Calculation The Relativistic and non-Relativistic Cross Sections of the Electrons Elastic Scattering by Some Atoms

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Abstract:

Partial wave analysis was employed to solve Schrodinger and Dirac equations to calculate non-relativistic and relativistic cross sections, respectively. We have chosen five groups from the periodic table and two atoms for each to show the generality of the theoretical model in applications. The differential and total cross sections were calculated and compared with the available data, and the agreement was very good for most the systems we worked on.

Keywords:. Cross Sections Calculation; Electrons Elastic Scattering; Relativistic and non-Relativistic.

حساب المقاطع العرضية النسبية وغير النسبية للأستطارة المرنة للإلكترونات بواسطة بعض الذرات

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الخلاصة:

تم الاستعانة بطريقة الموجة المجزئة باستخدام معادلتي شرودنجر و ديراك لحساب المقاطع العرضية النسبية والغير النسبية على التوالي .وقع اختيارنا على خمسة مجاميع من الجدول الدوري وتمت الدراسة على ذرتين من كل مجموعة لتبيان عمومية استخدام النموذج النظري في التطبيقات .نستعرض في هذه الدراسة كل من المقاطع العرضية الكلية والتفاضلية والتي تمت مقارنتها مع ما توفر من قراءات، وقد كان التوافــق بين حساباتنـــــا وهذه القـــراءات جيـدة جـــداً لمعظــــم الانظـمة التي عملنا عليهـا.

الكلمات المفتاحية: حساب المقطع العرضي; الأستطارة المرنة للألكترونات; النسبية وغير النسبية..

1. Introduction

The field of scattering process of electron-atom grow had an increasable attention during the last few years. The elastic scattering of charged particles that interacting with natural atoms is very important in which we deal with the cascade distribution of electrons in the target produced from elementary incident particle strike[1].

The electron elastic scattering with neutral atoms is of great importance in wide range of applications such as from radiation processing, radiation sensor x-ray photo electron spectroscopy[2] and plasma physics[3].

Theoretically, difficulties in electron scatters by atoms arises from the exchange effects between the projectile and electrons of the atom-target by its Coulomb field. The approximation methods give many solutions for electron-atom collision problem . All of them showed that the difficulties sharply increases with the increase of the atomic number for an atom [4].

A large angle of scattering ,which is in turn responsible for the back scattering and spreading of the projectile beam from the atoms[5] elastic cross section of the electron from neutral atoms, has been studied by many researchers . Sienkiewicz [6]used Dirac equation for an energy range beginning with 25eV and over; with an exact exchange treatment whereby he include the polarization potential. McEachram and stauffer[7] included the relativistic equation of Dirac-Fock and the no-local potential of exchange and a large range potential of polarization. Haberlamd and Fritsch[8],used the Kohn-Sham approximation method which in turn included the relativistic effects.

2.Theory

We used Schrodinger and Dirac equations where we used the partial wave

analysis to calculate the scattering differential and total cross section. This methods provides a complete description of elastic scattering of electrons by atoms using the partial wave analysis with non-relativistic (Schrodinger) and relativistic (Dirac) equations.

2.1.Schrodinger equation

Schrodinger equation mentioned above predicts that wave functions can form standing waves, called stationary states (also called "orbitals", as in atomic orbitals or molecular orbitals[9].The Hamiltonian itself is not dependent on time explicitly.

$$H\psi = E\psi \qquad (1)$$

When the Hamiltonian operator acts on a certain wave function ψ, and the result is proportional to the same wave function ψ, then ψ is a stationary state, and the proportionality constant, E, is the energy of the state ψ. Hamiltonian operator[9]:

$$H = -\frac{i\hbar^2}{2\mu}\nabla^2 + V(r) \qquad (2)$$

When μ is the particle's reduced mass, $V(r)$ is the effective potential , and $\frac{i\hbar^2}{2\mu}\nabla^2$ equals kinetic energy.

From equ.(1) and equ.(2) and one can obtain the general time-independent Schrodinger equation[9]:

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right]\psi(r) = E\psi(r) \qquad (3)$$

The elastic scattering of non-relativistic particles with kinetic energy E is described by the scattering amplitude $f(\theta)$ defined by[10]:

$$f(\theta) = \sum_{l=0}^{\infty} F_l\, P_l\,(\cos\theta) \qquad (4)$$

where θ is the polar scattering angle, $P_l(\cos\ \theta)$ are the Legendre polynomials, and:

$$F_l = \frac{1}{2ikn}(2l+1)[exp(2i\delta_l) - 1] \qquad (5)$$

Atomic units (a. u.) will be used throughout this monograph. They are such that $\hbar = m = e = 1, k = (2E)^{\frac{1}{2}}$ is the momentum of the projectile, (δ_l) denoted is the Schrodinger phase shift of order l, which is obtained from the solution of the radial equation[11].

The differential cross-section per unit solid angle is given by

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \qquad (6)$$

The total elastic cross-section σ and the transport (or momentum transfer) cross section σ_{tr} are defined by[10]

$$\sigma \equiv 2\pi \int_0^{\pi} \frac{d\sigma}{d\Omega} \sin\theta \, d\theta \qquad (7)$$

And:

$$\sigma_{tr} \equiv 2\pi \int_0^{\pi} (1 - cos\theta) \frac{d\sigma}{d\Omega} \sin\theta \, d\theta \qquad (8)$$

2.2.Dirac equation

In particle physics, the Dirac equation is a relativistic wave equation derived by British physicist Paul Dirac in 1928.The equation also implied the existence of a new form of matter, antimatter, previously unsuspected and unobserved and which was experimentally confirmed several years later[12].

