Probing collision dynamics of atoms, ions and molecules via electron impact ionization

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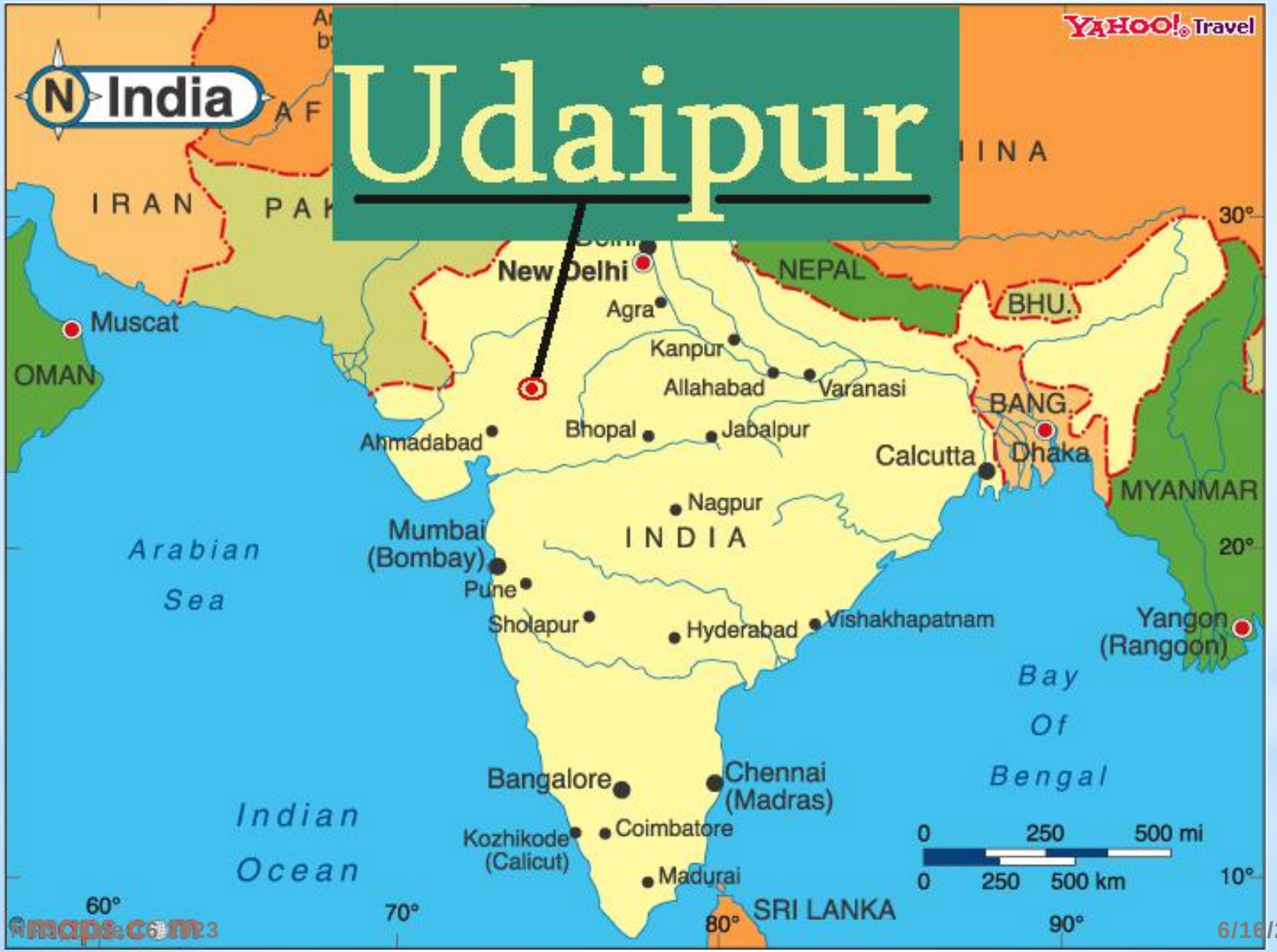
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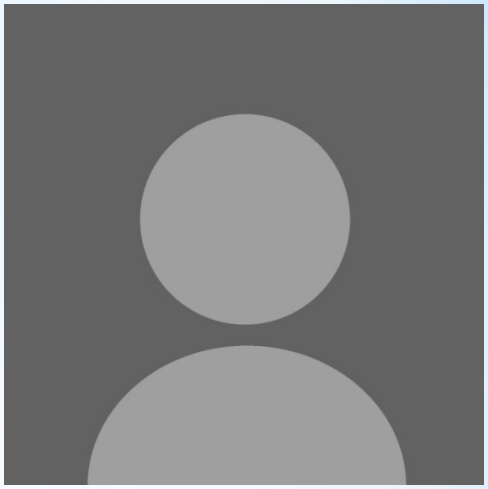

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D.K. Mani, IIT Delhi

- INTRODUCTION
- KINEMATICS and GEOMETRY – ionization process
- THEORY
- RESULTS

  TDCS for Ar, Xe, W, W+

  TICS for W, W+ and Be

  TDCS for N_2, H_2O and CO_2

- Conclusions
- Outlook

Introduction

Scattering – Important tool to know the structure of targets (Rutherford et al. (1909)).

Electron impact ionization – Important in many physical processes (The first theoretical paper on electron impact ionization of atoms - by Sir J. J. Thompson "**Ionization by moving electrified particles**".)

- everyday processes both natural and man made are driven by collision between charged particle and atoms /or molecules
- Atomic and subatomic micro world information
- Interaction of complex target with charged projectile
- Development of Quantum Mechanics
- Recent advancement in experimental technique.

Applications

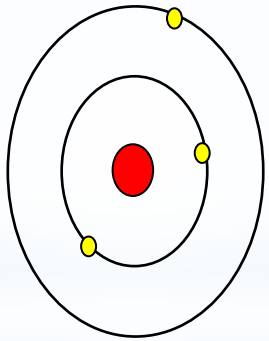
Few applications of a fundamental collision process;

* plasma physics - Fusion Plasma, Industrial Plasmas
* astrophysics
* atmospheric modeling - Stellar and Planetary Atmospheres
* discharge physics and radiobiology.

However, there are many more

What happens when target (atom, ion or molecule) is hit by a projectile?

Projectile



Scattering processes

There are basically following electron-atom scattering processes:

Elastic scattering : $A+B \rightarrow A+B$

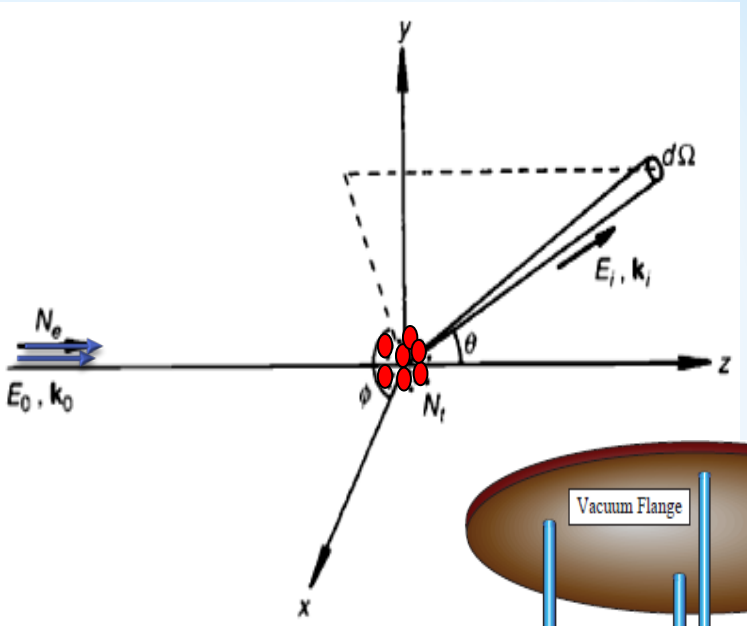
Inelastic scattering : $A+B \rightarrow A^{\#}+B$

Excitation processes : $A+B \rightarrow A^{*}+B$

Ionization processes : $A+B \rightarrow A+B^{+}$

Electron-Electron exchange:

$\mathbf{A^{+}+B \rightarrow A+B^{+}}$



Scattering cross sections

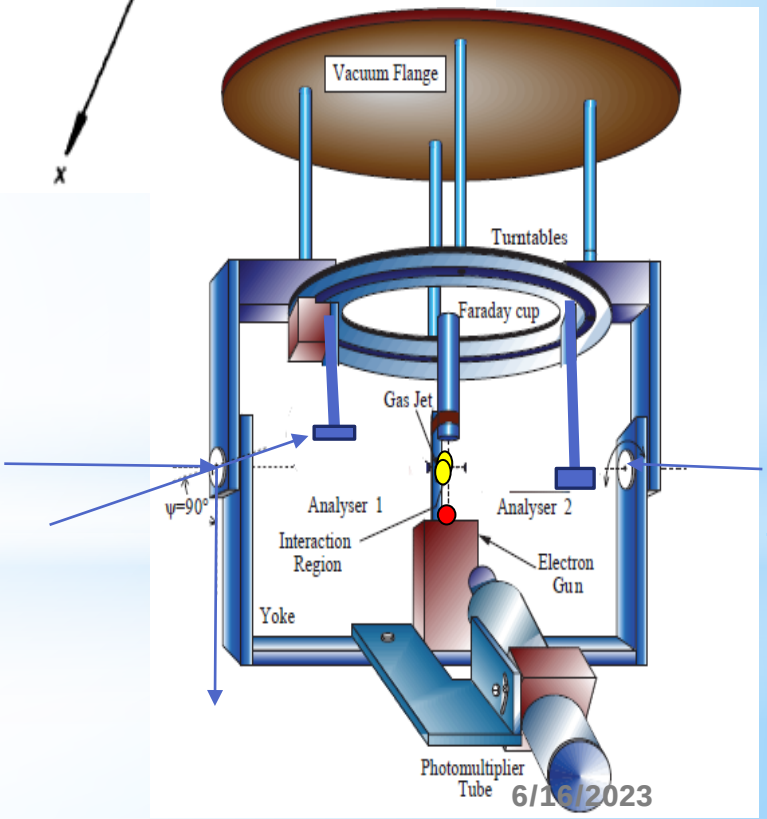
The collision which take place betv projectile and a target is conveniently described in terms of a cross section.

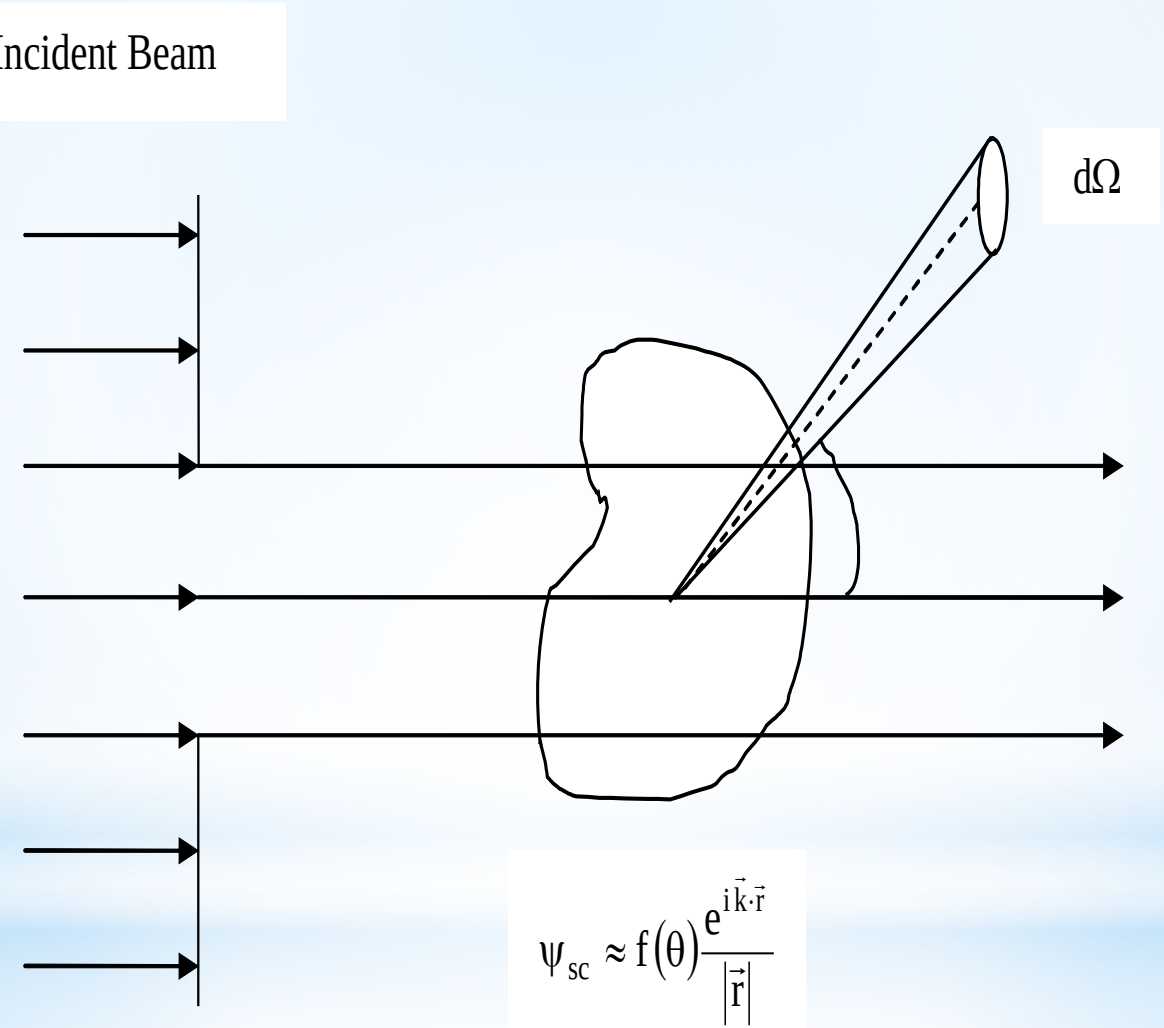
singly differential cross section (SDCS) $\sigma = \int \frac{d\sigma}{d\Omega} d\Omega$

double differential cross section (DDCS) $\sigma = \int \frac{d^2\sigma(\theta)}{d\Omega dE} dE d\Omega$

triple differential cross section (TDCS) $\frac{d^3\sigma}{d\Omega_1 \, d\Omega_2 \, dE_1}$

five- fold differential cross section $\frac{d^5\sigma}{d\Omega_1 d\Omega_2 d\Omega_s dE_1 dE_2}$



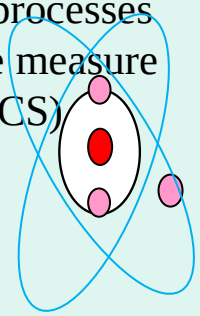


$$\psi_{sc} \approx f(\theta)\frac{e^{i\vec{k}\cdot\vec{r}}}{|\vec{r}|}$$

(e, 2e) Processes

Definition :- An electron impact single ionization, which is referred to as (e, 2e) processes. In order to gain information about the (e, 2e) ionization process, we measure the triple differential (TDCS) or fully differential cross section (FDCS).

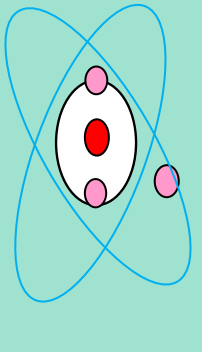
$$e^- + A \rightarrow A^+ + e^- + e^-$$



(e, 3e) Processes

Definition :- An electron impact double ionization, which is referred to as (e, 3e) processes. In order to gain information about the (e, 3e) ionization process, we measure the Five-fold differential cross section (FDCS) .

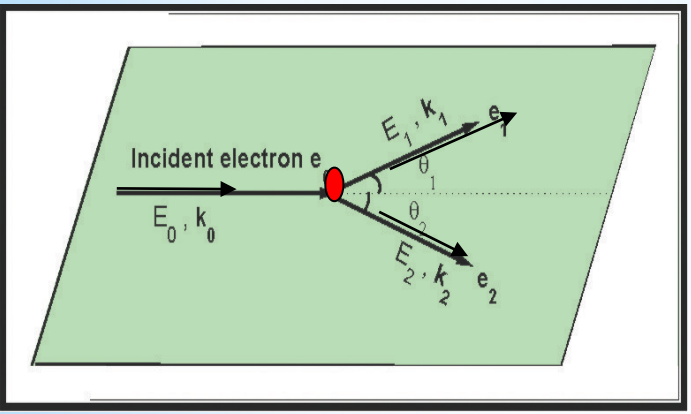
$$e^- + A \rightarrow A^{++} + e^- + e^- + e^-$$



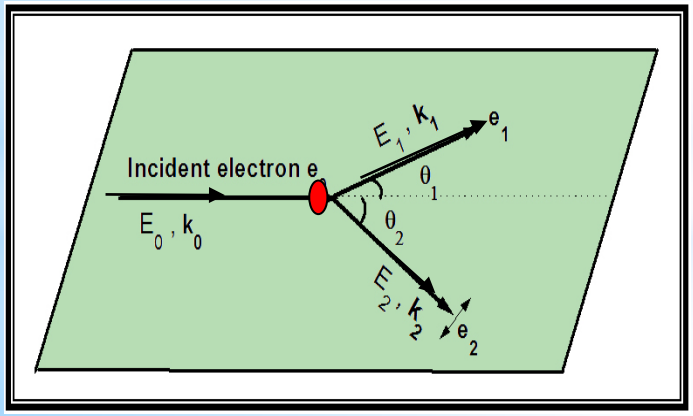
Motivation:- Theoretical modeling of few-body dynamics such as electron impact ionization is very challenging since the few-body problem is one of the most fundamental unsolved problems in physics.

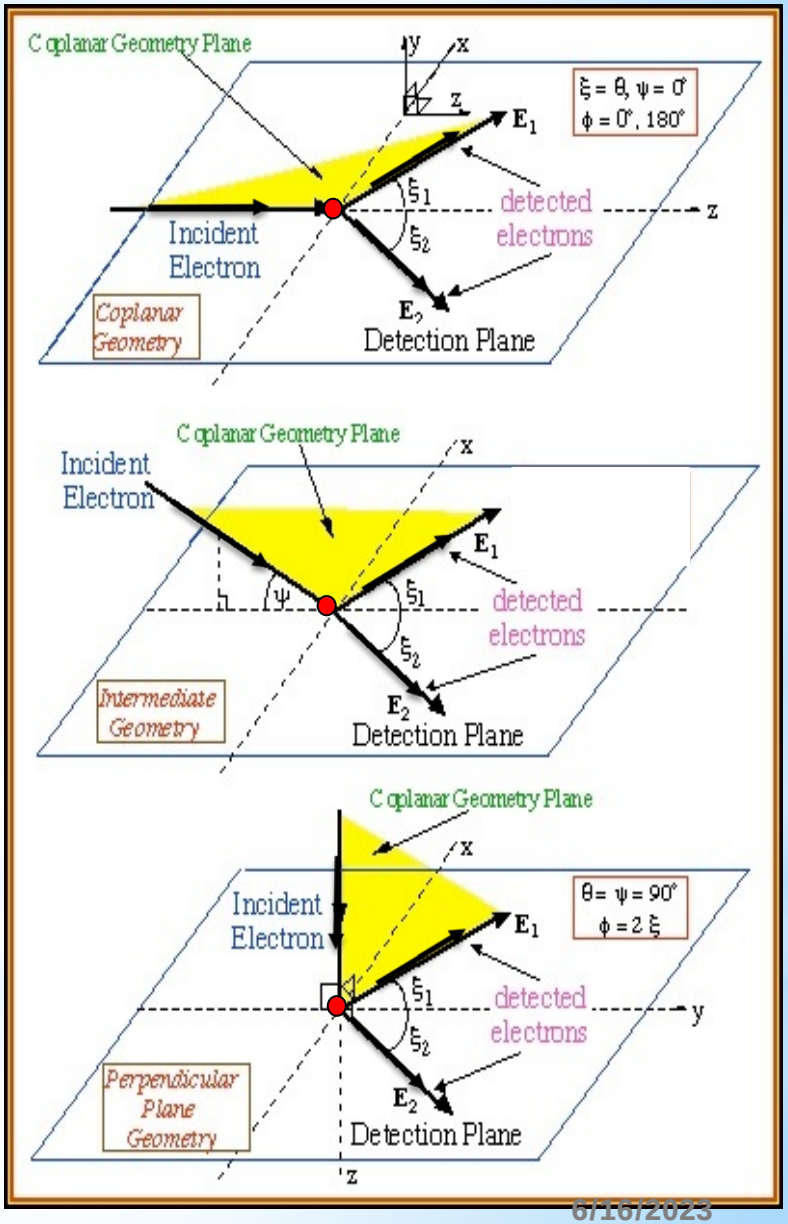
Kinematics

Coplanar symmetric kinematics :-

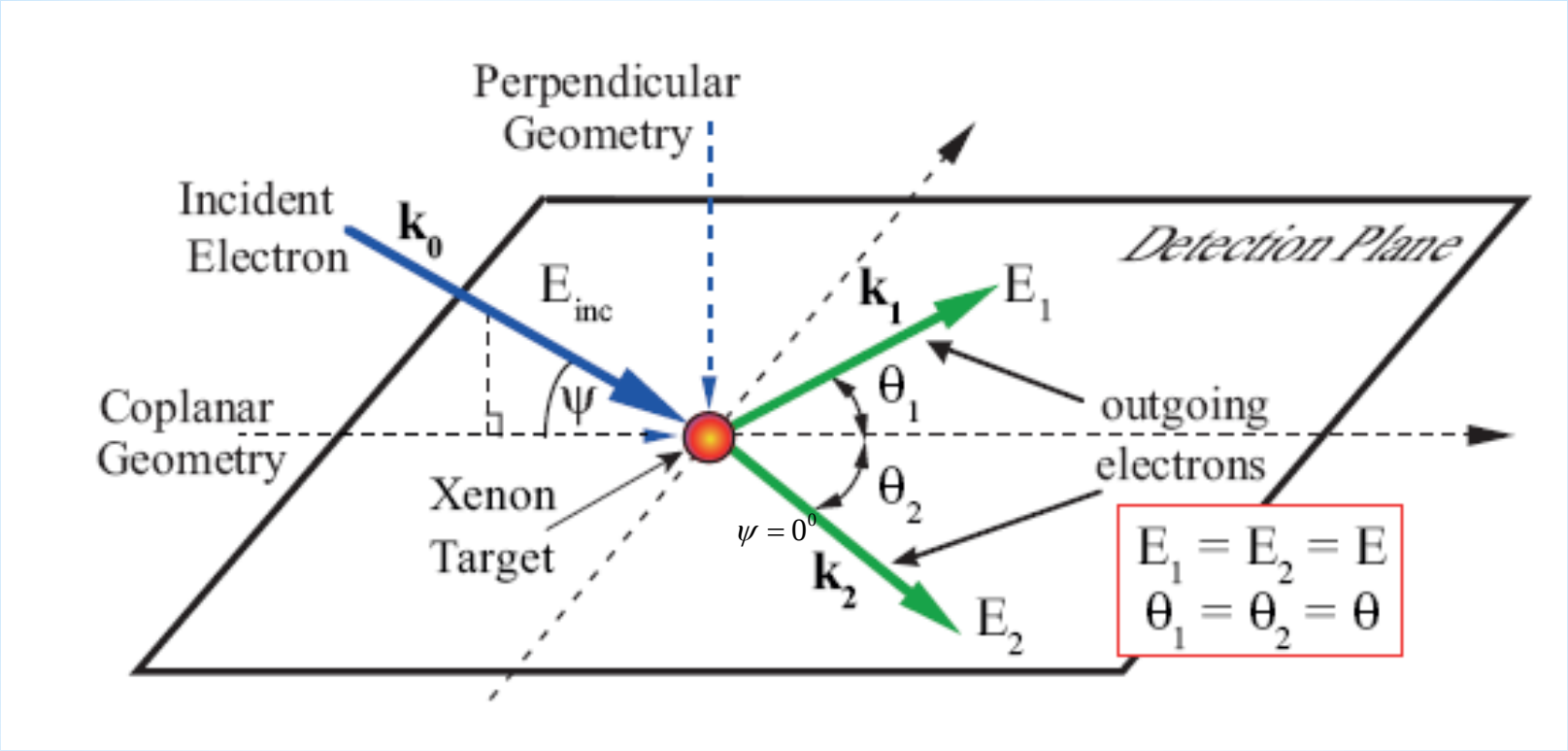


Coplanar asymmetric kinematics:-



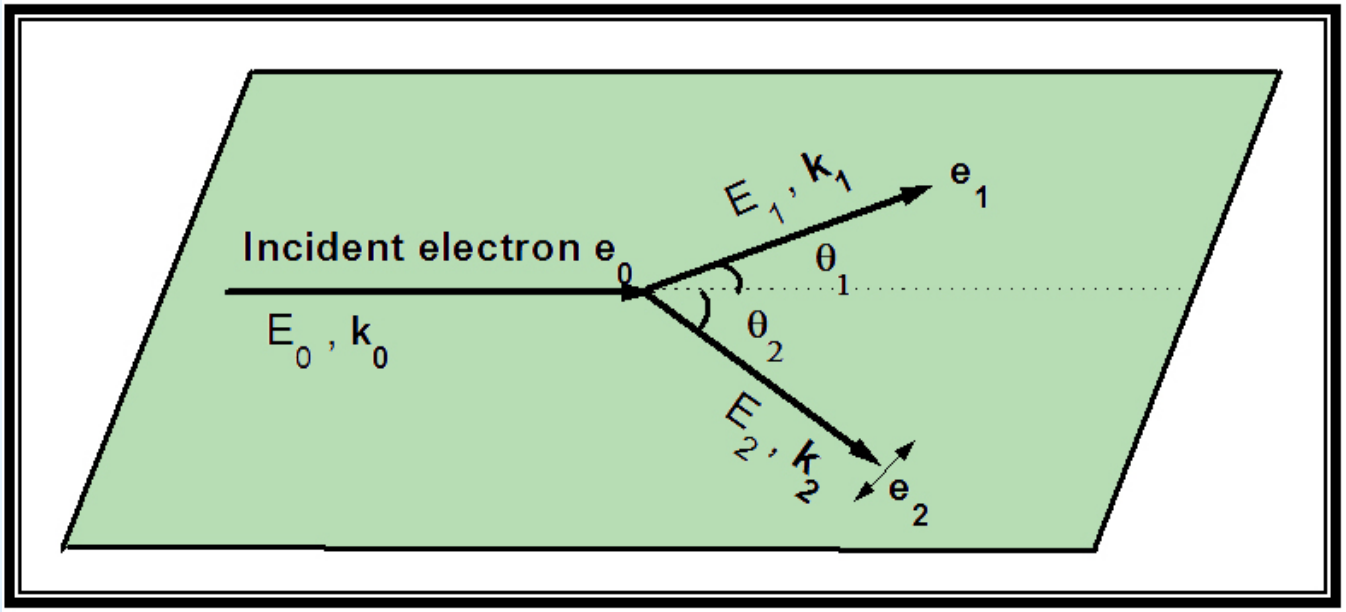


Patel et al. Phys. Rev. A **105, 032818 (2022)**



The incident electron momentum can be moved from being in the detection plane to being perpendicular to this plane

$$e^-(E_{0,}\,\boldsymbol{k_0}) + A \rightarrow A^+ + e^-(E_1, \boldsymbol{k_1}) + e^-(E_2, \boldsymbol{k_2})$$



(e, 2e) – Coincidence technique

Delivers most precise data for the study of ionization by electron impact

(e, 2e) measurements – **Differential cross sections** (DCS) which depends on all three momenta

In the electron impact single ionization process, an incident electron of linear momentum k_i and energy E_i ionizes the target (atom / ion) and the two emerging electrons are described by the linear momentum and energy (k_f, E_f) and (k_e, E_e), where the scattered (primary) electron is specified by subscript ‘f’ and the ejected (secondary) electron is specified by subscript ‘e’.

The energy conservation principle states;

$$E_i = E_f + E_e + E_b \qquad (1)$$

where E_b is the energy of the bound electron.

The momentum conservation equation is

$$k_i = k_e + k_f + k_r$$

Momentum transfer from incident electron to target is given by

$$K = \left| k_i - k_f \right|$$

The triple differential cross section (TDCS) for the electron impact single ionization, which is the probability of single ionization, is expressed in atomic units as

$$\frac{d^3\sigma}{d\Omega_f\, d\Omega_e\, dE_f} = (2\pi)^4 \frac{k_f k_e}{k_i} \sum_{av} \left| T(k_f, k_e, k_i) \right|^2 \qquad (2)$$

The expression in Eq. (2) includes a sum over final and average over initial magnetic and spin state degeneracy. The T matrix in Eq.(2), which is the subject of approximation, includes interaction between the incident and target electrons and the nucleus.

