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THE TRANS FORMATIVE FUTURE OF ELECTRON IMPACT IONIZATION STUDIES FOR ZINC ATOM

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Abstract:

This study decisively investigates the ionisation cross-section of the zinc atom resulting from electron impact. Utilizing a semi-empirical approach, we analyze the ionisation process across a comprehensive energy value from the threshold up to 5120 eV, employing electron impact mass spectrometry. Our computational calculations yield a robust graph that clearly illustrates the strong correlation between energy and the cross section. Furthermore, we systematically examined the fragmented ions of the zinc atom such as $\mathrm{Zn}^{+}, \mathrm{Zn}^{++}, \mathrm{Zn}^{+++}, \mathrm{Zn}^{++++}, \mathrm{Zn}^{+++++}$and accurately calculated their total ionization cross section (TICS). Our TICS results align closely with the previous findings of Jaspreet Kaur and Dhanoj Gupta et al (1993), demonstrating a significant degree of agreement. This research underscores the importance of fundamental processes that have far-reaching applications in plasma physics, material science, and astrophysics**.**

Keywords: Electron Impact, Cross section, Ionisation, Zinc atom and Zinc fragments.

1. Introduction:

The interaction of atoms with electrons forms the foundation for significant advancements across various fields, including atmospheric science, plasma physics, and astrophysical sciences. Central to this interaction is a parameter known as Q_{ion}, which defines the probability of an atom being ionised upon colliding with an electron. In systems with more than two particles, the Schrodinger equation becomes impractical, necessitating the use of approximations in theoretical methods. The validity of these approximations can be effectively assessed by comparing them with established experimental results. Electron impact ionisation (EII) of atoms and molecules serves as a crucial method for delving into the complexities of many-body problems (Bhatt P, Kumar S 2021).

EII stands out as a fundamental process in modern atomic physics due to its intricate nature. The complexity of electron-atom scattering during ionisation stems from various factors, including coupling effects, target polarisation, and resonances. Recent breakthroughs have shed light on many-electron correlations in the bound states of atoms and molecules. Typically, theoretical calculations of electron-ionisation cross sections for atoms and molecules rely on approximation methods that are both physically realistic and numerically manageable (Younger, S.M. 1985).

Positively charged ions play a critical role in stimulating plasma polymerisation (Economou, D.J 2017), significantly affecting combustion rates (Prager, J. et al 2007 ,Chen B. et al.2019), and are vital in plasma etching (Donnelly, V.M. et al 2013). To develop effective plasma models, it is essential to comprehend electron ionisation as a result of both total and partial ionisation processes (Carbone E.et al. 2021,Mohr, S. et al.2021, Hagelaar, G.J.M. et al 2005). The modified binary encounter Bethe model allows for the determination of ionisation cross sections through electron impact for both complex and simple systems (Kim, Y.K.; Rudd, M.E. 1994, Sharawat ritu et al. 2022, Akhilesh Vanketesh and Francis Robicheaux2020, Rui QIU et al. 2023, A. Y. Elizarov and I. I. Tupitsyn 2007, P.G. Burke, A.J. Taylor 1965) . Various approaches, such as the R-matrix with pseudo states (Pindzola M and Robicheaux F 2000), convergent close-coupling (Fursa D and Bray I 2008) , and time-dependent close-coupling (Colgan J et al 2001), are utilized to compute cross sections for different elements. The exterior complex scaling (ECS) approach employed by Baertschy et al. (2001) effectively addresses the three-body problem beyond significant approximations.

Recent studies have focused on K-shell ionisation cross sections for zinc, conducted by Wu Y. et al.(2010) and Tang Chang-huan et al. (1999), while Xie L. et al. (2020) explored electron impact excitation of zinc. Additional research, including work by Rogers et al.(1982) and Gopaljee et al. (1993), has contributed to the understanding of EII, while electron impact excitation in zinc-like atoms was examined by Tapasi Das et al. (2012), and the integral cross section by Robert McEachran et al.(2020), M.S. Pindzola et al. (1991) investigated electron impact excitation, and significant insights into total ionisation cross sections (TICS) for zinc were presented by Jaspreet Kaur and Dhanoj Gupta et al (2015), alongside direct excitation cross sections studied by S. Inaba et al.(1986) Photoionisation of zinc was also addressed by M. Stener and P. Decleva(1997).