The Dirac equation in the form originally proposed by Dirac is

$$\left(\beta mc^2 + C\left(\sum_{n=1}^{3} \alpha_n \;\; p_n\right)\right)\psi = E\psi \qquad (9)$$

where ψ is the wave function for the electron of rest mass m with space-time coordinates x and t, α and β are the usual 4 X 4 Dirac matrices. The p_1, p_2 and p_3 are the components of the momentum, understood to be the momentum operator in the Schrödinger equation. Also, c is the speed of light, and $\hbar$ is the Planck constant divided by 2π. These fundamental physical constants reflect special relativity and quantum mechanics, respectively[12].

Elastic scattering of relativistic spin $\frac{1}{2}$ particles is described by the direct and spin-flip scattering amplitudes, f(θ) and g(θ), defined by [10].

$$f(\theta) = \sum_{l=0}^{\infty} F_l \, P_l \, (\cos\theta) \qquad (10)$$

$$g(\theta) = \sum_{l=0}^{\infty} G_l \, P_l^1 (\cos\theta) \qquad (11)$$

Where θ is the scattering angle, $P_l^1(\cos\theta)$ are the associated Legendre functions,

$$F_l = \frac{1}{2ik} \{(l+1)[\exp(2i\delta_{l+}) - 1] + l[\exp(-2i\delta_{l-}) \, 1]\} \qquad (12)$$

$$G_l = \frac{1}{2ik} \{\exp(2i\delta_{l-}) - \exp(-2i\delta_{l+})\} \qquad (13)$$

And $\boldsymbol{\delta_{l+}}, \boldsymbol{\delta_{l-}}$ are the phase shifts of order $l. k$, which stands for the momentum of the projectile related to its kinetic energy E through [10]:

$$K^2 = E(E + EC^2)/c^2 \qquad (14)$$

Where c is the speed of light in the vacuum. For each value of the orbital angular momentum l (except l = 0), there are two phase shifts corresponding to the two possible values of the total angular momentum j = $I \pm \frac{1}{2}$, Following Walker[13], the notation $\delta_{la}$with $a \equiv 2(j - l)$ for the phase shifts is used. These are obtained from the solution of the Dirac radial equation [11].The differential cross-section per unit solid angle $\frac{d\sigma}{d\Omega}$ for scattering of unpolarized electrons [10, 13]:

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2 \qquad (15)$$

The total cross-section (7) are now given by the series[10] **:**

$$\sigma = 4\pi \sum_{l=0}^{\infty} \frac{1}{2l+1} (|F_l|^2 + l(l+1)|G_l|^2 \quad (16)$$

3. Results and discussion

In this paper, we presented relativistic (Dirac) and non-relativistic (Schrodinger) differential and total cross sections for electrons scattering from ten atoms, (Cu, Ag, Ga, In, Zn, Hg, Si, Pb, P, Sb) atoms at several energies, which in turn belong to five groups in the periodic table .Our results were compared with the available theoretical and experimental data. Also the total cress sections (TCS's) were presented here for each of those systems.

Here, the authors depend on the non-relativistic (Schrodinger) and relativistic (Dirac) equations in the plane wave analysis. The phase shifts (δ_l) were computed numerically by integrating on the radial part of the wave function .

The aim of this research is to make a comparison between the non-relativistic and relativistic effects resulting from differential and total cross section at low and intermediate energies .Our results showed a good agreement with theoretical and experimental data with which it has been compared with **.**

In fig.(1), we made comparisons for the present work of the differential cross section for Cu atom at the electron incident energies (20 , 60, and 100)eV. The agreement was very good with the theoretical of Yousif Al-Mulla [14] and good with the experimental measurements of Trajmar et al.[15]. The total cross section for Cu was compared with the measurement of Trajmar et al. [15]and the agreement was very good.

In fig.(2) our results of DCS for Ag atom were compared with the theoretical and experimental data of Toisc [16] at 100eV ,and data of Jablonski et al.[17]at (100 and 2000)eV. The agreement at 100 was good at (0-40^{o}) and became very good after this degree. For (1000 and 2000)eV, the agreement was excellent .The TCS for Ag atom were compared with the experimental and theoretical data of Toisc[17]. The agreement was very good with the experiment at the energy range (10-40)eV ,and very good with the theory at energy rang (60-110)eV.

In fig.(3), we made comparisons for the present work of the differential cross section for Zn atom at the electron incident energies (25eV). The agreement was very good with the Dirac data but with Schrodinger was good. When the comparisons (100, 200)eV , the agreement was excellent with the data of McGarrah et al. [18]. The total cross section for Zn-atom was compared with the calculation of McGarrah et al.[18] and the agreement was very good.

In fig.(4), our results of DCS for Hg-atom were compared with the theoretical data of Jablonski et al. [17] and the experimental measurement of Holtkamp et al. [19] at (150eV ,300 and 5000)eV. The agreement are excellent .The TCS's for Hg-atom was compared with experimental data of Zubek et al. [20]and the agreement was very good.

In fig.(5), we made comparisons for the present work of the differential cross section of Ga atom at the electron incident energies (500,1000 and 2000)eV. The agreement was excellent with the theoretical of Ozturk et al.[21] . The total cross section for Ga was compared with the theoretical data of Ozturk et al. [21], and the agreement was very good.

In fig.(6), we made comparison for the present work of the differential cross section for In-atom at the electron incident energies (500, 1000 and 2000)eV. The agreement was excellent with the theoretical data of Ozturk et al.[22] . The total cross section for Ga was compared with the theoretical data of Ozturk et al.[22]and agreement was good.

