

Projectile charge effects on the differential cross sections for the ionization of molecular nitrogen by positrons and electrons

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3 **Projectile charge effects on the differential cross sections for the ionization of molecular**
4 **nitrogen by positron and electron**
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24 **Abstract**
25

26 Triply differential cross sections (TDCS) are reported for the positron and electron impact
27 ionization of molecular nitrogen at 250 eV projectile energy. The TDCSs have been calculated
28 in the distorted wave Born approximation formalism using the orientation averaged molecular
29 orbitals. The present attempt is helpful to analyze the recent measurements [Phys. Rev. A **93**,
30 032710 (2016)] and study the effect of projectile charge in the ionization of molecular target.
31 The TDCS trends are compared for the positron and electron impact ionization in terms of binary
32 and recoil intensities, binary lobe positions for different values of energy loss. The binary
33 emission of electron is enhanced for positron impact however the nearly same recoil emission is
34 observed for positron as well as electron impact. Significant discrepancies are observed from the
35 measurements in terms of relative binary intensity for positron and electron impact.
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I. Introduction

Ionization of atoms and molecules by electron impact has been studied since the initial experimental work [1] with a special emphasis on the study of triple differential cross section (TDCS), which provides important information about the collision dynamics. Later, the complete kinematics of the ionization process during and after the collision has been learnt through the powerful experimental techniques; Cold Target Recoil Ion Momentum Spectroscopy (COLTRIM) [2] and Recoil-ion Momentum Spectroscopy (RMS) [3]. Many of the experimental efforts have been for the atomic targets, mostly inert gases [4]. From last few years there has been growing interest to investigate the collision dynamics of molecular targets. The closely spaced energy levels of different molecular states and the orientation of the molecule make it difficult to measure the TDCS and it is also challenging for the theoretical models to describe the molecular ionization due to multi-center nature of the target wave functions. Despite of this, TDCS studies have been done for the molecular targets ranging from simple diatomic molecules to more complex molecules, few may be listed as H_2 [5-7], N_2 [8-13], O_2 [14], H_2O [15-17], CH_4 [18-20], $HCOOH$ [21]. Complex molecules of biological interest such as DNA analogues [22], pyrimidine [23], thymine [24] etc. have also been investigated. Distorted wave and time-dependent close coupling approaches have been used to calculate the cross sections for the molecular hydrogen target and both the approaches have been successful to describe the features of TDCS [5, 25-26]. Variants of distorted wave formalism have been applied for the electron impact ionization of various molecular targets (see [27] and references cited in) and mixed degree of agreement has been achieved with the measurements, most of the time good agreement in the binary lobe region with certain discrepancies in the recoil scattering description [9].

Recently ionization by antiparticle impact such as positrons has been studied experimentally as well as theoretically. Such type of studies are helpful to understand the similarities or differences between antiparticle-matter and particle-matter interactions and are also helpful to obtain certain information which cannot be obtained only by the study of electron impact processes [28-29]. Differential studies with positrons are desirable to understand the collision dynamics in comparison with projectiles such as electrons or protons of same energy as well as to probe the effect of projectile charge and mass on the collision dynamics. Due to technical problem of low signal intensities the measurements for positron impact differential cross sections

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3 have been less in comparison to the electron impact. To begin with single differential [30] and
4 double differential cross sections [31-32] have been reported for the positron impact ionization.
5 In few later attempts more single and double differential cross section results for the positron
6 impact single as well as double ionization were obtained [33-34]. Various theoretical efforts
7 have been made to study the positron impact ionization of atomic hydrogen [35-38]. Structures
8 in the triply and doubly differential ionization cross sections of atomic hydrogen have been
9 identified [35] and the cross sections have been found to depend on the description of three-body
10 system [35-36]. The ionization of atomic hydrogen by fast positrons has been studied in the
11 presence of laser field [37] and recently study based on two center approach to fully differential
12 positron impact ionization of hydrogen has been reported [38].

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14 First triple differential cross sections were measured for the positron impact ionization of argon
15 atoms in coincidence with both the outgoing particles moving in forward direction [39]. Results
16 of TDCS with wider range of emission angles have been reported for argon atoms [40-42].
17 Theoretical efforts based on the distorted wave formalism tried to analyze the differential cross
18 section trends of positron impact ionization for the measurements reported [43-44]. Recent
19 review details the progress and methods used in studying the inelastic interactions between
20 positrons and atoms [45].

21
22 In the last decade, there has been increased interest to investigate the positron impact collision
23 dynamics of molecular targets with emphasis on obtaining the information which are
24 inaccessible by the study of electron impact only. There have been few attempts to measure
25 positron impact fully differential cross sections for molecular targets. Triply differential study of
26 positron impact ionization of H_2 molecules have been reported for the forward emission of
27 scattered and ejected particles [46-47]. These efforts also verified the presence of broad peak in
28 the ejected electron spectrum attributed to the process referred as electron capture to the
29 continuum (ECC). Very recently de Lucio and DuBois [12] reported the triply differential cross
30 section measurements for the positron and electron impact ionization of nitrogen molecules at
31 250 eV projectile energy. Apart from the recent experimental study [12], no other study is
32 available for the positron and electron induced differential cross sections for N_2 molecules at
33 same kinematical conditions, however electron impact TDCSs have been measured for the nearly
34 same projectile energy [13]. Further to mention that, total cross sections have been calculated
35 for the positron [48] and electron impact [49] ionization of N_2 molecule in the distorted wave
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Born approximation (DWBA) approach and reasonable degree of agreement has been obtained with the measurements.