It is important to note that while Kaur and Gupta conducted their research from threshold to 1000 eV, our investigation extends to ionisation cross sections (ICS) for zinc fragmented ions with TICS from threshold to 5120 eV, a previously unexplored area as shown in table 1. Our results, derived from the semi-empirical modified Jain and Khare model, show significant validity at both low and high energies. The agreement observed at low energy highlights an aspect that has not been previously studied, and our findings at high energy stand out since even Kaur and Gupta did not venture into this range.

2. Research Methodology:

The modified Jain Khare model's ionisation cross-section is provided by

$$\sigma_C = \sigma_{CBB} + \sigma_{CMB} + \sigma_t$$

What is known as the Bethe Cross Section σ_{CPB} is

$\sigma_{CBB} = \frac{ST_r^2}{(t+j)}\int_{I_r}^{E_r}\frac{1}{\xi^3}\ln\left(\frac{\xi}{P}\right)\, d\xi$

Because of traverse interaction Mott cross section σ_{CMB} is termed as

$$\sigma_{CMB} = \frac{S}{(t+j)} \times \left[\left(1 - \frac{2}{t+1} + \frac{t-1}{2t^2}\right) + \left(\frac{5-t^2}{2(t+1)^2} - \frac{1}{t(t+1)} - \frac{t+1}{t^2}\ln\left(\frac{t+1}{2}\right)\right)\right]$$

While transverse interaction (σ_t) cross section is given as

$$\sigma_t = \frac{ST_r^2}{NR(t+j)}K^2(\ln(1-\lambda^2)+\lambda^2)$$

Here, S and t is stated as

$$t = \frac{E_r}{T}, \qquad S = \frac{4\pi R^2 N a_0^2}{T^2}$$

Where, v and c are the incidence and light velocity ratios, λ is the result and R is Rydberg energy and K^2 is total dipole matrix squared for ionization, which is termed as

$$K^2 = \int_{I_{nl}}^{\phi_{max}} \frac{Rdf(\phi,0)}{\phi d\phi}\, d\phi$$

Relativistic energy E_r of incident electron moving with velocity v and having rest mass m

$$E_r = \frac{1}{2}mv^2 = \frac{1}{2}mc^2\left(1 - \frac{1}{\left(1+\frac{E}{mc^2}\right)}\right)$$

$$T = \frac{1}{2}mv^2 = \frac{1}{2}mc^2\left(1 - \frac{1}{\left(1+\frac{I}{mc^2}\right)}\right)$$

T is the electron's kinetic energy moves at speed v and I is binding energy of atom.

And, relationship between Bethe collision parameter (b_{nl}) and K^2 is termed as

$$b_{nl} = \frac{TK^2}{Z_{nl}R}$$

The atom's nl subshell's electron counts is denoted by Z_{nl}. Taking $Z_{nl} = N$ and putting the value of $K^2$from expression (5) in expression (4),

$$\sigma_t = -\frac{Sb_l}{(t+j)}(\ln(1-\lambda^2)+\lambda^2)$$

With Continuum Optical Oscillator Strength (COOS) ${}^{df}/_{d\phi} = N\,{}^{I}/_{\varphi^2}$, value of Bethe collision parameter (b_{nl}) is equal to 0.5 for all atoms as it does not depend on atomic number. So, present approximate form of COOS is not Known.

$$b_{nl} = \alpha a^{-\gamma}$$

$$P = 0.5mc^2\left(\left(E_r(E_r-\xi)\right)^{1/2} - \left((E_r-\xi)(E_r-\xi+2mc^2)\right)^{1/2}\right)^2$$

$$P = \frac{\xi^2}{4}\left(\frac{1}{2}mc^2 + \frac{1}{E_r}\right)$$

$$\sigma_{CBB} = \left(\frac{S}{t+j}\right) \times \left(0.4431\left(1-\frac{1}{t^2}\right) - 0.5\ln\left(\frac{1}{t}+\frac{T_r}{2mc^2}\right) + \frac{1}{2t^2}\ln\left(1+\frac{E_r}{2mc^2}\right)\right)$$

3. Result and Discussion:

In present paper, impact ionization of Zinc atom was studied by impact of electron in the energy range from threshold to 5120 eV. And results were observed for Zinc atom fragmented ions like $Zn^{+}, Zn^{++}, Zn^{+++}, Zn^{++++}$, Zn^{+++++} and its TICS was also studied.

