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K-shell ionization cross sections of transition and non metals by electron impacts

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Abstract. The theoretical model, developed by Khare, has been modified to calculate the total cross sections for K-shell ionization of 12 atom targets (C, N, O, Al, Fe, Se, Ag, Sb, Ho, Au, Bi, U) due to electron impact at incident electron energy from ionization threshold to 1 GeV. The various calculated cross sections are in remarkable agreement with available experimental data and other theoretical cross sections.

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Key words: ionization cross section, atoms, electron impact, K-shell

1 Introduction

Electron impact ionization cross sections for K-shell ionization are needed for modeling of radiation effects in materials, in biomedical research and modeling of fusion plasmas in tokomaks. The electron impact ionization cross sections find important applications in fields such as mass spectrometry, radiation science, semiconductor physics, atmosphere physics, astrophysics, x-ray laser and fusion research. The computed data on cross sections are necessary in studying the problems of radiative association. Over the past five decades, many experimental and theoretical studies have been carried out to estimate the electron impact K-shell ionization cross section by various groups.

In this paper, we have modified the Khare *et al.* [1] model for K-shell ionization. First of all, the classical formula for K-shell ionization is given by Gryzinski [2], which provides a fairly good description over a wide energy range except near the threshold region. This formula was further modified by Deutsch *et al.* [3] for atomic ionization cross sections covering the whole energy range. Their formula uses weighted sum of the squared radii of the maximum charge

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density of the electron subshells. The final expression involves a number of parameters which are different for s, p and d bound electrons and are different from those given by Gryzinski. An additional relativistic factor was also introduced empirically by the above authors to fit the theoretical cross sections with experimental data. Later on, quantum mechanically the theory based on the Plane Wave Born Approximation (PWBA) [4–6] and Distorted Wave Born Approximation (DWBA) [7] came into light.

In ultrarelativstic energy region, Scofield [7] employed the first Born approximation (FBA), in which he represented incident and scattered electrons by plane waves, obtained by solving the free particle Dirac equation and the active electron of each target, moving in a central field, was also treated relativistically. His cross sections exhibit a nice agreement with the experimental data at ultrarelativstic energies. However, these methods fail at impact energies near threshold of ionization. Hombourger [8] calculated the K shell ionization cross sections by proposing a relativistic empirical expression through an analysis of experimental data for atoms ($6 \leq Z \leq 76$). For the electron impact ionization cross sections, Bell *et al.* [9] have developed analytical formulae, referred as BELL formulae, involving species-dependent parameters. Casnati *et al.* [10] proposed another empirical model to describe cross sections for ($6 < Z < 79$).

Khare *et al.* [4–6] have calculated the electron impact ionization cross sections for K-shell for a numbers of atoms. They have employed the PWBA with corrections for exchange, coulomb and relativistic effects. In 2000 Kim *et al.* [11] proposed the relativistic version of the BEB model [12]. Kim *et al.* [11] and Santos *et al.* [13] calculated the cross sections for K-shell ionization of atoms by using their relativistic BEB formula.Recently many researchers like Haque *et al.* [14], Uddin *et al.* [15], Patoatry *et al.* [16], Huo [17], Talukder *et al.* [18] etc. have calculated the K shell ionization cross sections by modifying the different model from threshold to ultrarelativistic energy range.

In 1999 Khare *et al.* [1] proposed a model, referred as Khare [BEB] model, to calculate the ionization cross sections for molecules This model has been developed by combining the useful features of PWBA [19] and BEB model of Kim and Rudd [12], where $(1-\omega/E)$ was replaced by (E_r/E_r+I+U), ω is the energy lose suffered by incident electron in the ionizing collision, E_r is the relativistic kinetic energy of incident electron, I is the ionization energy, U is the average kinetic energy of bound electron. Here $I+U$ represent the increase in kinetic energy of the incident electron due to its acceleration by the field of the target nucleus. Furthermore, they have employed the useful features of the Binary Encounter Bethe models of Kim and Rudd [12]. Kim and Rudd [12] have used the COOS $df/d\omega = NI/\omega^2$ and dropped the contribution of exchange to Bethe term. Although Bethe and Mott cross-sections in Khare *et al.* [1] model are different corresponding cross-sections of Kim [BEB] model but the total ionization cross sections obtained in both model are very close to each other.

For the positron and electron impact Khare *et al.* [5] have calculated the deacceleration and acceleration energy of the coulomb field of the bare nucleus for the hydrogen like atom. They have shown that the coulomb energy $E_c = hI/[1+F(x)]$, where $h = 4n^2/[3n^2 - l(l+1)]$, n and l are the principal quantum number and angular quantum number respectively, $F(x)$ is the function of the $x = 2Zr_-/a_0$, Z and a_0 are the atomic number and Bohr radius. r_- is the shortest distance from the centre of the atom at which electron or positron reaches in the collision process. They have taken $r_- = 0$, so $F(x) = 0$ for the electron.

