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Compton Profile Investigation for Aluminum (Al)

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ABSTRACT
This paper presents a study on the Compton Profile (CP) for aluminum in the face-centered cubic (fcc) crystal structure. Renormalized -Free Atom (RFA) model has been used to calculate the CP for the (3s-3p) subset of configurations. It is found that the RFA calculation for the ($3s^2$-$3p^1$) configuration provides a better agreement with experimental values and the Plane Wave Generalized Gradient Approximation (PW-GGA) than the free atom model. CP was chosen for all values within the momentum region (P_Z= 0→7a.u) and compared the theoretical results with the available experimental values. The results were in good agreement with the available experimental values.

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تحقيق منحنى كومبتون لعنصر الالمنيوم (Al)

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الملخص

يتضمن هذا البحث دراسة منحنى كومبتون (CP) لعنصر الالمنيوم (Al) ذات التركيب البلوري الممركز الجسم (fcc)، تم استخدام نموذج اعادة معايرة الذرة الحرة (RFA) لحساب منحنى كومبتون (CP) للتكوين الالكتروني (3s-3p)، وجد ان التكوين الالكتروني ($3s^1$-$3p^1$) ضمن حسابات نموذج اعادة معايرة الذرة الحرة (RFA) كأفضل تكوين الكتروني عند مقارنته مع القيم العملية المتوفرة وكذلك مع بيانات (PW-GGA) وبيانات نموذج الذرة الحرة. تم اختيار منحنى كومبتون لجميع القيم ضمن منطقة الزخم من (P_z=0→7a.u.)، وتمت مقارنة النتائج النظرية مع القيم العملية المتوفرة. كانت النتائج متوافقة بشكل جيد مع القيم العملية المتوفرة.

الكلمات المفتاحية:

منحنى كومبتون , نموذج اعادة معايرة الذرة الحرة, استطارة كومبتون.

1- Introduction:

Aluminum is a metallic element with the chemical symbol Al and atomic number (Z = 13). The phenomenon of Compton scattering, or the inelastic scattering of X-rays as the diffraction of these rays is used for the purpose of knowing the physical properties of materials and gamma-rays via electrons, is strongly associated with the electron density distributions. The movement of targeted electrons strongly corresponds with the Compton spectrum's line-broadening [1,2]. The spectrum produced by the broadened line shape is called Compton Profile (CP). Compton Scattering (CS) method is a renowned approach for investigating materials electrical characteristics [3,4]. It is widely recognized that CS is a versatile method for validating exchange and correlation potentials through electron momentum density [5]. This process involves the transfer of energy from an energetic photon to an electron, resulting in inelastic scattering [6]. The Electron Momentum Density (EMD) through its dependence on the ground-state wave functions and fitting procedure for extracting EMD properties from the Electron Density (ED) has been recently suggested [7,8], which has a historical background dating back to the discovery of X-rays and gamma-rays by Roentgen and one of the main mechanisms for gamma-ray production is the nonlinear Compton scattering [9]. CS is a unique and versatile technique to test usefulness of various exchange and correlation energies through the electron momentum densities [10]. X-rays involving electrons at high energies and transfers of momentum are scattered inelastic by Compton profiles [11]. CS has been shown to be an advantageous tool in obtaining bulk sensitive quantitative information on electronic structure [12]. The separate particles assumption is used in normal CS computations from atomic to represent electrons as distinct objects in a successful potential controlled through the electron-nucleus connection [13]. CP has a wide variety of applications, rang from clinical as in radiobiology and radiation therapy to photonuclear reactions in nuclear physics [14]. CS is an incoherent process relying on the interaction of an electron with an incident photon, it is now authenticated that electron CS can show an way to directly measurement momentum distributions of the electrons in a molecule [15]. It is well established that measuring the CP constitutes one of several direct approaches for exploring an object's ground-state electronics [16]. Compton profile $J(P_Z)$ can be defined as: can provide information about the projection of electronic momentum density on the scattering wave vector. J(Pz) is written as by [17].

$$J(P_Z) = n(p)dp_x dp_y \quad (1)$$

Where p_x, p_y represents the momentum components in the x and y directions relative to the Cartesian coordinates, whereas the direction of z corresponds towards the combination of the collision and scattered wave trajectories. The valence electron's spherical averaging is then merged together with free atom central contributions [18] to yield the complete Compton profile. Over the past years, researchers have made an exceptional effort to study the CP for aluminum, such as [19,20,21].

The aim of the study is to find the electronic momentum density n(p) of the CP for the aluminum element and to know the best electronic configuration using the RFA model, and to compare the results obtained theoretically with the available experimental values.