Table 1: TICS values for Zinc by impact of electron

Electron energy ICS (10^{-16} cm^2) (eV) fragmented ions

eV	Zn+	Zn++	Zn+++	Zn++++	Zn+++++	TIC
13	0.009902					0.009902
14	0.039556	0.05385	0.018638	0.000899		0.112943
15	0.124481	0.170348	0.104503	0.068408	0.053928	0.522068
50	2.11181	2.07318	1.9889	1.93983	1.90781	10.02153
60	2.16362	2.12556	2.0533	2.01174	1.97708	10.3313
65	2.1668	2.129	2.06165	2.02314	1.98897	10.36956
70	2.15971	2.12366	2.06067	2.02484	1.99029	10.35917
100	2.0928	2.00041	1.95547	1.93066	1.90089	9.81671

500	0.912083	0.907171	0.900203	0.89704	0.891783	4.568176
1000	0.559522	0.557458	0.554507	0.553315	0.55119	2.775992
1500	0.411536	0.410271	0.408455	0.407782	0.406512	2.044556
2000	0.32865	0.327739	0.326444	0.325971	0.32506	1.633864
2500	0.275144	0.274451	0.273433	0.273081	0.272384	1.368493
3000	0.237505	0.236941	0.236114	0.235832	0.235281	1.181673
3500	0.209497	0.209025	0.208327	0.208103	0.20766	1.042612
4000	0.187763	0.187358	0.186764	0.186574	0.186183	0.934642
4500	0.170377	0.170017	0.16951	0.169363	0.169008	0.848275
5000	0.15613	0.155819	0.155355	0.155219	0.154901	0.777424
5100	0.153579	0.153274	0.152833	0.152697	0.152403	0.764786
5120	0.153079	0.152776	0.152337	0.152202	0.151908	0.762302

Figure 1 clearly demonstrates the ICS value about the energy value from threshold up to 5120 eV, showcasing a peak value of 2.1668 at 65 eV. Notably, all other fragmented ions also exhibit higher peak values at approximately the same energy level.