In fig.(7), we made a comparisons for the present work for the differential cross section of Si-atom at the electron incident energies (70,500 and 1000)eV. The agreement was very good with the theoretical data of Meredith et al. [5].The total cross section for Si-atom was compared with theoretical data of Meredith et al.[5] ,and the agreement was good.

In fig.(8), our results of DCS's for Pb atom were compared with the experimental data of Tosic et al.[23] and the theoretical data Kumar et al.[24] at (60, 80 100)eV. The agreement was excellent with theoretical data but good with experimental measurement .The TCS,s for Pb-atom were compared with experimental data of Tosic et al.[23] and the theoretical data of Fink et al.[25].The agreement was very good with theory, good with experiments ,but the behavior was the same.

In fig.(9), we made comparisons for the present work of the differential cross section for P-atom at the electron incident energies (50, 500 and 1000)eV. The agreement was very good with the theoretical data of of Ozturk et al.[22] .The total cross section for P-atom was compared with the theoretical data of Ozturk et al.[22] and the agreement was very good.

In fig.(10), we made comparisons for the present work (P.W) of the differential cross section for Sb atom at the electron incident energies (5001000and 2000)eV. The agreement was very good with the theoretical data of of Ozturk et al.[22].The total cross section for P-atom was compared with the theoretical data of Ozturk et al.[22] , and the agreement was very good.

The reason for using five groups in our study is to know with what kind of atoms the model we had depend will be more successful, and also to see if our approximation method will be valid in this work by made a comparison with other approximation methods.

4.Conclusions

We noticed through this research that the Dirac method agrees with the results of other research more than the Schrodinger method. This accuracy is due to the relative values Dirac introduced in his calculations such as the energy and relative velocity of the particle projectile on the target atom. In addition the interaction spin-orbital and spin-flip effects.

In general, the comparison between our calculated data were very good for most of those systems. From what was presented, we can conclude that at low and intermediate energies the agreement was good, especially at the small angle and there was some shifting between our data and those which we compared with due to that at low energy the electrons penetrating to the centrifugal barrier is so weak, which in turn effects the phase shift making it decreasing rapidly .However at high energies, the incident electrons will have the ability to penetrate into the region of scattering, and then we noticed that the agreement become very good.

The action of the cross section in our calculations was obvious started with maximum values at the small angles and then begin to decrease with the increasing of the scattering angle. Also we noticed that in most figures we had done, that the action of the cross section was smooth in its behavior with no resonance action, and this is because the whole process is elastic.

The total cross section result was in general very good for all atoms except for Ag atom, where the agreement was good with experiment at low energies, and good with the theory at the intermediate energies.