In present investigation we have replaced $(U+I)$ by $hI/[1+F(x)]$, attraction by target nucleus, in denominator of the Khare BEB model for K-shell ionization. Here I is the ionization energy with relativistic correction. Furthermore, we have taken the finite values of $F(x)$ for electron impact. The values of h and $F(x)$ are obtained by fitting on reliable experimental data.

2 Theory

In Khare [BEB] model [1], the ionization cross section is given by

$$\sigma_T = \sigma_{PBB} + \sigma_{PMB} + \sigma_t, \tag{1}$$

where the Bethe cross section

$$\sigma_{PBB} = \frac{SI_r^2}{(t+f)} \int_{I_r}^{E_r} \frac{1}{\omega^3} \ln\left(\frac{\omega}{Q_-}\right) d\omega. \tag{2}$$

Mott cross section

$$\sigma_{PMB} = \left(\frac{s}{t+f}\right) \times \left[\begin{array}{c} \left(1 - \frac{2}{t+1} + \frac{t-1}{2t^2}\right) + \left(\frac{5-t^2}{2(t+1)^2} - \frac{1}{t(t+1)}\right) \\ -\left(\frac{t+1}{t^2} \ln\left(\frac{t+1}{2}\right)\right) \end{array}\right], \tag{3}$$

and the cross section due to transverse interaction is

$$\sigma_t = -\frac{SI_r^2}{NR(t+f)} M^2 \left(\ln(1-\beta^2) + \beta^2\right). \tag{4}$$

For the incident electron of the rest mass m and velocity v, the relativistic energy E_r is

$$E_r = \frac{1}{2} m v^2 = \frac{1}{2} mc^2 \left(1 - \frac{1}{\left(1+\frac{E}{mc^2}\right)^2}\right), \tag{5}$$

$$I_r = \frac{1}{2} m v_b^2 = \frac{1}{2} mc^2 \left(1 - \frac{1}{\left(1+\frac{I}{mc^2}\right)^2}\right), \tag{6}$$

and

$$f = \frac{h}{1+F}, \tag{7}$$

F is fitted by the equation $F = \xi Z$, where $\xi = 0.018$ and $h = 1.77$ are fitting parameter for the K-shell ionization.

The relation between M^2 and Bethe collision parameter (b_{nl}) is given by

$$b_{nl}=\frac{I_r M^2}{z_{nl} R}, \tag{8}$$

where Z_{nl} is the number of electrons in the (nl) subshell of the atom. Taking $Z_{nl}=N$ and putting the value of M^2 from Eq. (8) in Eq. (4), we get

$$\sigma_t=-\frac{s b_{nl}}{t+f}\left(\ln(1-\beta^2)+\beta^2\right). \tag{9}$$

With COOS $df/d\omega=NI/\omega^2$, we get the value of Bethe collision parameter (b_{nl}) is equal to 0.5 for all atoms that does not depend on Z. This is because at present the appropriate form of the COOS is not known. It will be conveinent to take the value of the Bethe parameter b_{nl} in the Khare parameters [6]. The value of b_{nl} in the Khare parameters is given by

$$b_{nl}=\alpha p^{-\gamma}, \tag{10}$$

where $p=I/I_s$, $I_s=Z_s^2 R$, $Z_s=Z-s$ is the effective atomic number and the Khare parameters are $\alpha=0.285$ and $\gamma=1.70$.

The recoil energy Q_- is given by

$$Q_-=0.5mc^2\left(\left(E_r(E_r-\omega)\right)^{\frac{1}{2}}-\left((E_r-\omega)(E_r-\omega+2mc^2)\right)^{\frac{1}{2}}\right)^2. \tag{11}$$

It is due to the assumption that a large contribution to the integral comes from the small values of ω. Hence for $\omega \ll E$, we obtain from Eq. (11)

$$Q_-=\frac{\omega^2}{4}\left(\frac{1}{2}mc^2+\frac{1}{E_r}\right). \tag{12}$$

Now putting this into Eq. (2) and evaluating the integral we obtain

$$\sigma_{PBB}=\left(\frac{S}{t+f}\right)\times\left(0.4431\left(1-\frac{1}{t^2}\right)-0.5\ln\left(\frac{1}{t}+\frac{I_r}{2mc^2}\right)+\frac{1}{2t^2}\ln\left(1+\frac{E_r}{2mc^2}\right)\right). \tag{13}$$

After putting the values of σ_{PMB}, σ_t and σ_{PBB} from Eqs. (3), (9) and (13) into Eq. (1), the K-shell ionization cross sections are obtained for atom.