2- Theoretical Calculations: RFA model

The purpose of using computer programs such as RFA is to explain the accuracy of these programs in finding the values under study, such as the CP. Our theoretical calculations were made for the CP of Al(fcc) using the RFA models. By using the calculate wave equation for Hartree-Fock (HF), the CP was calculated for the electrons in the 3s shell of Al(fcc) [22]. As for the remaining electrons (3s-3p), the values of the CP shape have been taken from tables of Biggs et al. [18]. Our final results for the CP have been normalized to (5.98765) electrons, which is equivalent to the region of free atom CP derived from tables of Biggs et al. [18] in the range of (P_z=0→7 a.u).

RFA model involves truncating the atomic wave function at the Wigner-Seitz radius and renormalizing it to one electron per unit volume within the Wigner-Seitz sphere, yielding an approximate crystal wave function. This approach was first introduced by Chodorow [23].

The new wave function $R_{nl}(r)$ is given by.

$$R_{nl}(r) = \begin{cases} N_{nl}^{-2}\ R_{nl}^{atomic(r)} & r \le R_0 \\ 0 & r > R_0 \end{cases} \qquad (2)$$

Here $R_{nl}^{atomic(r)}$ is the atomic radial wave function for the state with quantum number $n\ and\ l\ and\ N_{nl}^{-2}$ is defined by

$$N_{nl}^{-2} = \int_0^{R_0} \left|R_{nl}^{atomic(r)}\right|^2 r^2 dr \qquad (3)$$

This new wave function is then used in theoretical calculations. The effect of normalization is the largest for electrons in the s shell, because it almost contains a charge (5 %) within the Wigner-Seitz sphere. As for the electrons in the d shell, this percentage is about (95 %). For this region, the effect of the calibration process on it is almost imperceptible.

3- Results and Discussion:

The theoretical results of the Compton profile J(P_Z), which were obtained in the final form after all calculations and corrections were made, were given in Table (1). Three arrangements were chosen for the CP theoretically, which are ($3s^{1.8}$- $3p^{1.2}$) , ($3s^{1.9}$-$3p^{1.1}$) and ($3s^2$-$3p^1$) respectively, were compared with the Free Atom (FA) model ($3s^2$-$3p^1$) as well as data (PW-GGA). All the values of the CP have been normalized to the area under the curve (5.98765) within the momentum region (P_z=0→7a.u.).

When we compare the different calculated and experimental result of [24] Compton profile shown in Table 1, we notice that in the extremely high momentum region (P_z >4.0a.u.), all possible values are nearly identical. This is since only electrons from the core participate in this region, so a similar model remains employed in all situations. It is worth noting that the outcomes agree well with the results of the experiment.

In the momentum region (P_z=0→0.3a.u.), we can observe that a free atom concept has the greatest disparity. Overall, the PW-GGA and RFA parameters are significantly flatter. For the momentum region P_z <0.4a.u. We can see that RFA values for ($3s^2$-$3p^1$) are lower than the (PW-GGA ,$3s^{1.8}$- $3p^{1.2}$, $3s^{1.9}$-$3p^{1.1}$) results, but as the momentum increases beyond 0.6 a.u., the trend is reversed, and the ($3s^2$-$3p^1$) values are higher than those from (PW-GGA ,$3s^{1.8}$- $3p^{1.2}$, $3s^{1.9}$-$3p^{1.1}$). At P_z =0.5a.u., the calculated results of ($3s^2$-$3p^1$, $3s^{1.9}$-$3p^{1.1}$) are equal.

Comparing the free atom model with other results, we can see that in the low momentum region, the free atom ($3s^2$-$3p^1$) values are higher than the PW-GGA values, but beyond P_z>0.4 a.u., the trend gets PW-GGA measurements are greater than free atom measurements. At Pz > (3, 4, 5) a.u., the values of both models become similar (see Fig 1). Fig 2 illustrates the comparison of the free atom results with experimental [24] Compton profile for Al.

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Table 1: Our theoretical Compton profile results for Al were compared to the experimental values [24], and all quantities were expressed in atomic units. These values were normalized to (5.98765) electrons.