TDCS (eq. 2) for the ionization is written in terms of direct and exchange amplitude as

$$\frac{d^3\sigma}{d\Omega_f\, d\Omega_e\, dE_i} = (2\pi)^4 \frac{k_f k_e}{k_i} \sum_{m=-l}^{l} \left(|f|^2 + |g|^2 - \mathrm{Re}\left(f^* g \right) \right)$$

where

$$f = \left\langle \chi_f^{(-)}(k_f, r_f)\, \chi_e^{(-)}(k_e, r_e) \left| v_{fe} \right| \chi_i^{(+)}(k_i, r_f)\, \chi_b(r_e) \right\rangle$$

$$g = \left\langle \chi_f^{(-)}(k_f, r_e)\, \chi_e^{(-)}(k_e, r_f) \left| v_{fe} \right| \chi_i^{(+)}(k_i, r_f)\, \chi_b(r_e) \right\rangle$$

The second order Born term is given as

$$f_{B2} = \left\langle \chi_1^{(-)}(\boldsymbol{k_a}, \boldsymbol{r_a}) \chi_2^{(-)}(\boldsymbol{k_b}, \boldsymbol{r_b}) \middle| V G_0^+ V \middle| \psi_i \chi_0^{(+)}(\boldsymbol{k_i}, \boldsymbol{r_a}) \right\rangle$$

Where G_0^+ is Green's function having the form;

$$G_0^+ = \frac{1}{E_0 - H + i\varepsilon}$$

here H is the Hamiltonian of the target atom defined by

$$H = -\frac{\nabla^2}{2} \pm \left(\frac{z}{r_a} - \frac{1}{|\boldsymbol{r_a} - \boldsymbol{r_b}|} \right)$$

where the symbol $\pm$ is for the projectile charge, E_0 represents incident energy and $\varepsilon \to 0^+$.

* The initial-state distorted waves are generated in the equivalent local ground state potential of the atom.
* The final-state distorted waves and are obtained in the equivalent local ground state potential of the ion.
* Hartree-Fock orbitals for the bound target state
  * E. Clementi and C. Roetti, At. Data Nucl. Data Tab. 14, 177 (1974).
  * A. D. McLEAN and R. S. McLEAN, At. Data Nucl. Data Tab. **26**, 287 (1981).

$$\left|\chi^{(+)}(\boldsymbol{k_0},\boldsymbol{r_1})\right\rangle = \sqrt{\frac{2}{\pi}}\,\frac{1}{k_0\,r_1}\sum_{L,M} i^{L}\,e^{i\sigma_L}\,u_L(k_0,r_1)\,Y^{*}_{L,M}(\hat{k}_0)\,Y_{L,M}(\hat{r}_1)$$

$$\left\langle\chi_1^{(-)}(\boldsymbol{k_1},\boldsymbol{r_1})\right| = \sqrt{\frac{2}{\pi}}\,\frac{1}{k_1\,r_1}\sum_{L',M'} i^{-L'}\,e^{i\sigma_{L'}}\,u_{L'}(k_0,r_1)\,Y^{*}_{L',M'}(\hat{k}_1)\,Y_{L',M'}(\hat{r}_1)$$

$$\left\langle\chi_2^{(-)}(\boldsymbol{k_2},\boldsymbol{r_2})\right| = \sqrt{\frac{2}{\pi}}\,\frac{1}{k_2\,r_2}\sum_{L'',M''} i^{-L''}\,e^{i\sigma_{L''}}\,u_{L''}(k_2,r_2)\,Y^{*}_{L'',M''}(\hat{k}_2)\,Y_{L'',M''}(\hat{r}_2)$$

Modified spin-averaged static-exchange potential of Riley and Truhlar (1975)

$$V_E(r) = \frac{1}{2}\left[E + V_D(r) - \left\{ (E + V_D(r))^2 - 2\pi\rho(r)^2 \right\}^{\frac{1}{2}} \right]$$

The distorting potentials

$$V_D(r) = \sum_{nl} N_{nl} \int dr' \left[u_{nl}(r') \right]^2 / r_>$$

where $r_>$ is the greater of r and r' and N_{nl} is the number of electrons in each orbital nl. where $\rho(r)$ is the electron density.

Ref.:- Riley M. E. and Truhlar D. G., "Approximations for the exchange potential in electrons scattering," J. Chem. Phys. 63, 2182 (1975).

The TDCS expression including Post Collision Interaction (PCI)

$$\frac{d^3\sigma}{d\Omega_1\, d\Omega_2\, dE_1} = M_{ee}(2\pi)^4 \frac{k_1 k_2}{k_0} \sum_{m=-l}^{l} \left(|f_{nlm}|^2 + |g_{nlm}|^2 - \mathrm{Re}\left(f^*_{nlm}\, g_{nlm} \right) \right)$$

Correlation-polarization potential

N. T. Padial and D. W. Norcross, Phys. Rev. A 29, 1742 (1984).
J. P. Perdew and A. Zunger, Phy. Rev. B 23, 5048 (1981).

PCI

S. J. Ward and J. H. Macek, *Phys. Rev. A*49, 1049 (1994).

Positron impact ionization

- For the positron impact ionization there is no exchange amplitude
- The distorted waves for the incident and scattered positrons are generated in the static potential of the atom (target).
- The distorted waves for the ejected electron is generated in the static exchange potential of the ion.

Total Ionization Cross Section (TICS)

Using partial wave expansion and performing angular integrations the total ionization cross section is given by

$$\sigma(E_i) = \frac{16}{\pi E_i} \int_0^E dE_e \sum_{l_i, l_e, l_f} (2L+1) |F|^2$$

where l_i, l_f are electron orbital angular momentum quantum numbers in incident and final channels respectively, l_e is the ejected electron quantum number and L is the total orbital angular momentum. Energies obey the conservation defined

F is the ionization amplitude, can be written as

$$F = \sum_{\lambda} f_{\lambda}(l_b l_i l_e l_f L) \langle \chi_b \chi_i | V | \chi_e \chi_f \rangle_{\lambda}$$

Total Ionization Cross Section (TICS)

The total ionization cross sections have been calculated in two variants of distorted wave approximation (DWA) namely Cowan structure calculation and HULLAC code.

The Hartree-Fock target wave function and Hartree potential with semi-classical exchange and correlation correction has been used for the semi relativistic DWA calculations with Cowan formalism.

Ionization cross sections using Cowan formalism have been calculated in fine-structure and configuration mode.

We have also used Modified Khare and modified Kim BEB Methods to calculate the TICS

Ref.:

R. D. Cowan, The Theory of Atomic Structure and Spectra (Univ. of Cali. Press, Berkeley, 1981).

A. Bar-Shalom, M. Klapisch, and J. Oreg, J. Quant. Spec. Radiat. Transf. 71, 169 (2001).

M. E. Riley and D. G. Truhlar, J. Chem. Phys. **63**, 2182 (1975).

Why W

- **W** - the tungsten (W) and tungsten based materials have been recommended as one of the materials to be used as plasma facing components for the International Thermonuclear Experimental Reactor (ITER) [1] and the Demonstration Power Station (DEMO) as these materials have thermo-physical properties suitable for fusion application [2-4].

[1] G. Federici, Phys. Scr. **T124**, 1 (2006).

[2] S. Wurster et al., J. Nucl. Mater. **442**, S181 (2013).

[3] J. de Prado et al., Mater. Des. **112**, 117 (2016).

[4] J. W. Coenen et al., Phys. Scr. **T167**, 014002 (2016).

Why W

- Tungsten is already in use as plasma facing components in tokamaks such as JET [5] and ASDEX-Upgrade [6].
- In the fusion devices the tungsten and related materials may exhibit high melting temperature, strong resistance against sputtering and shorter penetration depth etc.

[5] M. Groth et al., Nucl. Fusion **53**, 093016 (2013).

[6] M. Mayer et al., Phys. Scr. **128**, 106 (2007).

Why Be

- **Be** - recommended as surface materials in ITER project
- Erosion of the Be walls will occur when it is in contact with the hot plasma containing hydrogen and its isotopes [7, 8].
- This leads to the formation of gas-phase Be in various charge states and of Be hydrides, i.e. BeH_2. The presence of these species in the fusion edge and diverter plasmas influences them due to electron collision processes
- There is not much cross section information available concerning Be and its hydrides up to now.

[7] R. Doerner, M.J. Baldwin, D. Buchenauer, G. De Temmerman, D. Nishijima, J. Nucl. Mater. **390**, 681 (2009)

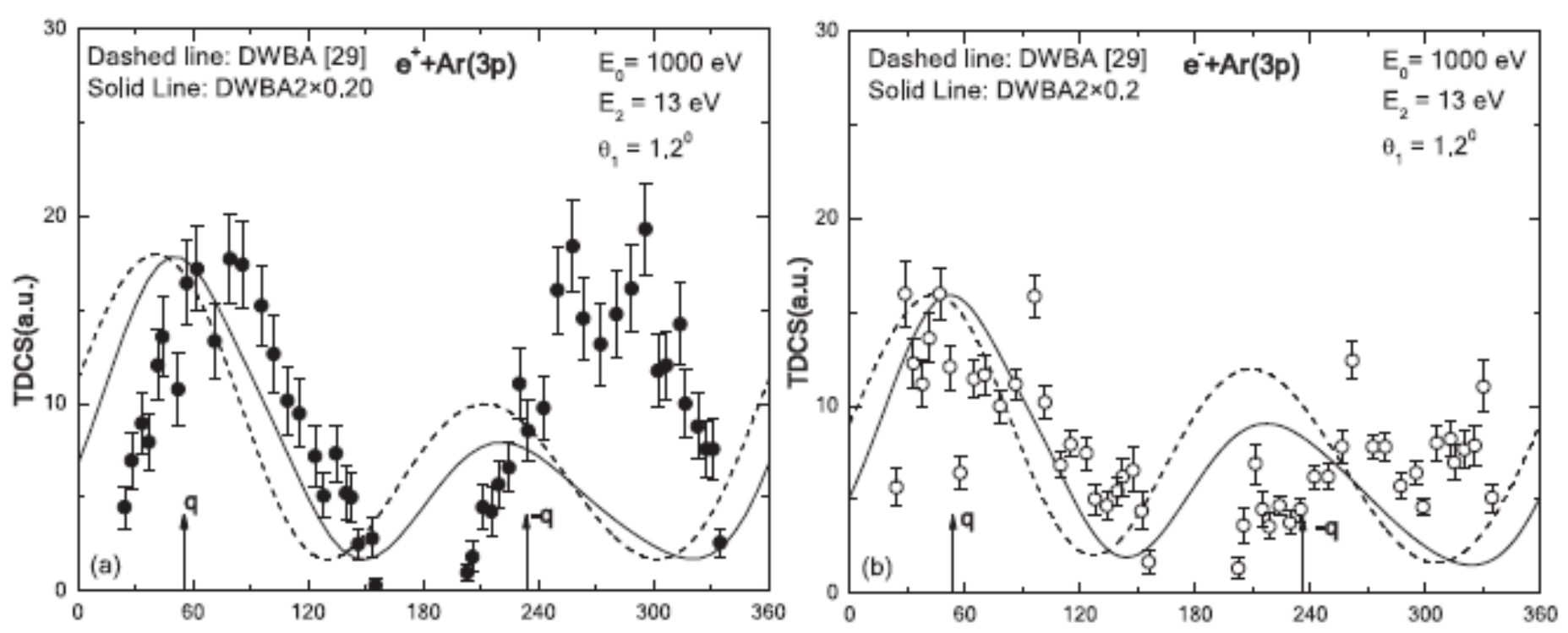
[8] C. Bjorkas, K. Vortler, K. Nordlund, D. Nishijima, R. Doerner, New J. Phys. **11**, 123017 (2009)

W and Be

* Electron induced processes such as excitation and ionization are prevalent in such magnetic fusion devices in a wide range of energies with significant variation of temperature and density.

* A reliable data base is required for the electron impact ionization and excitation cross sections for W and Be atoms and their charged states to model the electron induce interactions and understand the spectroscopy involved.

Results – Coplanar ionization of Ar (3p) atoms



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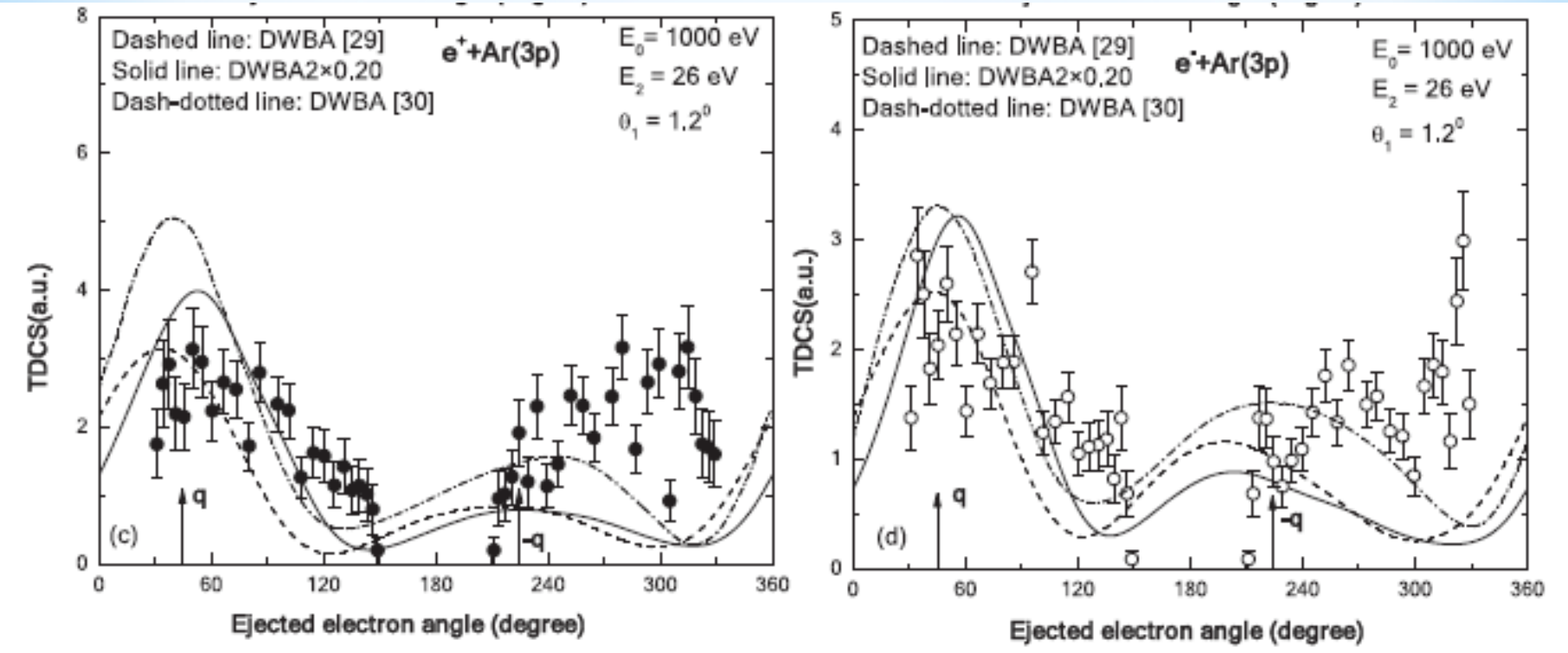
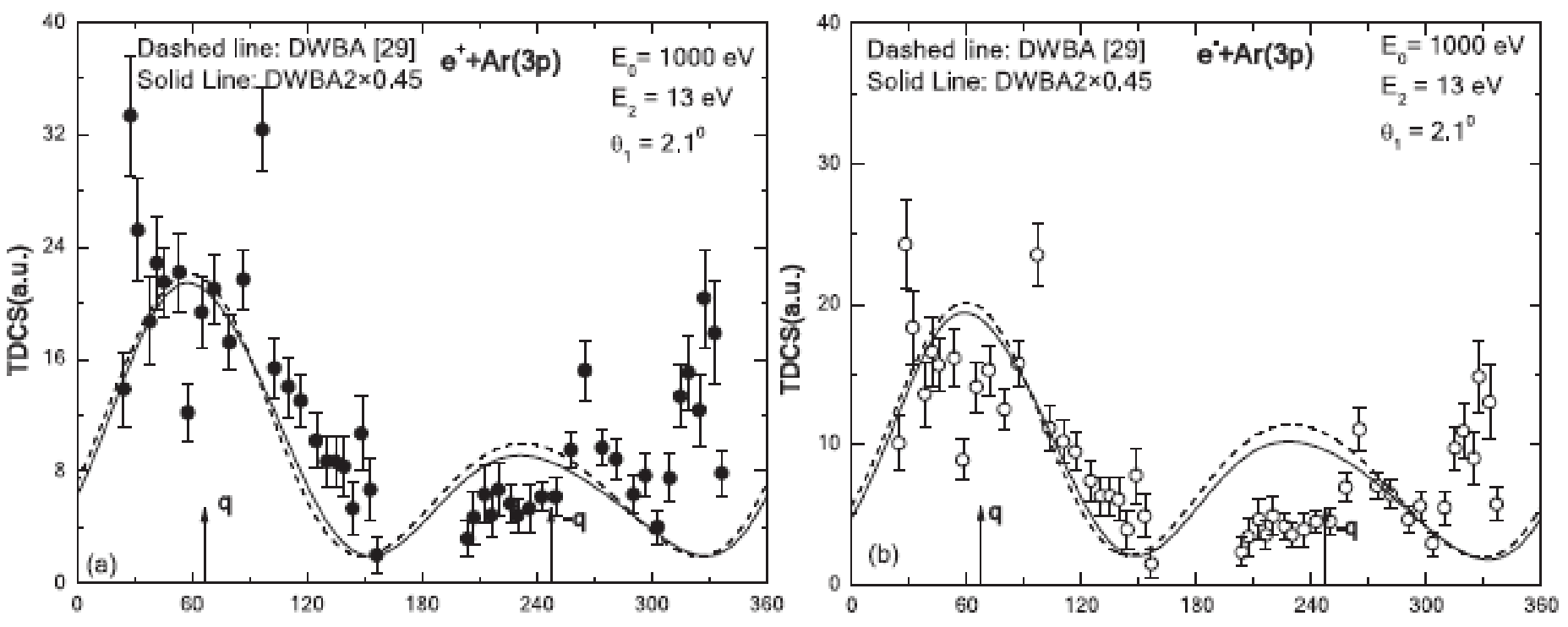
Results – Coplanar ionization of Ar (3p) atoms



Results – Coplanar ionization of Ar (3p) atoms



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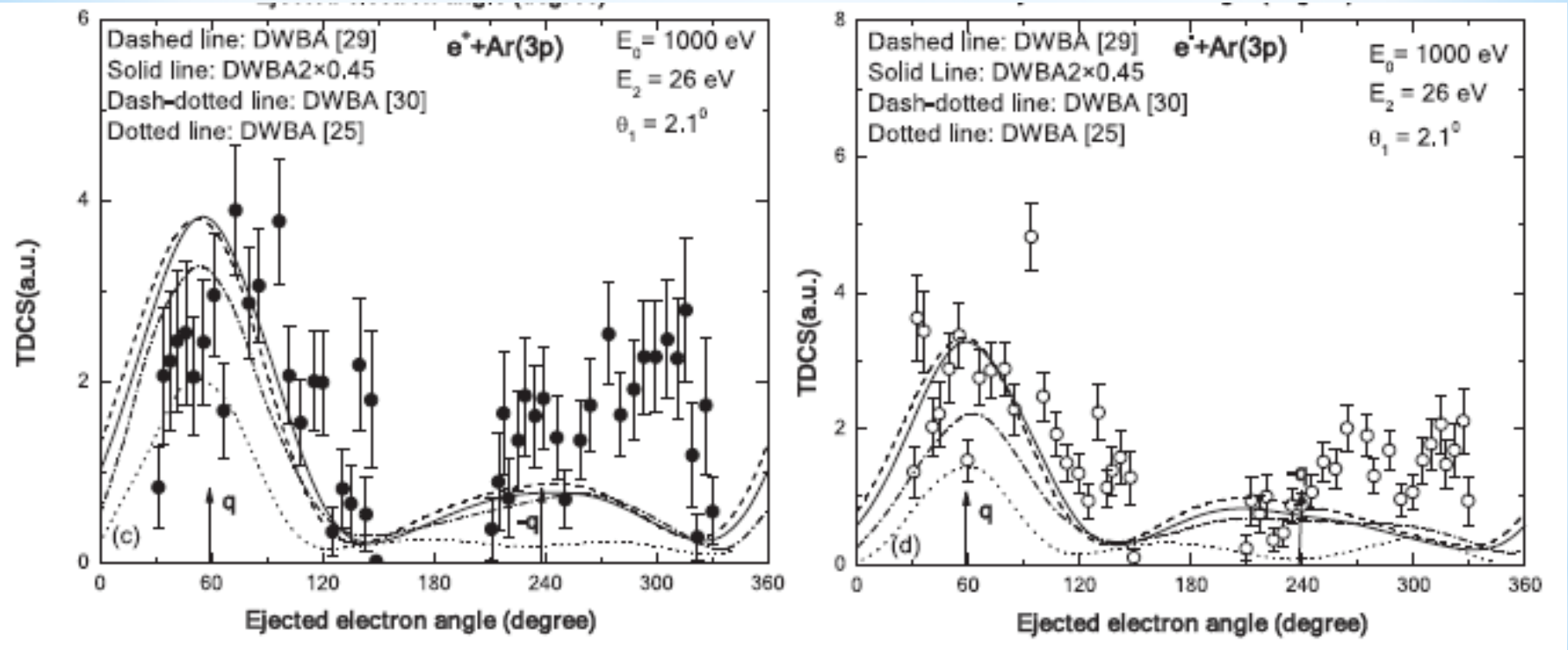

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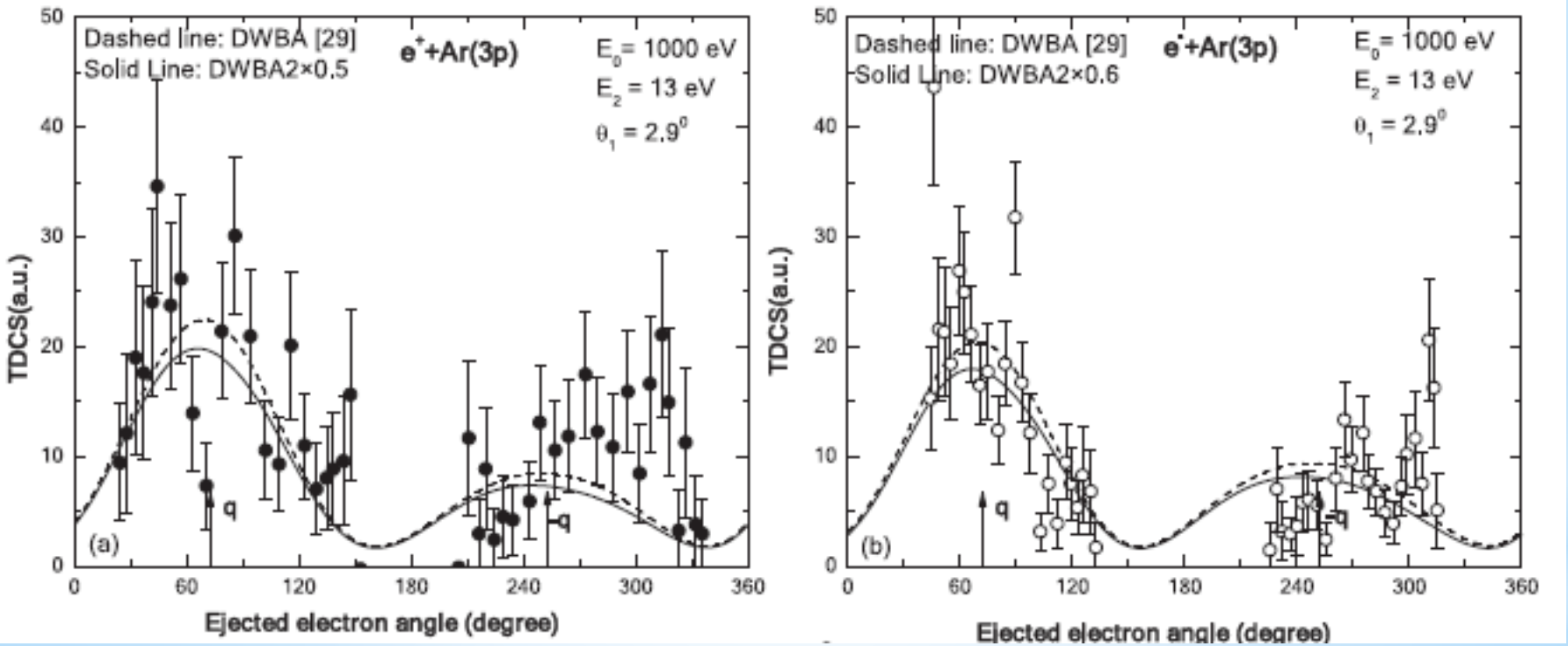

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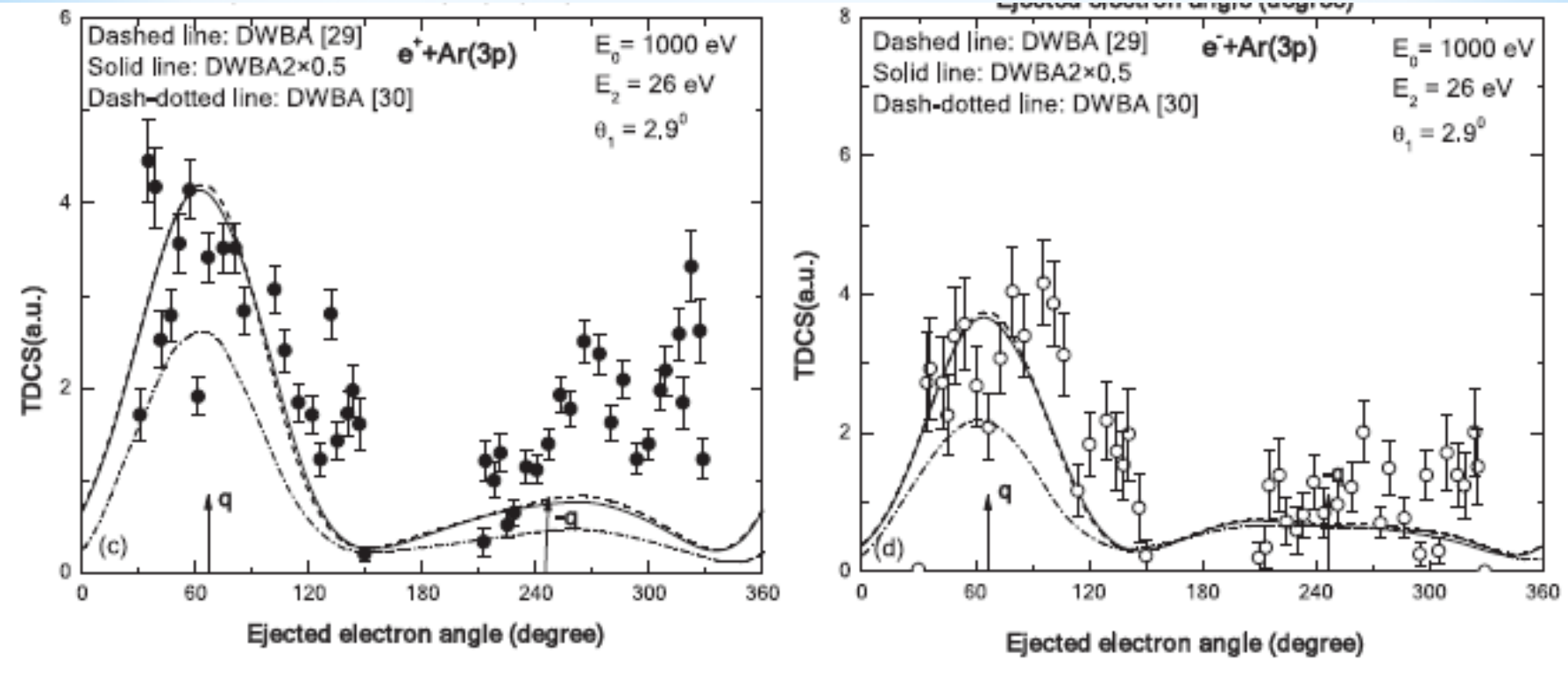
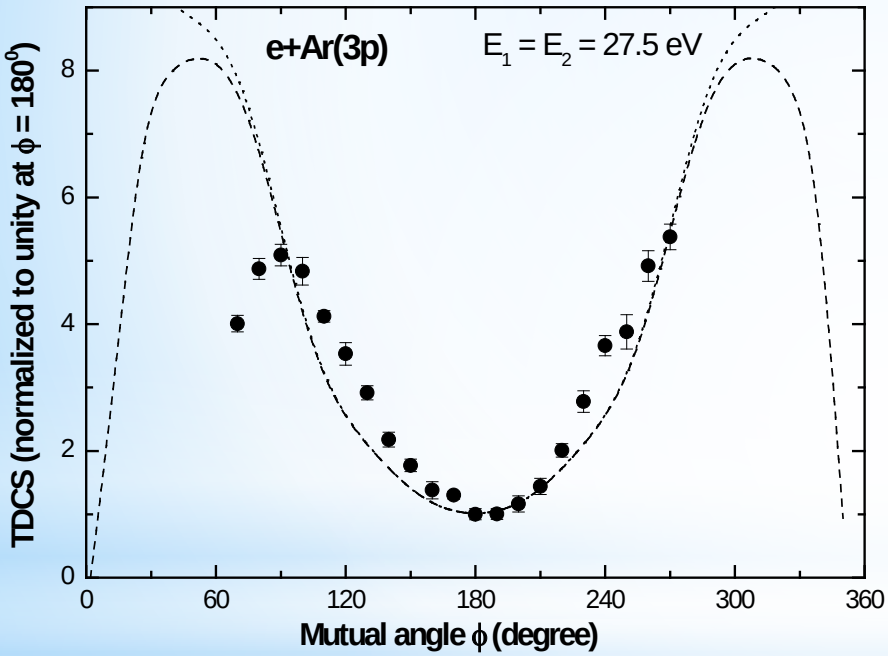
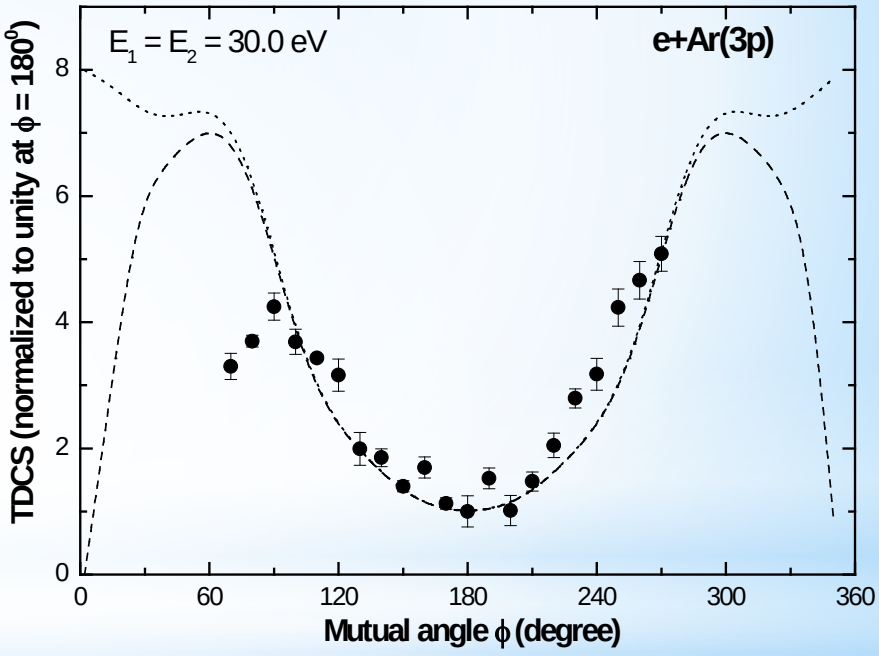


Table 1
Momentum transfer values and directions for the single ionization of Ar (3p) at 1 keV projectile energy.