In this paper, we have

$A=4\pi a_0^2 R^2$, $R=$ Rydberg energy,
$a_0=$ first Bohr radius, $N=$ number of electrons,
$I=$ ionization thresholds, $m=$ rest mass of electron,
$E_r=$ relativistic energy, $v=$ incident velocity,
$c=$ velocity of light, $Q_-=$ recoil energy,
$\omega=$ the energy loss,
$M^2=$ total dipole matrix squared for the ionization.
$Z_s=$ the effective atomic number,
$s=$ screening parameter,
$v_b=$ the speed of an electron with thte kinetic energy I,
$\beta=$ the ratio of the incident velocity and the velocity of light.

3 Results and discussion

In the present investigation the K-shell ionization cross sections have been calculated for the twelve atoms by modifying the Khare [BEB] model [1] for incident energy varying from threshold ionization energy to high energy (GeV). The ionization potentials are taken from Desclaux [20] and Jolly *et al.* [21]. The parameter h and ξ have been obtained from fitting the experimental data of C, Au, and Bi targets by using the least square method. The sources of the experimental data are Tawara *et al.* [22] for carbon atom, Rester *et al.* [23], Davis *et al.* [24], Middlemann *et al.* [25], Berkner *et al.* [26] for gold atom and Hoffmann *et al.* [27] and Ishii *et al.* [28] for Bi atom. The ionization cross sections calculated by Bell *et al.* [9], Talukder *et al.* [18], Patoatry *et al.* [16], Huo [17], Haque *et al.* [14] and Uddin *et al.* [15] are not shown in the figures. The ionization cross sections for all atoms are compared with the available experimental and theoretical results as following.

Fig. 1 shows the comparison of present cross- sections for Carbon along with the experimental data given by Tawara *et al.* [22], Isaacson [29], Hink and Ziegler [30], Egerton [31] and theoretical results of Kim *et al.* [11], Casnati *et al.* [10], Hombourger [8]. The present cross-sections are in good agreement with the experimental data.

Fig. 2 shows the K-shell ionization cross-sections for nitrogen. The present cross- sections, Casnati *et al.* [10], Santos *et al.* [13] and Hombourger [8] agree well with experimental data

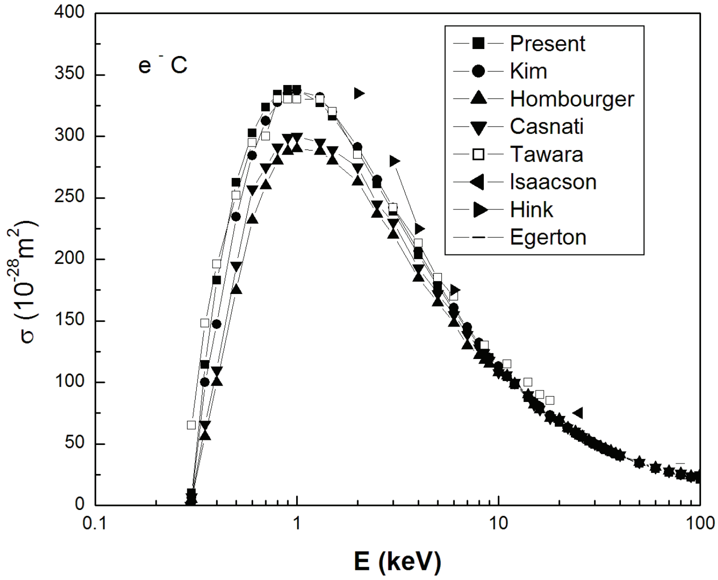

Figure 1: The figure compares the present theoretical electron impact ionization cross section and experimental electron impact ionization cross section for carbon (C). ■, present work; •, theoretical data by Kim *et al.* [11]; ▲, theoretical data by Hombourger [8]; ▼, theoretical data by Casnati *et al.* [10]; ◄, experimental data by Isaacson [29]; ►, experimental data by Hink and Ziegler [30]; —, experimental data by Egerton [31]; □, experimental data by Tawara *et al.* [22].