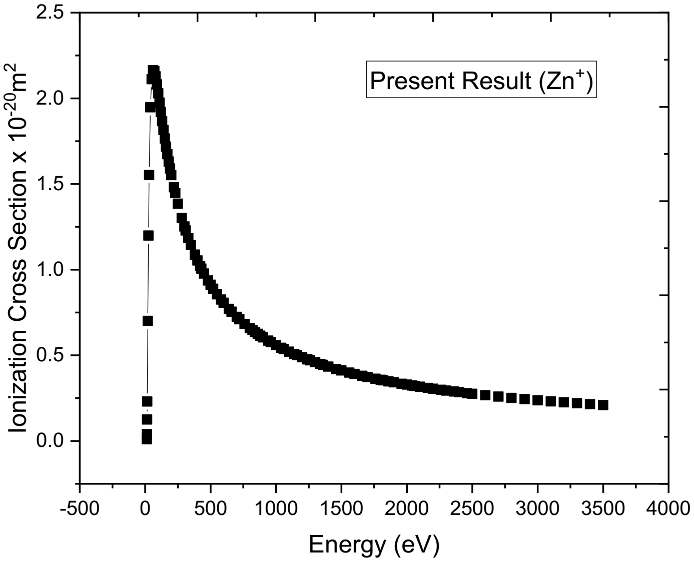

Figure 1

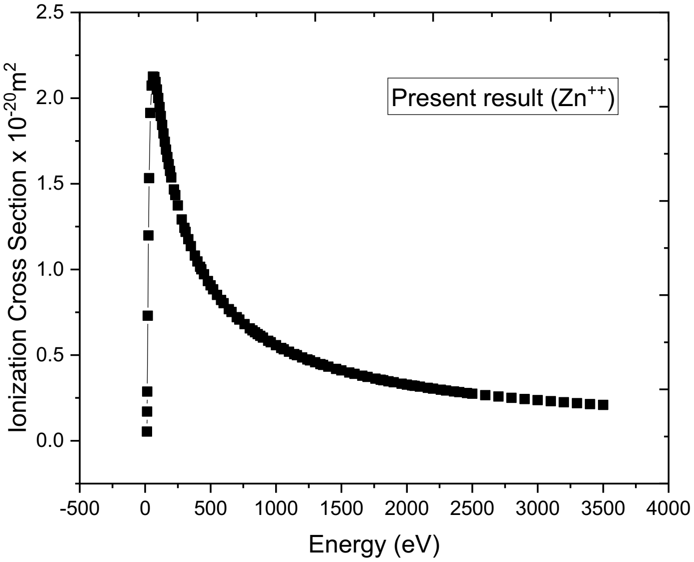

Figure 2

Figures 2 and 3 prominently illustrate the cross-section by EII value for Zn^{2+} and Zn^{3+} ions across the energy range from threshold to 5120 eV. Both ions exhibit peak cross-section values of 2.129 and 2.06165, respectively, achieved at the same energy level demonstrated by Zn^{+}.

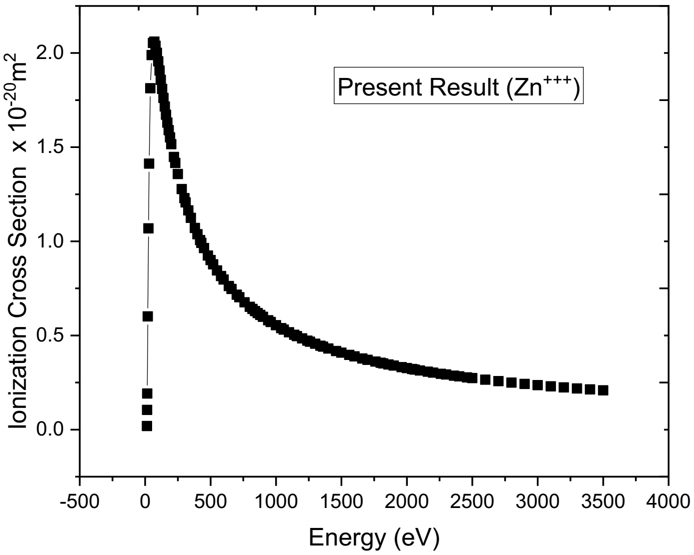

Figure 3

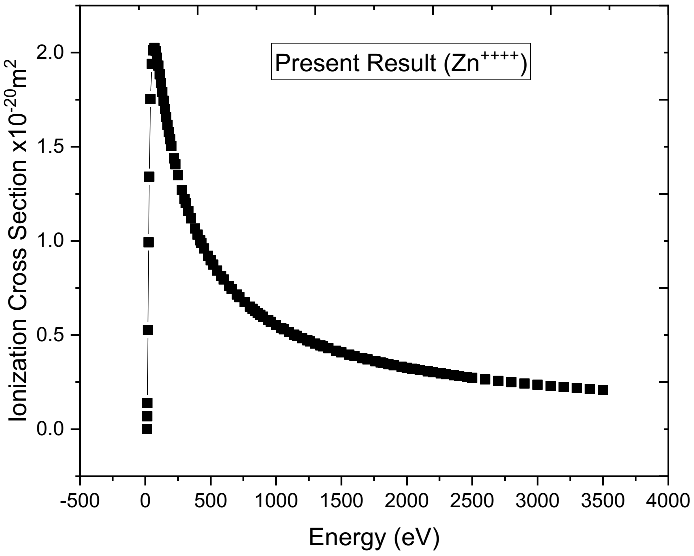

Figure 4

Fig 4th and 5th illustrate the cross-section by EII for Zn^{++++} *and* Zn^{+++++} ions across the energy value from threshold to 5120 eV. Both ions reveal impressive peak cross section values of 2.02484 and 1.99029 respectively at 70 eV.