Projectile	Ejected electron energy E_2	Scattering angle θ_1	Value of momentum transfer (q) (a.u.)	Expected Direction of momentum transfer (q), i.e. binary peak	Binary peak direction in DWBA	Binary peak direction in DWBA2	Binary peak direction in measurements
Electron	13 eV	1.2°	0.22	54.5°	44°	53°	52°
		2.1°	0.34	67.2°	61°	59°	54°
		2.9°	0.45	72.5°	69°	67°	64°
	26 eV	1.2°	0.25	43.8°	44°	56°	56°
		2.1°	0.36	58.7°	58°	59°	56°
		2.9°	0.46	65.7°	66°	65°	55°
Positron	13 eV	1.2°	0.22	54.5°	41°	51°	62°
		2.1°	0.34	67.2°	59°	58°	53°
		2.9°	0.45	72.5°	69°	66°	57°
	26 eV	1.2°	0.25	43.8°	34°	53°	54°
		2.1°	0.36	58.7°	52°	56°	61°
		2.9°	0.46	65.7°	64°	62°	56°

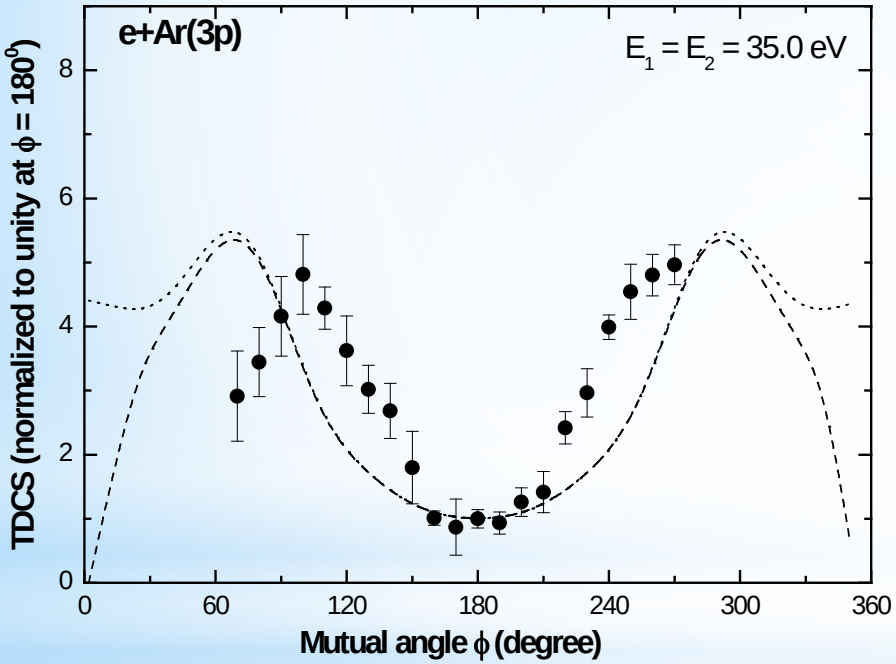
Results – Perpendicular Plane ionization of Ar (3p) atoms

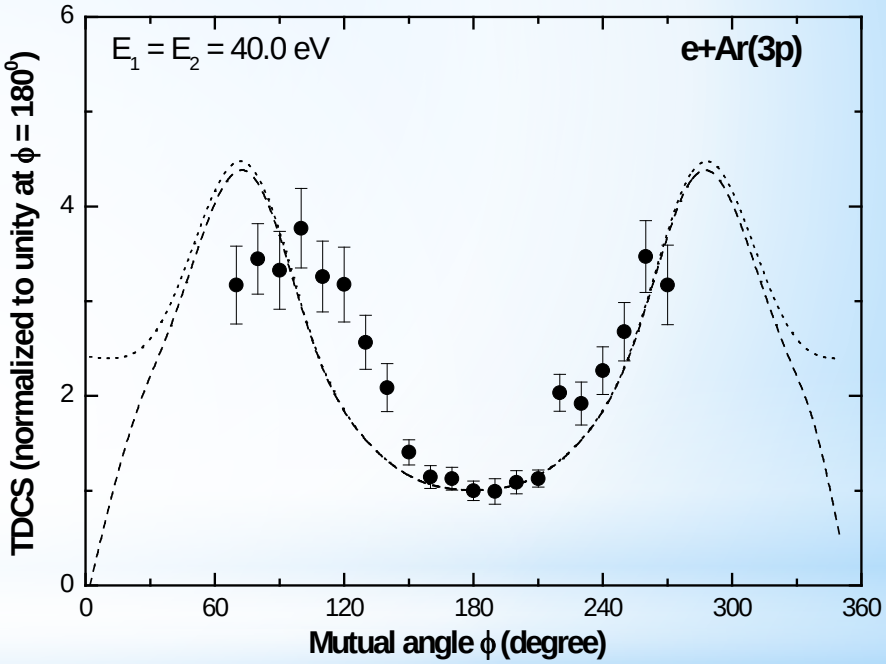




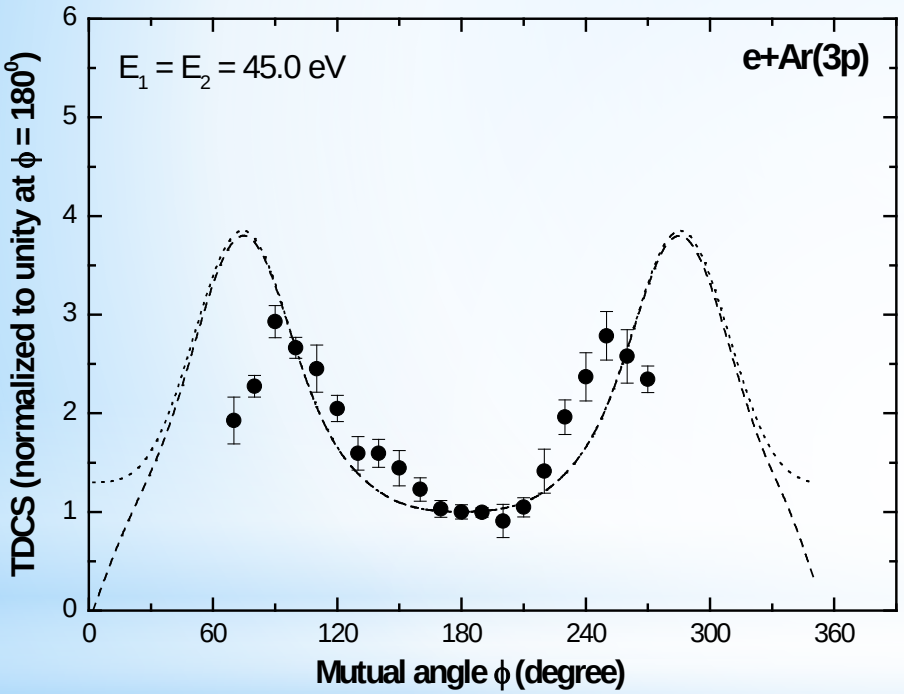
Experimental Data: Patel and Murray Phy. Rev. A **105, 042815 (2022)**

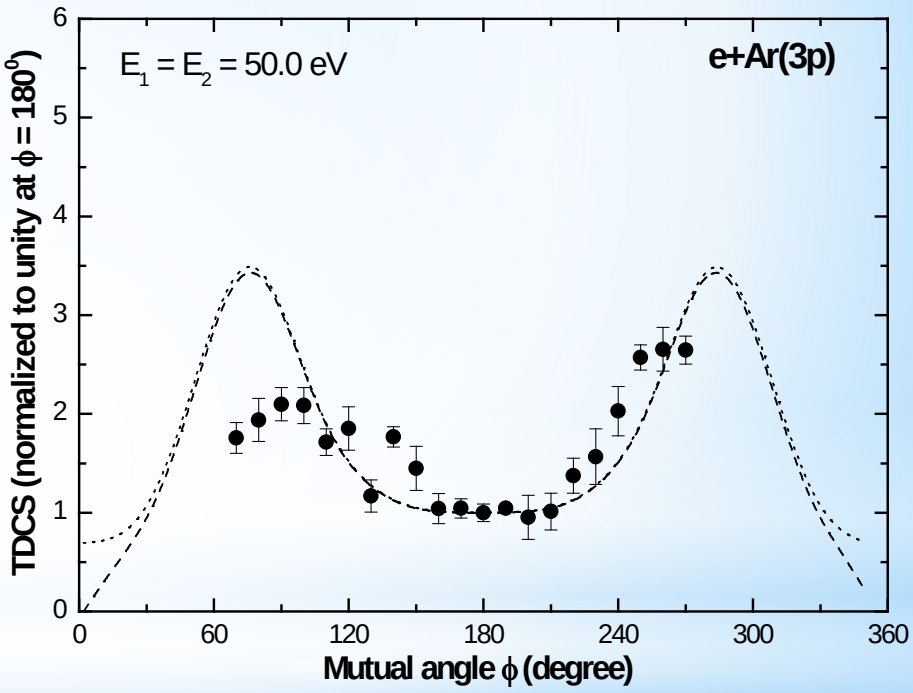
Results – Perpendicular Plane ionization of Ar (3p) atoms



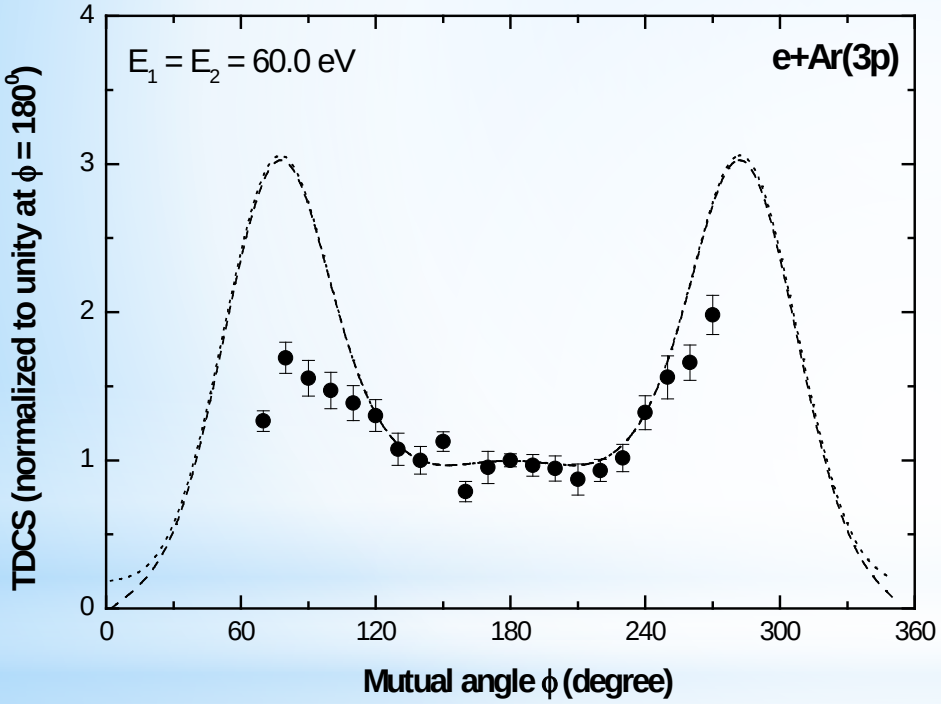


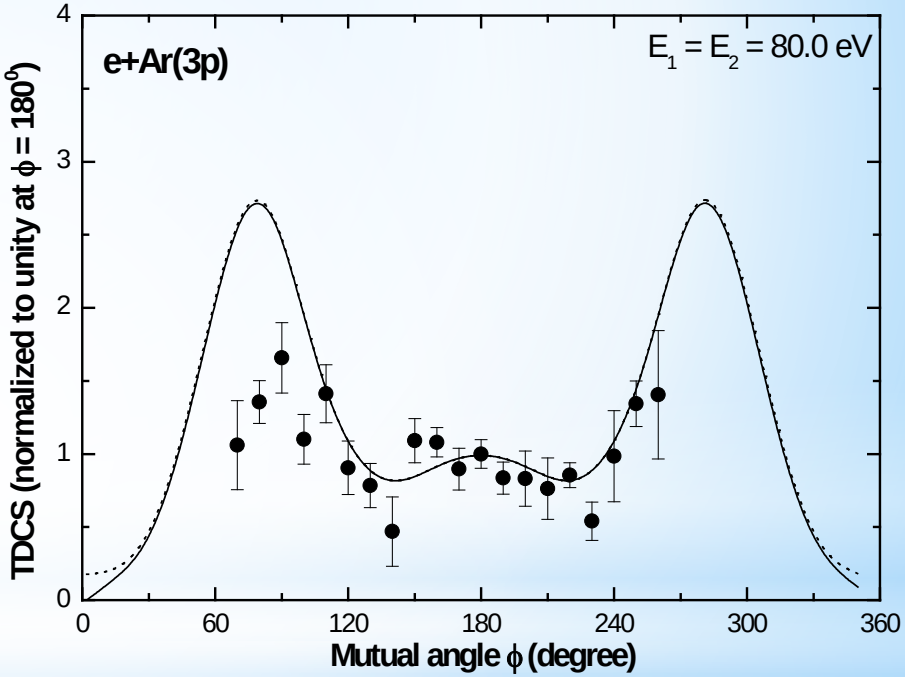
Results – Perpendicular Plane ionization of Ar (3p) atoms



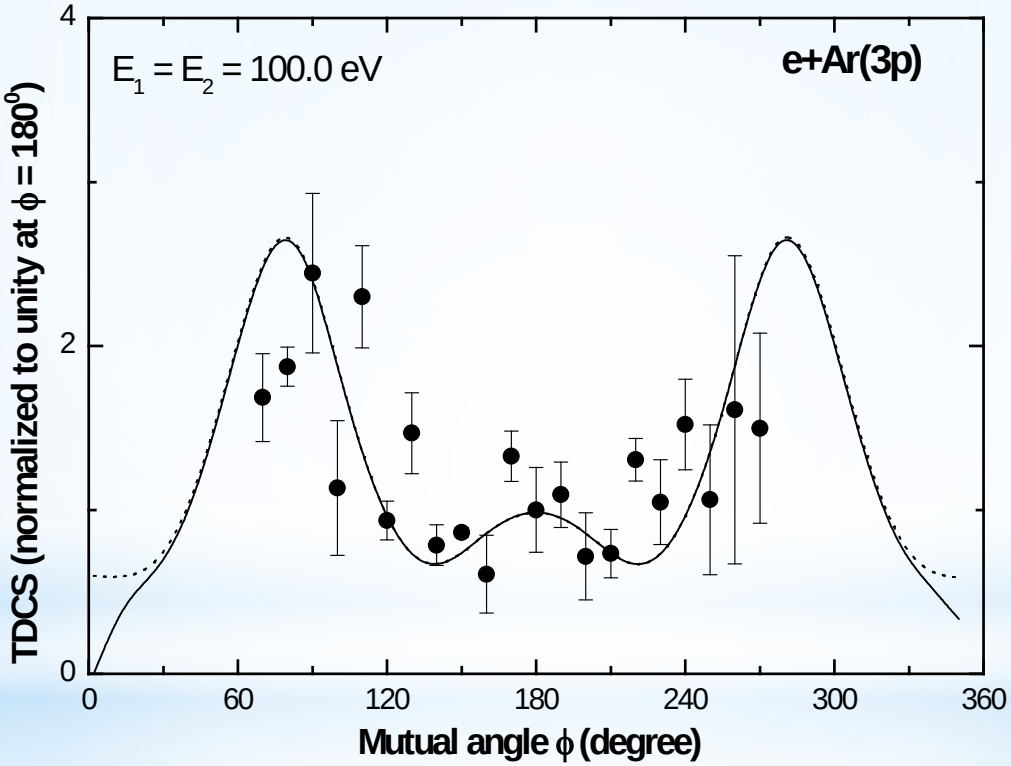


Results – Perpendicular Plane ionization of Ar (3p) atoms

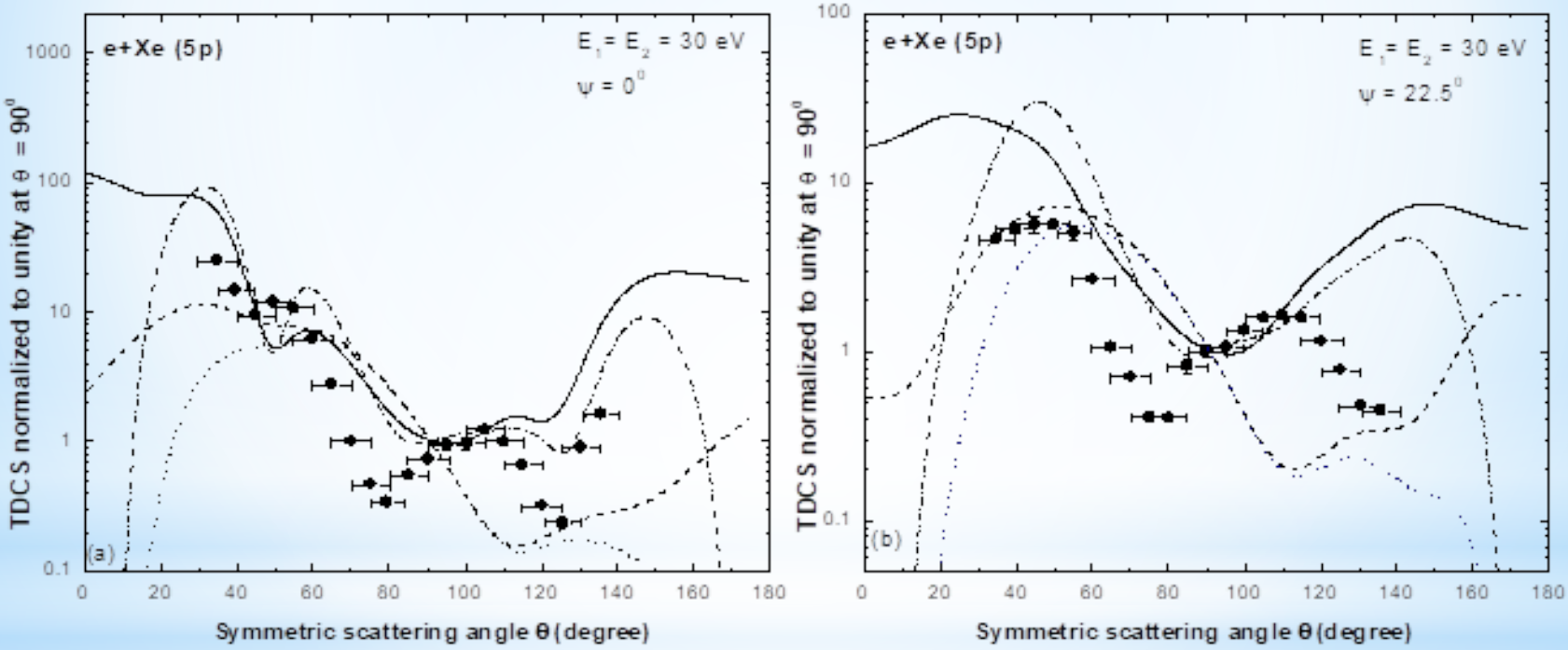




Results – Perpendicular Plane ionization of Ar (3p) atoms

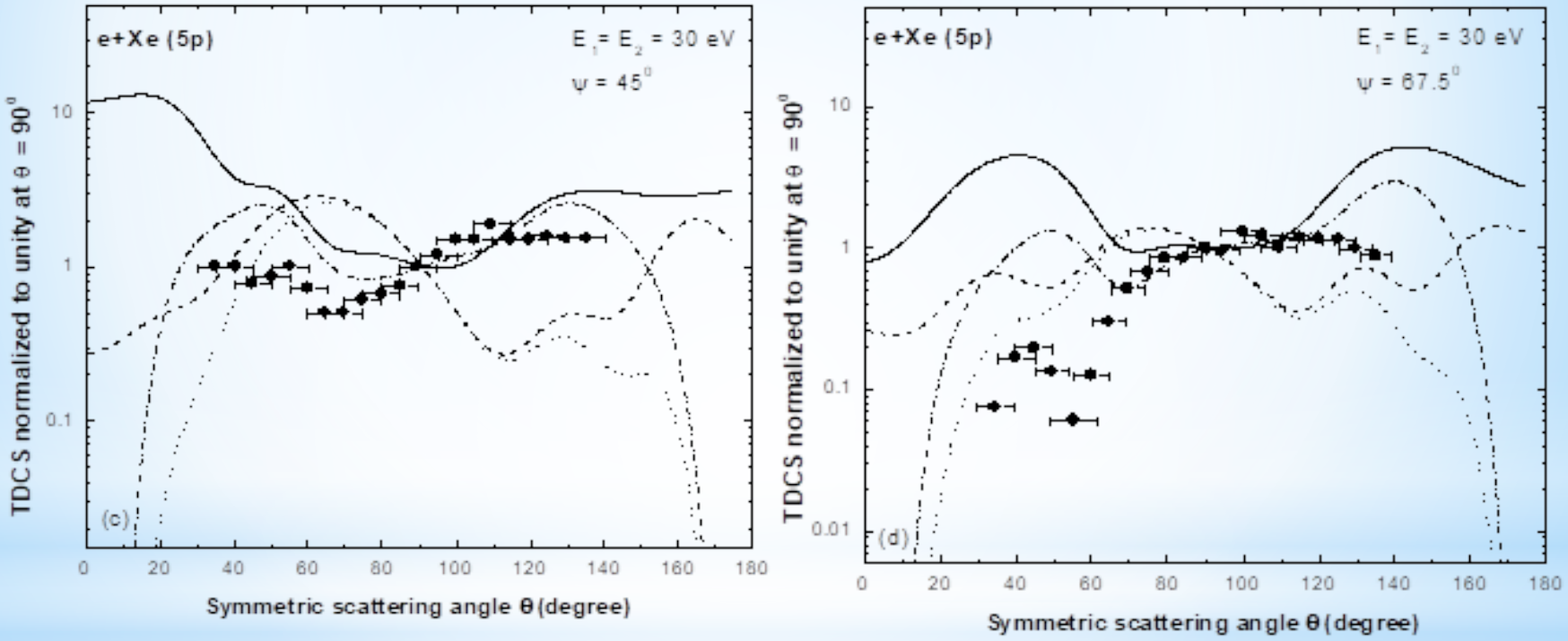


Results – Coplanar to Perpendicular Plane ionization of Xe (5p) at 60 eV above IP



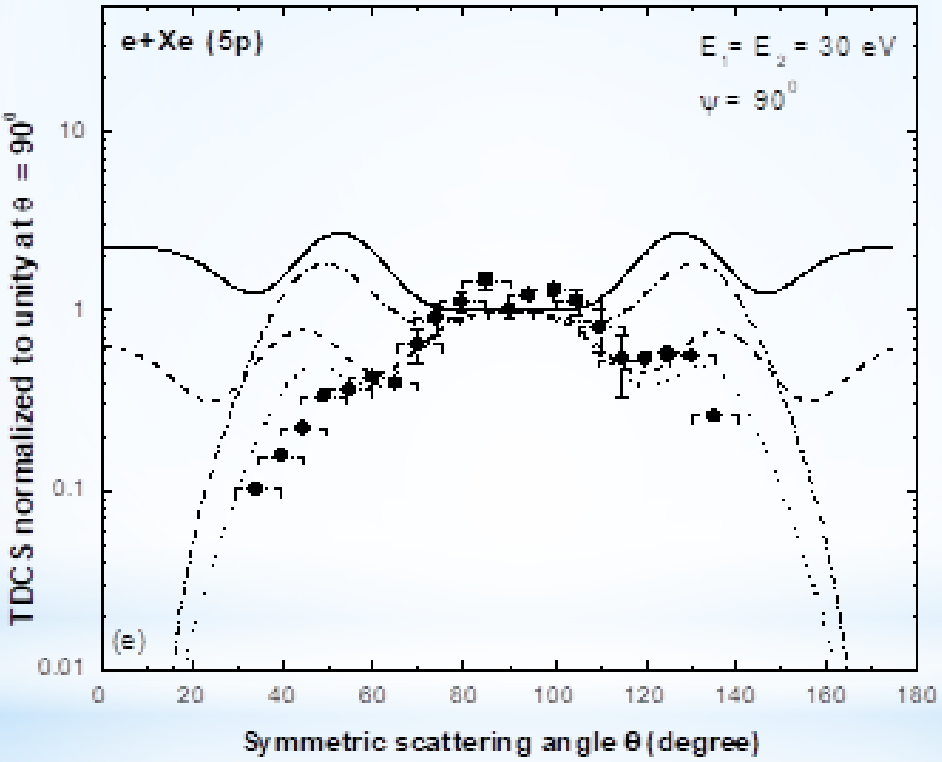
Experimental Data: Patel and Murray Phy. Rev. A **105, 032818 (2022)**

Results – Coplanar to Perpendicular Plane ionization of Xe (5p) at 60 eV above IP



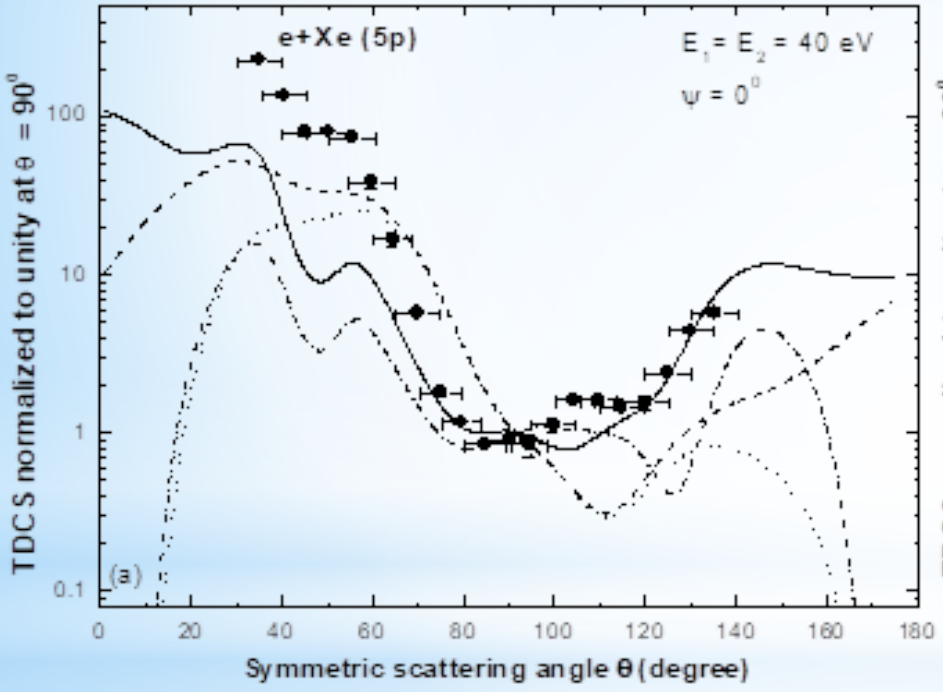
Experimental Data: Patel and Murray Phy. Rev. A **105, 032818 (2022)**