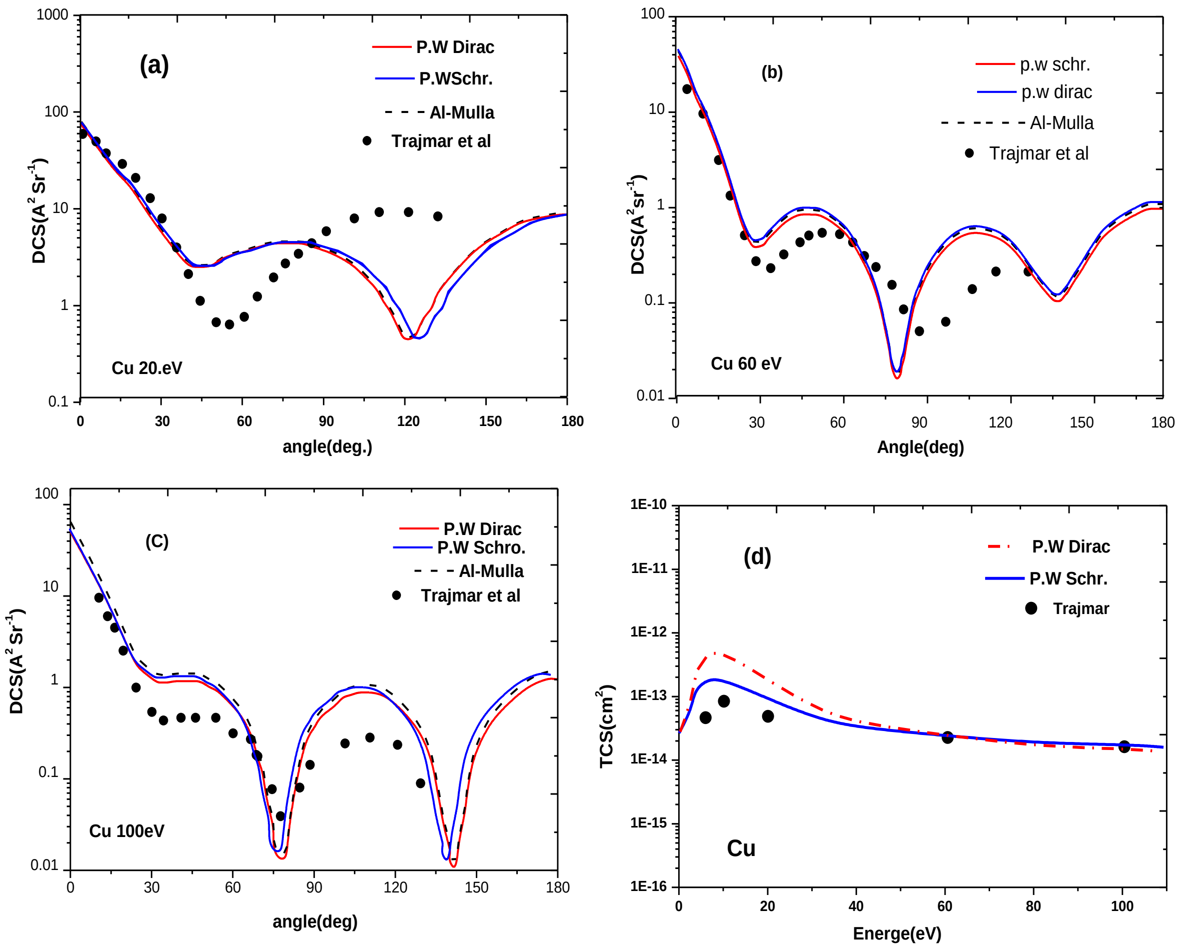

Fig. 1 Differential cross sections for the elastic scattering of electrons from copper (Cu)(a) 20eV (b) 60eV (c) 100eV and (d) total cross sections.

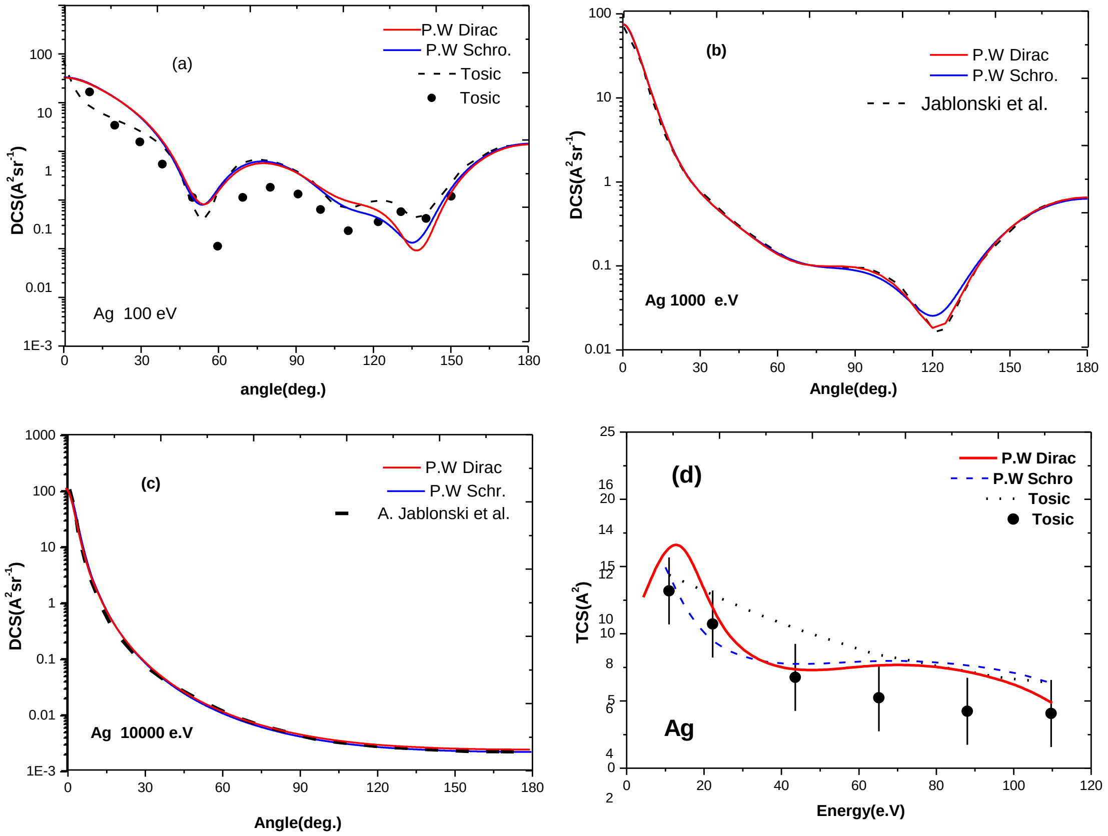

Fig. 2 Differential cross sections for the elastic scattering of electrons from silver (Ag) (a)100eV (b) 1000eV (c) 10000eV and (d) total cross sections.