We report the triple differential cross section (TDCS) results for the positron and electron impact ionization of nitrogen molecule at 250 eV projectile energy. We analyze the recent measurements [12] reported to study the projectile charge effect in the ionization of molecular nitrogen, following which no theoretical results are available to compare, to the best of our knowledge. We also calculate and compare the electron impact TDCS for ionization of N₂ molecules for the kinematical conditions of earlier measurements [13] in the nearly same energy regime (incident energy ≈300 eV) as the recent measurements [12]. TDCSs have been calculated in the distorted wave Born approach using the orientation averaged molecular orbital approximation, the atomic units ($\hbar = e = m_e = 1$) have been used.

II. Theory

The positron and electron induced TDCS may be written in the following form:

$$\frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_1} = (2\pi)^4 \frac{k_1 k_2}{k_0} \sum_{av} |T(k_1, k_2, k_0)|^2 \quad (1)$$

A projectile with energy E_0 and momentum k_0 collides with the target molecule and produces scattered and ejected particles with energies E_1 , E_2 and momenta k_1 , k_2 respectively in the outgoing channel, which are observed in coincidence. The energy conservation $E_0 = E_1 + E_2 + IP$ is followed, where IP is ionization potential of the target orbital. The transition matrix element (T) may be expressed in terms of the direct and exchange scattering amplitudes as;

$$|T|^2 = |f_{dir}|^2 + |f_{ex}|^2 - \text{Re}(f_{dir}^* f_{ex}) \quad (2)$$

where

$$f_{dir} = \langle X_1(k_1, r_1) X_2(k_2, r_2) \left| -\frac{Z}{r_{12}} \right| \psi^{OA}(r_2) X_0(k_0, r_1) \rangle \quad (3)$$

$$f_{ex} = \langle X_1(k_1, r_2) X_2(k_2, r_1) \left| -\frac{Z}{r_{12}} \right| \psi^{OA}(r_2) X_2(k_0, r_1) \rangle \quad (4)$$

here $Z = \pm 1$ is the charge of projectile (“+” for positron and “-” for electron). The incident particle is described by the distorted wave $X_0(\mathbf{k}_0, \mathbf{r}_1)$ and $X_1(\mathbf{k}_1, \mathbf{r}_1)$; $X_2(\mathbf{k}_2, \mathbf{r}_2)$ are the distorted wave-functions used for the scattered and ejected particles respectively, the particles 1 and 2 are exchanged in the expression of exchange amplitude (eq. 4). $\psi^{\text{OA}}(\mathbf{r}_2)$ is the initial bound state wave function for the molecular target which is approximated as the orientation averaged molecular orbital for the orbitals of N_2 molecule. The molecular wave functions have been calculated using the density functional theory with B3LYP/TZ2P basis set [50].

The initial state distorting potential representing the interaction between projectile and target molecular electrons constitutes the contribution from molecular nuclei and a spherical symmetric potential obtained by averaging over all orientations using B3LYP basis sets. The molecular charge density for the neutral molecule is obtained by

$$\rho(\mathbf{r}, \mathbf{R}) = \sum_{k=1}^m n_k |\psi^{\text{OA}}(\mathbf{r}, \mathbf{R})|^2 \quad (5)$$

where ‘m’ is the number of orbitals in the molecule and ‘ n_k ’ is the occupation number of the orbital. The average radial charge density is obtained by averaging eq. (5) over all orientations;

$$\rho^{\text{av}}(\mathbf{r}) = \langle \rho(\mathbf{r}, \mathbf{R}) \rangle.$$

The spherically symmetric static distorting potential is then obtained using the average radial charge density

$$U_{\text{el}}(\mathbf{r}_1) = \left\langle \int \frac{\rho^{\text{av}}(\mathbf{r}) d\mathbf{r}}{|\mathbf{r}_1 - \mathbf{r}|} \right\rangle. \quad (6)$$

We also calculate the TDCS using Coulomb potential in place of spherically symmetric potential of Eq. (6) for the smallest ejected electron energy ($E_2 = 6$ eV) to see the differences in the trends of TDCS.

As described above, the initial state static distorting potential is the sum of electronic contribution and nuclear contribution, i.e. $U_{\text{static}} = U_{\text{el}} + U_{\text{nuc}}$. The nuclear contribution (U_{nuc}) is obtained by placing the nuclear charge on a spherical cell having radius equal to the distance of nucleus from center of mass. The final state distorted potential is generated in the similar way constituting the nuclear contribution and spherically symmetric potential generated in the field of molecular ion. In addition to the static distorting potential the exchange distorting potential of

Furness and McCarthy [51], corrected by Riley and Truhlar [52] has been used to generate the total distorting potential;

$$U_E(\mathbf{r}) = 0.5[E_0 - U_{\text{static}}(\mathbf{r}) - \{[E_0 - U_{\text{static}}(\mathbf{r})]^2 + 4\pi\rho(\mathbf{r})\}^{1/2}] \quad (7)$$

For the positron impact ionization there is no exchange amplitude f_{ex} and following choices have been made. The distorted waves for the incident $X_0(\mathbf{k}_0, \mathbf{r}_1)$ and scattered $X_1(\mathbf{k}_1, \mathbf{r}_1)$ positrons are generated in the static potential of the molecular target, the distorted waves for the ejected electron $X_2(\mathbf{k}_2, \mathbf{r}_2)$ is generated in the static exchange potential of the molecular ion.