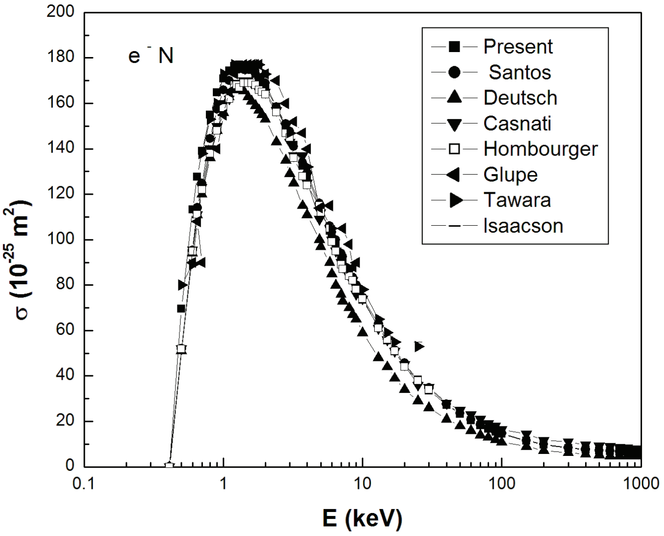

Figure 2: This figure showing the comparison of the present electron impact ionization cross section to experimental data for nitrogen (N). ■, the present work; •, theoretical data by Santos *et al.* [13]; ▲, theoretical data by Deutsch *et al.* [3]; ▼, theoretical data by Casnati *et al.* [10]; □, theoretical data by Hombourger [8]; ◄, experimental data by Glupe and Mehlhorn [32]; ►, experimental data by Tawara *et al.* [22]; —, experimental data by Isaacson [29].

measured by Tawara *et al.* [22] and Glupe and Mehlhorn [32] However theoretical results of Deutsch *et al.* [3] lie below the present calculations for $E > 1$ KeV. Experimental cross section measured by Isaacson [29] is higher than the theoretical cross sections.

In Fig. 3, the present cross sections for oxygen are compared with the experimental data of Glupe and Mehlhorn [32], Isaacson [29], Platten *et al.* [33], Tawara *et al.* [22] and theoretical results of Santos *et al.* [13], Casnati *et al.* [10], Deutsch *et al.* [3] and Hombourger [8]. The figure shows that the agreement between the experimental data and the present results is quite good.

In Fig. 4, we compare the present cross-sections with experimental cross sections measured by Hink and Ziegler [30], Hoffmann *et al.* [27], McDonald and Spice [34] and Kamiya *et al.* [35] and the theoretical calculations of Santos *et al.* [13] Casnati *et al.* [10], Deutsch *et al.* [3] and Hombourger [8] for Aluminum atom (Al). The present cross-sections are lower than the cross sections those measured by Hink and Ziegler [30] around the peak while at high energies they are in good accord with experimental data of Hoffmann *et al.* [27] and Kamiya *et al.* [35]. The cross sections measured by McDonald and Spice [34] lie below the present results at high energies. The ionization cross-sections obtained by Santos *et al.* [13], Hombourger [8] and Casnati *et al.* [10] are very close to present calculated cross sections.

The K-shell ionization cross sections for Fe atom have been shown in Fig. 5. The present theoretical values are in good agreement with experimental data of Luo *et al.* [36] and they agree with the experimental data of Llovet *et al.* [37] and Scholz *et al.* [38] over entire range

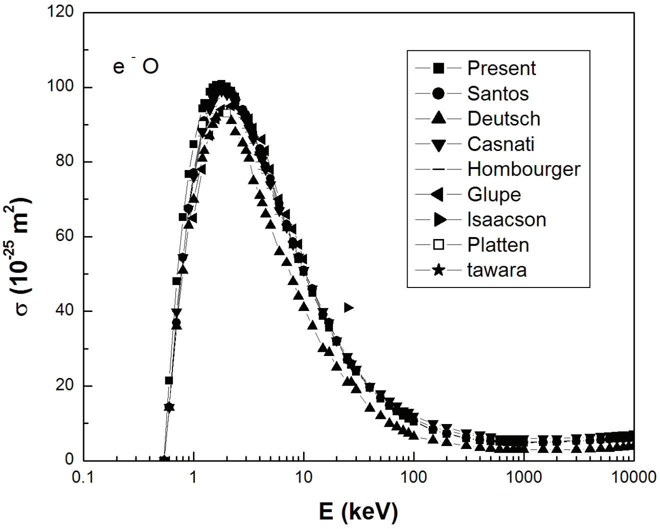

Figure 3: This figure compares of the present theoretical electron impact ionization cross section to experimental data for oxygen (O). ■, present work; •, theoretical data by Santos *et al.* [13]; ▲, theoretical data by Deutsch *et al.* [3]; ▼, theoretical data by Casnati *et al.* [10]; —, theoretical data by Hombourger [8]; ◄, experimental data by Glupe and Mehlhorn [32]; ►, experimental data by Isaacson *et al.* [29]; □, experimental data by Platten *et al.* [33] *, experimental data by Tawara *et al.* [22].

