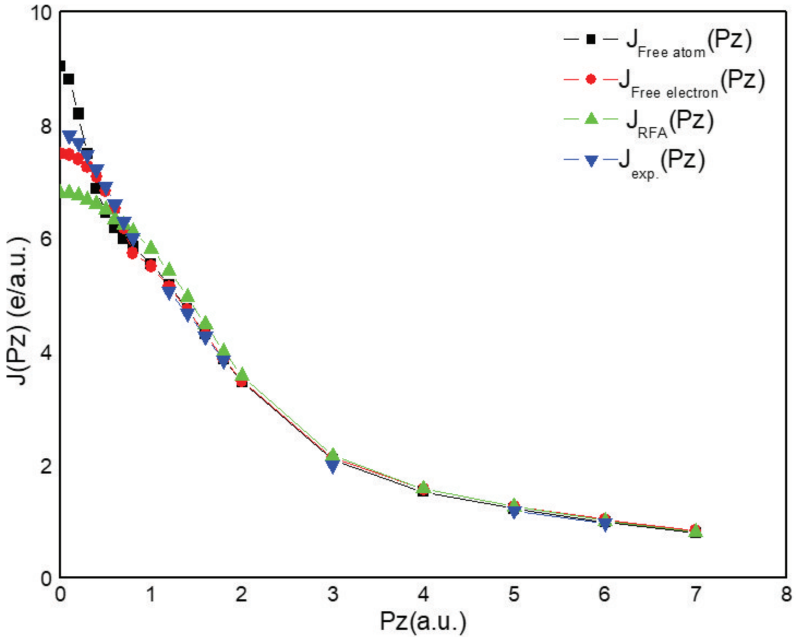
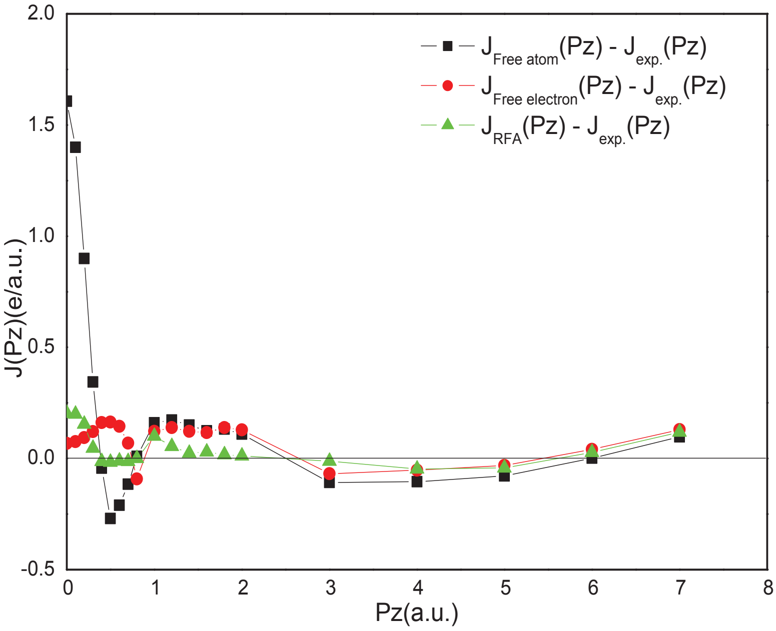


Fig (1): comparison of theoretical with the approved experimental data (Chu-Nan Chang,1989) of (Cd).



Fig(2): difference between theoretical computation and experimental profiles (Chu-Nan Chang et al, 1989) of (Cd).

Table (2) : given the theoretical Compton profiles results of semiconductor compound (CdS) with available experimental measurements (Heda et al,2007). All the values are measured in atomic mass units.

P_Z (a.u.)	$J(P_Z)$ (e/a.u.)			
	Superposition model for CdS			Exp.(Hada et al,2007)
	Free Atom	Free electron	RFA	
0	14.14	12.392	11.908	11.949±0.03
0.1	13.85	12.339	11.872	11.877
0.2	13.12	12.178	11.752	11.667
0.3	12.17	11.876	11.513	11.456
0.4	11.24	11.414	11.163	11.165
0.5	10.41	10.781	10.679	10.650
0.6	9.71	10.043	10.091	10.150
0.7	9.1	9.223	9.538	9.665
0.8	8.56	8.347	8.994	9.076
1	7.63	7.853	7.980	8.033±0.023
1.2	6.86	6.973	7.089	7.087
1.4	6.17	6.219	6.308	6.261
1.6	5.55	5.578	5.636	5.639
1.8	5	5.007	5.037	5.111
2	4.5	4.505	4.520	4.471±0.015
3	2.785	2.814	2.826	2.863±0.011
4	1.976	2.026	2.028	1.995±0.008
5	1.516	1.564	1.553	1.549±0.006
6	1.19	1.229	1.216	1.188±0.005
7	0.94	0.971	0.960	0.933±0.004