In order to see the effect of screening the TDCSs have been calculated for the scattered particle in both the atomic potential and ionic potential, however the ejected electron is treated in the potential of residual ion in both cases. For the lowest ejected electron energy case ($E_2 = 6$ eV) the TDCSs have also been calculated by including correlation-polarization potential $V_{\text{CP}}(\mathbf{r})$ in the distorting potential. The correlation-polarization potential $V_{\text{CP}}(\mathbf{r})$ is given as follows;

$$\begin{aligned} V_{\text{CP}}(\mathbf{r}) &= V_{\text{SR}}^{\text{Corr}}(\mathbf{r}), \quad r \leq r_0 \\ &= -\frac{\alpha_d}{2r^4}, \quad r > r_0 \end{aligned} \quad (8)$$

where the fundamental form of the short range correlation and long range polarization potential has been approximated by means of local density functional theory [53, 54]. α_d is dipole polarizability of the target and $V_{\text{SR}}^{\text{Corr}}(\mathbf{r})$ is short range correlation potential [53]. The point r_0 is the intersection of the short range correlation and long range polarization potential, we have ensured the smooth matching of potentials at r_0 .

The Coulomb interaction between the two outgoing particles has been treated by the Ward-Macek approximation [55], which has been found to give good agreement with the experimental data at lower energies and also reduces the computational difficulty [56].

The Ward-Macek factor is given by

$$M_{\text{ee}} = N_{\text{ee}} \left| F_1(-i\lambda_3, 1, -2ik_3 r_{3\text{ave}}) \right|^2 \quad (9)$$

Where $N_{\text{ee}} = \frac{\gamma}{e^\gamma - 1}$ is the Gamow factor, $\gamma = -\frac{2\pi}{|\mathbf{k}_1 - \mathbf{k}_2|}$

$$\lambda_3 = -\frac{1}{|k_1 - k_2|} \text{ and } r_{3\text{ave}} = \frac{\pi^2}{16\varepsilon} \left(1 + \frac{0.627}{\pi} \sqrt{\varepsilon \ln \varepsilon} \right)^2. \quad (9)$$

ε is the total energy of the two exiting electrons. The sign of γ and λ_3 are changed for the PCI calculation of positron impact.

The DWBA formalism along with the orientation averaged molecular orbital approximation is capable to produce reliable TDCS results at the incident electron energy 250 eV used in the present study [11, 56]. The DWBA has been very successful at the higher energies [9], however the DWBA with PCI effects have been found successful at the intermediate energies also [56]. The DWBA is useful in describing the complex multicenter and multi-orientation problem of molecular ionization as it can be applied for any energy and any size molecule and effects such as PCI makes it suitable for the lower energies also [56]. The orientation averaged molecular orbital approximation used in the present investigation has been found to be successful for the symmetric molecular states (see [56] and references cited in) and is useful to give the first estimates for the positron impact ionization of molecular nitrogen, however the calculation with proper average over all orientations of molecular target using DWBA formalism is computationally challenging.

III. Results and Discussion

The triply differential cross section (TDCS) measurements for the positron impact ionization of nitrogen molecules have been reported for the first time [12]. The measurements of electron impact TDCSs are also reported for the same kinematical conditions and the trends of TDCSs obtained through the experimental study for positron and electron ionization of nitrogen molecules are compared in terms of relative binary and recoil peak intensities, relative positions of binary peaks. We report the results of TDCS for the positron and electron impact ionization of molecular nitrogen for the same kinematical conditions used in the recent measurements [12]. The TDCSs have been calculated in the distorted wave Born approach using the orientation averaged molecular orbital approximation for the ionization taking place from the $3\sigma_g$ orbital of N_2 .

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3 The TDCS results are presented at projectile energy 250 eV for different average ejected electron
4 energies at scattering angle 3^0 , through which the TDCS information is obtained for the
5 momentum transfer ranging from 0.27 to 0.44 a.u. The calculated TDCSs have been compared
6 with the corresponding measurements. The TDCS results are displayed for ejected electron
7 energy 12.4 eV in Figure 1. The solid curve in Fig 1(a) is plot for the positron impact ionization
8 and the solid curve in Fig. 1(b) is plot for the electron impact ionization, the scattered particle is
9 treated in ion potential in both cases. The dashed curves in both the frames are for the scattered
10 particles treated in atom potential. The solid red circles (Fig. 1a) and solid black circles (Fig. 1b)
11 are the experimental TDCS [12] for the positron and electron impact ionization respectively.
12 The measurements have been normalized to the positron TDCS (solid curve in Fig. 1a) in the
13 binary peak region for best visual fit while retaining relative normalization between electron and
14 positron impact. Binary and recoil regions are identified in the TDCS results, experimentally as
15 well as theoretically. The binary peak positions observed in the theoretical TDCS for the
16 positron as well as electron case are shifted towards lower values of ejected electron angle in
17 comparison to the measurements. It is observed that the binary electron emission is enhanced for
18 the positron impact ionization, which is similar as shown by the measurements. However, there
19 are discrepancies between theoretical results and measurements in the relative magnitude of
20 binary peak for positron and electron case. The recoil emission of electron is decreased for the
21 positron impact ionization in the calculations; in contrast to this the measurements have recoil
22 peak intensity slightly higher for positron impact case.