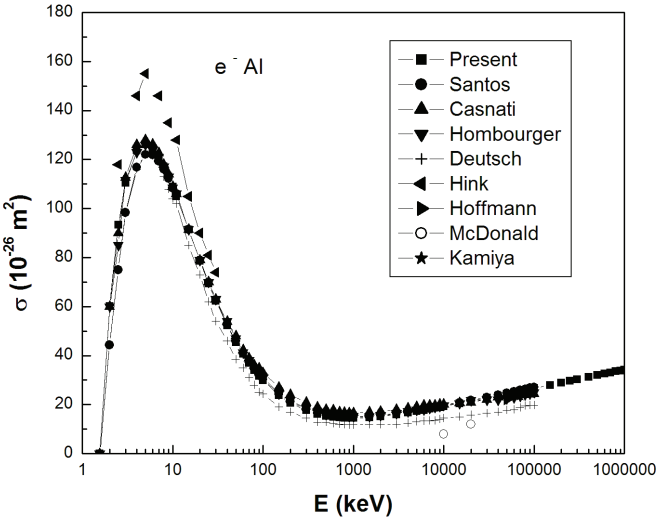

Figure 4: This figure compares of the present theoretical electron impact ionization cross section to experimental data for Aluminium (Al). ■, present work; •, theoretical data by Santos [13]; +, theoretical data by Deutsch *et al.* [3]; ▲ , theoretical data by Casnati *et al.* [10]; ▼, theoretical data by Hombourger [8]; ◄, experimental data by Hink *et al.* [30]; ►, experimental data by Hoffmann *et al.* [27]; ∘, experimental data by McDonald *et al.* [34]; *, experimental data by Kamiya *et al.* [35].

within 5%. However the data of He *et al.* [39] are higher than the theoretical values at the peak. Other theoretical values of Hombourger [8] are very close to present values. An

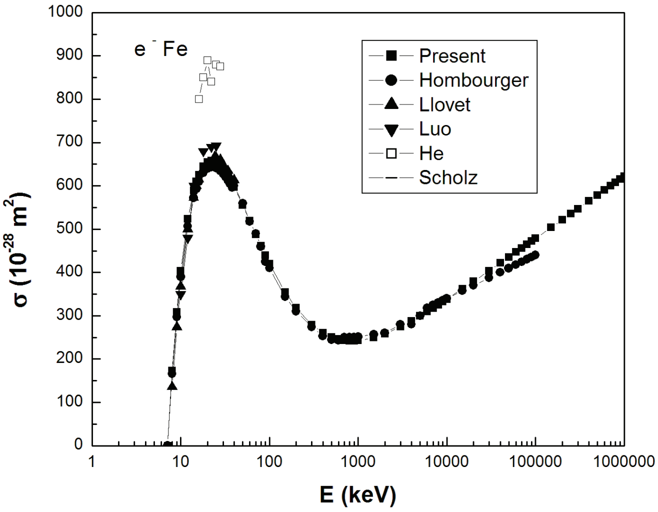

Figure 5: This figure showing the comparison of the present electron impact ionization cross section to experimental data for Iron (Fe). ■, the present work; •, theoretical data by Hombourger [8]; ▲, experimental data by Llovet *et al.* [37]; ▼, experimental data by Luo *et al.* [36]; □, experimental data by He *et al.* [39]; —, experimental data by Scholz *et al.* [38].

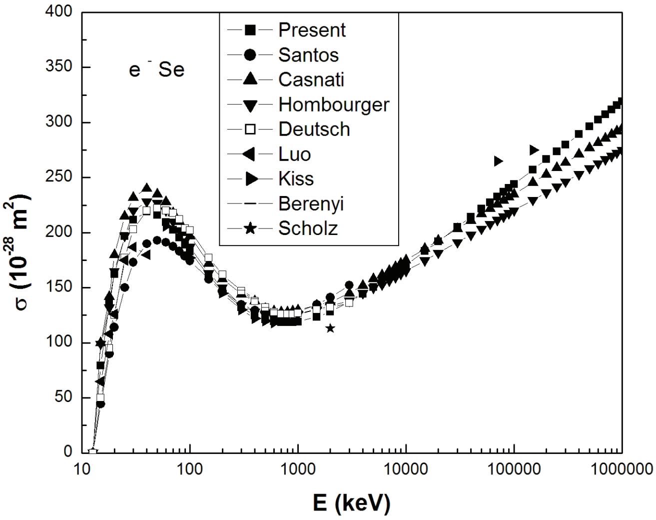

Figure 6: This figure showing the comparison of the present electron impact ionization cross section to experimental data for Se. ■, the present work; •, theoretical data by Santos *et al.* [13]; ▲, theoretical data by Casnati *et al.* [10]; ▼, theoretical data by Hombourger [8]; □, theoretical data by Deutsch *et al.* [3]; ◄, experimental data by Luo *et al.* [36]; ►, experimental data by Kiss *et al.* [41]; —, experimental data by Berenyi *et al.* [40]; *, experimental data by Scholz *et al.* [38].