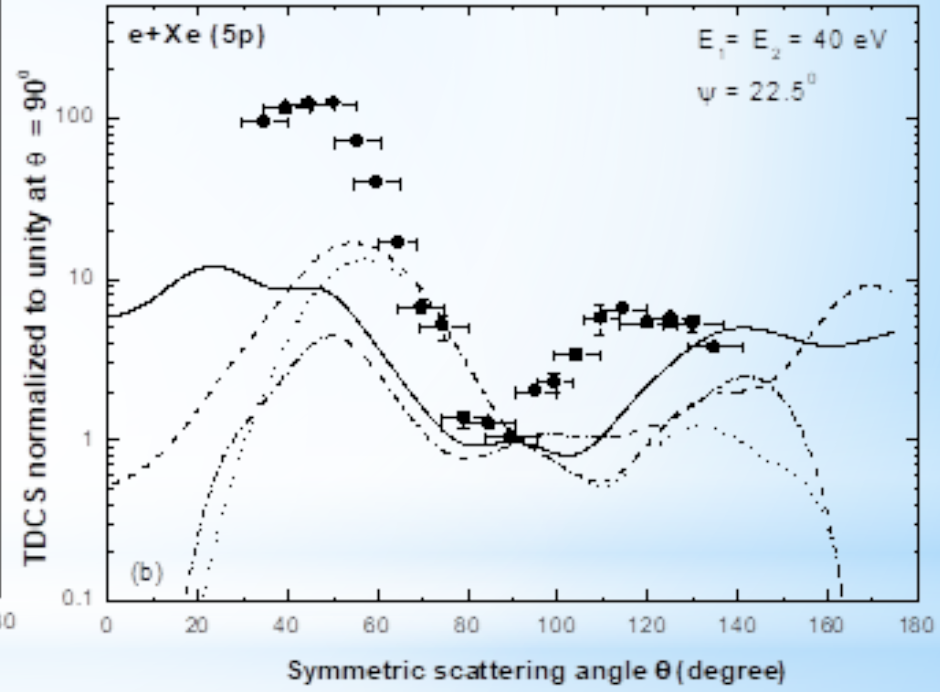
Results – Coplanar to Perpendicular Plane ionization of Xe (5p) at 60 eV above IP



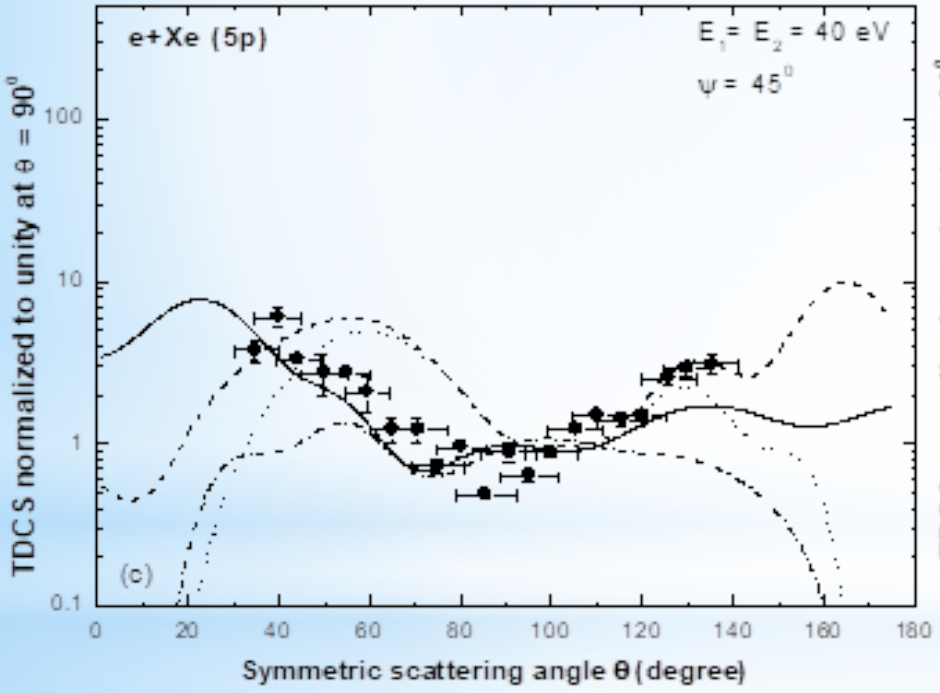
Experimental Data: Patel and Murray Phy. Rev. A **105, 032818 (2022)**

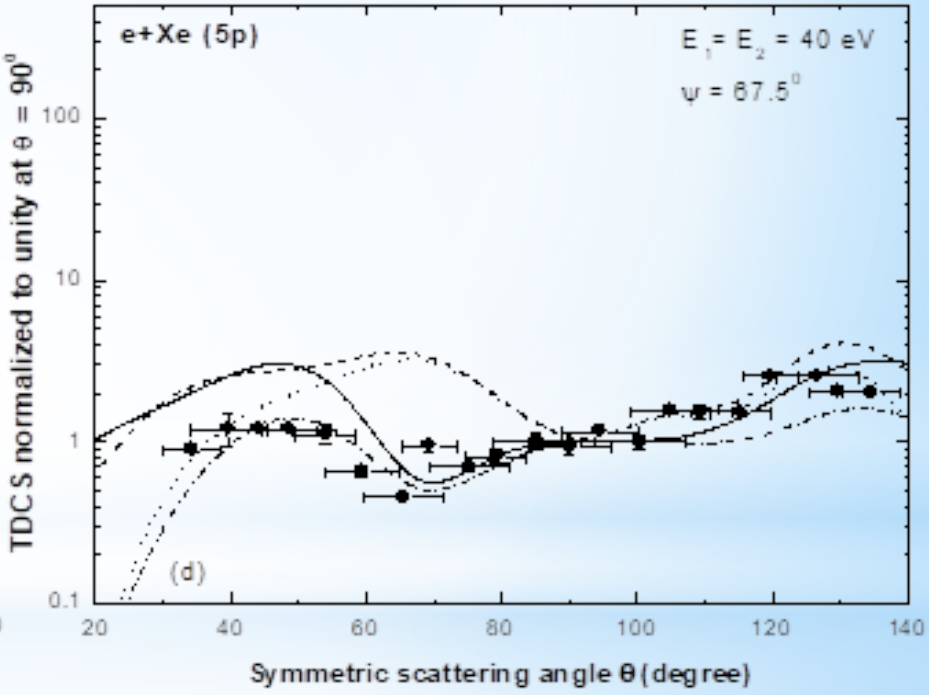
Results – Coplanar to Perpendicular Plane ionization of Xe (5p) at 80 eV above IP



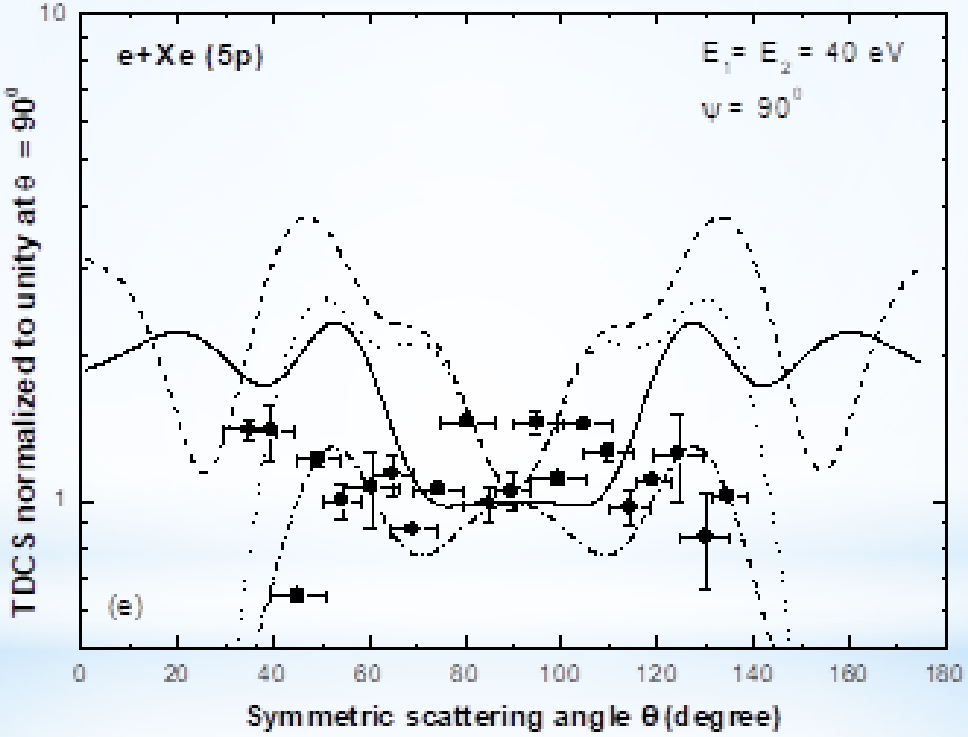


Results – Coplanar to Perpendicular Plane ionization of Xe (5p) at 80 eV above IP

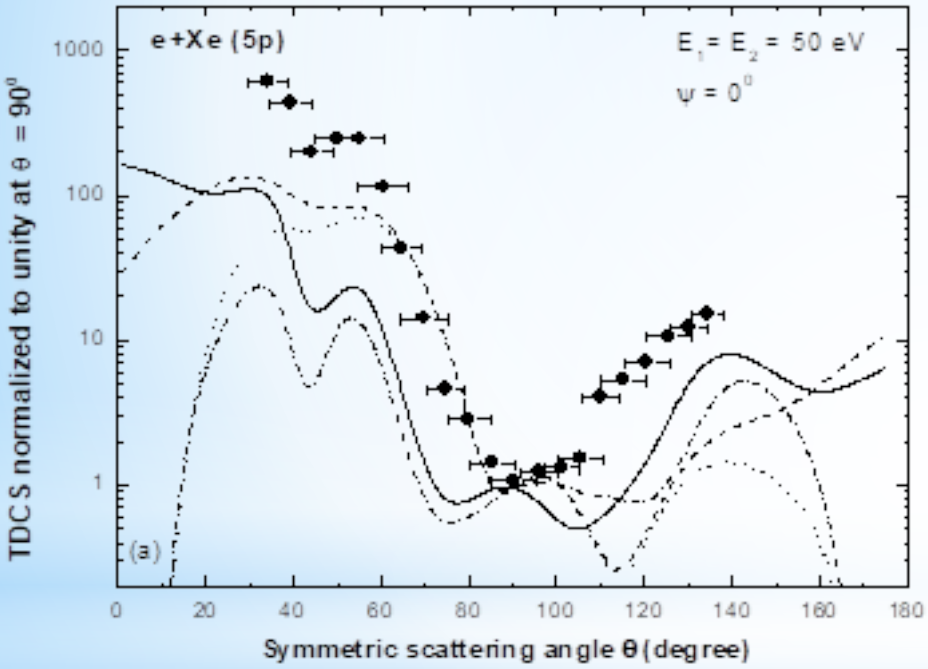


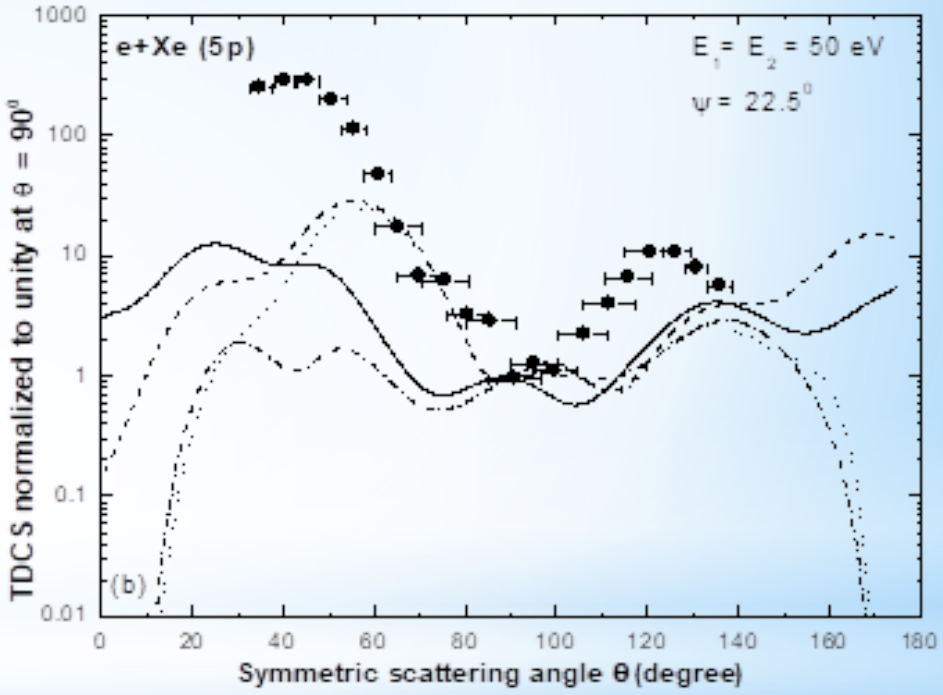


Results – Coplanar to Perpendicular Plane ionization of Xe (5p) at 80 eV above IP

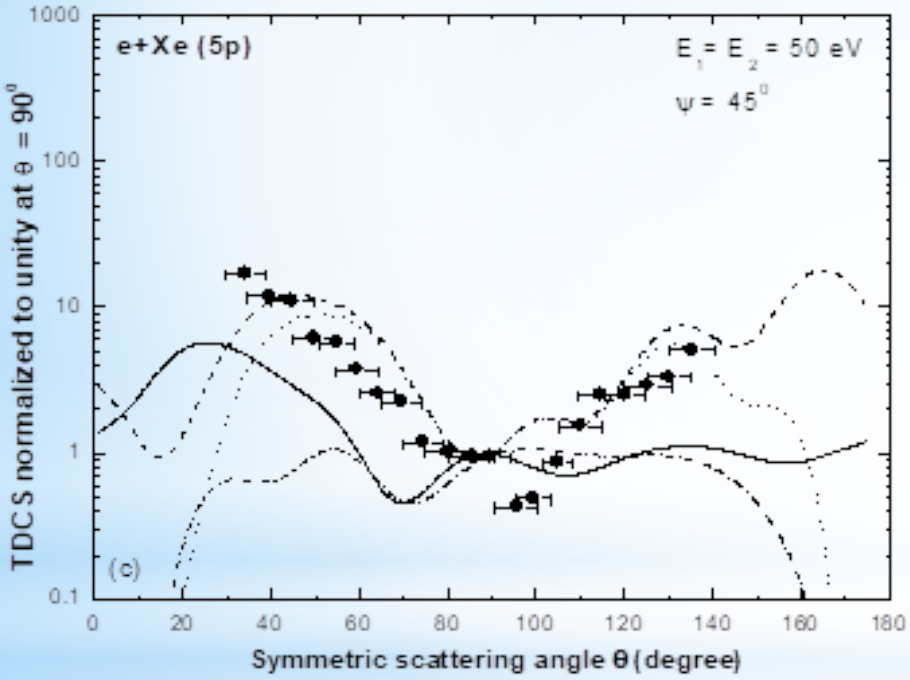


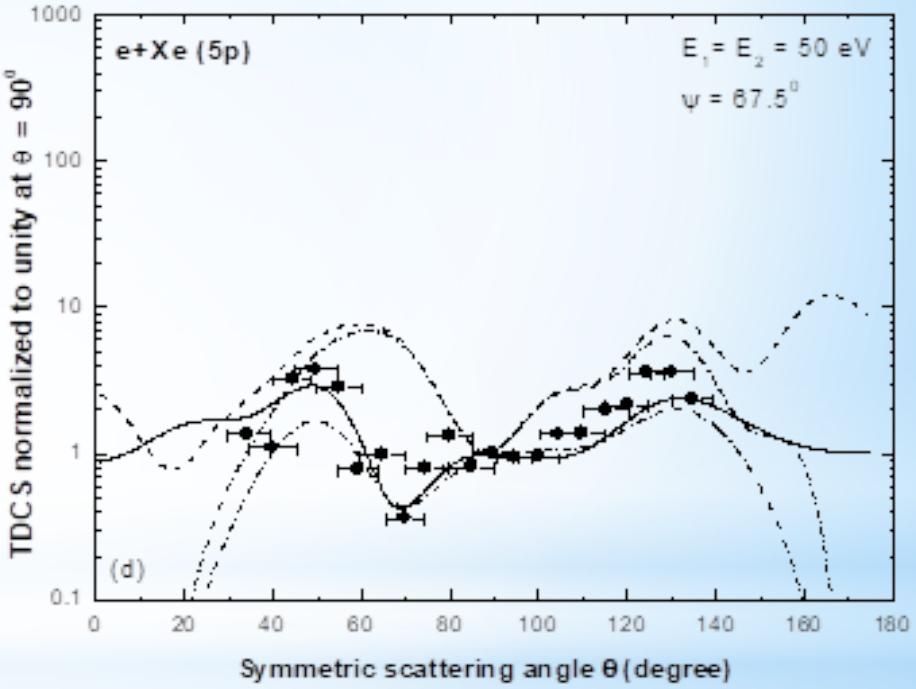
Results – Coplanar to Perpendicular Plane ionization of Xe (5p) at 100 eV above IP



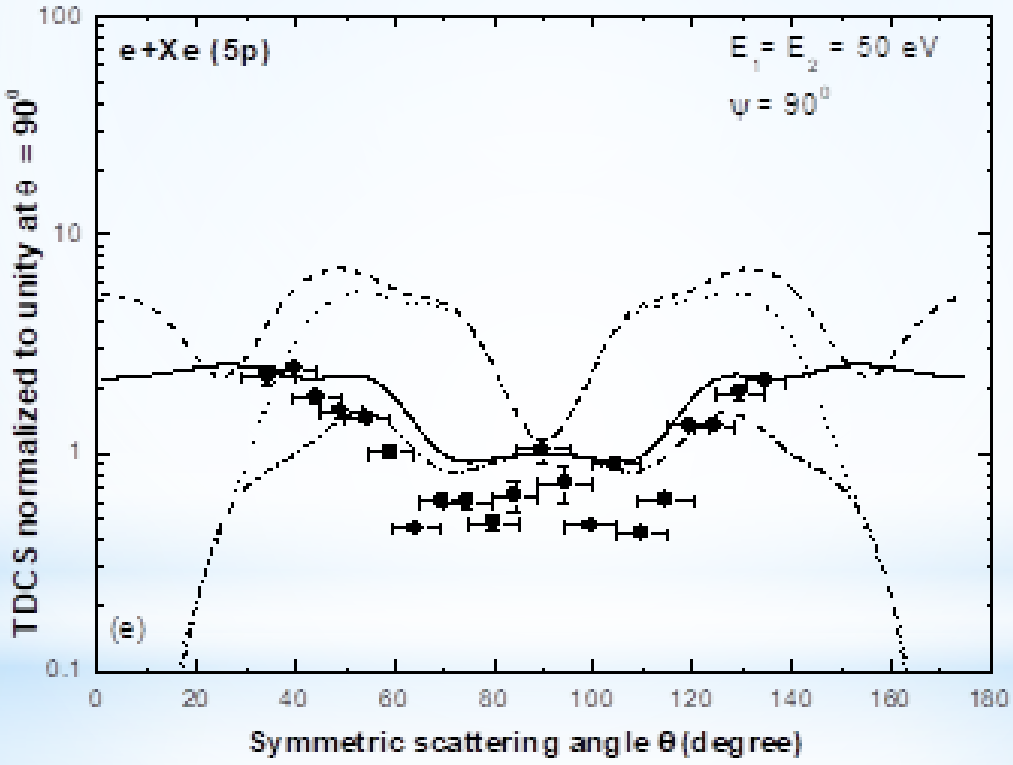


Results – Coplanar to Perpendicular Plane ionization of Xe (5p) at 100 eV above IP

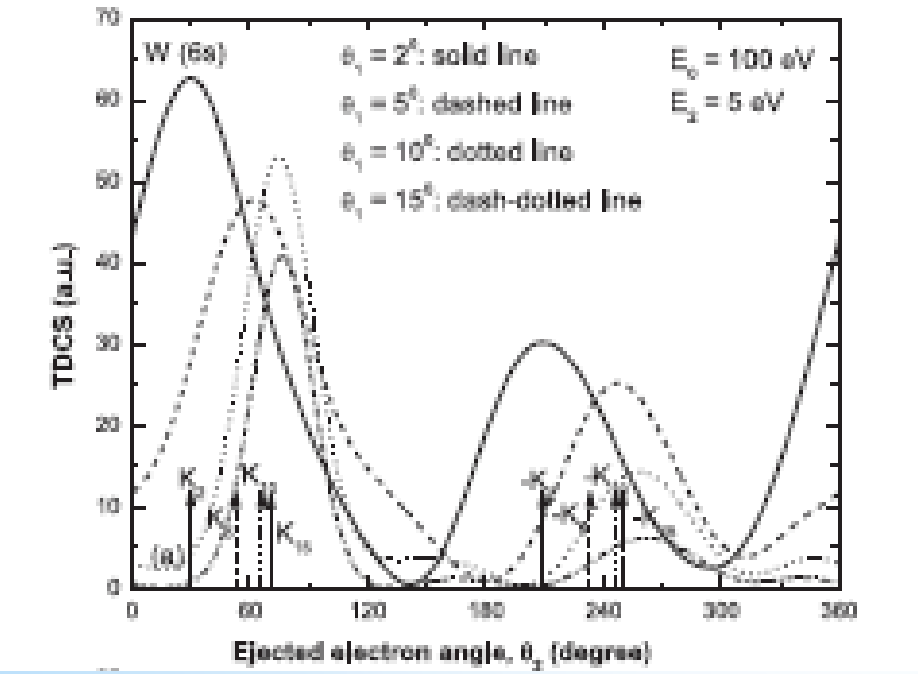


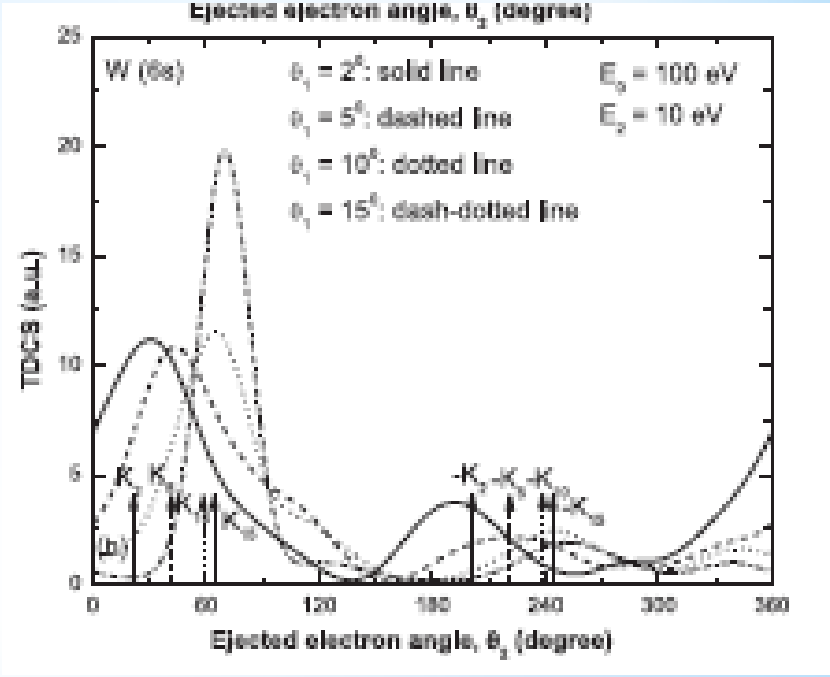


Results – Coplanar to Perpendicular Plane ionization of Xe (5p) at 100 eV above IP



Results – Coplanar Asymmetric Ionization of W (6s) atoms





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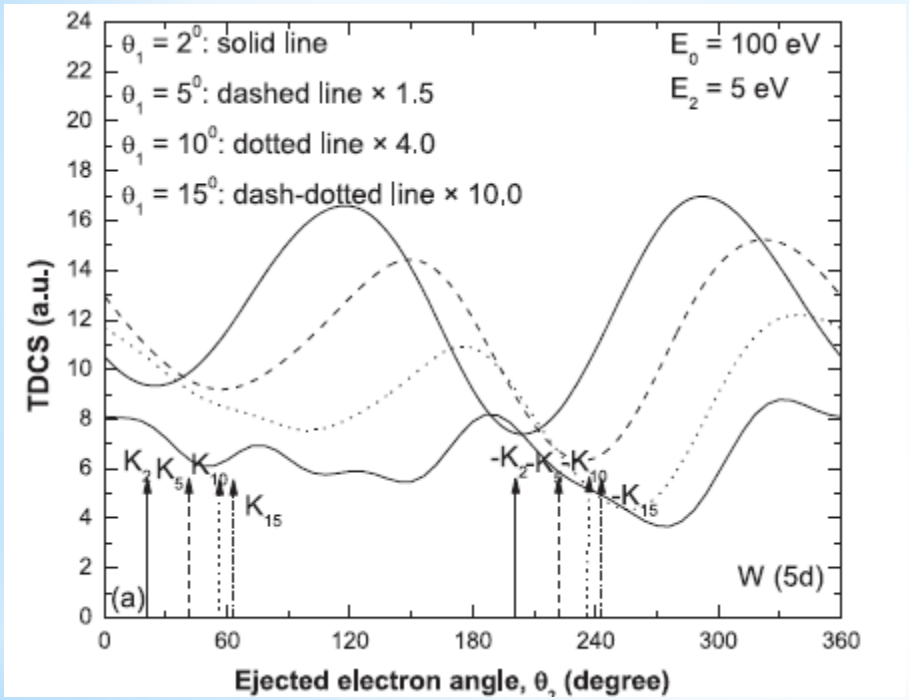
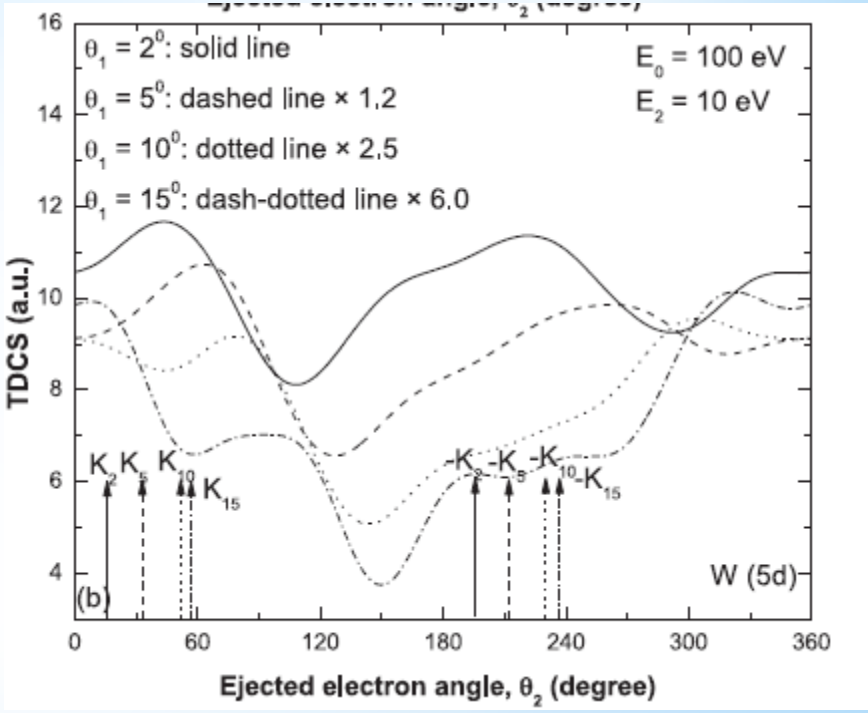
Results – Coplanar Asymmetric Ionization of W (5d) atoms