P_z (a.u.)	$J(p_z)$ (e/a.u.)					
	Free atom $(3s^2- 3p^1)$ [18]	PW-GGA [24]	Theory(RFA)			Expt. [24]
			Core +RFA $3s^{1.8}- 3p^{1.2}$	Core +RFA $3s^{1.9}- 3p^{1.1}$	Core +RFA $3s^2- 3p^1$	
0.0	5.15	3.880	3.934	3.858	3.808	3.871 ± 0.021
0.1	5	3.853	3.918	3.843	3.795	3.844
0.2	4.57	3.769	3.813	3.743	3.701	3.766
0.3	3.97	3.628	3.575	3.516	3.486	3.631
0.4	3.32	3.435	3.274	3.234	3.22	3.441
0.5	2.76	3.191	2.939	2.921	2.921	3.204
0.6	2.34	2.889	2.534	2.537	2.558	2.936
0.7	2.04	2.539	2.136	2.16	2.199	2.652
0.8	1.84	2.183	1.865	1.869	1.907	2.368
1.0	1.62	1.734	1.686	1.697	1.722	1.876 ± 0.013
1.2	1.49	1.531	1.546	1.559	1.584	1.554
1.4	1.38	1.419	1.424	1.436	1.461	1.361
1.6	1.26	1.303	1.305	1.316	1.337	1.236
1.8	1.14	1.182	1.184	1.195	1.215	1.113
2	1.03	1.063	1.066	1.075	1.094	1.011 ± 0.009
3	0.568	0.570	0.595	0.6	0.61	0.557 ± 0.007
4	0.322	0.323	0.338	0.341	0.346	0.324 ± 0.005
5	0.199	0.199	0.209	0.211	0.215	0.198 ± 0.003
6	0.199	0.133	0.14	0.142	0.144	0.134 ± 0.003
7	0.134	0.094	0.097	0.099	0.102	0.095 ±0.002

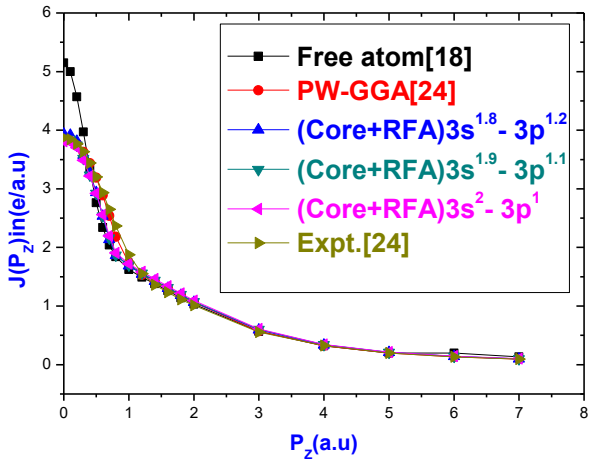

Fig 1: Comparison of the theoretical Compton profile (normalized to 5.98765 electrons) for Al with the experimental values [24].

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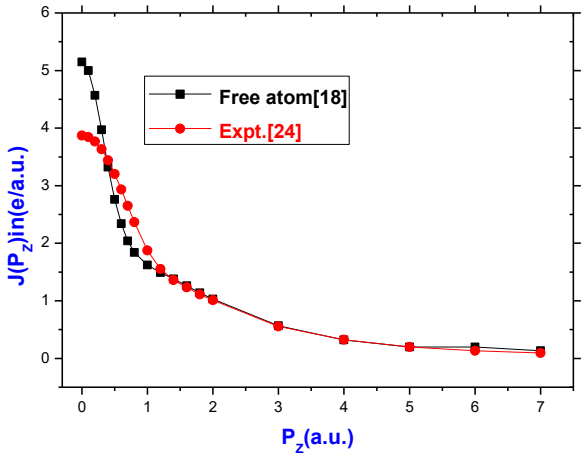

Fig 2: Comparison of the Compton profile results of the free atom model for Al with the experimental values [24].

Now to determine the best configuration of electrons, for every scenario, the overall square error of $\sum_0^{7\ a.u.}|\Delta J|^2$ a.u. was determined for each case in the range of (P_z =0→7 a.u.) by:

$$\left(\sum_0^7 \left(J_{Theo.}(p_z) - J_{exp.}(p_z)\right)\right)^2 = \sum_0^7 |\Delta J(p_z)|^2 \quad (4)$$

Figure 3 displays a graph of the distinction among the hypothetical (RFA only) and experimental [24] Compton profile of Al, whereas Fig 4 provides the graph of a discrepancy among the hypothetical (RFA only) and experimental [24] Compton profile of Al. In the region of low momentum, it can be observed that the ΔJ values PW-GGA, $3s^{1.9}$ - $3p^{1.1}$, $3s^{1.8}$ - $3p^{1.2}$– Exp, and $3s^2$ - $3p^1$-Exp are larger than ΔJ for $3s^2$ - $3p^1$-Exp. Moreover, the ΔJ values for $3s^2$ - $3p^1$-Exp are only similar to those in the low momentum region. However, the ΔJ values where (P_z>3 a.u.), free Atom-Expt is approximately the same as well. The values obtained from experiments are extremely similar to the predictions in the extremely high transference area (P_z>3 a.u.).