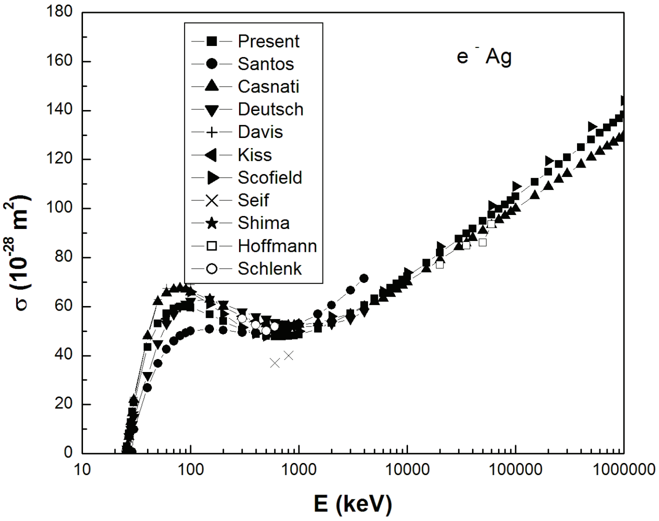

Figure 7: This figure showing the comparison of the present electron impact ionization cross section to experimental data for silver atom (Ag). ■, the present work; •, theoretical data by Santos *et al.* [13]; ▲, theoretical data by Casnati *et al.* [10]; ▼, theoretical data by Deutsch *et al.* [3]; + experimental data by Davis *et al.* [24]; ◄, experimental data by Kiss *et al.* [41]; ►, theoretical data by Scofield *et al.* [7]; -x-, experimental data by Seif *et al.* [43]; *, experimental data by Shima [42]; □, experimental data by Hoffmann *et al.* [27]; ∘, experimental data by Schlenk *et al.* [44].

examination of Fig. 6, which exhibits the cross sections for Se, shows the present theoretical values agree with the experimental data measured by Luo *et al.* [36], Berenyi *et al.* [40], Kiss *et al.* [41] and Scholz *et al.* [38]. The theoretical values of Hombouger [8], Deutsch *et al.* [3] and Casnati *et al.* [10] lie above at peak but for high energies they become lower than the present calculations. However other theoretical results by Santos *et al.* [13] are close to present results.

The present theoretical values for Ag shown in Fig. 7 are in good agreement with experimental data of Kiss *et al.* [41] over entire energy range. The difference between the theoretical values and the experimental values is usually less than the experimental error of 15%. Conversely, the data of Davis [24] are higher than the present values. The measured results of Hoffmann *et al.* [27], Shima [42], Seif *et al.* [43], and Schlenk *et al.* [44] are in good agreement with the obtained results. Present caculations and theoretical results of Santos *et al.* [13], Scofield [7], Deutsch *et al.* [3] and Casnati *et al.* [10] are maintained same shape till the peak.

The theoretical and experimental results of Sb have been shown in Fig. 8. The ionization cross sections in this case were measured by Kiss *et al.* [41] and Scholz *et al.* [38]. Present results are in good agreement within 5% of the experimental results of Kiss *et al.* [41] and Scholz *et al.* [38]. The theoretical calculations by Santos *et al.* [13], Casnati *et al.* [10], Deutsch *et al.* [3] and Hombourger *et al.* [8] do not agree with the experimental data.

Fig. 9 shows the ionization cross section for Ho atom. Present results are in good compar-

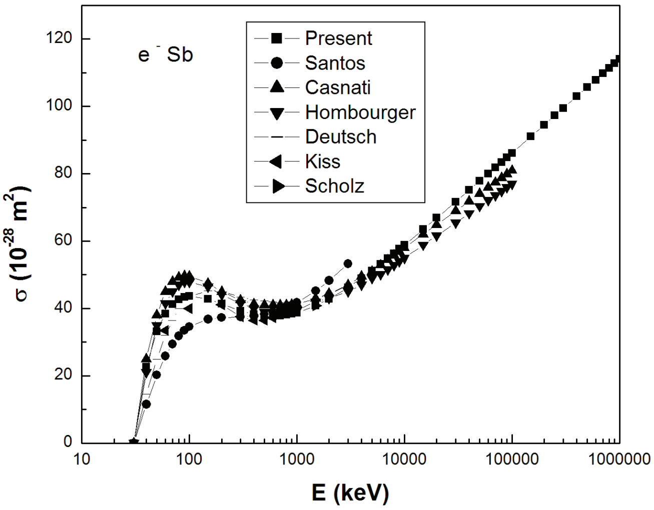

Figure 8: This figure showing the comparison of the present electron impact ionization cross section to experimental data for Sb. ■, the present work; •, theoretical data by Santos *et al.* [13]; ▲, theoretical data by Casnati *et al.* [10]; ▼, theoretical data by Hombourger [8]; —, theoretical data by Deutsch *et al.* [3]; ◄, experimental data by Kiss *et al.* [41]; ►, experimental data by Scholz *et al.* [38].