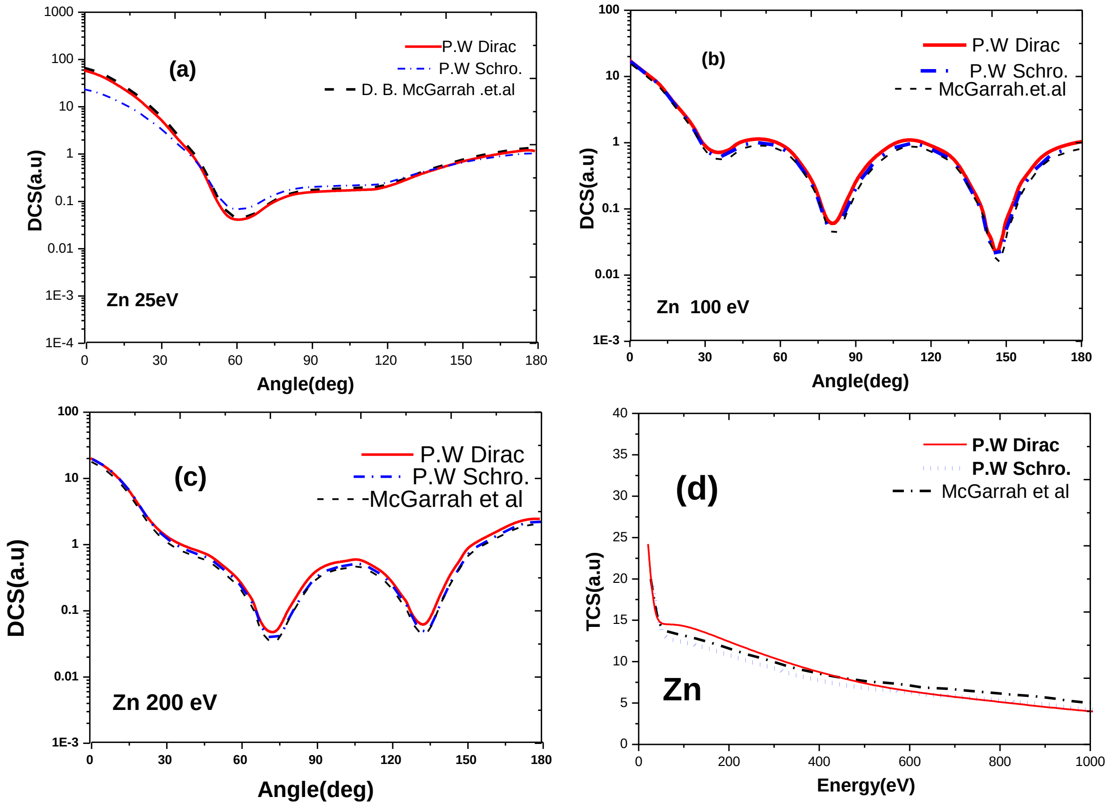

Fig. 3 Differential cross sections for the elastic scattering of electrons from zinc (Zn) (a)25eV (b) 100eV (c) 200eV and (d) total cross section.

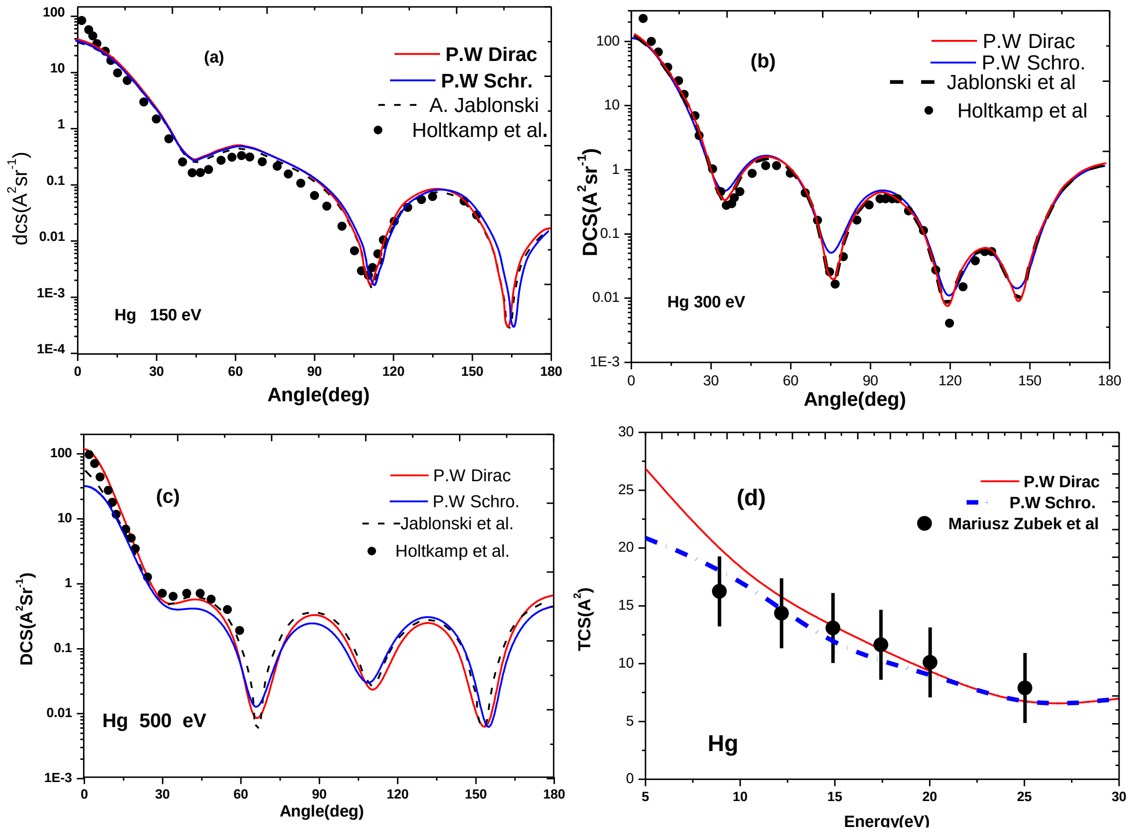

Fig. 4 Differential cross sections for the elastic scattering of electrons from mercury (Hg) (a)150eV (b) 300eV (c)500eV and(d) total cross sections.