In the high momentum region, the contribution of valence electrons is negligible, and the majority of the contribution comes from the inner-core electrons. The free-atom values provide a reasonable description of these inner-core electrons.

To determine the optimal electron configuration, the total square deviation $\sum_0^{7\ a.u.}|\Delta J|^2$ was calculated for each case in the (P_z =0→7a.u.) range. The resulting values for the ($3s^2$ - $3p^1$, $3s^{1.9}$ - $3p^{1.1}$, $3s^{1.8}$ - $3p^{1.2}$) configurations were 0.657032, 0.667634, and 0.738595, respectively (refer to Table 2). Therefore, the ($3s^2$ - $3p^1$) configuration appears to be the most suitable for accurately describing the Compton profile of Al in the high momentum region.

Table 2: Variance between calculated measured results of [24]

NO	Configuration	Different value
١	Core+RFA($3s^2$ - $3p^1$)	0.657032
٢	Core+RFA ($3s^{1.9}$ - $3p^{1.1}$)	0.667634
٣	Core+RFA ($3s^{1.8}$ - $3p^{1.2}$)	0.738595

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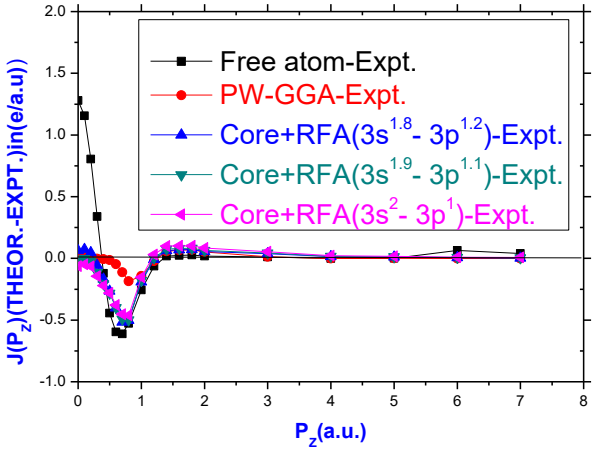

Fig 3: Comparison of ΔJ for different between Electronic Structures and Free atom results, With all theoretical values normalized to (5.98765) electrons.

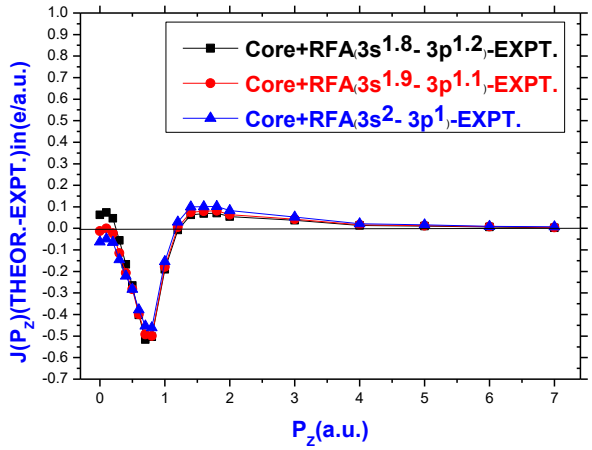

Fig 4: Comparison of ΔJ for different between Electronic Structures results, With all theoretical values normalized to (5.98765) electrons.

4- Conclusions

The scattering of electromagnetic waves with charged particles is called (Compton phenomenon), which can give us important information about the electronic structure of elements, alloys, and compounds. In other words, the Compton scattering experiments provide us with information about the Compton profile of the sample under study. The Compton profile $J(P_Z)$ of aluminum element (Al-Fcc) has been studied by the (RFA) model. The results obtained by this model were in good agreement with the available experimental values. The electronic configuration ($3s^2$-$3p^1$) was the best configurations with the available experimental values. Moreover, RFA model gives completely correct results for the characteristics of the band structure and provides clear explanations about the cohesive energy of the elements, and the successes achieved by RFA model compared to the available experimental results have proven that this model gives correct and accurate results in the theoretical calculations of the Compton profile.