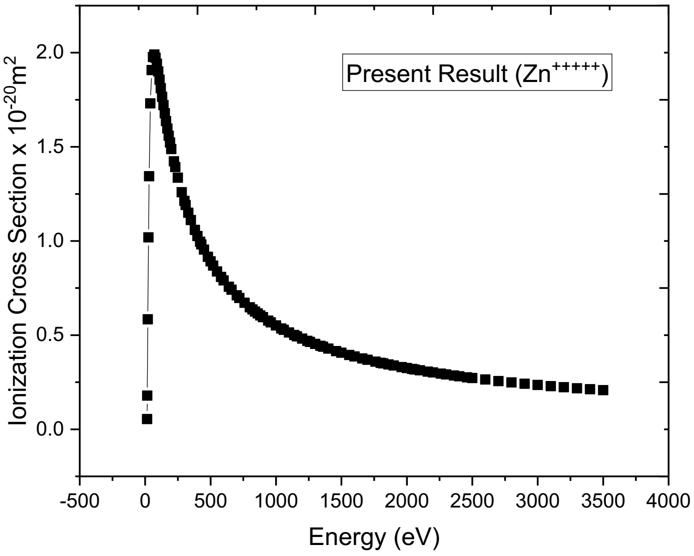

Figure 5

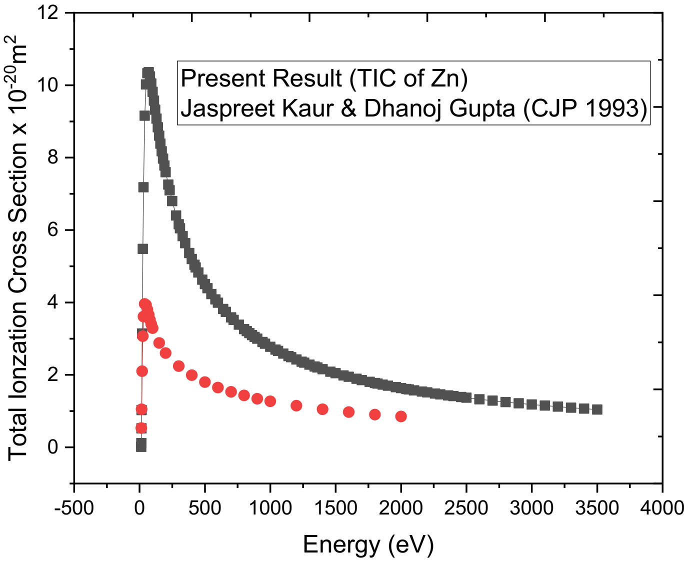

Figure 6

Fig. 6 gives the TICS value for the zinc atom and its fragmented ions. It also displays the cross-section's maximum value 10.36956 at 65 eV. And our results are compared with the previous results of Jaspreet Kaur and Dhanoj Gupta et al (2015) whose shows peak value of cross section is 3.96 at 40 eV. But our result shows higher peak value and it possibly shows the value at every point of energy but other result shows values at some points not on the every point of given energy range.

1) Conclusion:

Among the three theories—Modified Khare, Bethe, and Mott cross section—the Modified version of Jain and Khare provides the most accurate cross-section values for zinc atoms in EII. Our theoretical calculations employ a Semi-Empirical approach based on the modified Jain and Khare model. In this paper, we analyse the TICS of the zinc atom due to EII, across an energy value from the threshold up to 5120 eV, comparing our findings with those from previous studies by Jaspreet Kaur and Dhanoj Gupta et al (2015). Notable agreement is observed between our results and theirs. While their study indicates a peak TICS value of 3.96 eV, our results show a peak at 10.36956 eV. Furthermore, our findings are consistent across nearly the entire range of electron energy, whereas the results from Jaspreet Kaur and Dhanoj Gupta et al (2015) are limited to a narrower energy range. Overall, our results demonstrate strong alignment with previous findings at both low and high electron energy levels.

2) Future Scope:

This study of total ionisation cross section opens up numerous avenues for future research in atomic physics and applied fields. Key directions include:

- Plasma modelling and diagnostics: The ionisation cross-section data for zinc is super important for getting a handle on zinc containing plasma's used in variety of fields like semiconductor manufacturing, lightning technologies, fusion energy and astrophysics.
- Material science: We are diving into electron impact processes in zinc based materials like Zinc Oxide, which is important for optoelectronics and spintronics.
- Atmospheric and environmental science:While it’s a bit less common, zinc can also show up in atmospheric aerosols and studying its electron impact processes might help us understand their chemistry better.
- Fundamental atomic data for database:Collecting high quality experimental and theoretical data to contribute to international atomic database helps support the wider scientific community.

By exploring these areas, future research can materially advance our understanding of EII of zinc and its applications across various scientific domains.

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