ison with experimental data by Hoffmann *et al.* [27] and Ishii *et al.* [28]. Theoretical results of Hombourger [8] and Casnati *et al.* [10] lie above the calculated value at peak. However their cross sections are lower than the present values at high energies.

In Fig. 10, we have compared the data of Gold atom for K-shell. There are seven experimental data, named Davis *et al.* [24], Rester and Dance [23], Berkner *et al.* [26], Middleman *et al.* [25] Hoffmann *et al.* [27], Ishii *et al.* [28] and Seif *et al.* [43]. The present cross sections are in good agreement with those are measured by Rester and Dance [23], Hoffmann *et al.* [27], Ishii *et al.* [28]and Middleman *et al.* [25] within 12%. The experimental data measured by Seif *et al.* [43] are slightly higher than the present cross sections. The present cross-sections also agree with the experimental data of Davis *et al.* [24]. Present cross section is in well agreement with theoretical result by Scofield [7], while slightly differ from the theoretical values of Hombourger [8] and Casnati *et al.* [10]

The K-shell ionization cross sections for Bi have been shown In Fig. 11. The obtained results are in contrast with measured values of Hoffmann *et al.* [27], Ishii *et al.* [28] and Scholz *et al.* [38], while data by Middleman *et al.* [25] is slightly higher than the calculated values. Theoretical results of Hombourger [8] and Casnati *et al.* [10] do not agree with experimental data of Hoffmann *et al.* [27], Ishii *et al.* [28] and Middleman *et al.* [25] at high energies.

Fig. 12 shows the present total cross sections for uranium atom. Present calculations show a better agreement with the experimental data of Ishii *et al.* [28] and previous theoretical values of Scofield [7]. Again theoretical results of Hombourger [8] and Casnati *et al.* [10] do

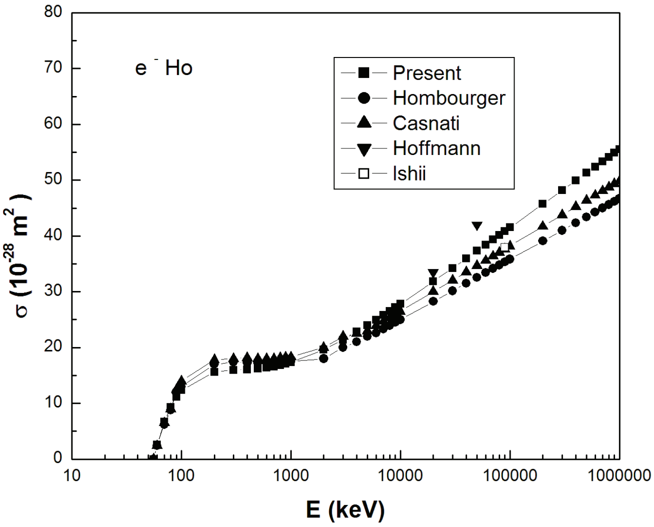

Figure 9: This figure showing the comparison of the present electron impact ionization cross section to experimental data for Ho. ■, the present work; •, theoretical data by Hombourger [8]; ▲, theoretical data by Casnati *et al.* [10]; ▼, experimental data by Hoffmann *et al.* [27]; □, experimental data by Ishii *et al.* [28].