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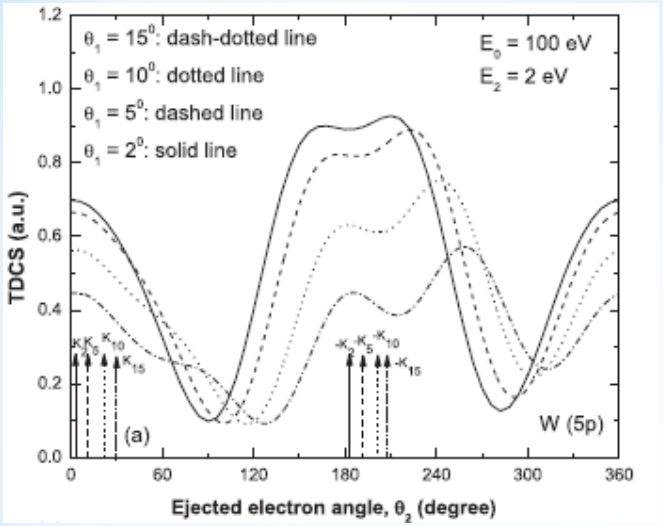
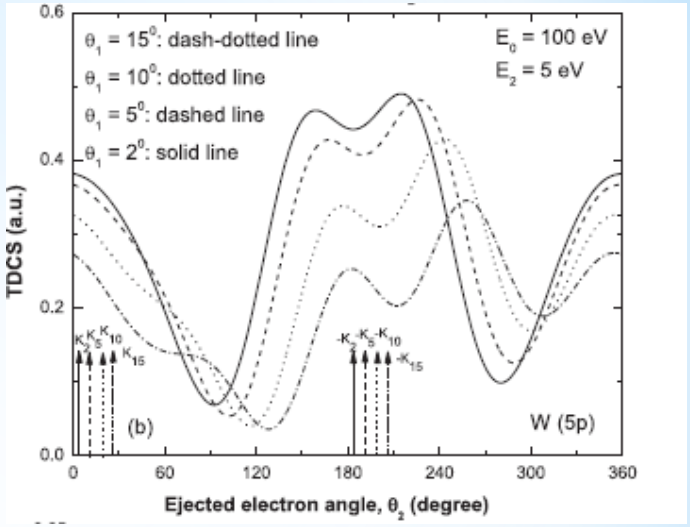
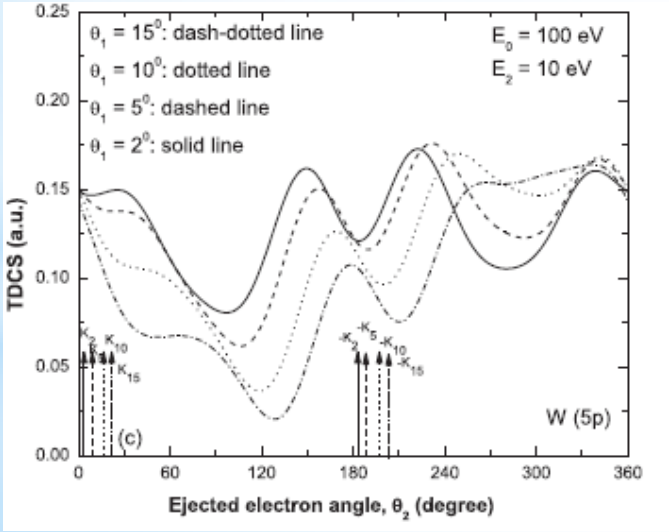
Results – Coplanar Asymmetric Ionization of W (5p) atoms







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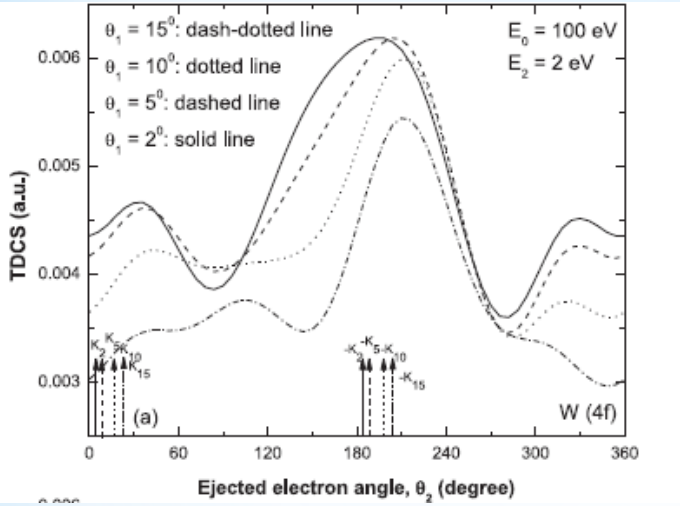
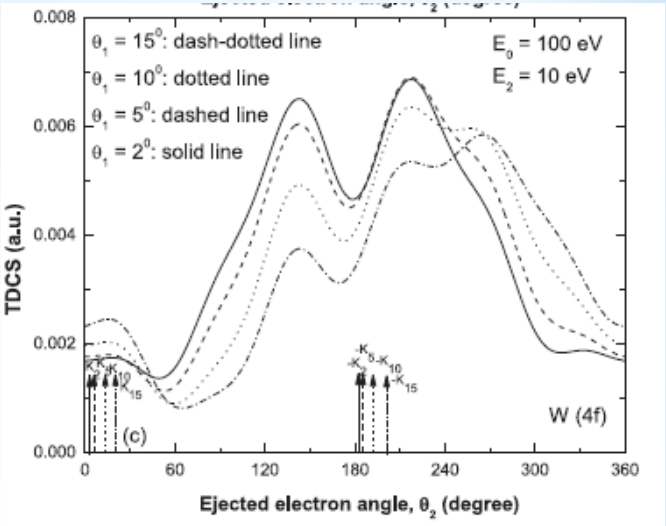
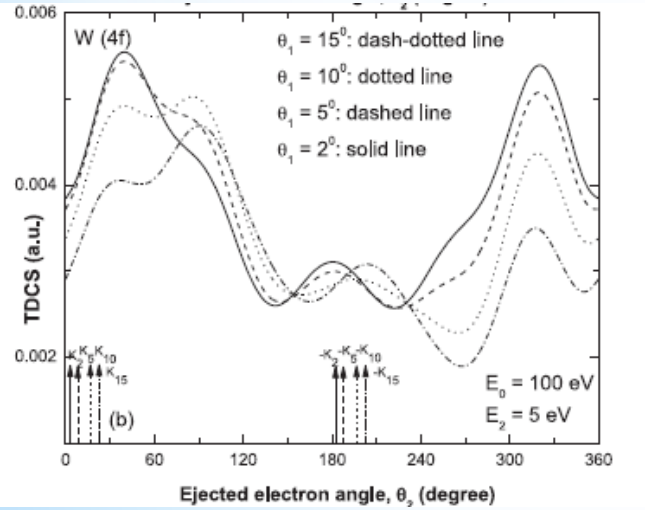
Results – Coplanar Asymmetric Ionization of W (4f) atoms







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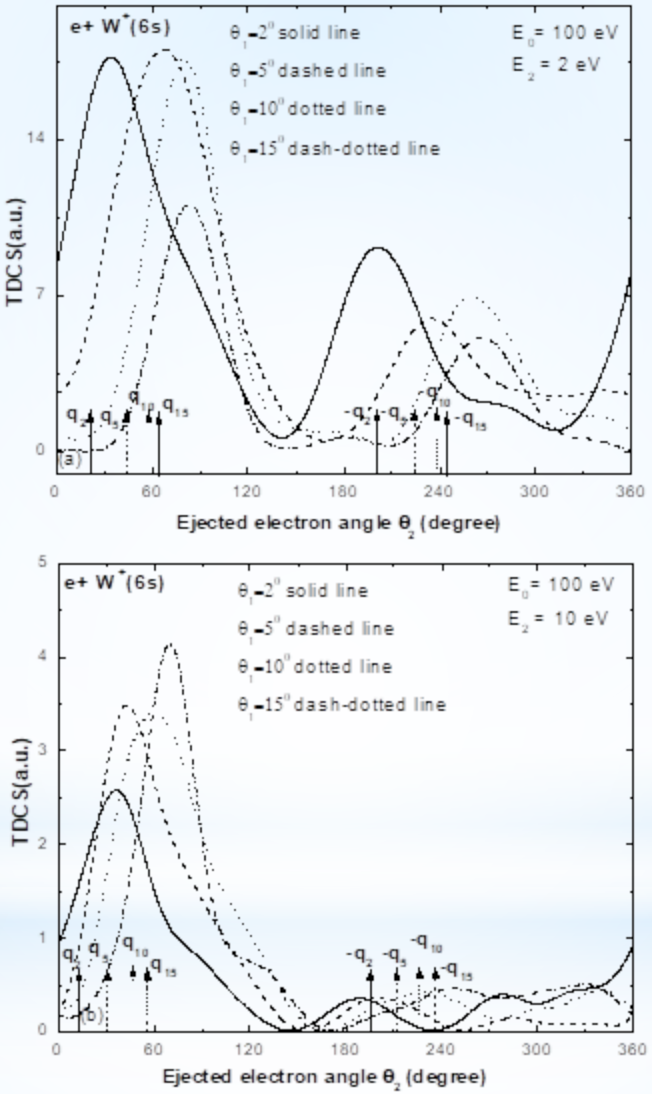
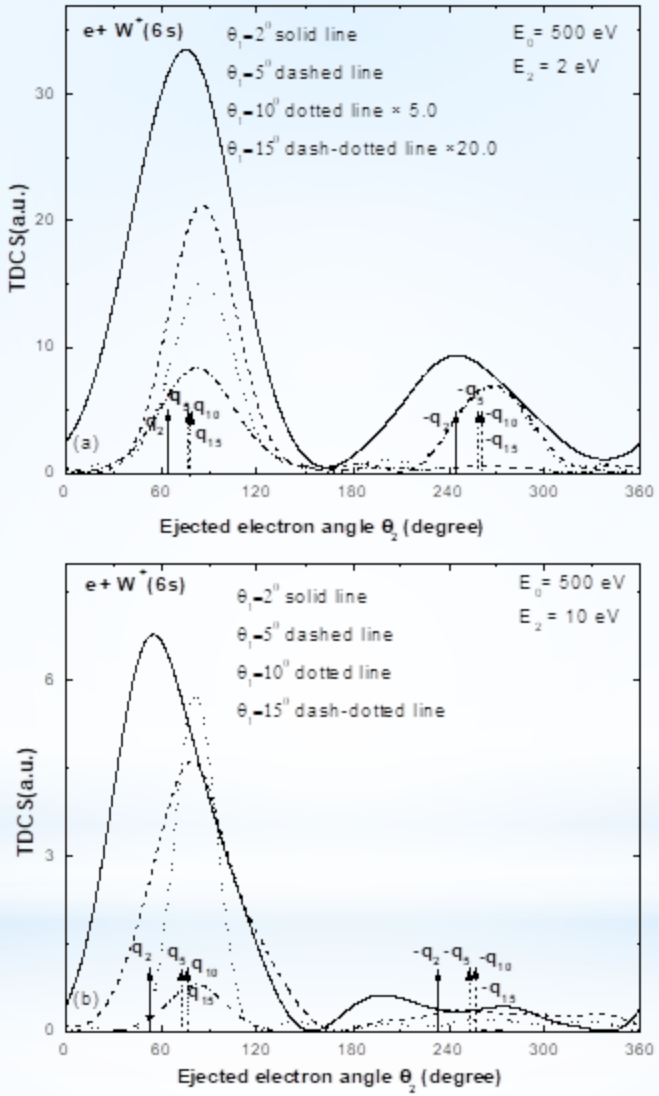
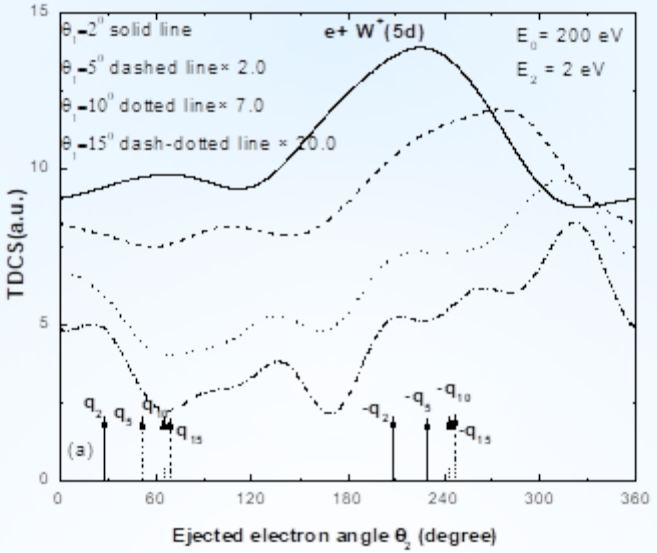
Results – Coplanar Asymmetric Ionization of W^+ ions

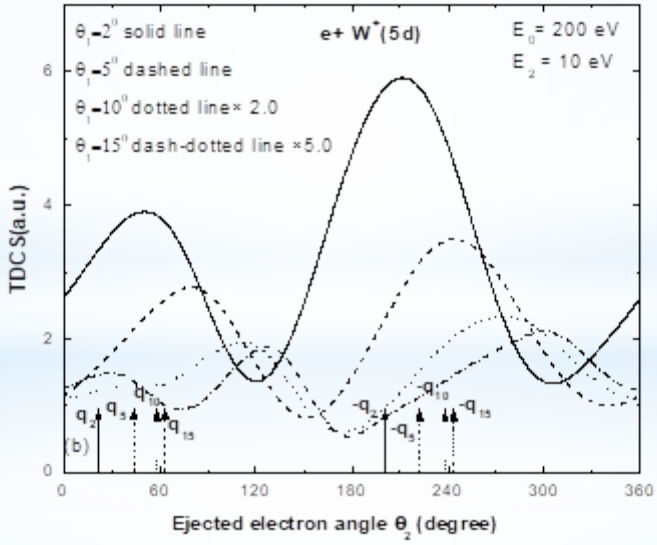


Results – Coplanar Asymmetric Ionization of W^+ ions

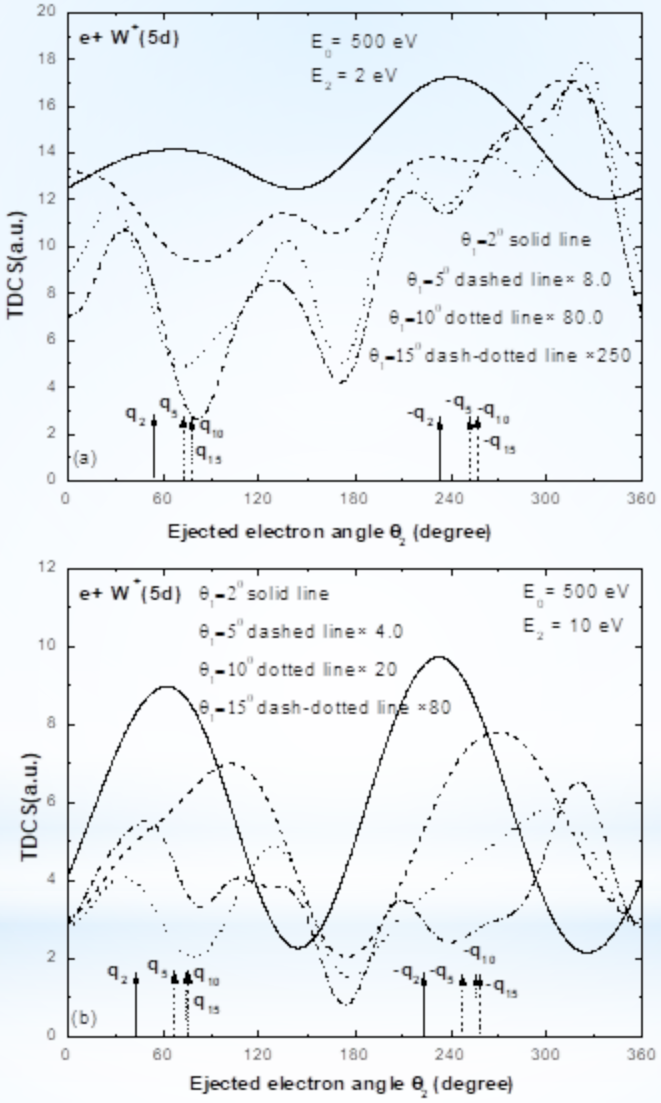


Results – Coplanar Asymmetric Ionization of W^+ ions

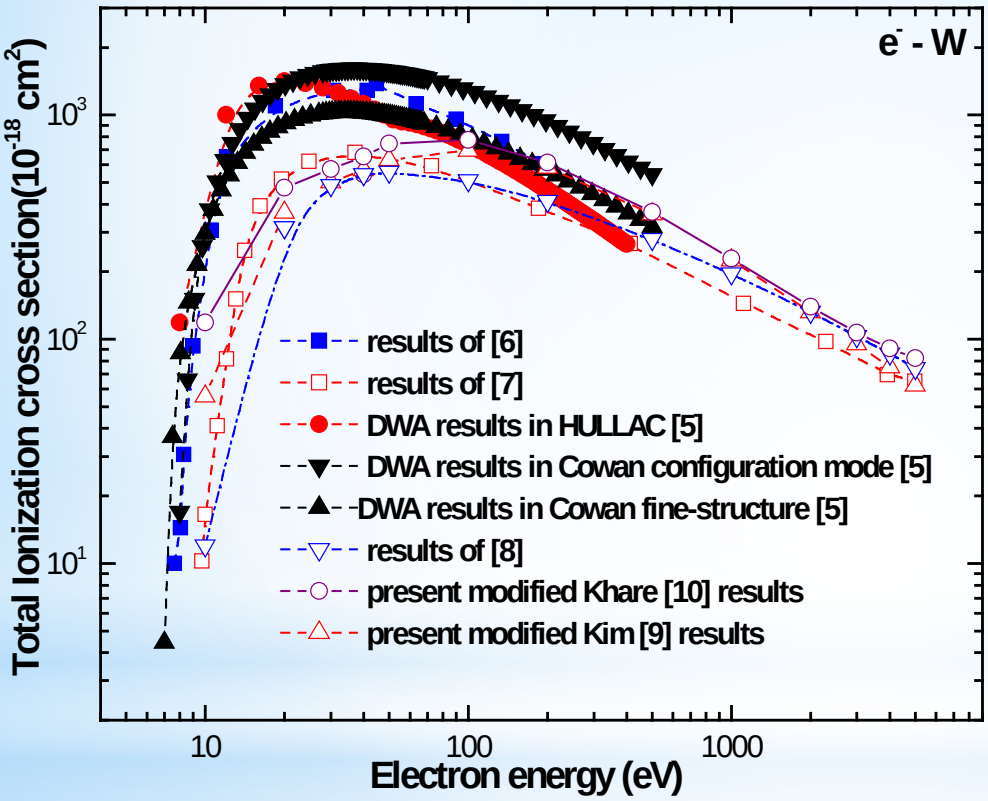




Results – Coplanar Asymmetric Ionization of W^+ ions



Results - Ionization cross sections for W atoms



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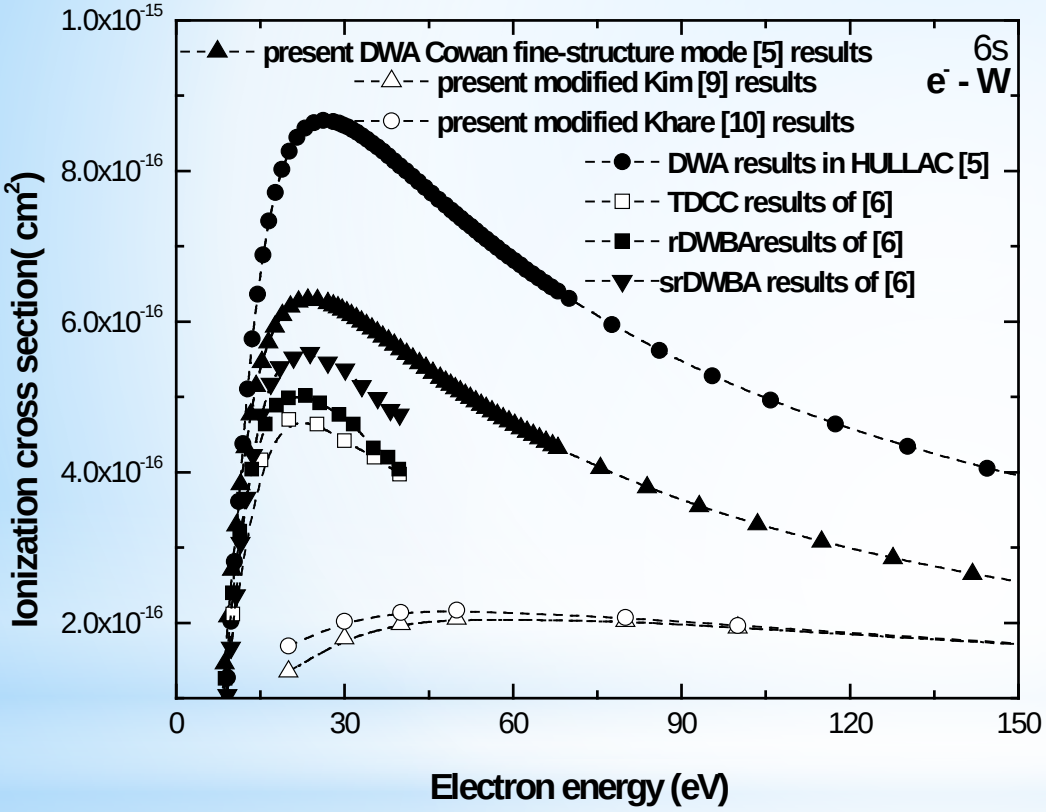
[5] G. Purohit, D. Kato and I. Murakami, Plasma and Fusion Research 13, 3401026 (2018). [6]M. S. Pindzola, S. D. Loch and A. R. Foster, J. Phys. B: At. Mol. Opt. Phys. 50, 095201 (2017).[7] F. Blanco, F. Ferreira da Silva, P. Limao-Vieira and G. Garcia, Plasma Sources Sci. Technol. 26, 085004 (2017).[8] B. Goswami, R. Naghma and B. Antony, Int. J. Mass Spectrom. 8, 372 (2014).[9]Y.K. Kim and M.E. Rudd, Phys. Rev. A 50, 3954–67 (1994).[10]S.P. Khare, M.K. Sharma and S. Tomar, J. Phys. B: At. Mol. Opt. Phys. 32, 3147 (1999).

Results - Ionization cross sections for W atoms



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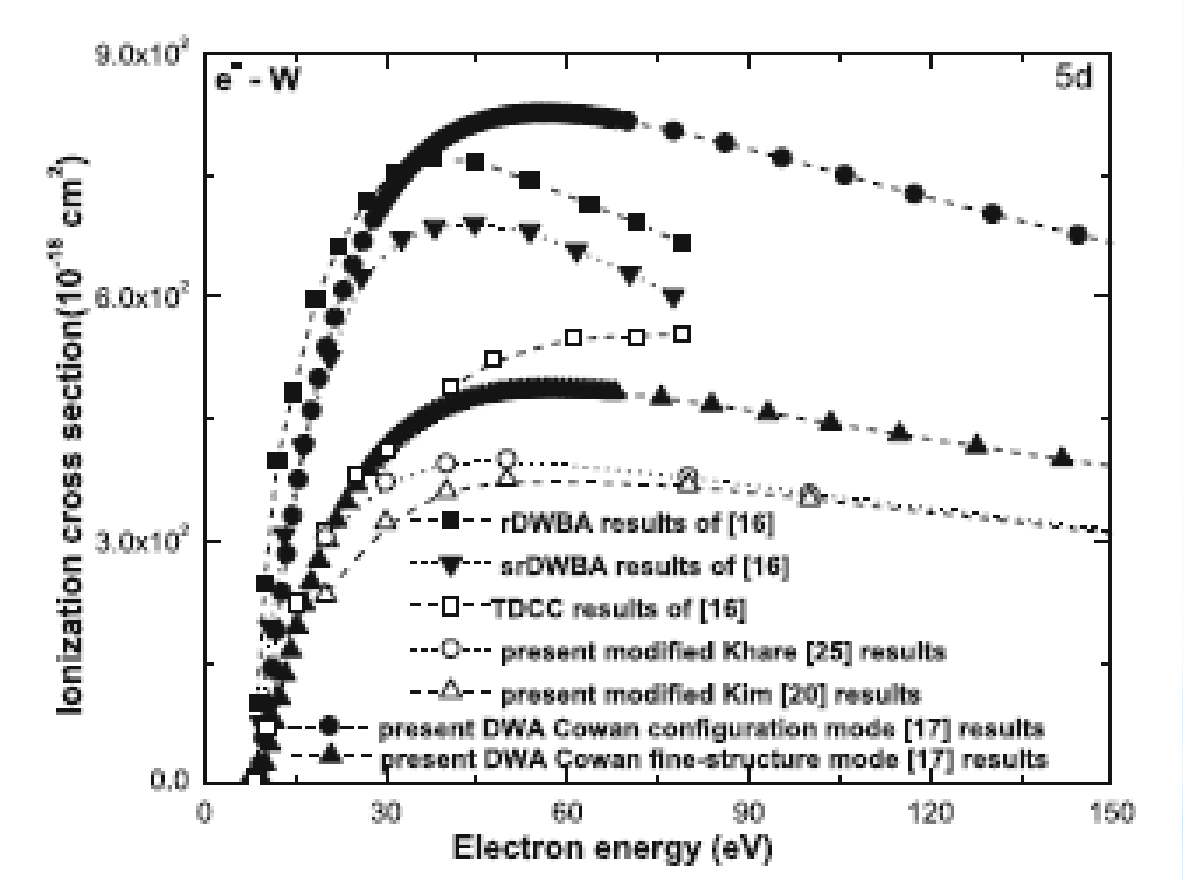
[5] G. Purohit, D. Kato and I. Murakami, Plasma and Fusion Research 13, 3401026 (2018). [6]M. S. Pindzola, S. D. Loch and A. R. Foster, J. Phys. B: At. Mol. Opt. Phys. 50, 095201 (2017).[7] F. Blanco, F. Ferreira da Silva, P. Limao-Vieira and G. Garcia, Plasma Sources Sci. Technol. 26, 085004 (2017).[8] B. Goswami, R. Naghma and B. Antony, Int. J. Mass Spectrom. 8, 372 (2014).[9]Y.K. Kim and M.E. Rudd, Phys. Rev. A 50, 3954–67 (1994).[10]S.P. Khare, M.K. Sharma and S. Tomar, J. Phys. B: At. Mol. Opt. Phys. 32, 3147 (1999).

