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Electron Momentum Density of Mos$_2$ using Compton Scattering Technique

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Abstract **- Electron momentum density for (MoS_2) were calculated and presented in this paper by using different models (RFA, FE and superposition) models, and compared with recent experimental data it shows a good agreement. To indicate wheter there are charge transfer of compound formation (Mo^{-x}) ($S^{+x/2}$)$_2$ the ionic model is adopted for number of arrangements, these supports transfer of 1.2 electrons from 3p state of each (S_2) atom to 4d state of (Mo).**

Keywords **- Superposition model, Compton profile, charge transfor, renormalized Free Atom (RFA), Free Electron (FE), Free Atom (FA).**

I. INTRODUCTION

The description of electronic charge in terms of the electron momentum density and it's study by Compton scattering was reviewed in 1977 [1]. The Compton effect is the inelastic scattering of a photon by an electron and it's a technique for obtaining an theoretical result of the electron momentum distribution in materials [2,3]. The scattering from a density of moving electron due to the motion of the target electrons is Doppler broadened. The Compton profile $J(P_Z)$ is defined as projection of the ground state electron momentum distribution n(p) onto the scattering vector and is given by [4]:

$$J(q) = \iint_{-\infty}^{+\infty} n\ (p_x p_y p_z)\, dp_x dp_y \qquad (1)$$

The impulse approximation show that the energy transfer is so larger than the electron binding energies. However the conditions imposed by the impulse approximation when using low gamma ray energies had made Compton profile measurements to be restricted to materials of low atomic number Z [5,6]. Require the use of high gamma ray energies to extend the applicability of Compton profile measurements to materials of higher atomic number Z while maintaining the validity of the impulse approximation by the photoelectric absorption [7]. The intercalation of Li in molybdenum dichalcogenides (MoS_2) has led to its use in Li batteries. They resist hole induced corrosion and work as catalysts. They are also to be good lubricants. Then electronic structure of MoS_2 with $NbSe_2$ has been calculated using ultraviolet photoemission measurements by McMenamin and spicer [8]. The linear combination of muffin tin orbitals method has been used for the determined of energy bands of MS_2 (M=Mo and Nb) by Kasowski [9]. In this paper, we report the ever theoretical Compton profiles of MoS_2. For the calculation of electron momentum density and theoretical Compton profiles we have used several models for this purpose.

II. THEORY

i) Renormalized Free Atom (RFA) model

The renormalized free atom suggest was the firstly to be used by [10] in RFA model starts with the Hartree Fock wave function, cuts them at the wigner - seitz radius and renormalized the wave function to one unit within this sphere to maintain charge neutrality. The Compton profile $J_{5s}(p_z)$ for 5s electrons, can be written by as:

$$J_{5s}(P_Z) = 4\pi \sum_{n=0}^{\infty} |\, \Psi_0^c(k_n)|^2\, G_n(P_Z) \qquad (2)$$

Where k_n is a reciprocal lattice vector and P_Z the projection of electron momentum along the scattering vector direction. $\Psi_0^c(k_n)$ is the Fourier transform of the wave function.

The wave function $R_{nl}(r)$ are given in the following formula:

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

Then the new wave function will be used in further computation , in this model the solid is constructed of individual atom approximately in the same shape in which they really enter the solid before bounding together.

As for the successes of this model beside Compton work [11] have view that this simple model gives correct estimates of band structure properties and also an explanation for cohesion in the transition metal series.
The $G_n(p_n)$ given as

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

For more details see Berggren [12].

- -s- electron

The procedure for calculating Compton profile is already published and here we have re-write equation for the purpose of completeness the momentum transform for a Bloch function of the cubic structures is written as :

$$\Psi_0^c(\vec{k}_n)=(2/\pi)^{1/2}k_n^{-1} \int_0^{r_0} dr\ r\ \sin(k_n r)[\emptyset_0^c(r)-\emptyset_0^c(r_0)] \qquad (5)$$

Then the Compton profile was calculated using equ.(3) to (5) for several cases selecting various (d-s) configuration.

The Compton profile values of "d" electrons and other core electrons were taken from Bigges [13].

i) Free Electron (FE) model

In case of an electronic properties equ. (1) reduces to the following form:

$$J_{5S}(P_Z) = 2\pi \int_{P_Z}^{\infty} dp\ n(\vec{p})\ p \qquad (6)$$

If we take the valence electron in the metal as a non reactive electron gas then the momentum distribution is :

$$n(\vec{p}) = \frac{n}{\frac{4}{3}\pi p_F^3} = \text{constant} \qquad (7)$$

n is number of free electron per position , the P_F is the Fermi momentum.