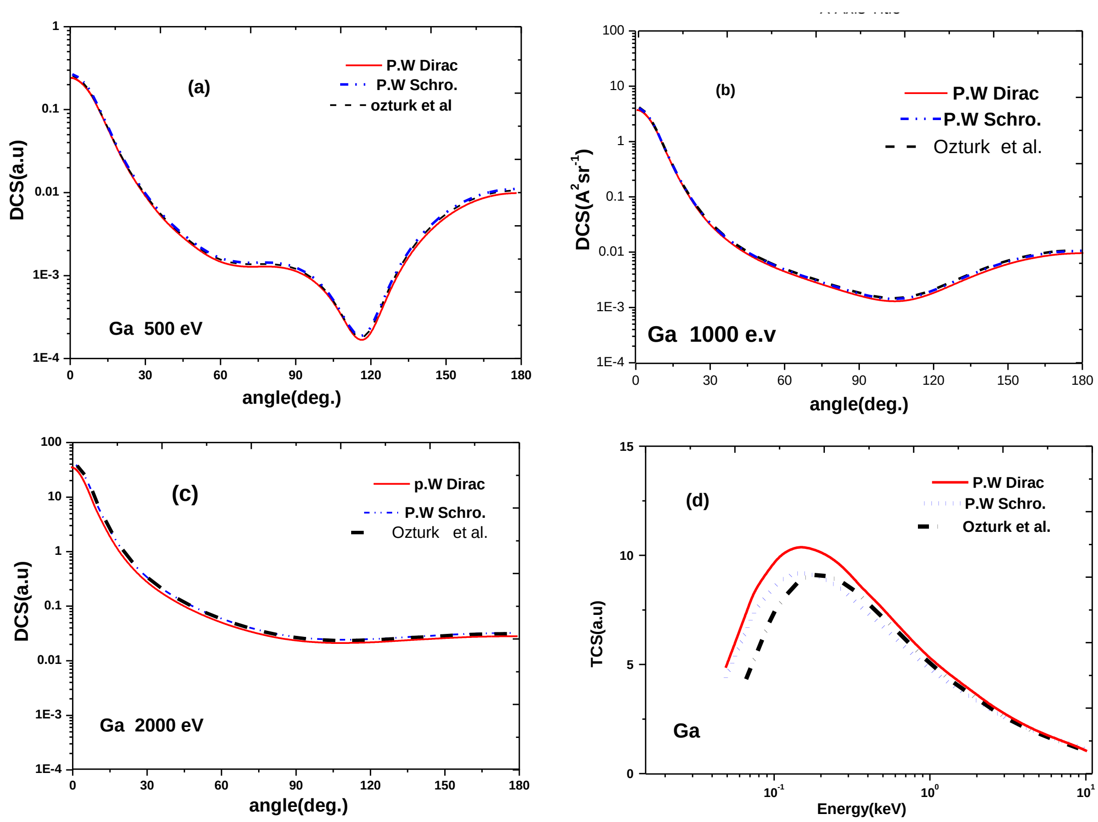

Fig. 5 Differential cross sections for the elastic scattering of electrons from gallium (Ga) (a)500eV (b) 1000eV (c) 2000eV and(d) total cross section.

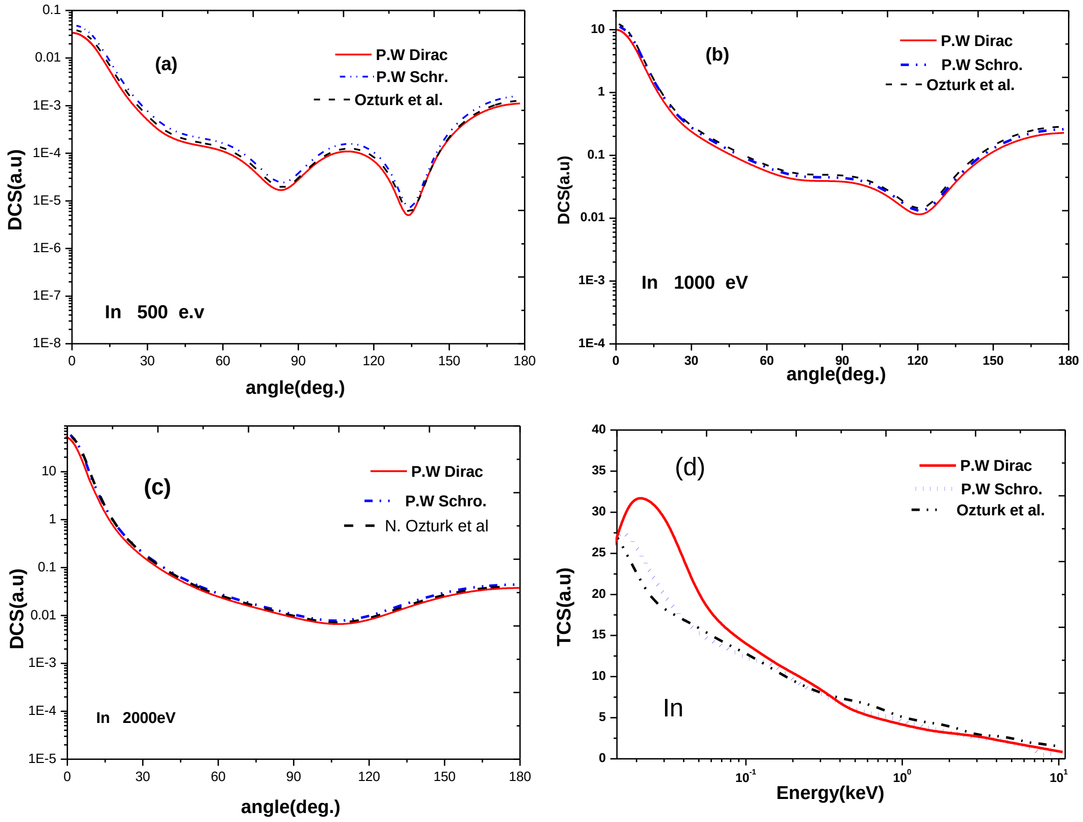

Fig. 6 Differential cross sections for the elastic scattering of electrons from indium (In) (a)500eV (b) 1000eV (c) 2000eV and (d) total cross section.