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38 The TDCS results calculated at ejected electron energies 6.0 eV and 24.7 eV are presented in
39 Figure 2. These calculations have been done at scattering angle 3^0 for momentum transfer 0.29
40 a.u. (Fig. 2a) and 0.42 a.u. (Fig. 2b). The calculated TDCS results have been compared with the
41 fits to the individual data obtained by [12] for best visual fit while retaining relative
42 normalization between electron and positron impact. At the small momentum transfer case (Fig.
43 2a) a large recoil peak is observed for both the positron and electron impact ionization in the
44 DWBA results, however still retaining the nature of trends; enhanced binary peak and smaller
45 recoil peak for the positron impact. The positron recoil peak in the calculated results is slightly
46 higher than electron impact at larger momentum transfer (Fig. 2b). The TDCS curves with and
47 without PCI are plotted for both the electron and positron impact case, the PCI has not been
48 found to change the trends of TDCS significantly with changes less than 1% (see the black solid
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3 and black dashed curves in Fig. 2a). For the higher momentum transfer (Fig. 2b) the recoil peaks
4 for the positron and electron impact ionization are of nearly same intensities, which are also
5 observed by the measurements. As observed previously there is certain discrepancy in the
6 theoretical results and measurements in terms of relative height of binary peaks for positron and
7 electron impact and also in terms of position of peaks.
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10 We have also calculated TDCS for the ionization of N_2 molecules using Coulomb potential in
11 place of the spherically symmetric potential of Eq. (6) and including correlation-polarization
12 potential in the distorting potential. We observe that using different forms of potentials do not
13 change the trends of TDCS significantly for both the electron as well as positron impact
14 ionization. The main discrepancy in the relative magnitude of binary peak for the electron and
15 positron impact still remains same. Changes in the magnitudes of TDCS are observed, the plots
16 including different forms of potentials are presented in Figure 3 for the lowest ejected electron
17 energy used in present study ($E_2 = 6$ eV). The three outer $3\sigma_g, 1\pi_u$ and $2\sigma_u$ valence orbitals of
18 nitrogen molecules have very near values of ionization potentials. We have calculated the TDCS
19 for the contribution from these individual orbitals at ejected electron energy 12.4 eV (Figures 4a,
20 4b) and 6.0 eV (Figures 4c, 4d). We observe that the major contribution to TDCS for both the
21 electron and positron impact is from $3\sigma_g$ orbital. The TDCS calculated for the $2\sigma_u$ orbital has
22 larger binary peak and smaller recoil peak however both the $3\sigma_g, 1\pi_u$ orbital TDCSs have
23 larger recoil and smaller binary peak ratio.
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38 The discrepancies in the binary peak positions and the intensities of binary and recoil lobes are
39 better visualized through the comparison shown in Figure 5, between the theoretical results and
40 the measurements. The direction of binary lobes for 250 eV positron and electron ionization of
41 molecular nitrogen are plotted as a function of momentum transfer in Figure 5(a). The
42 momentum transfer considered is ranging from 0.27 a.u. to 0.44 a.u. corresponding to various
43 energy loss cases considered in the measurements [12]. The blue solid triangles and red solid
44 circles are the experimental positions of binary lobes for electron impact and positron impact
45 respectively. The red solid line and blue dashed line are the binary positions observed by present
46 calculations for positron and electron impact respectively. The black dotted line is the binary
47 peak positions calculated according to the kinematic conditions. An addition of 10° angle has
48 been made in the theoretical binary peak positions for better comparison with measurements.
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3 The binary peak positions in the measurements are shifted towards higher values of ejected
4 electron angle in comparison to the directions predicted by theoretical results. The binary peak
5 in the measurements for electron impact is at higher ejected electron angle in comparison to
6 positron impact except few cases, however the present theoretical results show that the binary
7 lobe for positron impact is observed at higher ejected electron angles (solid red line in Fig. 5a).

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10 The experimental and theoretical values for the maximum binary and recoil intensities are also
11 compared as a function of momentum transfer in Figure 5(b). Both the experiments and
12 theoretical results show the increased binary emission of electron for positron impact ionization
13 (the solid red triangles and solid red line), however the theoretical relative intensity of binary
14 peak for electron impact is not as less as reported by the measurements (the blue solid line and
15 blue solid triangles). The measurements also show a higher recoil emission of electron for
16 positron impact ionization (hollow solid circles), the theoretical results show slightly higher
17 recoil peak intensity for electron impact for smaller momentum transfer (dashed red line).

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19 We have also calculated TDCS for the electron impact ionization taking place from the $3\sigma_g$
20 orbital of nitrogen molecule for the kinematical conditions of earlier measurements [13],
21 following which there are no other theoretical results available to compare to the best of our
22 knowledge. The DWBA results with OAMO are reported for the ejected electron energies 10 eV
23 (Figure 6a, 6b) and 18.4 eV (Figure 6c, 6d) and compared with the measurements [13]. The
24 measurements have been normalized to theoretical results for the best visual fit. The binary peak
25 for all the cases overestimate the experimental binary peak, however the binary to recoil peak
26 ratio improves at higher values of scattering angles. The experimental and theoretical peak
27 positions agree reasonably well except Fig. 6c.

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29 The differences in the trends of TDCS for the positron and electron impact ionization of nitrogen
30 molecules are attributed to mainly the exchange term in the Hamiltonian due to charge of
31 projectile. For the electron case there is exchange in the elastic scattering in the incident channel
32 and for the both the outgoing electrons also. The exchange amplitude is calculated and included
33 in the calculation of TDCS. For the case of positron impact there is no exchange amplitude and
34 the distorted waves for the positron are generated in the static potential of the nitrogen molecule,
35 however the distorted wave for the ejected electron is calculated in the static-exchange potential
36 of the molecular ion. The post collision interaction (PCI) is included using the WM factor for
37 both the electron and positron impact cases, the PCI is of opposite sign for positron case due to

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3 positron and electron in the outgoing channel. The role of PCI has not been found significant for
4 kinematics of the present calculations for both the electron as well as positron impact cases so
5 the exchange is the dominant effect responsible for the different trends of TDCS observed. The
6 TDCS curves including PCI and without PCI are plotted in Figure 2a for the smallest ejected
7 electron energy which show that the inclusion of PCI does not make significant change in the
8 trends of TDCS. We have calculated TDCS using atom potential as well as ion potential for the
9 scattered particle (Figure 1) as the scattered particle is faster than the ejected electron in the
10 kinematics used presently. Shift of the binary peak position towards higher ejected electron
11 angle and increase of magnitude is observed for the TDCS calculated in the ion potential for the
12 scattered particle.