Results – Ionization cross sections for W atoms



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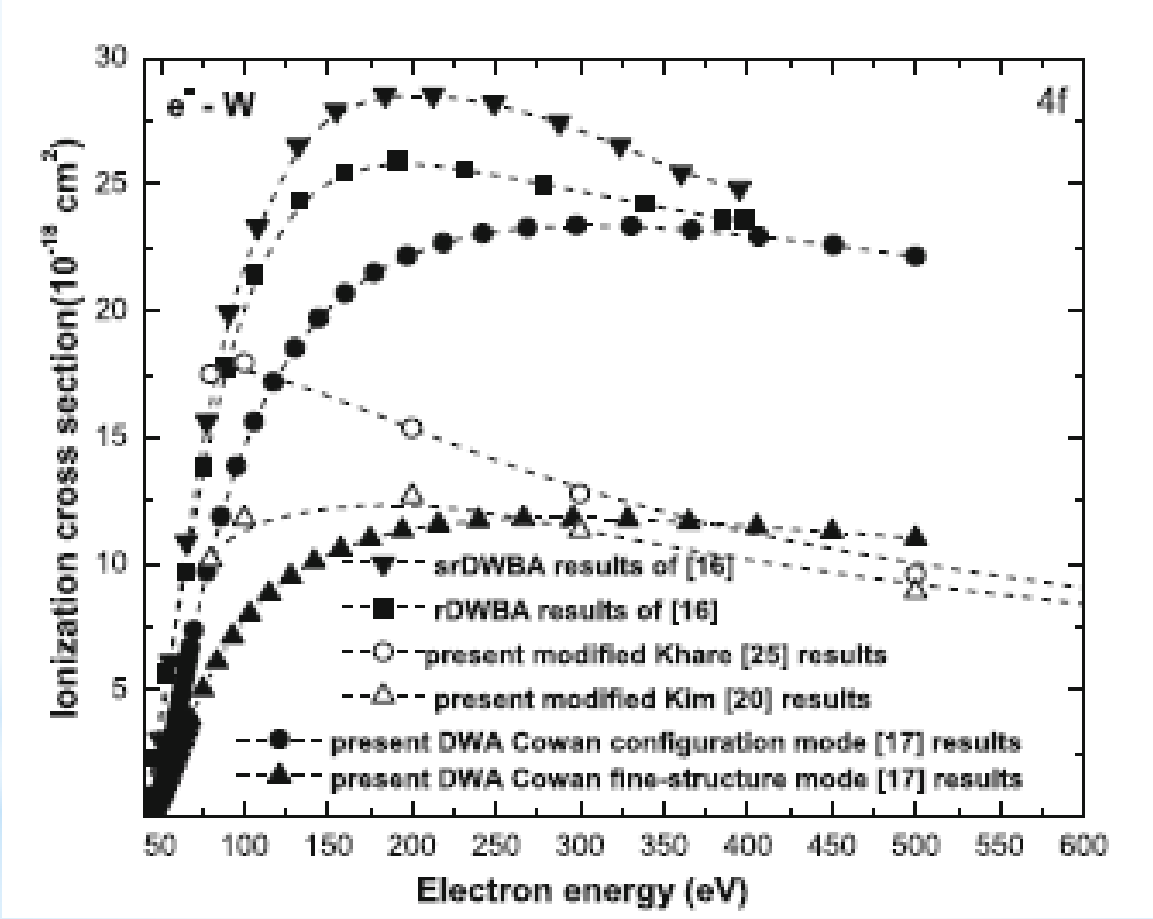
Results – Ionization cross sections for W atoms

Ionization cross sections of W atom 4f subshell



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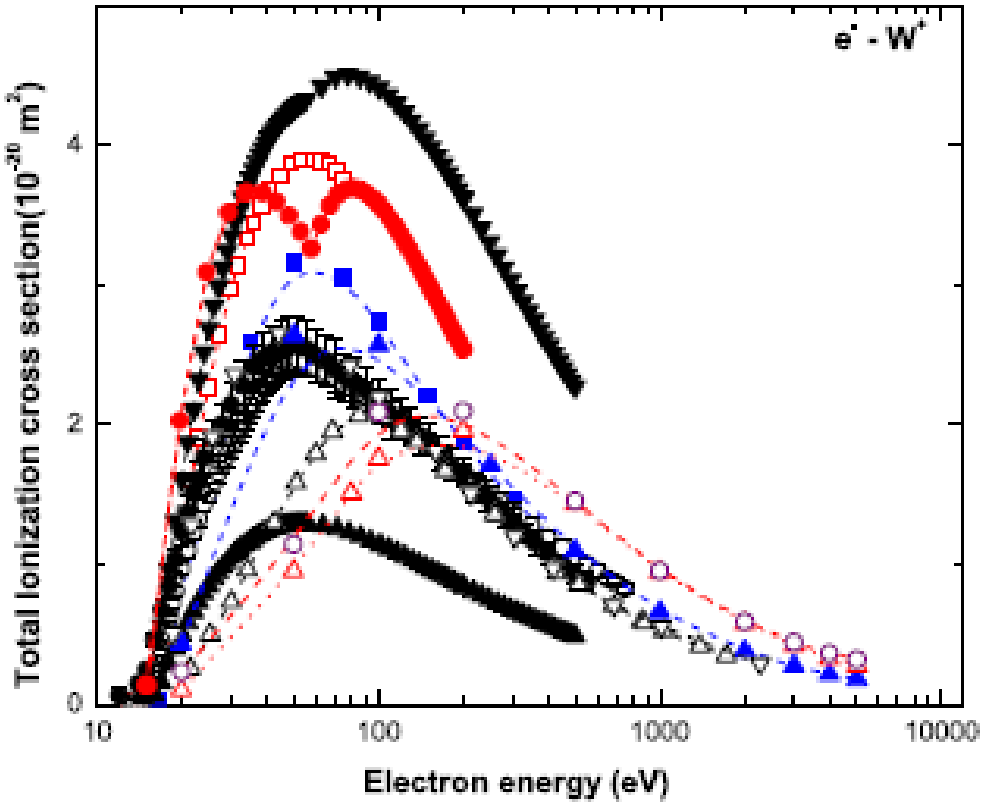
Results – Ionization cross sections for W^+ ions



Red solid circles: DWA results in HULLAC [Plasm. Fus. Res. **13,** 3401026 (2018)], black solid up- and down- triangles: DWA results in Cowan formalism with fine-structure and configuration mode [Plasm. Fus. Res. **13,** 3401026 (2018)]; blue solid squares: results of [J. Phys. B At. Mol. Opt. Phys. **44, 125201 (2011)**] and red hollow squares: results of [Phys. Rev. A **46, 2486** (1992)], Red hollow up triangles: present results in modified Kim [Phys. Rev. **A50, 3954-67 (1994)**] and purple hollow circles: present modified Khare [J. Phys. B At. Mol. Opt. Phys. **32, 3147 (1999)**] results;

solid black circles: measurements [J. Phys. B At. Mol. Opt. Phys. **28, 4853** (1995)]; black hollow circles: measurements [J. Phys. B At. Mol. Opt. Phys. **17, 2707 (1984)**]; blue up triangles: results of [Int. J. Mass Spectrom. **252, 213 (2006)**], black hollow up triangles: results of [Phys. Rev. A **20, 445 (1979)**] and black hollow down triangles: results of [Z. Phys. **216, 241 (1968)**]

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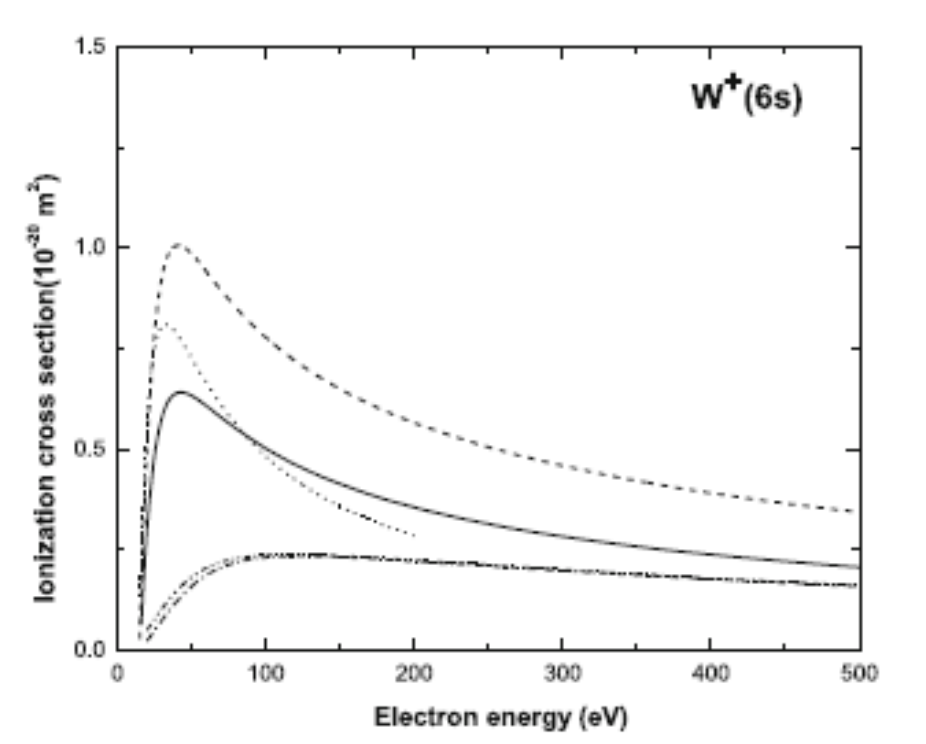
Results - Ionization cross sections for W^+ ions



Dotted Curve: DWA results in HULLAC [Plasm. Fus. Res. **13,** 3401026 (2018)],

Solid and dashed curves: DWA results in Cowan formalism with fine-structure and configuration mode [Plasm. Fus. Res. **13,** 3401026 (2018)];

Dash dotted line: present results in modified Kim [Phys. Rev. **A50, 3954-67 (1994)**] and Dash dot dotted line: present modified Khare [J. Phys. B At. Mol. Opt. Phys. **32, 3147 (1999)**] results;

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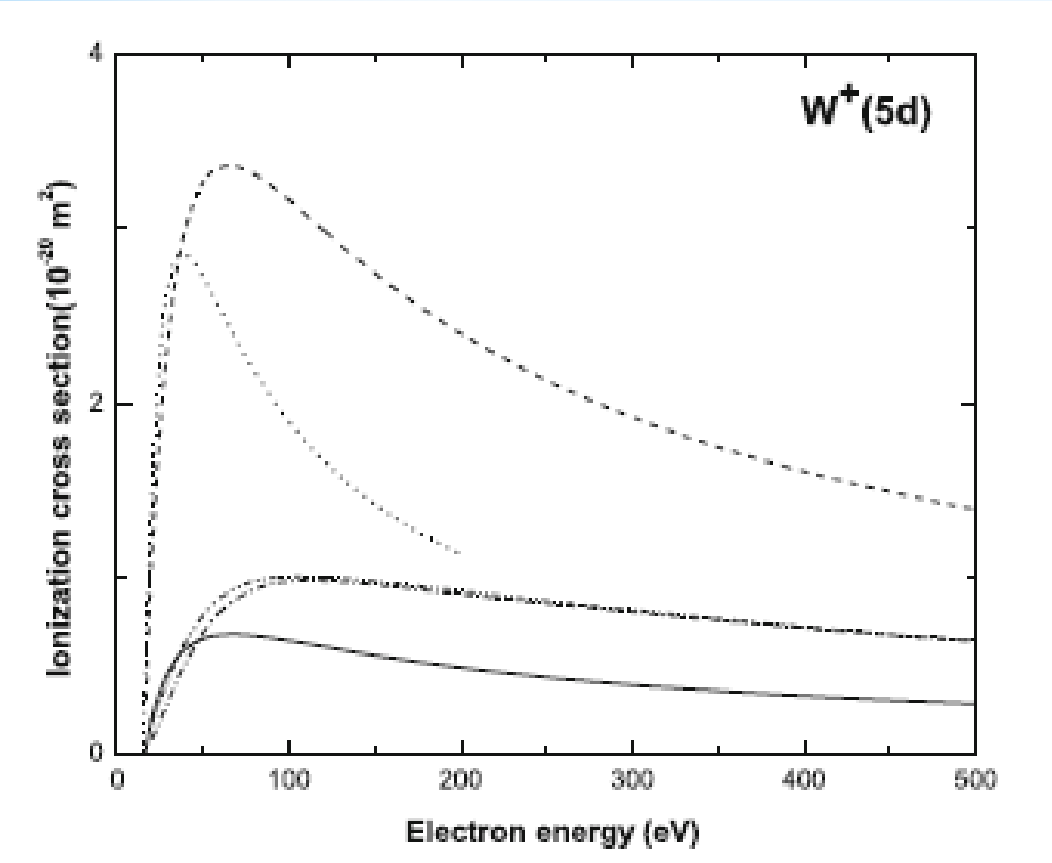
Results - Ionization cross sections for W^+ ions



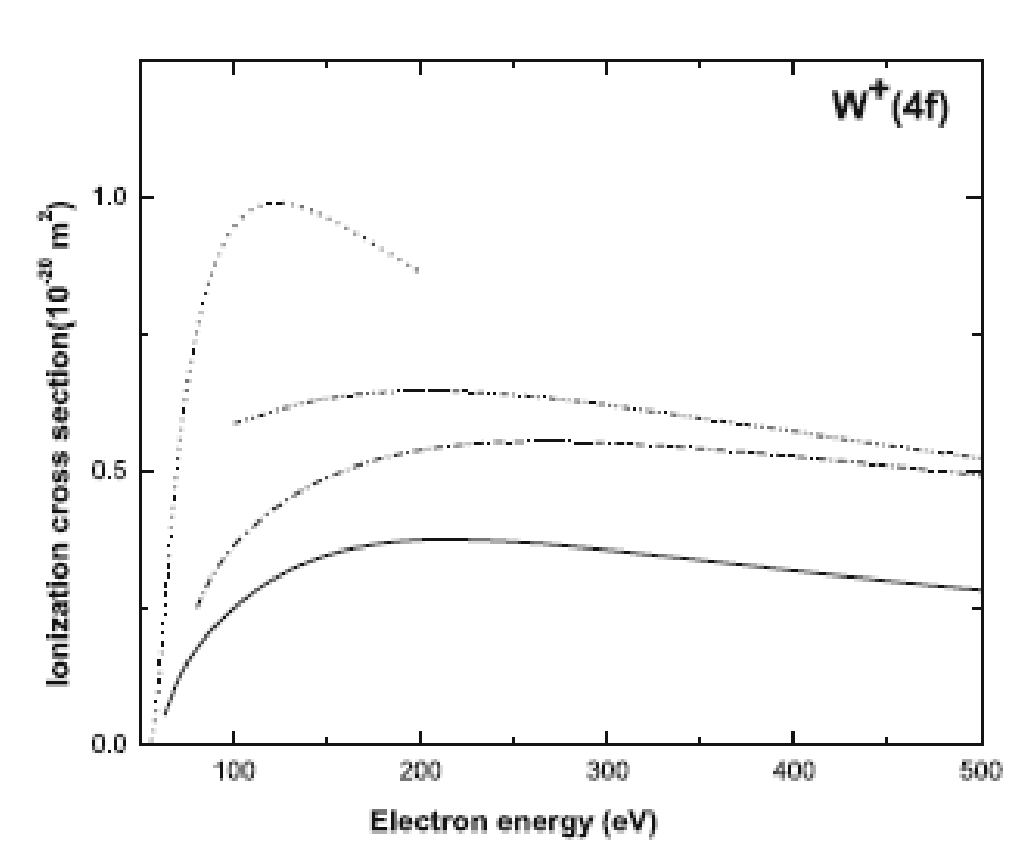
Dotted Curve: DWA results in HULLAC [Plasm. Fus. Res. **13,** 3401026 (2018)],

Solid and dashed curves: DWA results in Cowan formalism with fine-structure and configuration mode [Plasm. Fus. Res. **13,** 3401026 (2018)];

Dash dotted line: present results in modified Kim [Phys. Rev. **A50, 3954-67 (1994)**] and Dash dot dotted line: present modified Khare [J. Phys. B At. Mol. Opt. Phys. **32, 3147 (1999)**] results;

Purohit, Kato and Murakami, et al. Eur. Phys. J. D 75, 219 (2021)

Results - Ionization cross sections for W^+ ions



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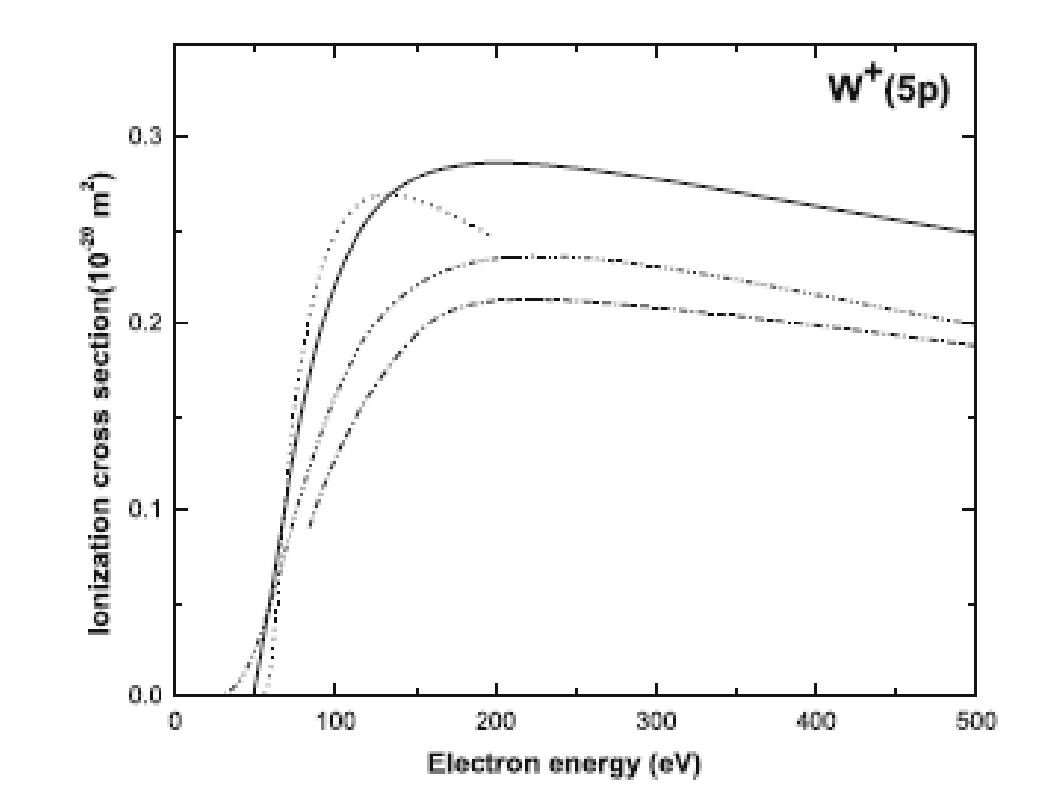
Purohit, Kato and Murakami, et al. Eur. Phys. J. D 75, 219 (2021)

Results - Ionization cross sections for W^+ ions



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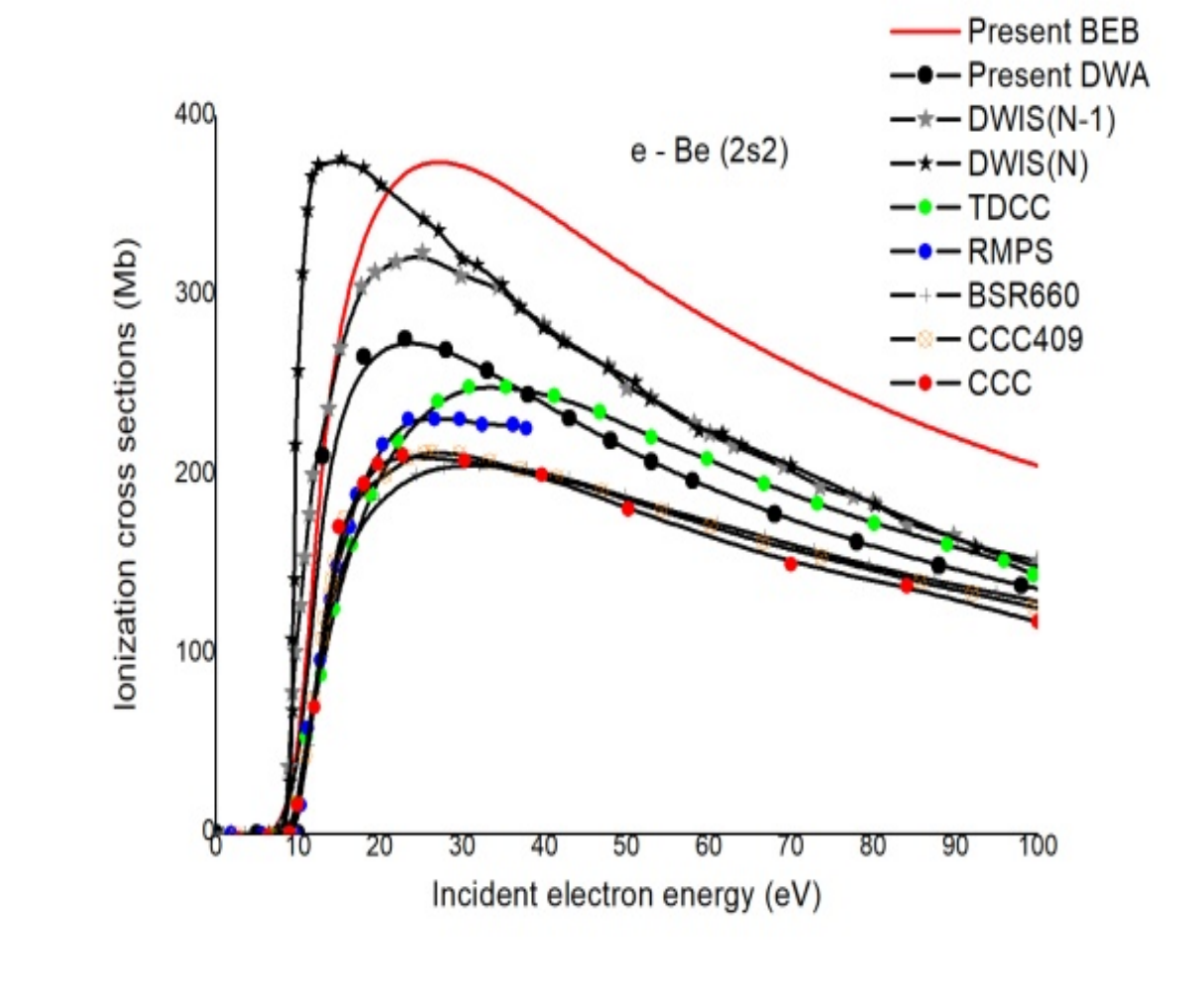
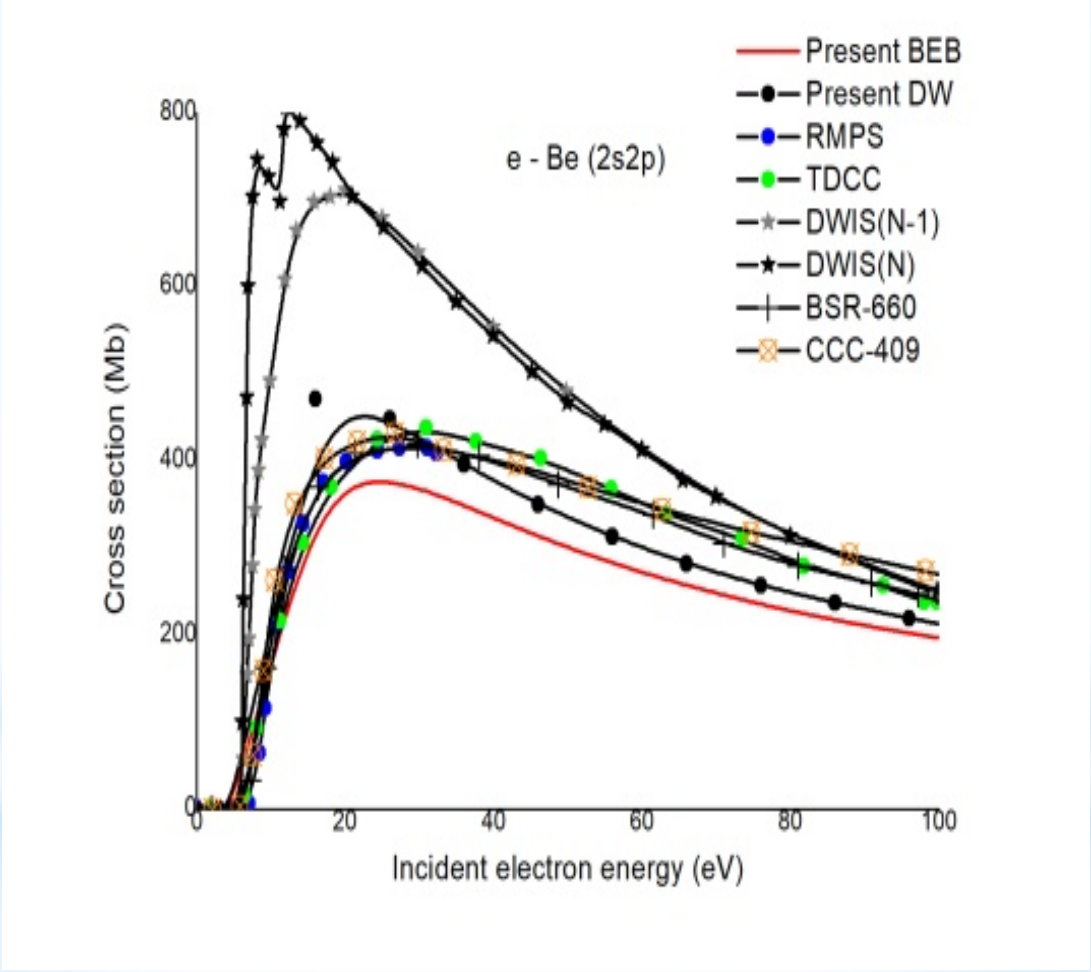
Purohit, Kato and Murakami, et al. Eur. Phys. J. D 75, 219 (2021)

Results - Ionization cross sections for Be ($1s^2$, $2s^2$)



Results - Ionization cross sections for Be ($1s^2 2s2p$)



Molecular targets – Difficulties?

A significant challenge - distributed nuclei.

Contrasts to atoms which have a single nuclear scattering centre - can be described using a spherical basis.

Molecular wave-functions - generally not spherical, the nuclei within the molecule providing multiple scattering centres.

Molecular targets – Difficulties?

So, there is a key challenge in developing an accurate multi-centered wave-function.

A further challenge arises - difficult to align the molecules (experimentally) prior to the collision, so the models must consider the random orientation of the targets for accurate comparison.

This becomes a computationally intensive problem, and so approximations are usually made to allow these calculations to become tractable.

TDCS for Molecules - DWBA with OAMO

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

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

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

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

$\psi^{OA}(r_2)$ is the initial bound state wave function for the molecular target which is approximated as the orientation averaged molecular orbital

The molecular wave functions for N_2 molecule have been calculated using the density functional theory with B3LYP/TZ2P basis set
[C. Lee, W. Yang and R. G. Parr, Phys. Rev. B 37, 785 (1988)]

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 post collision interaction (PCI) has been calculated using the Ward-Macek factor (M_{ee})

$$M_{ee} = N_{ee}\left|{}_1F_1(-i\lambda_3,1,-2k_3r_{3ave})\right|^2,$$

where

$$Nee = \frac{\gamma}{e^{\gamma}-1} \qquad \gamma = -\frac{2\pi}{|k_1-k_2|} \qquad \lambda_3 = -\frac{1}{|k_1-k_2|} \qquad r_{3ave} = \frac{\pi^2}{16\varepsilon}\left(1+\frac{0.627}{\pi}\sqrt{\varepsilon}\ln\varepsilon\right)^2$$

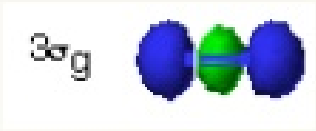
$$\varepsilon = \left(k_1^2 + k_2^2\right)/2$$

The TDCS expression including PCI

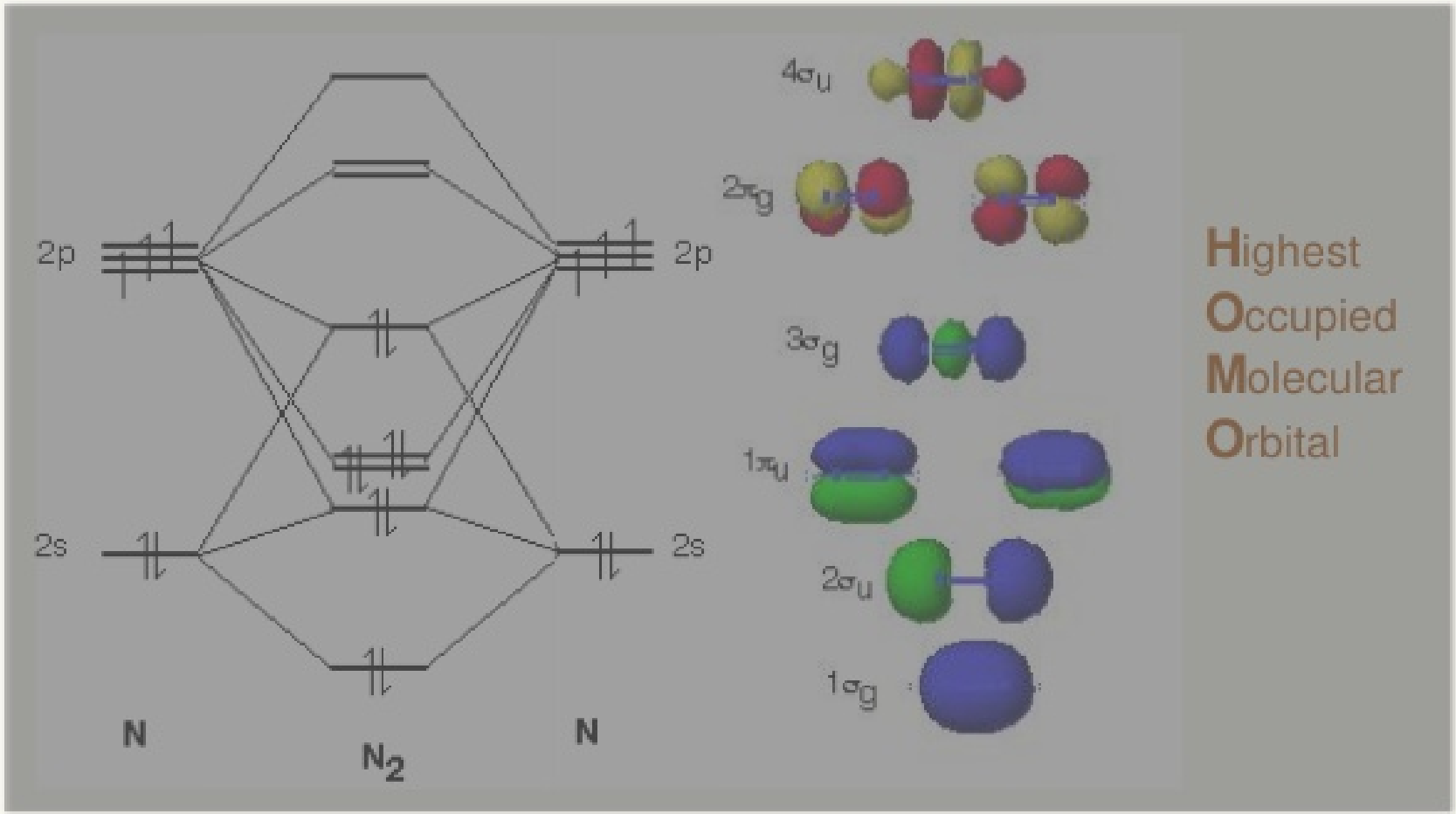
$$\frac{d^3\sigma}{d\Omega_1\, d\Omega_2\, dE_1} = M_{ee}(2\pi)^4 \frac{k_1 k_2}{k_0} \sum_{m=-l}^{l}\left(\left|f_{nlm}\right|^2 + \left|g_{nlm}\right|^2 - Re\left(f_{nlm}^{*}\, g_{nlm}\right)\right)$$