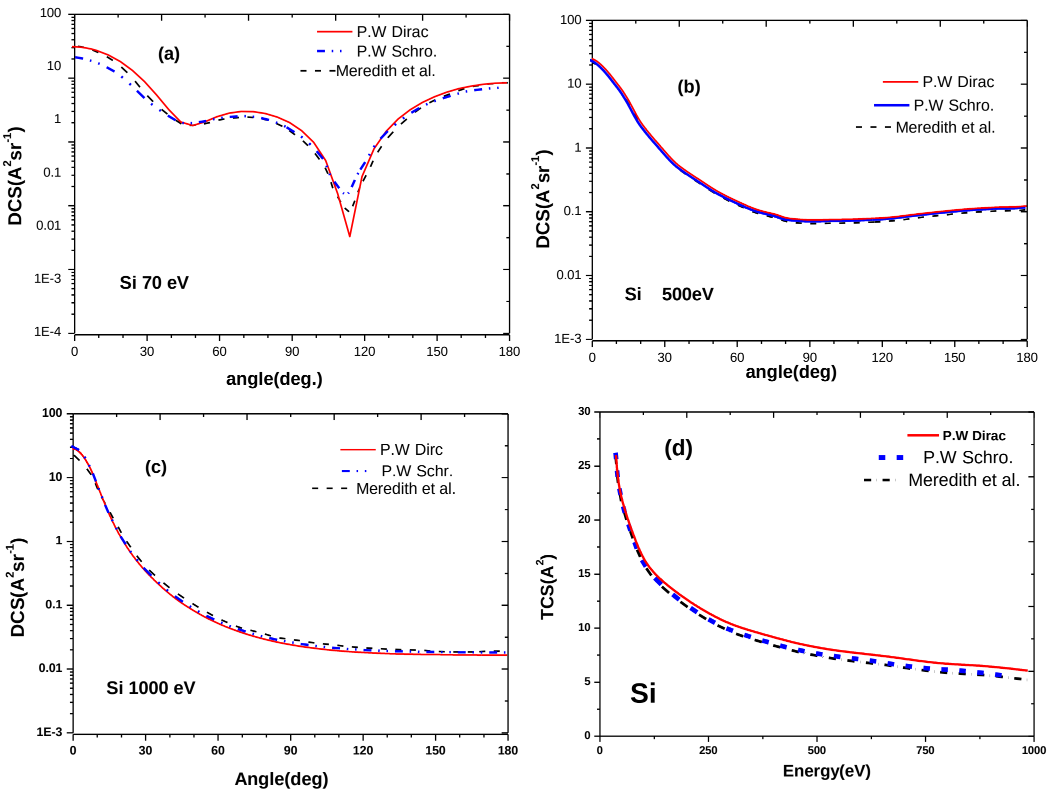

Fig. 7 Differential cross sections for the elastic scattering of electrons from silicon (Si) (a)70eV (b) 500eV (c) 1000eV and (d) total cross section.

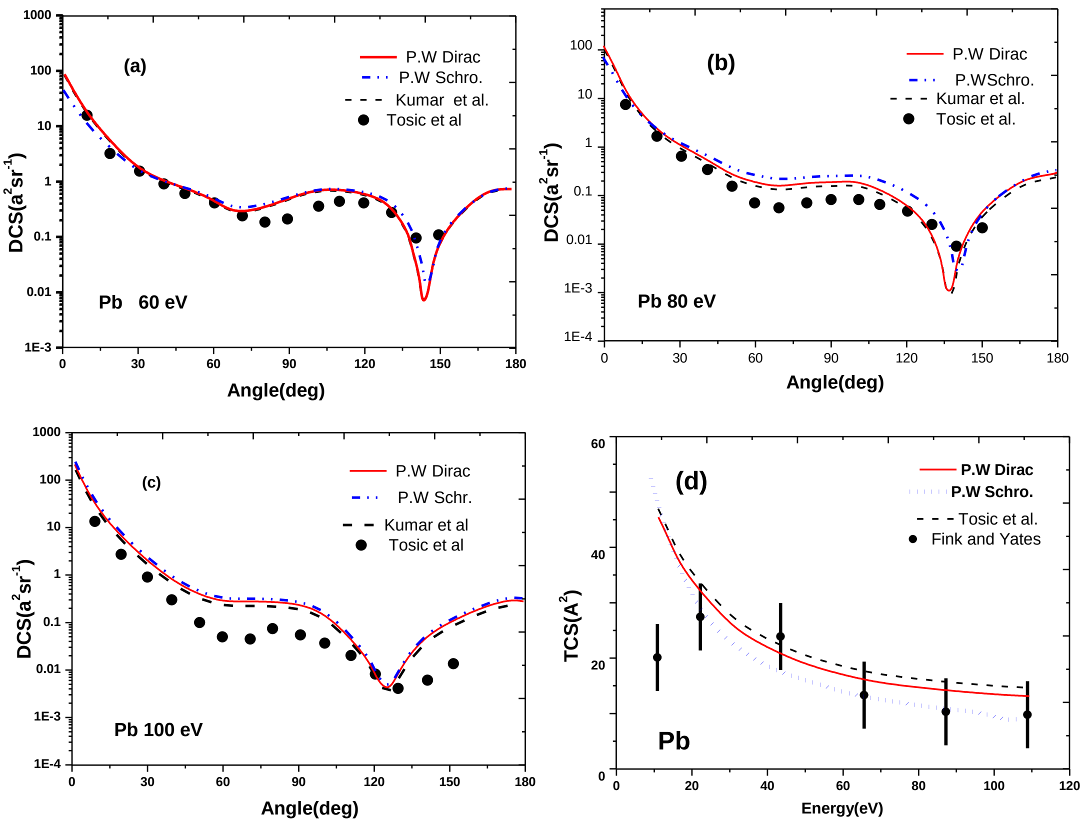

Fig. 8 Differential cross sections for the elastic scattering of electrons from lead (Pb) (a)60eV (b) 80eV (c) 100eV and (d) total cross section.