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20 The description of fully differential cross section for electron impact ionization of molecular
21 target is still an open problem and there are many un-answered questions. The theoretical
22 formalism used till date are basically based on the variants of distorted waves approach using
23 orientation averaged methods to describe the molecular target states, only few non perturbative
24 attempts has been made for hydrogen molecule [25-26]. Present attempt is able to describe the
25 trends of TDCS for positron and electron impact ionization of nitrogen molecules up to some
26 extent with points of agreement and disagreement with the measurements. The prime
27 disagreement lies in the relative magnitude of binary peak for the electron impact and the peak
28 positions. Larger binary peaks are observed in the present calculations for the electron impact
29 ionization which disagree with the measurements [12, 13]. The OAMO method used in the
30 present study has been found to be successful for the molecules such as H_2 and N_2 [11, 55],
31 particularly at the smaller momentum transfer conditions below unity. The results obtained for
32 the kinematics of present study have large degree of disagreement as described above. We have
33 also calculated TDCS using Coulomb potential as well as addition of polarization potential in the
34 distorting potential however the trends of TDCS have not varied significantly. The TDCS have
35 also been calculated to see the contribution of TDCS from the ionization of other valence orbitals
36 of nitrogen molecules, however the relative binary peak intensity for positron and electron
37 impact is not observed as in the measurements [12]. The disagreement with the measurements
38 in terms of binary to recoil peak ratio may be due to second order effects, particularly at the
39 lower ejected electron energies. The other possible reason for large discrepancies may be the use
40 of orientation averaged molecular orbital. The proper average (PA) over orientation-dependent
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3 cross-sections may be the other option which has been recently found to give better agreement
4 with the measurements for H₂O molecules [57], however the computational cost of proper
5 average method is exceptionally high requiring more than thousand processors. Calculations in
6 the second order Born approximation may also be tested in future. In absence of any other
7 theoretical results for analysis of the measurements [12, 13] and the large uncertainty in the
8 measurements reported (authors of [12] already cautioned for comparison on absolute scale and
9 authors of [13] have mentioned uncertainties in the absolute scale), the present effort in the
10 OAMO may give the predictions of theoretical TDCSs and provoke further theoretical attempts
11 with other forms of approximation such as PA as well as considering the second order Born
12 term.
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22 **IV. Conclusions**