S. J. Ward and J. H. Macek, *Phys. Rev. A*49, 1049 (1994).

MOLECULAR ORBITALS OF NITROGEN

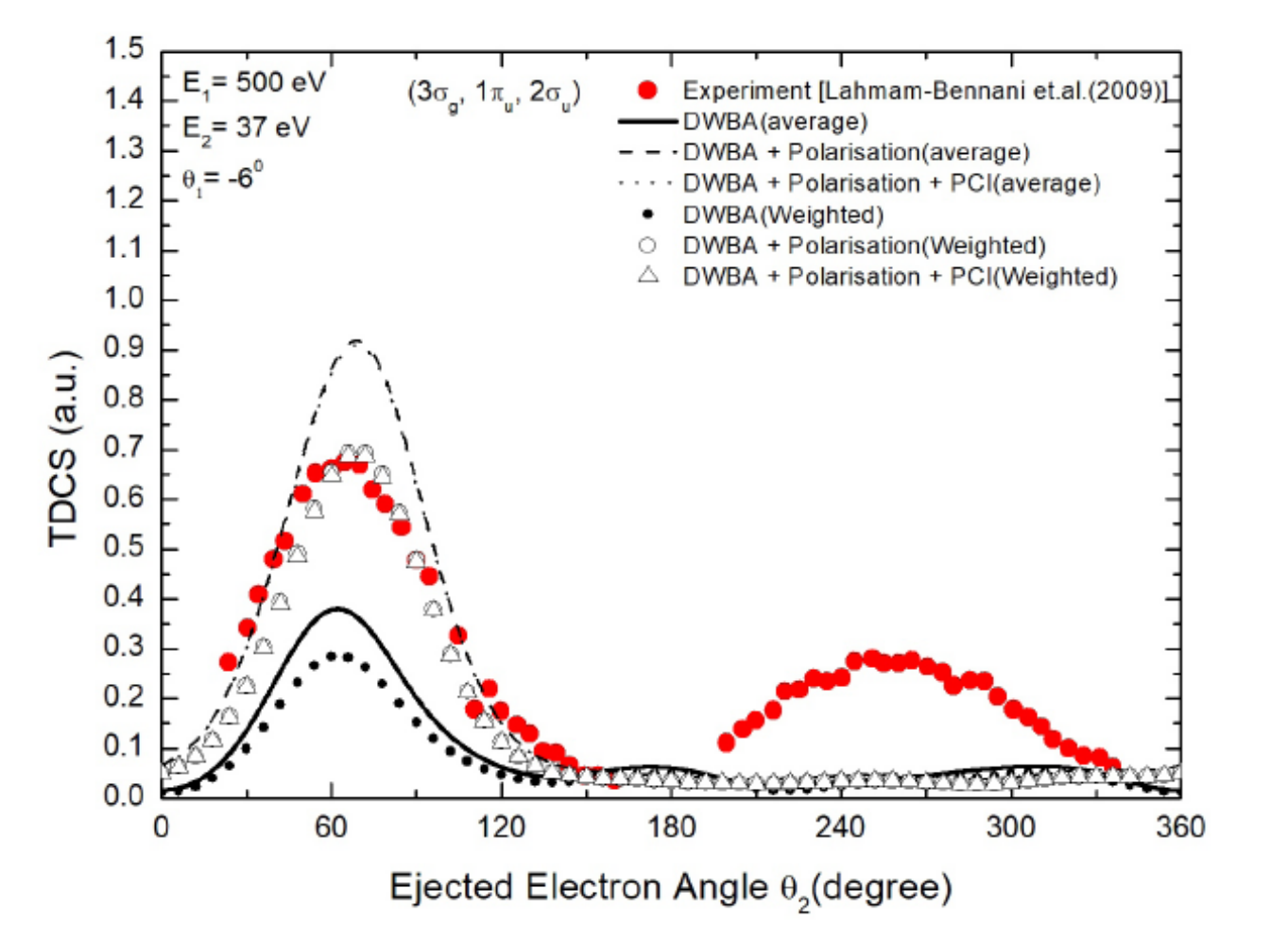


N_2 HOMO



Siriwardane. CHEM 281, *LA Tech*. www.chem.latech.edu (accessed 11 Oct. 2013).

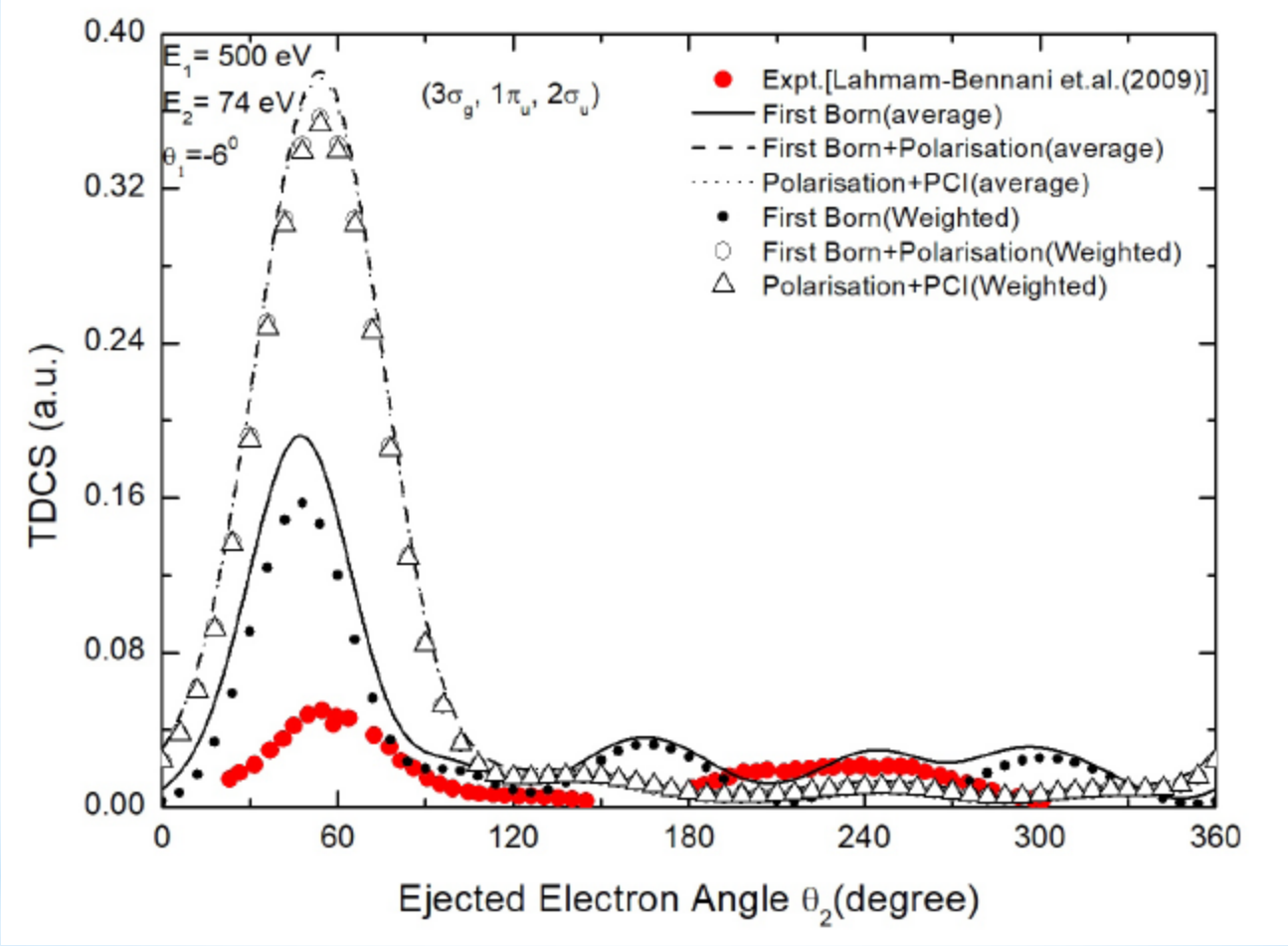
Results – Differential cross sections; N_2 molecules



Electron-impact TDCS for N2 molecule calculated for the weighted and average sum of the outer orbital $(3\sigma_g, 1\pi_u, 2\sigma_u)$. *The ejected electron energy is 37 eV. Kinematics and legends used are* displayed in the figure frame.

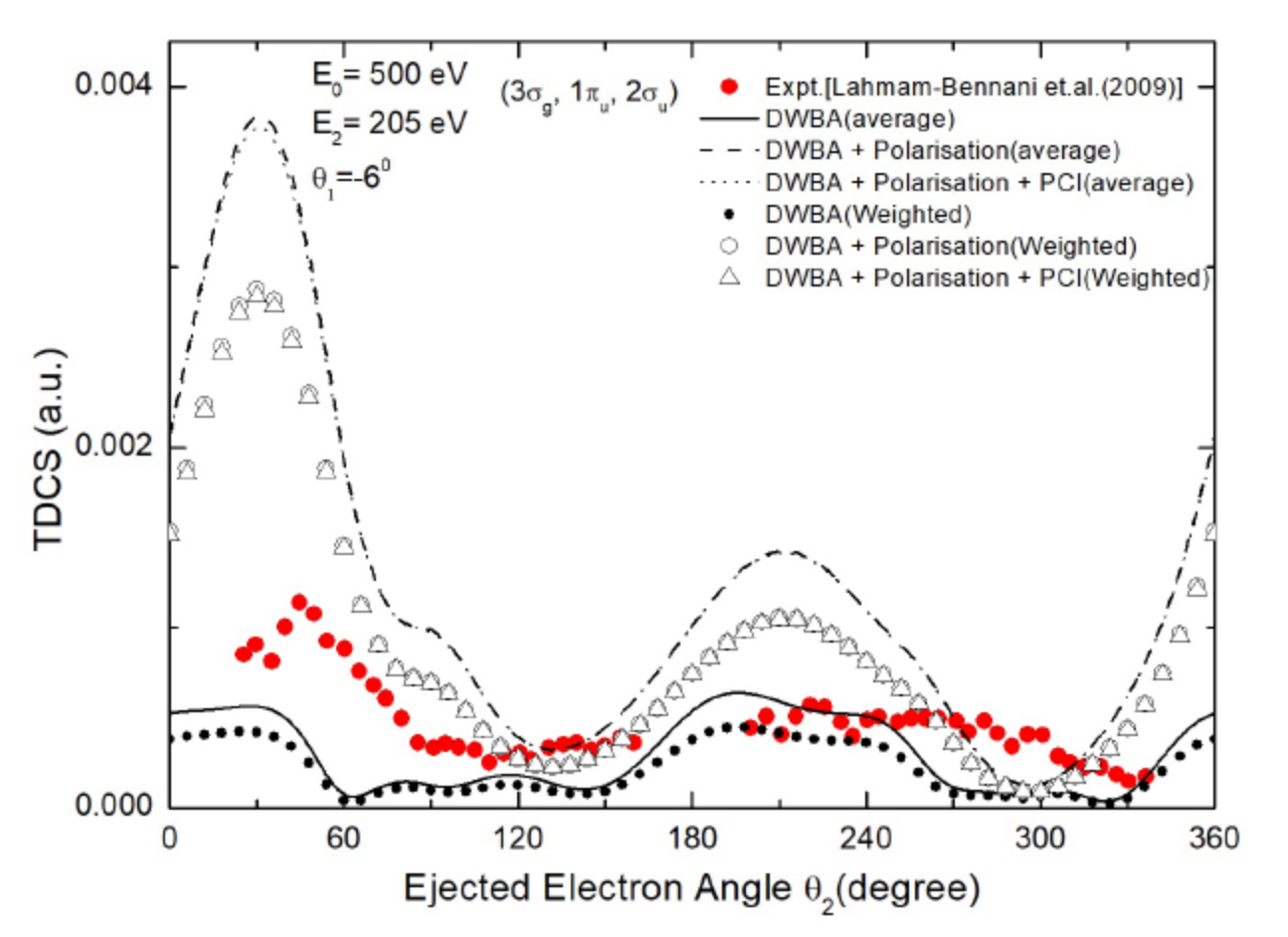
Pandey and Purohit Atoms 10 (2), 50 (2022)

Results - Differential cross sections; N_2 molecules



Electron-impact TDCS for N2 molecule calculated for the weighted and average sum of the outer orbital $(3\sigma_g, 1\pi_u, 2\sigma_u)$. *The ejected electron energy is 74 eV. Kinematics and legends used are* displayed in the figure frame.

Results - Differential cross sections; N_2 molecules



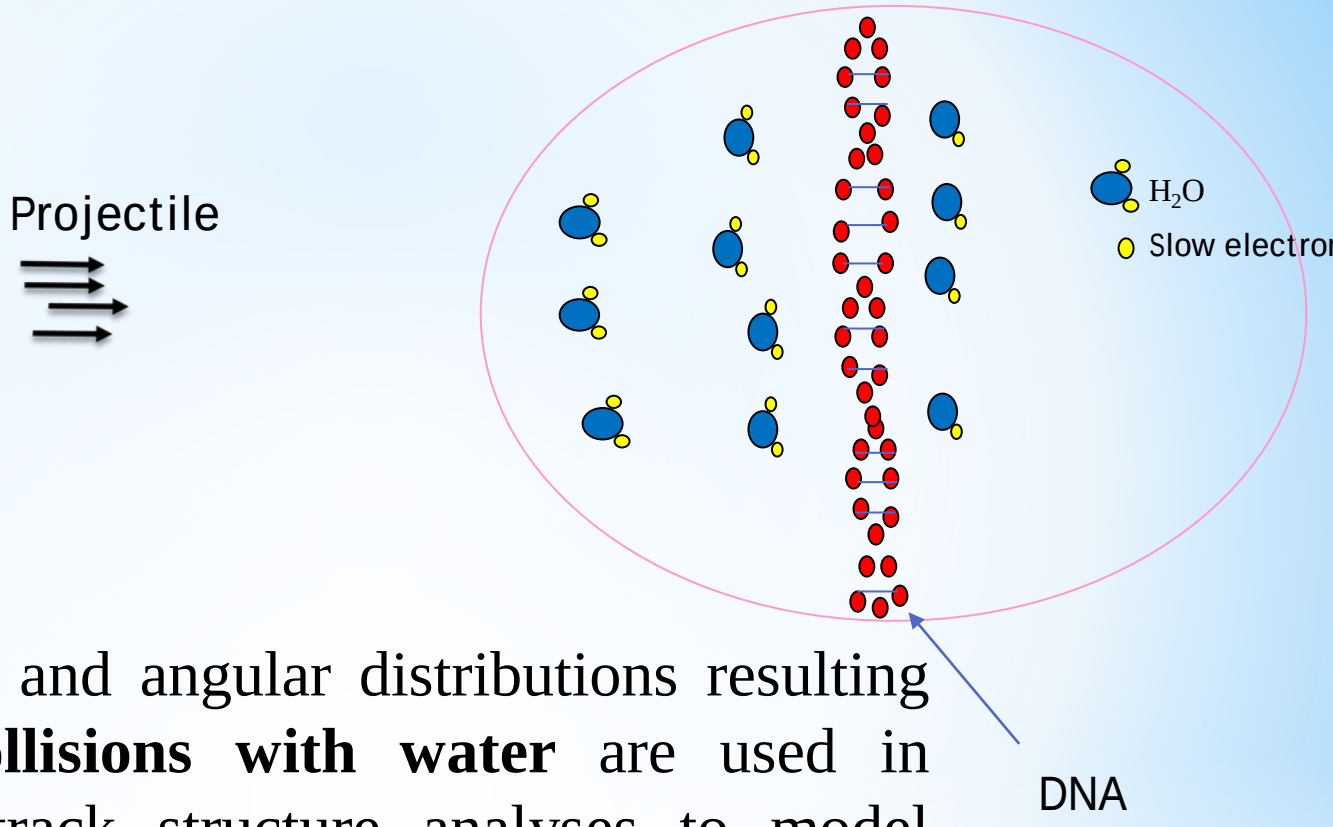
Electron-impact TDCS for N2 molecule calculated for the weighted and average sum of the outer orbital $(3\sigma_g, 1\pi_u, 2\sigma_u)$. *The ejected electron energy is 205 eV. Kinematics and legends used are* displayed in the figure frame.

Water Molecule

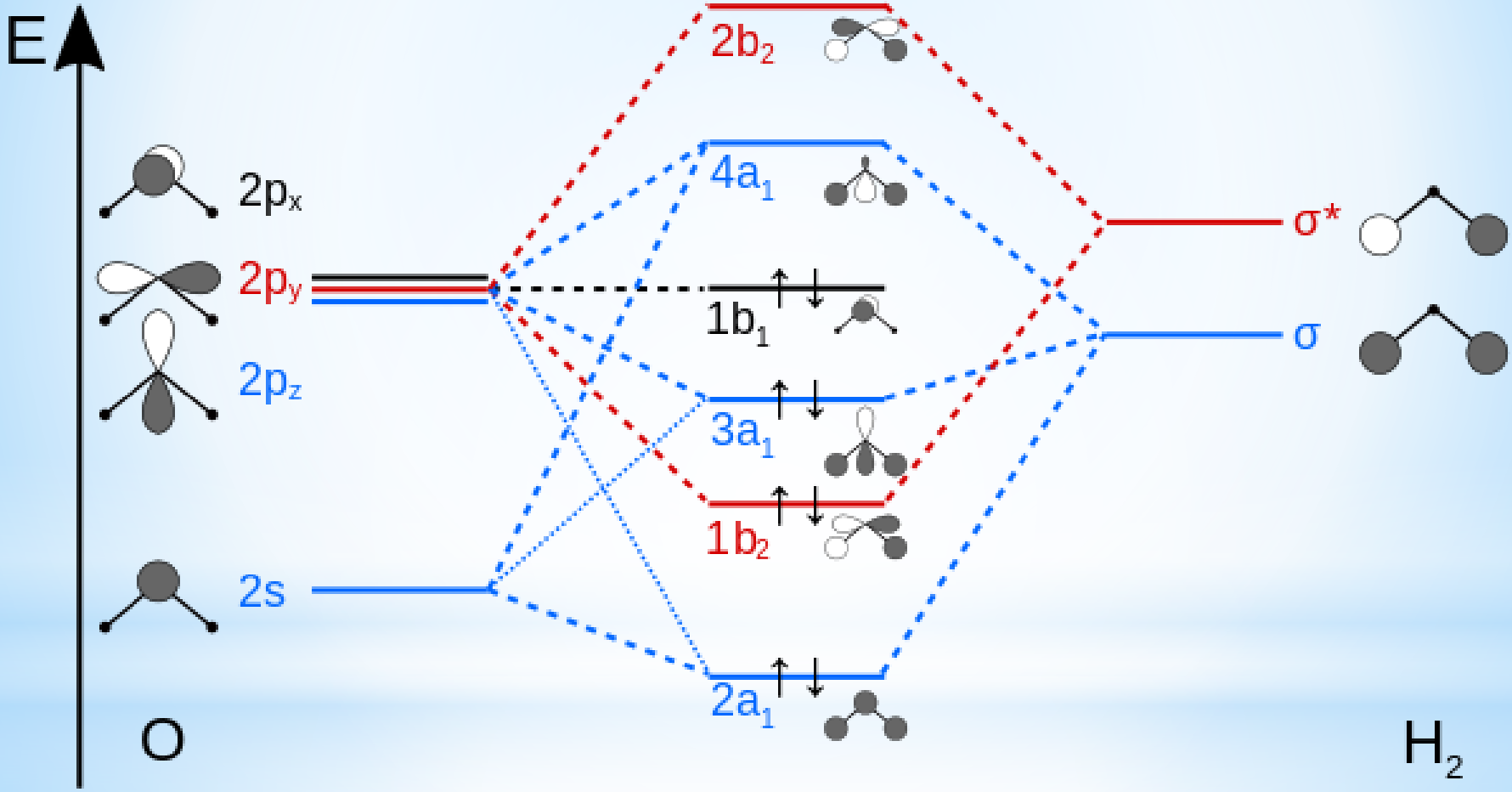
The third most abundant molecule on the earth - Of great importance in numerous multi-disciplinary research fields;

* Radiobiology where it is commonly used as surrogate of the living matter, the latter being composed of water for about 60% in mass.
* Energetic and angular distributions resulting from electron-induced collisions with water molecules are commonly used in charged particle track structure codes for modeling the radio-induced damages in biological samples.

* Particularly, the knowledge of the collision dynamics of low-energy electrons with biological systems remain crucial so as to develop robust numerical models of charged particle tracking in biological matter.



Energy deposition and angular distributions resulting from **electron collisions with water** are used in charged particle track structure analyses to model radiation damage in biological samples. These models are an active area of research since the observation that **high energy radiation that is used to treat cancers also liberates many low energy electrons, causing additional damage to cell DNA.**


E
2p_x
2p_y
2p_z
2s
O
2b_2
4a_1
1b_1
3a_1
1b_2
2a_1
σ*
σ
H_2

The TDCS in terms of second Born approximation is given as

$$\frac{d^3\sigma}{dk_f dk_e dE_e} = (2\pi)^4 \frac{k_f k_e}{k_i} \sum_{av} |f_{B1} + f_{B2}|^2,$$

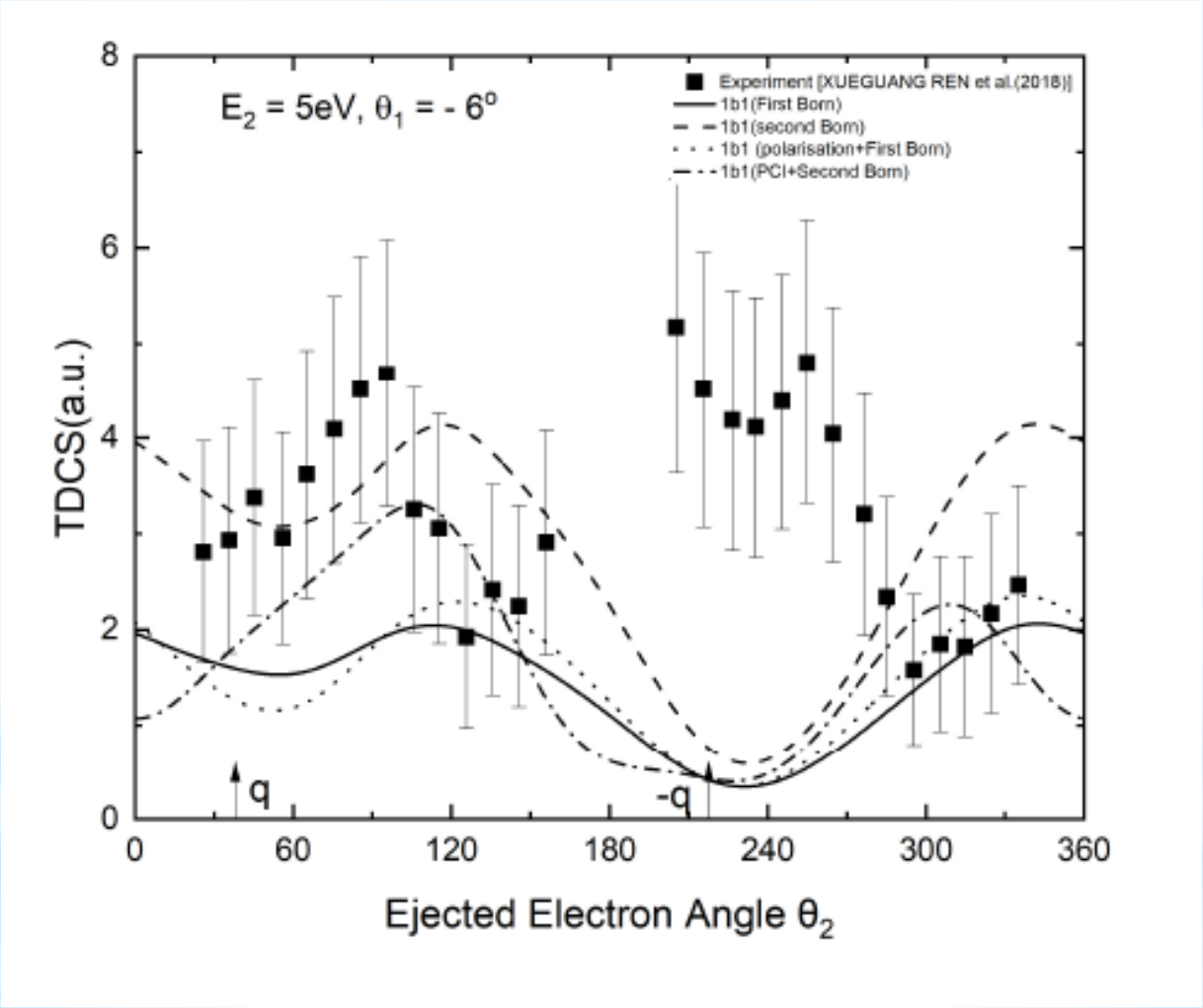
In DWBA, the first order term is calculated as follows:

$$f_{B1} = < \Psi_1(k_f, r_f)\Psi_2(k_e, r_i)| \pm \left(\frac{-Z}{r_f} - \frac{1}{|r_f - r_i|}\right)|\Phi_0(r_i)\Psi_i(k_i, r_f) >$$

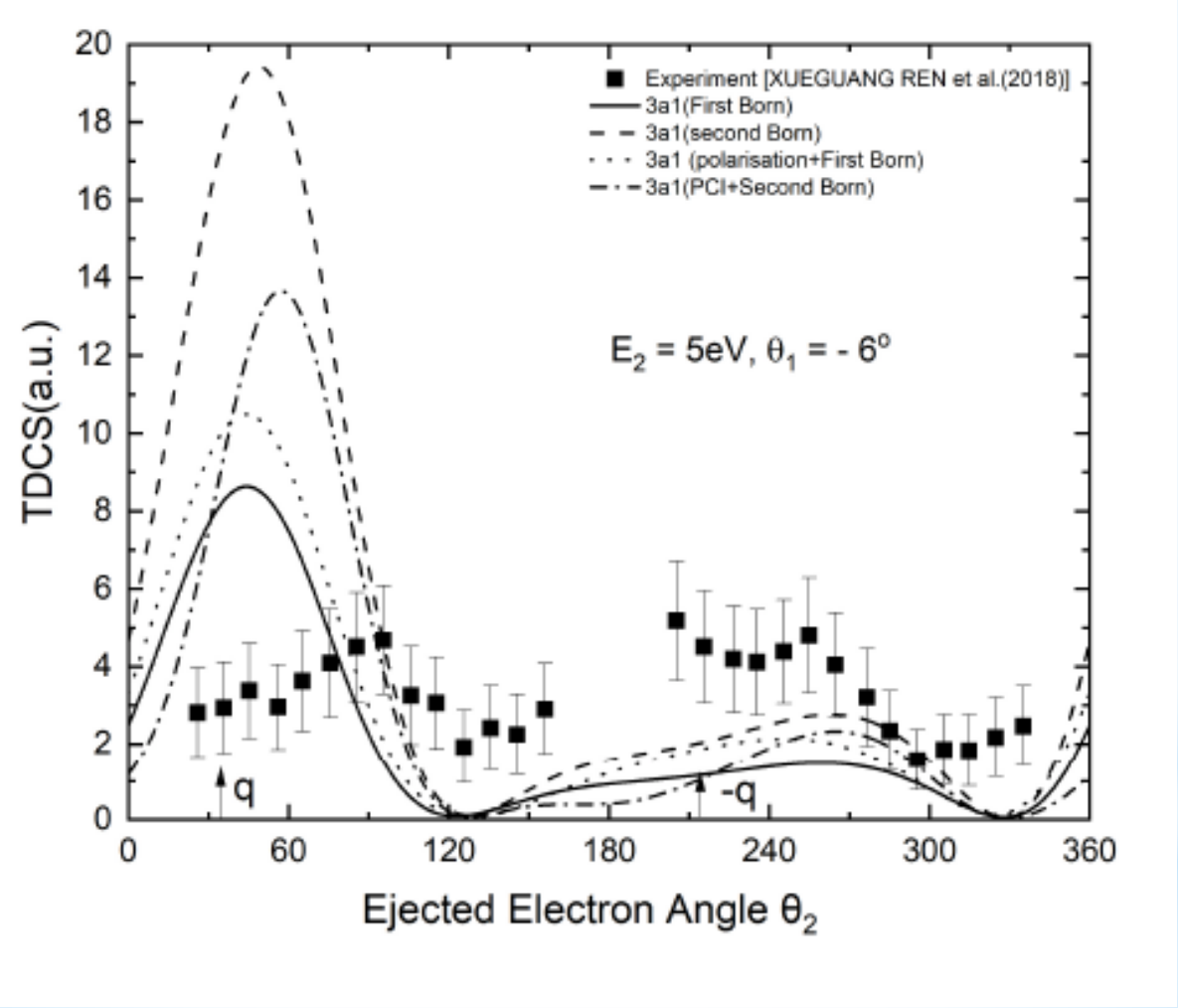
The second Born term in the DWBA is expressed by

$$f_{B2} = < \Psi^{(-)}(k_f, r_f)\Psi^{(-)}(k_e, r_i)|VG_0^+V|\Phi_0(r_i)\Psi_i^{(-)}(k_i, r_f) >$$