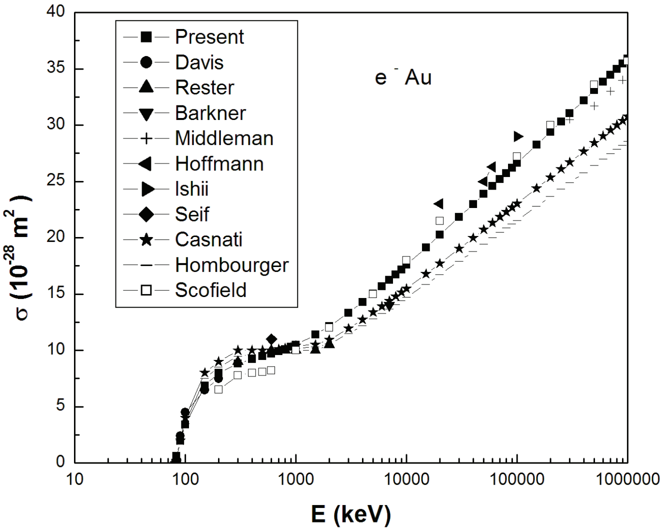

Figure 10: This figure showing the comparison of the present electron impact ionization cross section to experimental data for gold atom (Au). ■, the present work; •, experimental data by Davis *et al.* [24]; ▲, experimental data by Rester *et al.* [23]; ▼, experimental data by Barkner *et al.* [26]; + experimental data by Middleman *et al.* [25]; ◄, experimental data by Hoffmann *et al.* [27]; ►, experimental data by Ishii *et al.* [28]; ♦, experimental data by Seif *et al.* [43]; *, theoretical data by Casnati *et al.* [10]; —, theoretical data by Hombourger [8]; □, theoretical data by Scofield *et al.* [7].

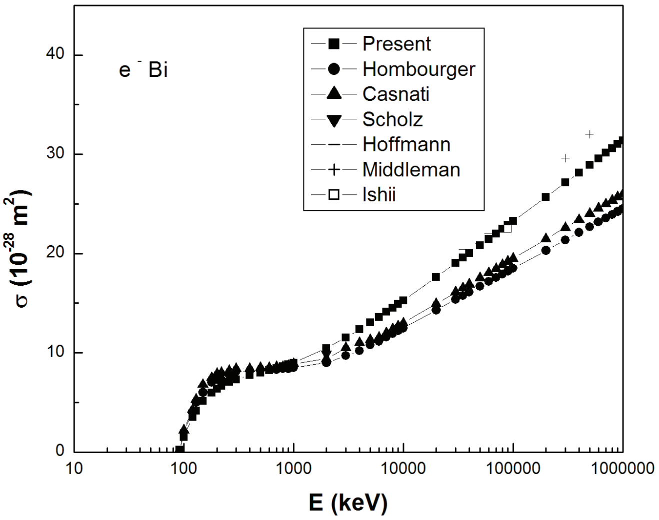

Figure 11: This figure showing the comparison of the present electron impact ionization cross section to experimental data for Bi. ■, the present work; •, theoretical data by Hombourger [8]; ▲, theoretical data by Casnati *et al.* [10]; ▼, experimental data by Scholz *et al.* [38]; —, experimental data by Hoffmann *et al.* [27]; +, experimental data by Middleman *et al.* [25]; □, experimental data by Ishii *et al.* [28].

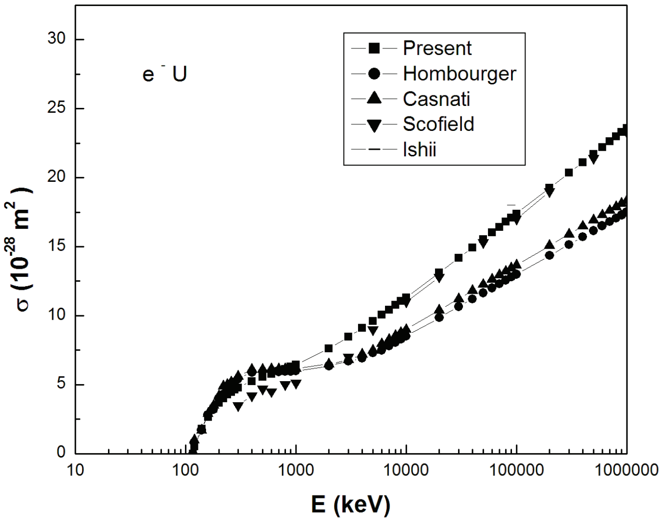

Figure 12: This figure showing the comparison of the present electron impact ionization cross section to experimental data for uranium atom (U). ■, the present work; •, theoretical data by Hombourger [8]; ▲, theoretical data by Casnati *et al.* [10]; ▼, theoretical data by Scofield [7]; —, experimental data by Ishii *et al.* [28].

not agree with experimental data.

4 Conclusion

The proposed model, an extension of the Khare *et al.* [1] model for the electron impact ionization of molecules, are examined for K-shell ionization on 12 atomic targets in the range $Z = 6-92$ up to ultrarelativstic incident energies. The present study investigates an almost complete picture of electron impact ionization cross section for these atoms at low and high energy range. The calculated cross sections are compared with the available experimental and theoretical data. We conclude that a slight modification in Khare *et al.* [1] model have considerably improved the agreement between the experimental and theoretical data. Present method has been successfully tested for a number of molecular targets [45–47]. The modified formulae have great versatility of obtaining electron impact cross sections for a great variety of molecules and atoms. The application of the present model is to extend the calculations to other targets and to inner atomic shells is in progress.

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