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25 In conclusion, present study gives insight of the positron and electron impact interactions with
26 the molecular nitrogen and the effect of the exchange term in the Hamiltonian due to the sign of
27 projectile on the collision dynamics. The trends of TDCS are extracted as a function of
28 momentum transfer through various energy loss values. The effect of reversal of the direction of
29 Coulomb field between the projectile and molecular target is studied through the relative
30 intensities of binary lobe for positron and electron impact and the directions of the binary lobes.
31 There are points of agreement and disagreement between the theoretical and experimental results
32 with large discrepancies. Both the theory and measurements show enhanced binary emission of
33 electron for positron impact ionization. Nearly same recoil intensities for positron and electron
34 impact are observed for the higher momentum transfer both in the theoretical and experimental
35 results. There are significant discrepancies in the relative magnitude of binary lobes for electron
36 impact case. The binary lobe positions obtained by the theoretical results are shifted towards
37 lower values of ejected electron angles in comparison to the experimental positions. TDCSs
38 have also been calculated with different forms of interaction potential and TDCS contributions
39 from other valence orbitals have also been investigated however the prime discrepancy of
40 overestimated binary peaks for electron impact is not resolved. Future efforts with second order
41 distorted wave Born approximation and proper average may be useful to further investigate the
42 trends of TDCS for the N₂ molecules in comparison with the available measurements.
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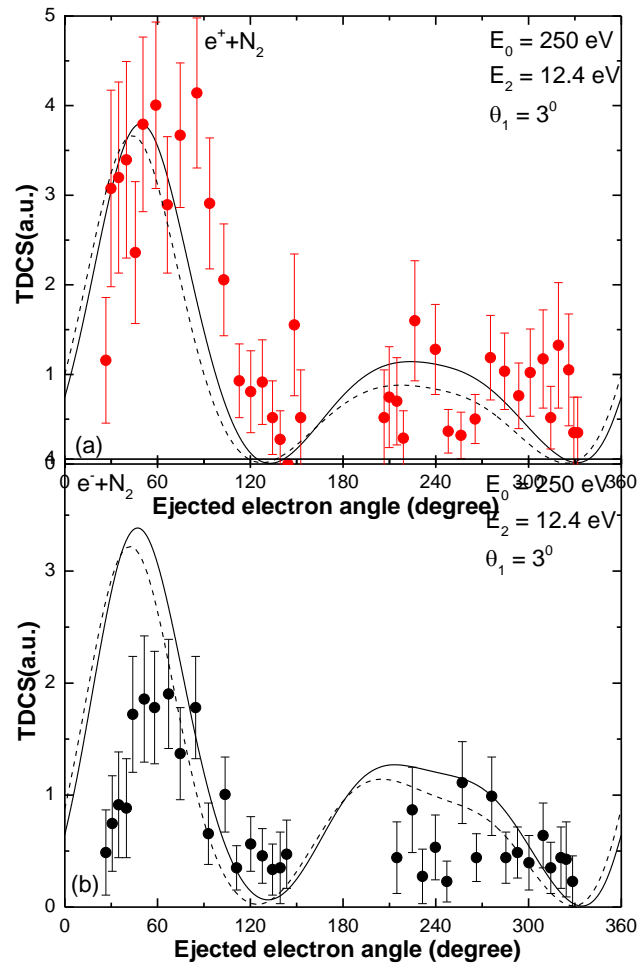
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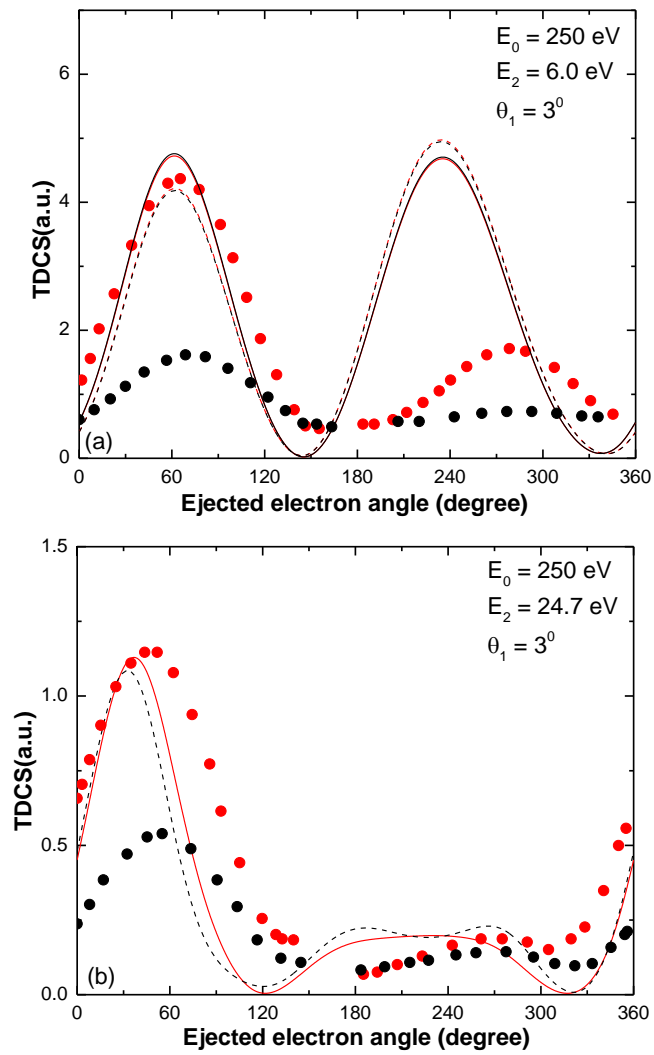
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16 Figure 1: TDCS plotted as a function of ejected electron angle for the ionization of N₂
17 molecule at projectile energy 250 eV, ejected electron energy 12.4 eV and
18 scattering angle 3⁰ (a) positron impact ionization, red solid circles: measurements
19 [12]; solid and dashed lines: DWBA results with scattered particle in ion and
20 atom potential respectively (b) electron impact ionization, black solid circles:
21 measurements [12]; solid and dashed lines: DWBA results with scattered particle
22 in ion and atom potential respectively. Measurements have been normalized to
23 positron curve for best visual fit while retaining relative normalization between
24 electron and positron impact.
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27 Figure 2: TDCS plotted as a function of ejected electron angle for the ionization of N₂
28 molecule at projectile energy 250 eV and scattering angle 3⁰ (a) ejected electron
29 energy 6.0 eV, black solid and red solid curves: DWBA results for positron with
30 and without PCI respectively; black dashed and red dashed curves: DWBA results
31 for electron with and without PCI respectively; red solid circles: fits to
32 measurements [12] for positron impact and black solid circles: fits to
33 measurements [12] for electron impact (b) ejected electron energy 24.7 eV, red
34 solid and black dashed curves: DWBA results for positron and electron impact
35 respectively, other legends are same as (a). Fits to measurements have been
36 normalized to positron curve for best visual fit while retaining relative
37 normalization between electron and positron impact.
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41 Figure 3: TDCS plotted as a function of ejected electron angle for the ionization of N₂
42 molecule at projectile energy 250 eV, ejected electron energy 6.0 eV and
43 scattering angle 3⁰; red solid and red dashed curves: DWBA results for positron
44 and electron impact in spherically symmetric averaged potential; black solid and
45 black dashed curves: DWBA results for positron and electron impact in Coulomb
46 potential; blue solid and blue dashed curves: DWBA results for positron and
47 electron impact in spherically symmetric averaged potential with inclusion of
48 polarization potential; red solid circles: fits to measurements [12] for positron
49 impact and black solid circles: fits to measurements [12] for electron impact. Fits
50 to measurements have been normalized to positron curve for best visual fit while
51 retaining relative normalization between electron and positron impact.
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3 Figure 4: TDCS plotted as a function of ejected electron angle for the ionization of N_2
4 molecule at projectile energy 250 eV from different orbitals; solid curve: $3\sigma_g$;
5 dashed curve: $1\pi_u$; dotted curve: $2\sigma_u$ (a, c) positron impact and (b, d) electron
6 impact; red solid circles: measurements (a) and fits to measurements (c) [12] for
7 positron impact; black solid circles: measurements (b) and fits to measurements
8 (d) [12] for electron impact. Measurements and fits to measurements have been
9 normalized to solid black curve for positron impact for best visual fit while
10 retaining relative normalization between electron and positron impact.
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16 Figure 5: (a) Binary lobe angles plotted as a function of momentum transfer, red solid line
17 and blue dashed line: present DWBA results with addition of 10^0 for positron and
18 electron impact respectively; black dotted line: results calculated from kinematics;
19 red solid circles: measurements [12] for positron impact and blue solid triangles:
20 measurements [12] for electron impact (b) binary and recoil intensities plotted as
21 a function of momentum transfer, red solid curve and red dashed curve:
22 theoretical binary and recoil intensities for positron impact; blue solid curve and
23 blue dashed curve: theoretical binary and recoil intensities for electron impact; red
24 solid triangles and red hollow triangles: experimental binary and recoil intensities
25 for positron impact [12]; blue solid triangles and blue hollow triangles:
26 experimental binary and recoil intensities for electron impact [12]. Measurements
27 for binary intensity have been normalized to the red solid curve for positron
28 impact for best visual fit and the other measurements have been plotted retaining
29 the relative normalization.
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33 Figure 6: TDCS plotted as a function of ejected electron angle for the electron impact
34 ionization of N_2 molecule. Solid curve: DWBA results with OAMO; black solid
35 circles: measurements [13]. Measurements have been normalized to solid curve
36 for best visual fit. Kinematics is displayed in each frame.
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**Figure 1**