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References

1. Mendonça, J. T., and Haas, F. (2023). Compton scattering of plasmons. *Physica Scripta*, *98*(6), 065603.
2. Fathi, S. J. (2021). Properties and Electrical of Nano composite (Ni_1-xSrxFe12O19) prepared by sol-gel. Samarra Journal of Pure and Applied Science, 3(4), 134-147.
3. Darweesh, S. Y., Jumaa, I. H., and ALYAR, H. (2023). Effect of Repeated Additions of Silica Nanoparticles on the Physical Properties of Nickel. *Samarra Journal of Pure and Applied Science*, *5*(2), 104-117.
4. Mohammed, F. M., Salih, S. H., and Mohammed, S. A. (2018). A study of electron momentum density in Ti_Al system. *Tikrit Journal of Pure Science*, *23*(4), 96-101.
5. Meena, Seema Kumari, and B. L. Ahuja. (2018) Electronic structure and electron momentum densities of Ag_2CrO_4. *AIP Conference Proceedings*. Vol. 1953. No. 1. AIP Publishing LLC, AIP Conf. Proc. 1953, 110026-1–110026-4.
6. Joshi, Ritu, Jagrati Sahariya, and B. L. Ahuja. (2011) Compton scattering study and electronic properties of vanadium carbide: A validation of hybrid functional. *Physica B: Condensed Matter* 406.10: 2007-2012.
7. James, A. D., Sekania, M., Dugdale, S. B., and Chioncel, L. (2021). Magnetic Compton profiles of Ni beyond the one-particle picture: Numerically exact and perturbative solvers of dynamical mean-field theory. *Physical Review B*, *103*(11), 115144.
8. Ghaleb, A. M. (2018). Investigation of electronic structure for β-Zr in the (s-d) subshell. *Tikrit Journal of Pure Science*, *21*(6), 126-131.
9. Gu, Y. J., Klimo, O., Bulanov, S. V., and Weber, S. (2018). Brilliant gamma-ray beam and electron–positron pair production by enhanced attosecond pulses.*Communications Physics*, *1*(1), 93.
10. Meena, Seema Kumari, et al. (2019) Performance of hybrid exchange-correlation potential for photocatalytic silver chromate and molybdate: LCAO theory and Compton spectroscopy. *Physica B: Condensed Matter* 560: 236-243.
11. Heda, N. L., et al. (2010) Electronic properties and Compton profiles of molybdenum dichalcogenides. *Journal of Physics and Chemistry of Solids* 71.3: 187-193.
12. Ruotsalainen, K. O., Inkinen, J., Pylkkänen, T., Buslaps, T., Hakala, M., Hämäläinen, K., and Huotari, S. (2018). The isotropic Compton profile difference across the phase transition of VO 2. *The European Physical Journal B*, *91*, 1-6.
13. Kaliman, Z., K. Pisk, and R. H. Pratt. (2011) Compton scattering from positronium and validity of the impulse approximation. *Physical Review A* 83.5: 053406:
14. Khalaf, M., and Kaminer, I. (2023). Compton scattering driven by intense quantum light. *Science Advances*, *9*(1), eade0932.
15. Onitsuka, Y., Tachibana, Y., and Takahashi, M. (2022). Asymptotic behavior of the electron-atom Compton profile due to the intramolecular H-atom motion in H 2. *Physical Chemistry Chemical Physics*, *24*(33), 19716-19721.

16. Cooper, M. J. (1985). Compton scattering and electron momentum determination. *Reports on Progress in Physics*, *48*(4), 415.
17. Khera, S., S. Mathur, and B. L. Ahuja. (2007) Electronic structure of hafnium: A Compton profile study. *Pramana* 68: 91-98.
18. Biggs, F., Mendelsohn, L. B., and Mann, J. B. (1975). Hartree-Fock Compton profiles for the elements. *Atomic data and nuclear data tables*, *16*(3), 201-309.
19. Felsteiner, J., Fox, R., and Kahane, S. (1972). Symmetry of the Compton profile of polycrystalline aluminum. *Solid State Communications*, *11*(5), 635-638.
20. Cooper, M., Pattison, P., Williams, B., and Pandey, K. C. (1974). The Compton profile of aluminium. *Philosophical Magazine*, *29*(6), 1237-1243.
21. Aguiar, J. C., Di Rocco, H. O., and Mitnik, D. (2013). Experimental Compton profiles of Be, Al and Ti and comparisons to generalized gradient approximation calculations. *Journal of Physics and Chemistry of Solids*, *74*(10), 1341-1348.
22. Clementi, E., and Roetti, C. (1974). Roothaan-Hartree-Fock atomic wavefunctions: Basis functions and their coefficients for ground and certain excited states of neutral and ionized atoms, Z≤ 54. *Atomic data and nuclear data tables*, *14*(3-4), 177-478.
23. Chodorow, M. I. (1939). The band structure of metallic copper. *phys. Rev*, *55*, 675.
24. Sharma, G., et al. (2011) Compton profile and charge transfer study in intermetallic Ti–Al system. *Intermetallics* 19.8 :1107-1114.