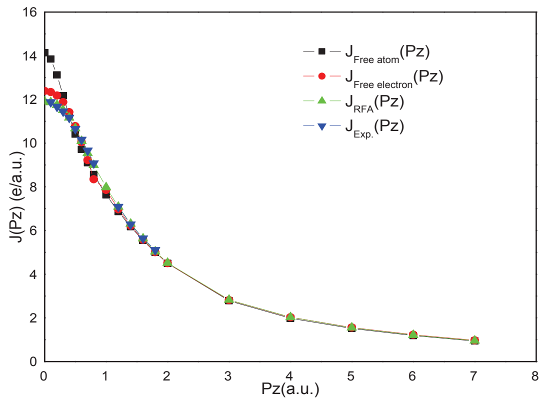


Fig (3): comparison of theoretical with the approved experimental data (Heda et al,2007) for (CdS).

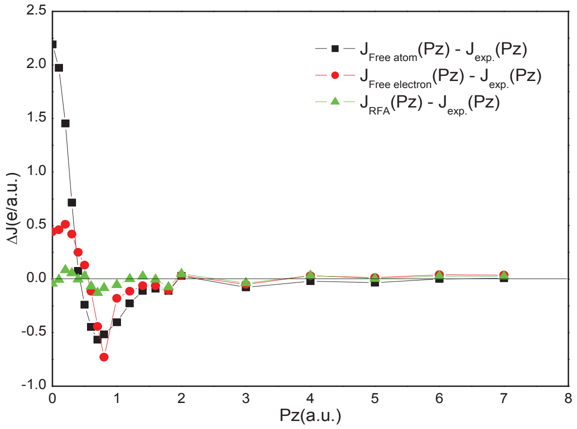


Fig (4) : difference square between theoretical computation and experimental profiles (Heda et al, 2007) of (CdS).

4. Conclusions

The different theoretical Compton profiles are obtained by using various models for the two constituent metals of (CdS) was compared with available experimental results, theoretical profile calculated by using superposition model for the CdS, it was seen that the present RFA work is relatively in best agreement with the resent experimental values of the zinc blende compound (Heda et al, 2007). The ionic model supports a transfer of 0.8 electrons from 4d shell of Cd atom to 3p shell of S atom on compound formation.

References

Berggren, K.F, Manninen, S., and Paakkari, T., Phys. Rev. B552516(1973).

Berggren, K.F. Phys.Rev.B6 2156-61,(1972).

Bigges, L., Mendelsohn, L., Mann, J.B., At. DataNucl. Data Tables. 1975,16,201.

Chu-Nan Chang, Loo Kok Ngai, and Bey-Bey Li Vol. 27, No. 6 (1989).

Cooper, M.J., Mijnarends, P.E., Shiotani, N., Sakai, N., Bansil, A., Oxford Science Publications, New York, 2004.

Cooper, M. J., Rep. Prog. Phys. 48, 415 (1985)

Emsley, John (2001). Nature's Building Blocks. Oxford: Oxford University Press. pp. 262–266.

Filatova, E. O., Andre, J. M., Yu Taracheva, E., Tvaladze, A. J., Kraizman, V. L., Novakovich, A. A. and Vedrinskii, R. V., J. Phys.: Condens. Matter 16, 4597 (2004).

Heda, N. L., Mathur, S., Ahuja, B. L., and Sharma, B. K., Phys. Stat. Sol. (b) 244,No. 3, 1070- 1081 (2007).

Kaplan, I.G., Barbiellini, B., Bansil, A., Phys. Rev. B 68 (2003) 235104.

Lide, R., David, ed. (1994). CRC Handbook of Chemistry and Physics. 4. Chemical Rubber Publishing Company. p. 18.

Lincot, D., Gary Hodes Chemical Solution Deposition of Semiconducting and Non-Metallic Films: Proceedings of the International Symposium The Electrochemical Society, (2006) ISBN 1- 56677 -433- 0.

Manninen, S., Sharma, B.K., Paakkari, T., Rundqvist, S., and Rishardson, M.W., (1981) Phys. Stat. Sol. (b)107, 749.

Saunders, V. R., Dovesi, R., Roetti, C., Orlando, R., Zicovich-Wilson, C. M., Harrison, N. M., Doll, K., Civalleri, B., Bush, I. J., D'Arco, Ph., and Llunell, M., CRYSTAL 2003, User's Manual (University of Torino, Torino, 2003).

Wright, K. and Gale, J. D., Phys. Rev. B 70, 035211 (2004).