**Figure 2**

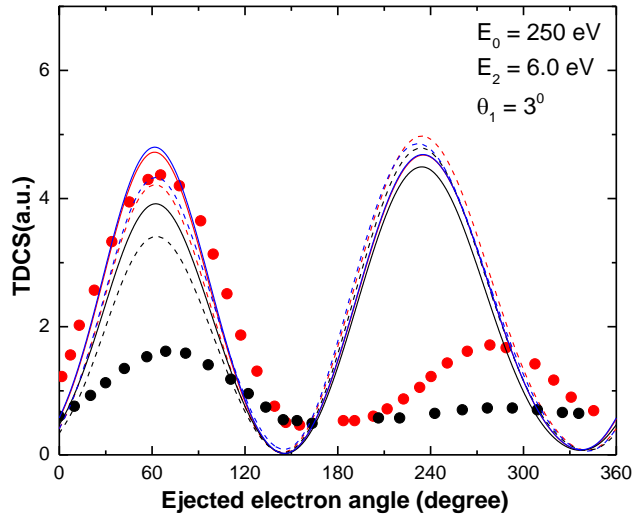


Figure 3

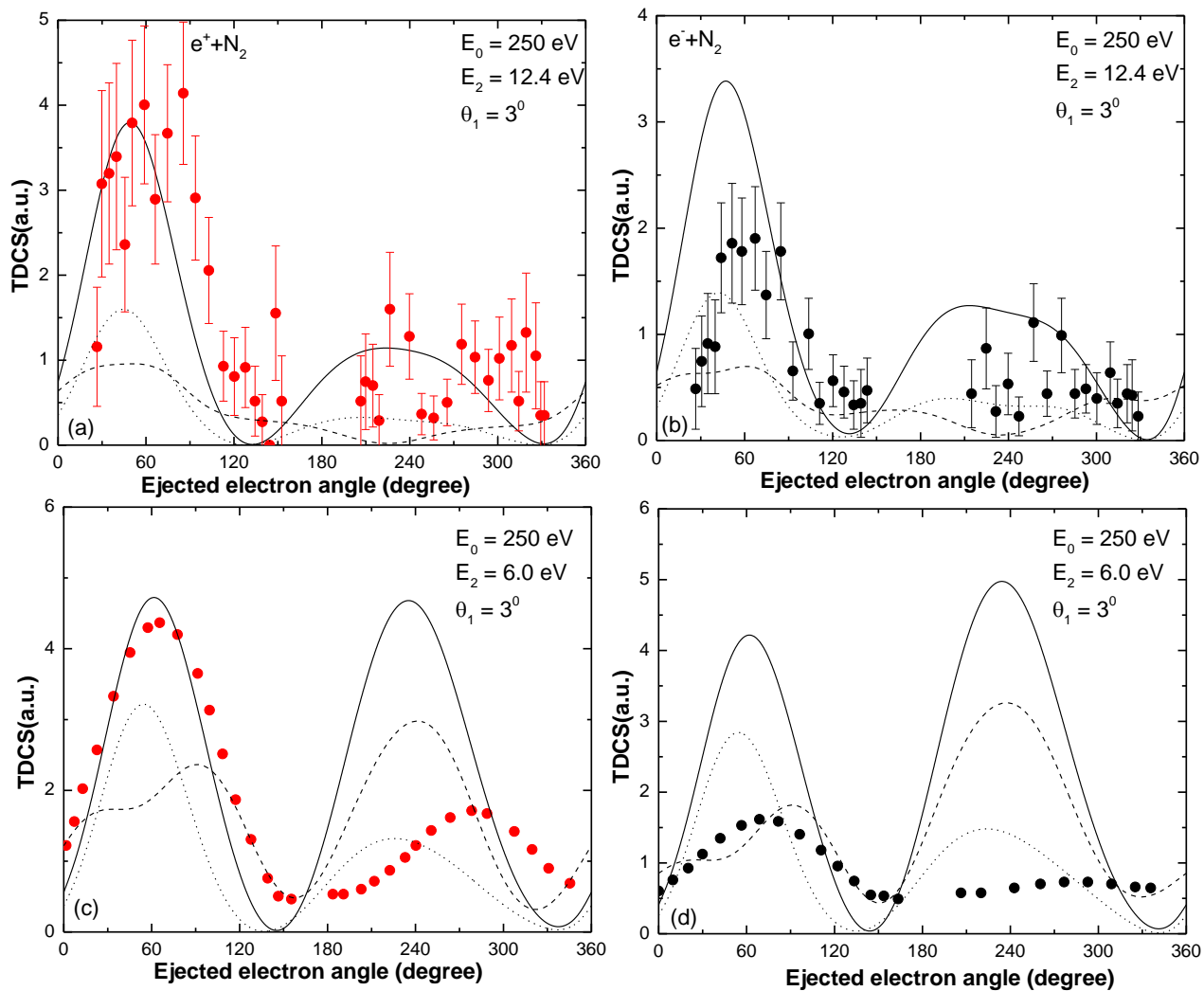