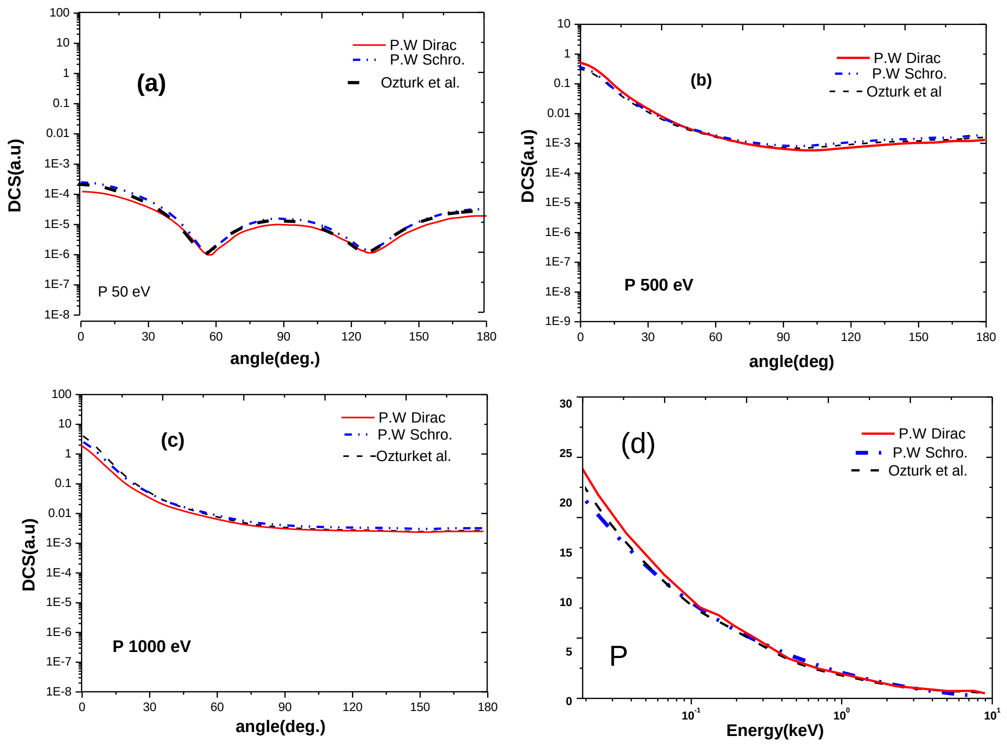

Fig. 9 Differential cross sections for the elastic scattering of electrons from phosphorus (P) (a)50eV (b) 500eV (c) 1000eV and (d) total cross section.

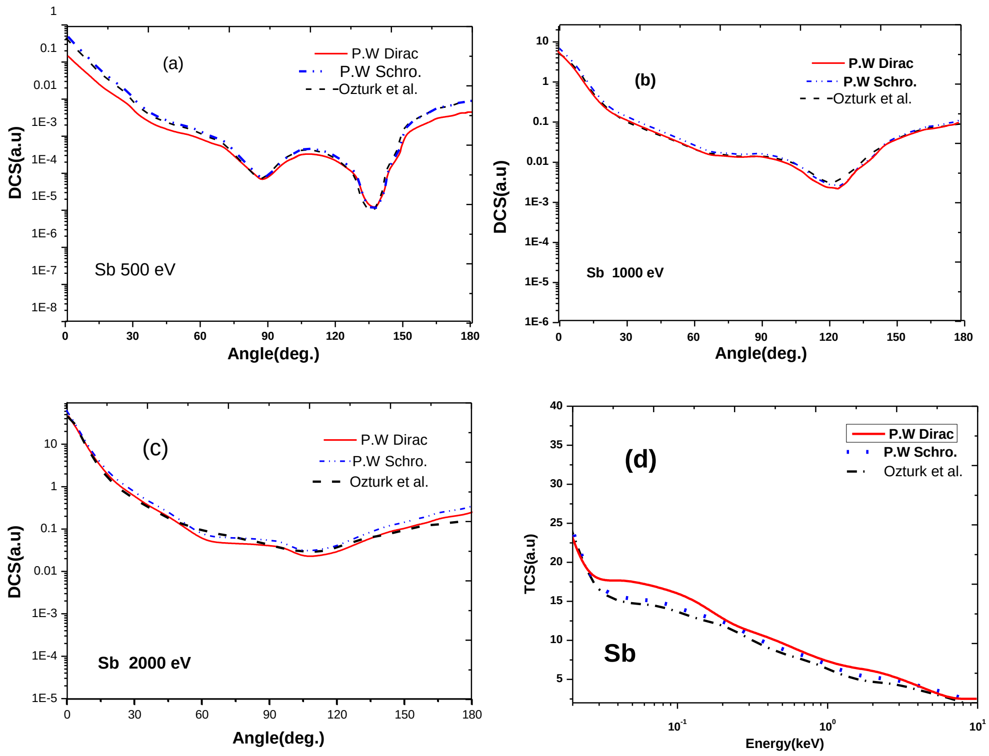

Fig. 10 Differential cross sections for the elastic scattering of electrons from antimony (Sb) (a)500eV (b) 1000eV (c)2000eV and (d) total cross section.

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