Substitution of n(p) from equ.(7) to equ.(6) give:
$$J_{5S}(P_Z) = \frac{3n}{4\pi P_F^3}(p_F^2 - p_z^2) \qquad \text{for } P_Z \le P_F \qquad (8)$$

ii) Superposition (S.P) model

The formula of the Compton profile of given compound $J^{sup.}(p_z)$ of (MoS_2) is as follows :

$$J^{SUP.}(P_Z) = J^{Mo}(P_Z) + J^{S}(P_Z) \qquad (9)$$

$J^{Mo}(P_Z)$ and $J^{S}(P_Z)$ are the calculated Compton profiles of Mo and S metals respectively. The $J(P_Z)$ values of constituent metals Mo and S were taken from the present work. For the sake of comparison the obtained theoretical values for Mo and S were convoluted with the Residual-Instrument-Function (RIF) for the purpose of appropriate comparison with the experiment because no deconvolution execution removes the instrumental expanding totally due to statistical noise always present in the experiment [14].

III. RESULTS AND DISCUSSION

i) Superposition for MoS_2

The theoretical values of Compton profiles for MoS_2 are calculated by employing the best electron arrangement ($4d^5\ 5s^1$) for Mo by using RFA, FE and FA models for more details about this metal can be found elsewhere [15] also we take the Compton profile values of free atom for S from Biggs et al.[13] to get the theoretical Compton profile of MoS_2, we used the relation.

$$J_{sup.}^{x}(P_Z) = J_{theo.}^{Mo/e-}(P_Z) + J_{theo.}^{S/e+}(P_Z) \qquad (10)$$

Where x varied from 0 to 2 in the step of 0.1. All the theoretical values and experimental normalized to an area under curve (84.005) being the number of electrons from 0 to 6 a.u. The final results of total Compton profile are presented in table (1) the 1st column included momentum zone (p_z), the 2nd column represents Free atom $J(P_Z)$ values , the 3rd column shows Free electron results , the 4th column included the best arrangement of RFA values and the final column are the experimental data [16].

Fig. 1 shows comparison between the calculated (theoretical) and measured (experimental) values [16]. When $P_Z<0.5$a.u. it is seen that the RFA theoretical superposition of MoS_2 results are lower than free electron and free atom values, but at ($1>P_Z > 0.6$) a.u. the trend is reverse and the RFA theoretical superposition of MoS_2 results are higher than (free electron , free atom). To show the differences more clearly the differences $\Delta J=(J_{Theo.}- J_{Exp.})$ are plotted as shown in figure (2) to select the best theoretical models by applying the superposition model which salisfy the experimental results, the summation Del square are done i.e. $\sum_{p_z=0\text{a.u.}}^{6\text{a.u.}} |\Delta J|^2$ and it is found that the values found to be (19.18796, 4.6309 , 1.30496) for (Free Atom , Free Electron , RFA).

ii) Charge transfer for MoS_2

The simple ionic model were applied to check whether there are any charge transfer between the two metals constituent of MoS_2 .

Case 1: when complete transfer of valence electrons to sulfur 3p orbitals of S_2 was considered:

$$J(P_Z)[(Mo)^{+5}\ (S^{-2})^{2.5}] = J(P_Z)\{[2s^2...4d^0]\ Mo + [1s^2...3p^9]S_2\} \qquad (11)$$

The Compton profiles for different orbital's were taken from tables of Biggs et al. [13]. To get the contribution of S^{-2}, 2.5 electrons were added to 3p orbital's of S increasing their contribution appropriately.

Case 2: partial ionicity here we started with the experimental $J(P_Z)$ profile of Mo and find out the contribution for each values electron by subtracting the corresponding core contribution and dividing by the number of valence electrons. This contribution after proper multiplication was removed from the contribution of metallic constitutions and then the contribution due to S^{-1} was added as discussed in case 1 that is :

$$J(P_Z)\text{exp.}\{2s^2.....4d^5\} - J(P_Z)\text{core}\ \{2s^2.....4p^6\} = J(P_Z)\text{valence} \qquad (12)$$

$$J(P_Z)\text{for one valence electron} = J(P_Z)\text{valence}/5 \qquad (13)$$

The results shows that in both cases the theoretical $J(P_Z)$ are far away from experimental values, hence we try a partial fractional charge transfer from S_2 to Mo in MoS_2 compound, the results support the transfer of 1.2 electrons from 3p orbital of S_2 to 4d orbital of Mo.

IV. CONCLUSIONS

In this paper we have report the charge transfer in MoS_2 compound by using the simple ionic model the amount of charge transfer is 1.2 electrons from S atom to Mo atom which detect that bonding in MoS_2 is ionic (or less covalent). Which is agree with experimental data.

V. ACKNOWLEDGMENT

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VI. REFERENCES

[1] B. G. Williams, (Mc Graw-Hill, London, 1977) p.11.

[2] B. Williams. - New York: McGraw-Hill, 1977.

[3] M.J. Cooper Rep. Prog. Phys. 1985. - Vol. 48. -P. 415.

[4] P. Eisenberger, P.M. Platzmann Phys. Rev.- 1970. - Vol. A2. - P. 415.

[5] A. Andrejczuk, L. Dobrzynski, E. Zukowski J. Phys.: Condens. Matter. - 1992. - Vol. 4. - P. 2735.