Figure 4

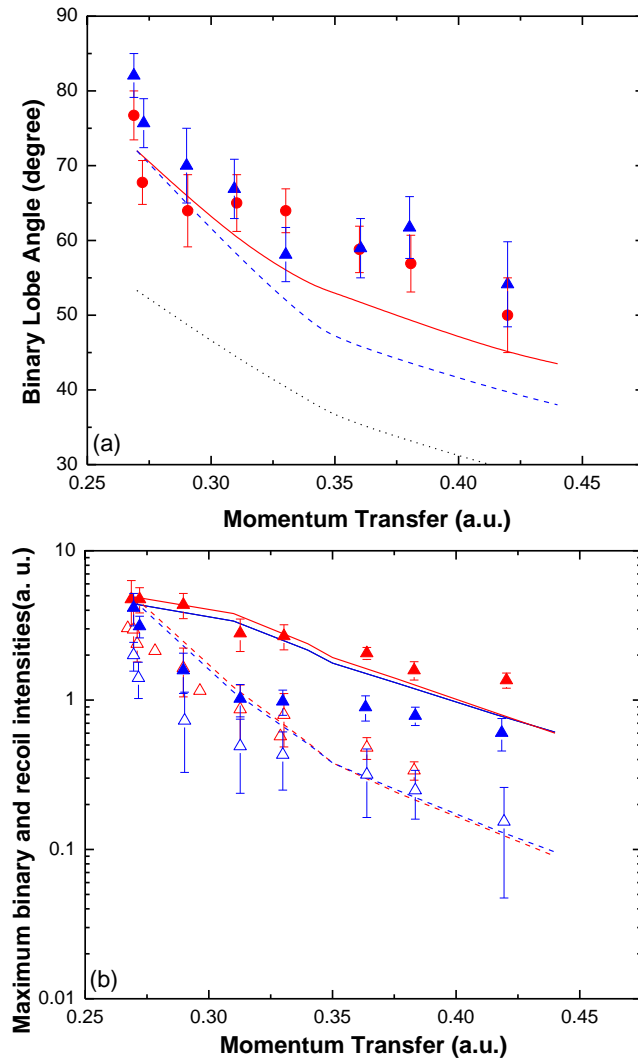
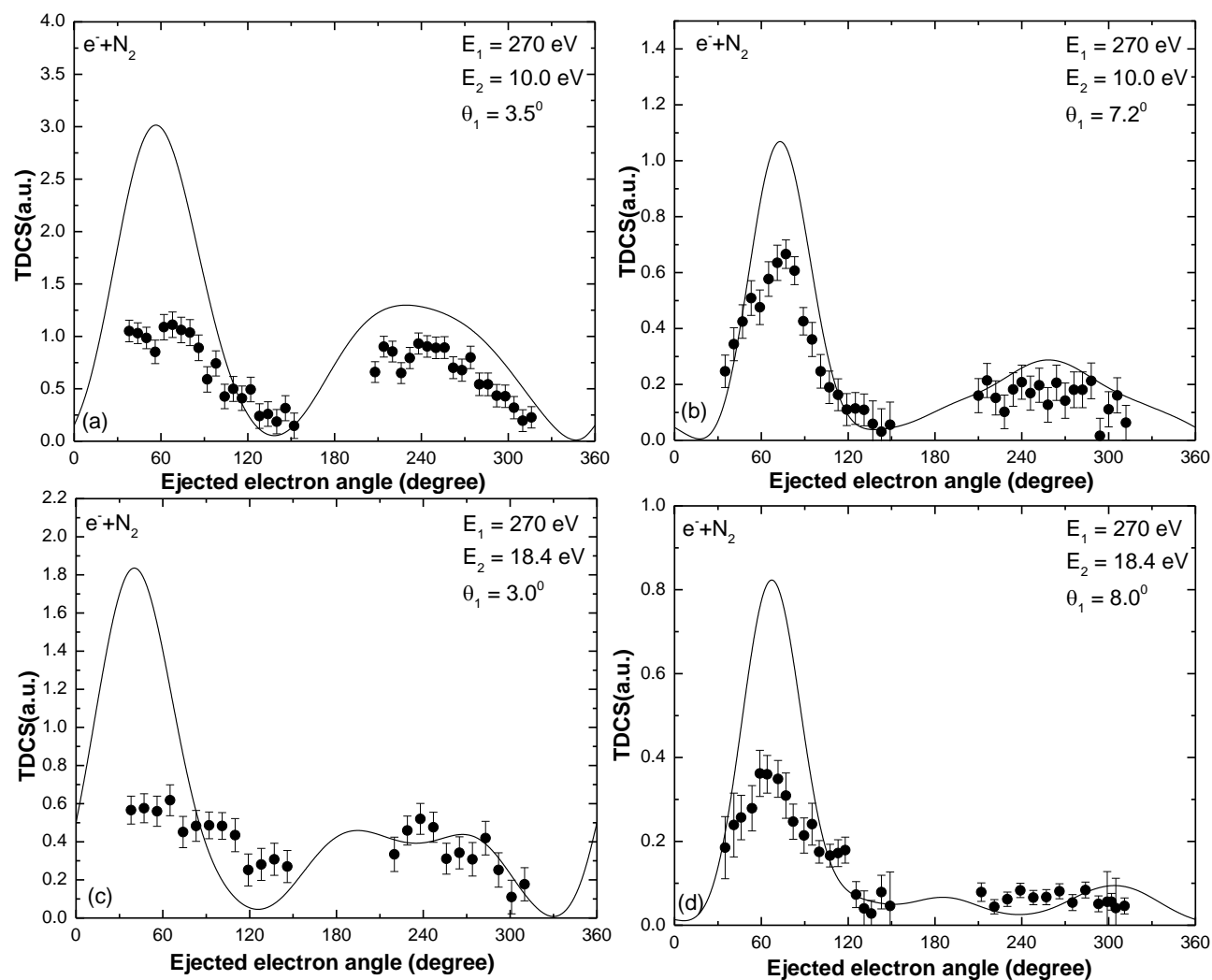


Figure 5

**Figure 6**