[6] B.L. Ahuja, M.D. Sharma, B.K. Sharma Physica Scripta. - 1998. - Vol. 58. - P. 185.

[7] B.L. Ahuja, M.D. Sharma Pramana - J. Phys. - 2005. - Vol. 65, No. 1. - P. 137 - 145.

[8] J.C. McMenamin, W.E. Spicer, Phys. Rev. Lett. 29 (1972) 1501.

[9] R.V. Kasowski, Phys. Rev. Lett. 30 (1973) 1175.

[10] M. Chodorow, (1939),Phys .Rev,55,675.

[11] D.N Timms and M. J. Cooper 48a:343,(1993).

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

[13] L. Bigges, L. Mendelsohn, J.B. Mann, At. Data Nucl. Data Tables. 1975,16,201.

[14] T. Paakkari and S. manninen , (1974) J. Phys. F. , 4 , L 133.

[15] F.M. Mohammed, A.S. Jassim, Sh.A. Shaaban and F.I. Rashid, accepted in Australian journal of basic and applied sciences (AJBAS) to be published and appear in, vol. 12, No. 5 mid of june (2018).

[16] N.L. Heda, ALPa Dashora, Ambica Marwal, Yamini Sharma,S.K. Srivastava Gulzar Ahmed, Rajesh Jain, B.L. Ahuja "J. Phys. Chem. of solids" 71(2010), 187-193.

TABLE I

Different theoretical Compton profiles values by using the superposition model for (MoS2) with the available experimental data [16] in atomic mass units (a.u.)

P_Z (a.u.)	$J(P_Z)$			
	Superposition model			Exp. [16]
	Free atom	Free electron	RFA MoS_2	
0	18.68	16.419	16.046	16.071±0.034
0.1	18.34	16.336	15.982	15.976
0.2	17.54	16.070	15.774	15.752
0.3	16.51	15.582	15.369	15.405
0.4	15.46	14.893	14.783	14.973
0.5	14.38	13.990	14.002	14.419
0.6	13.28	12.884	13.049	13.684
0.7	12.2	11.722	12.271	12.806
0.8	11.16	10.578	11.168	11.885
1	9.3	9.440	10.030	10.076±0.024
1.2	7.86	8.081	8.048	8.426
1.4	6.73	6.981	6.916	7.046
1.6	5.89	6.115	6.043	6.078
1.8	5.25	5.406	5.338	5.341
2	4.75	4.854	4.795	4.865±0.013
3	3.26	3.290	3.269	3.270±0.009
4	2.372	2.393	2.382	2.393±0.007
5	1.732	1.739	1.730	1.734±0.005
6	1.265	1.274	1.266	1.258±0.004

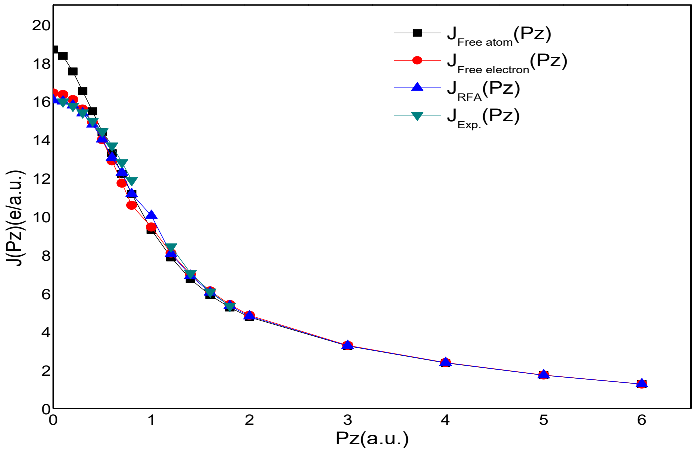

Fig 1. Comparison of theoretical results for Compton profiles with the experimental measurements [16] for MoS_2.

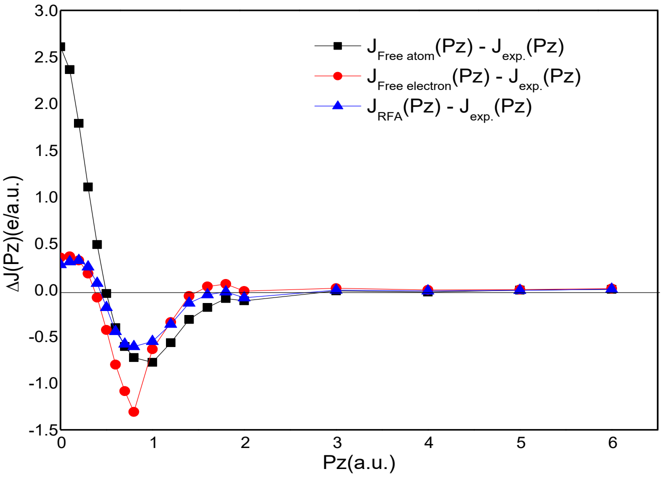

Fig 2. Difference between theoretical Compton profiles and available experimental data [16] of MoS_2.