Results – Electron impact TDCS for H_2O molecules at 81 eV – Coplanar geometry



Results – Electron impact TDCS for H_2O molecules at 81 eV – Coplanar geometry



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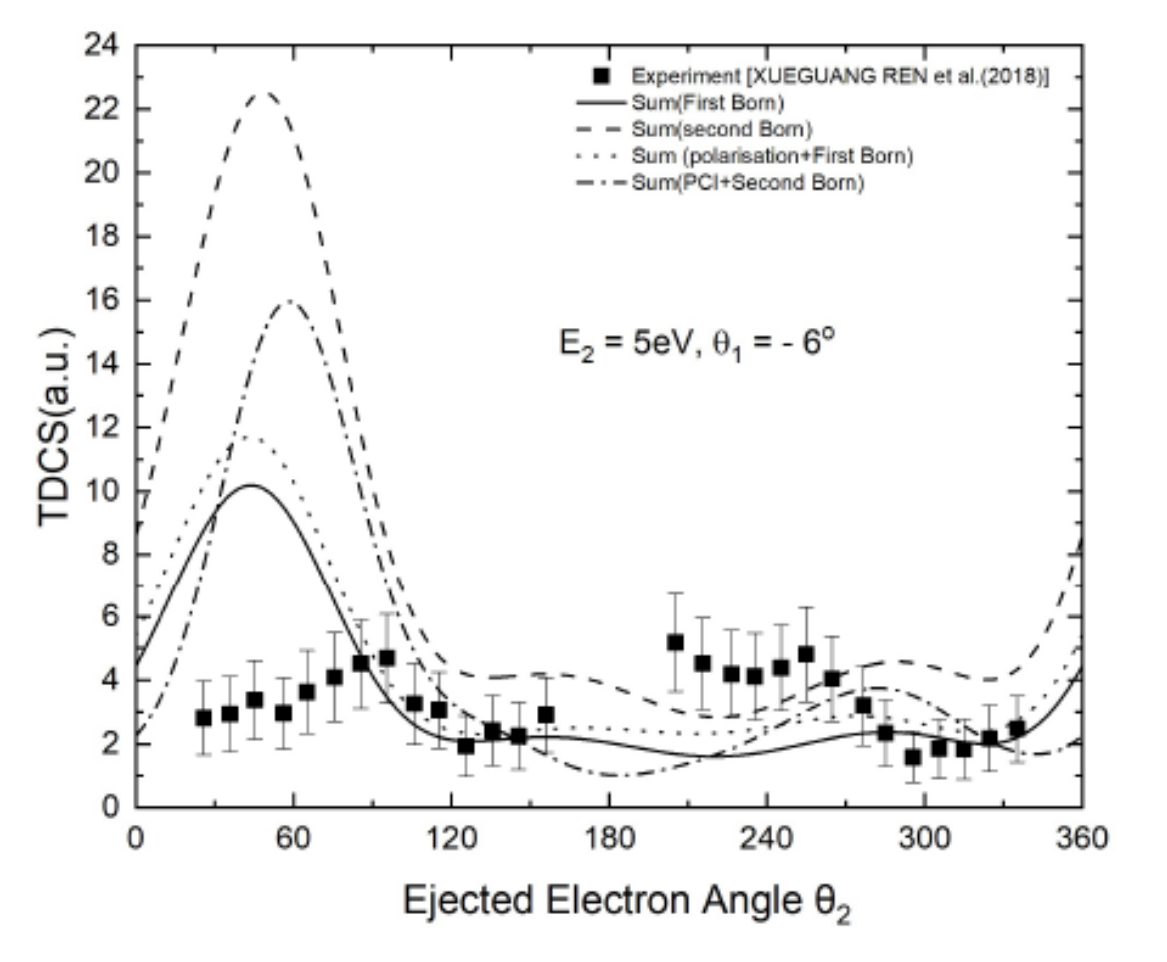

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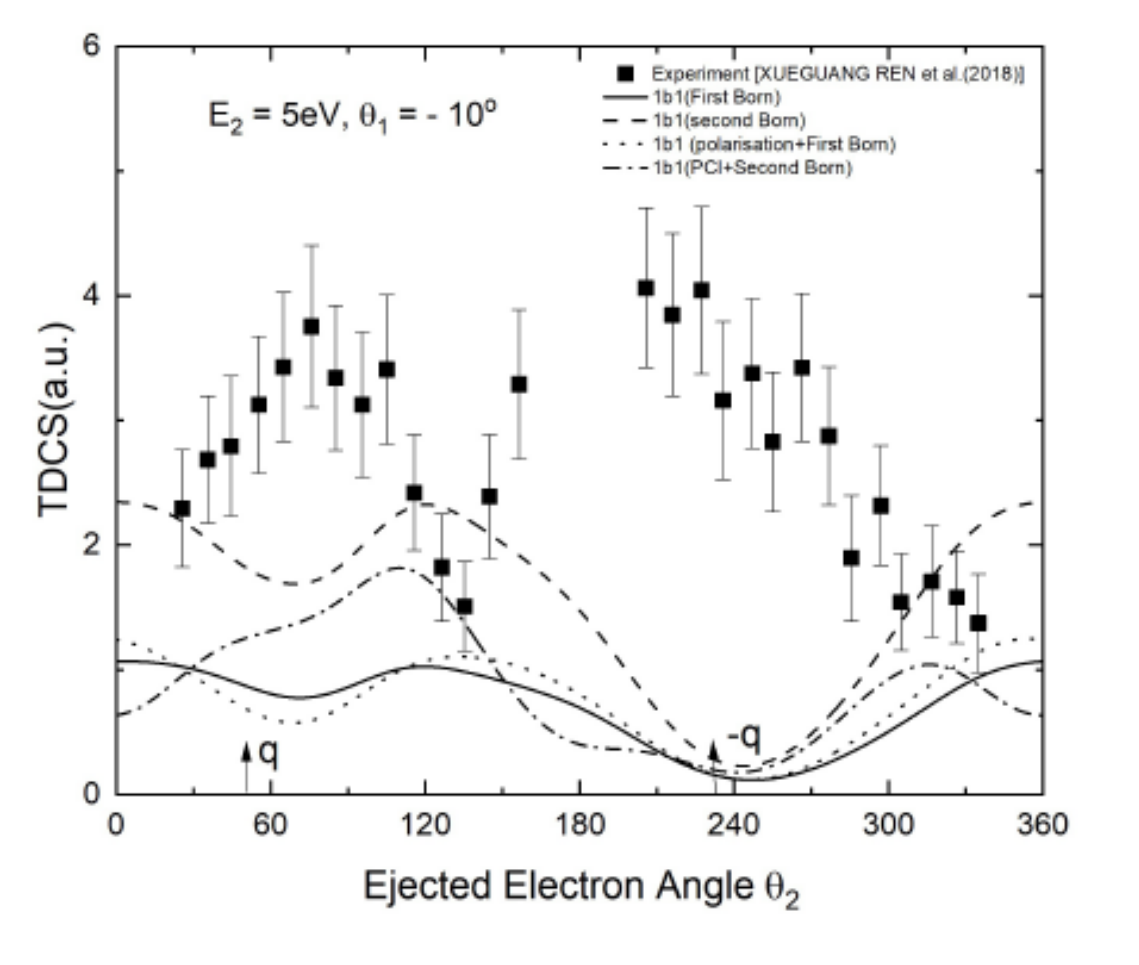
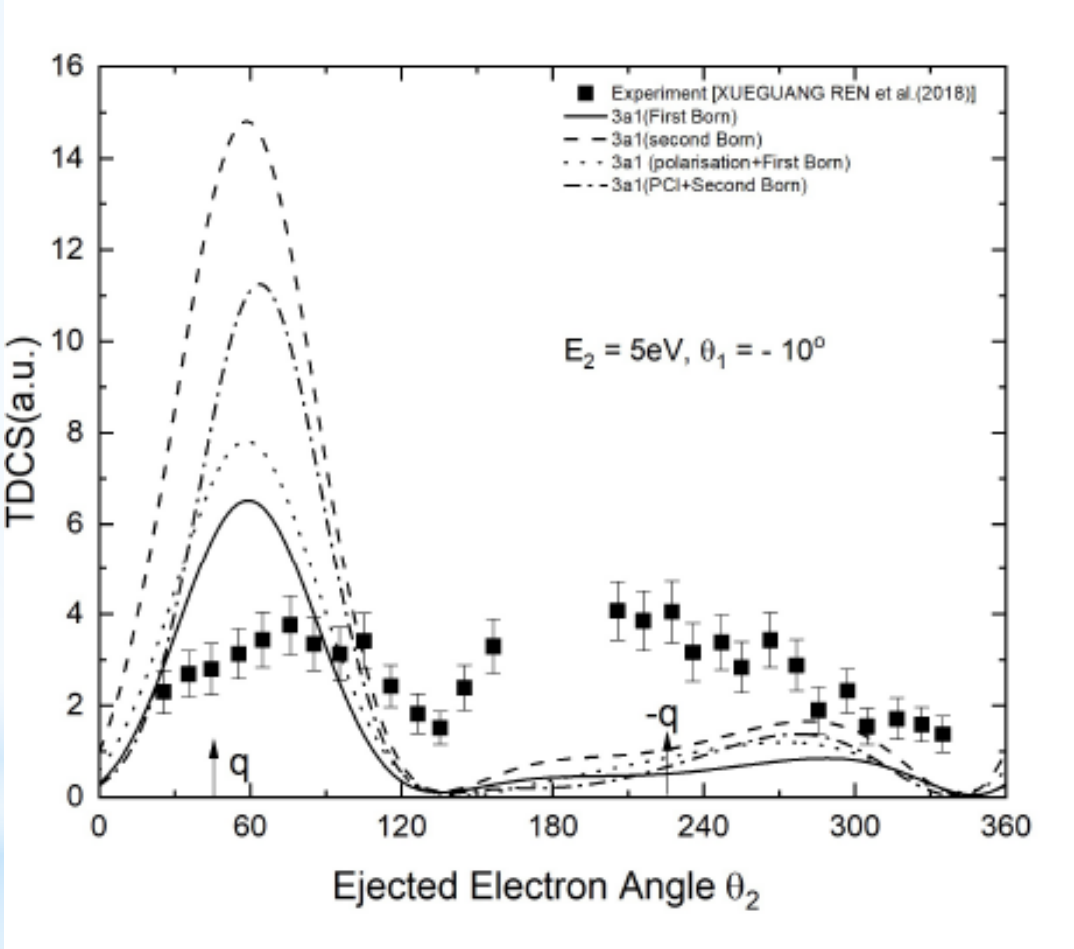
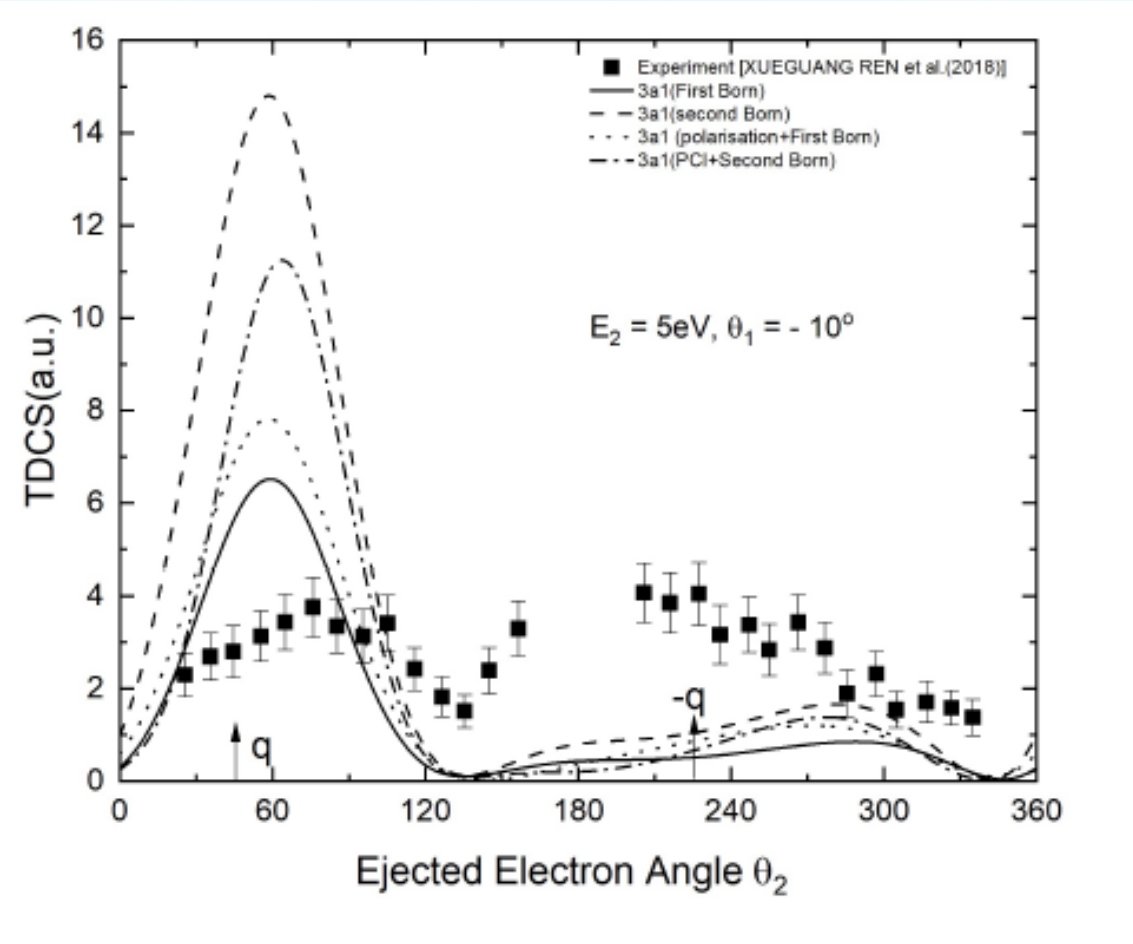


Results – Electron impact TDCS for H_2O molecules at 81 eV



Results – Electron impact TDCS for H_2O molecules at 81 eV



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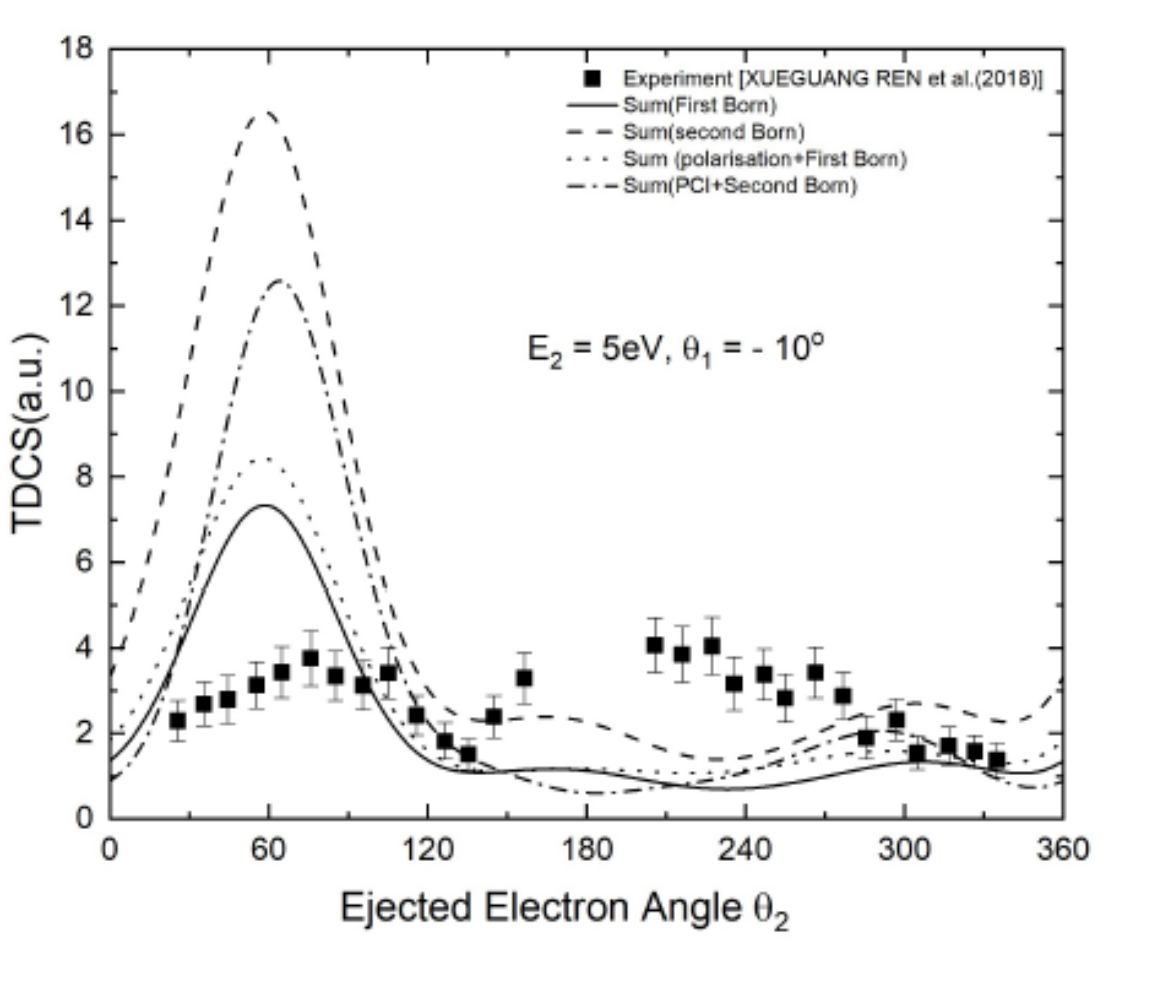

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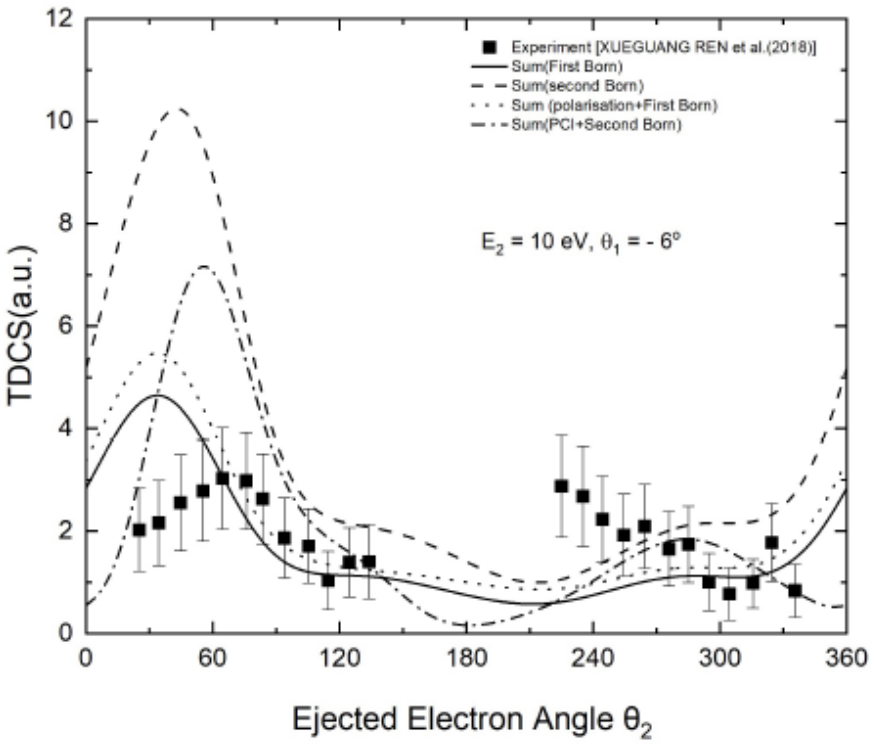
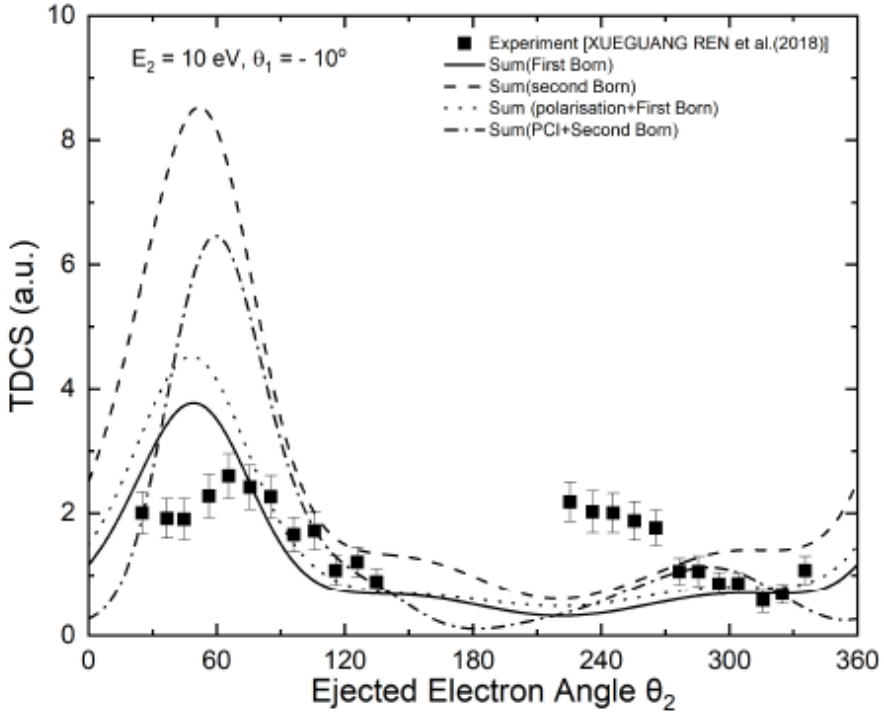
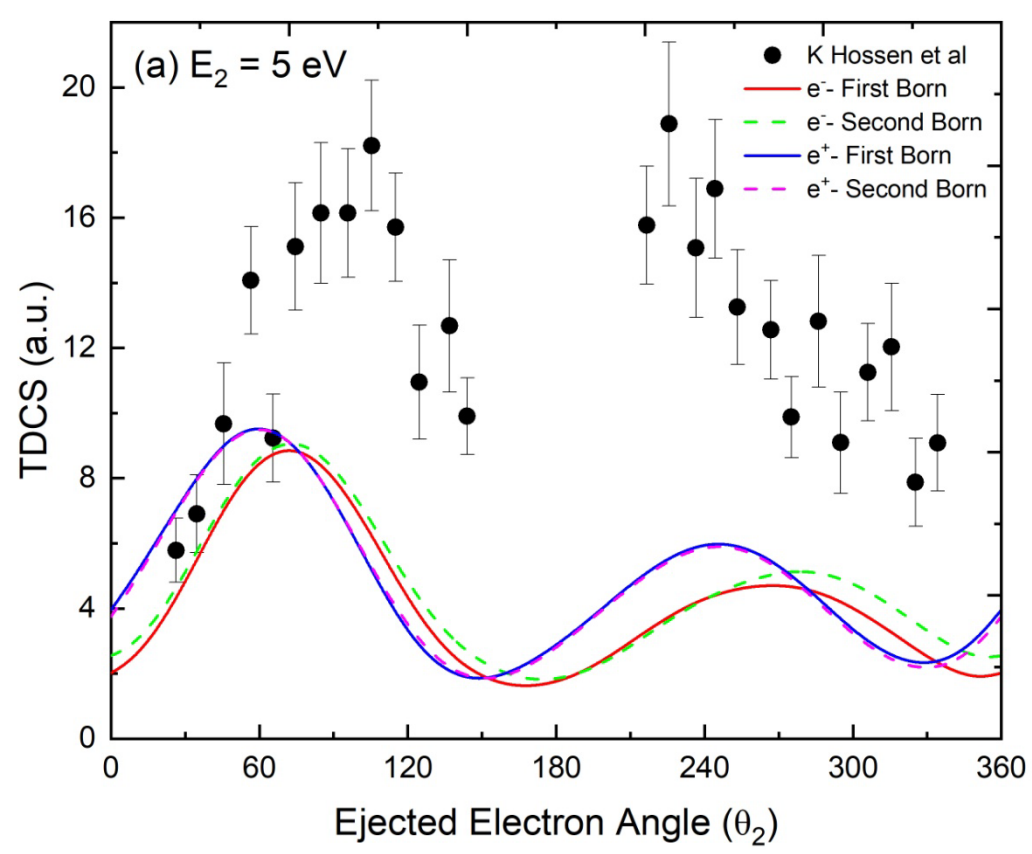




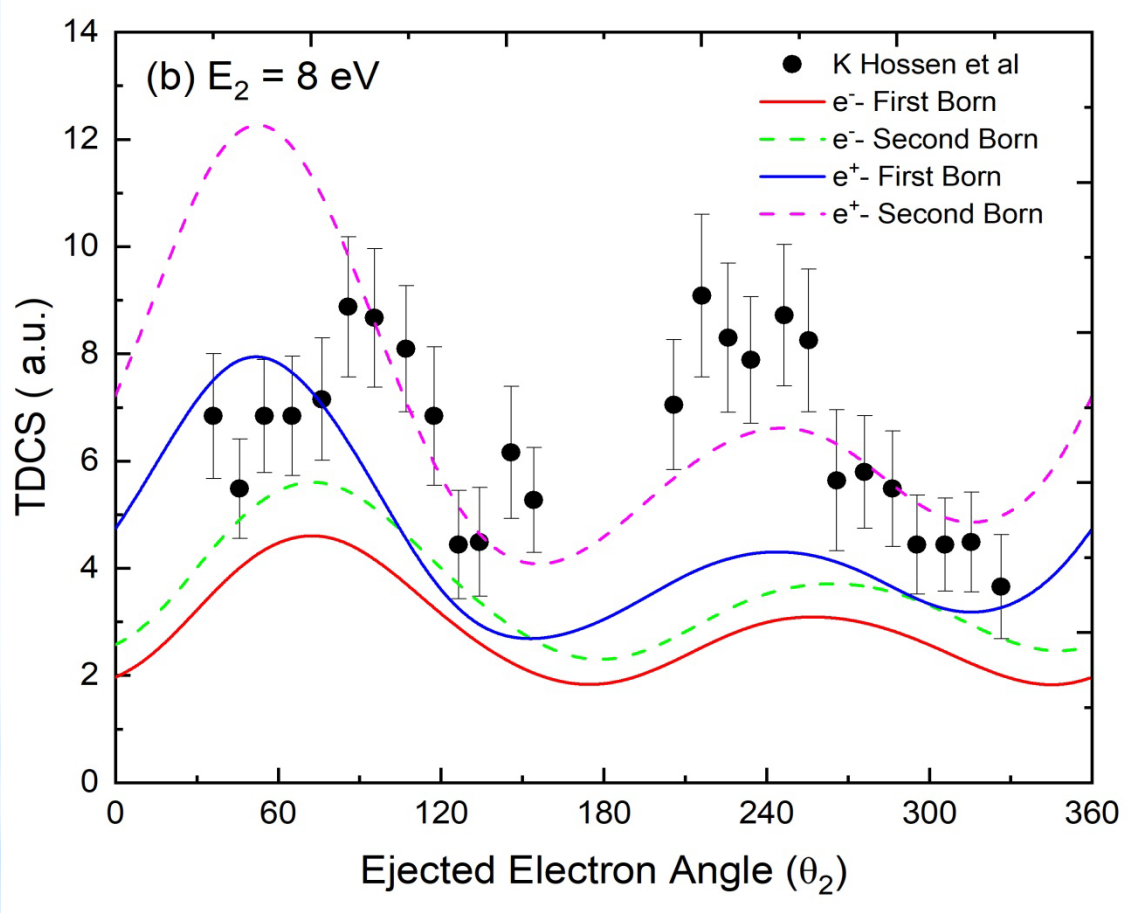
Exp. - X. Ren, S. Amami, K. Hossen, E. Ali, C. Ning, J. Colgan, D. Madison, and A. Dorn *Phys. Rev. A* ***95***, 022701(2017)

Results – Electron and positron impact TDCS for CO_2 molecules at 100 eV



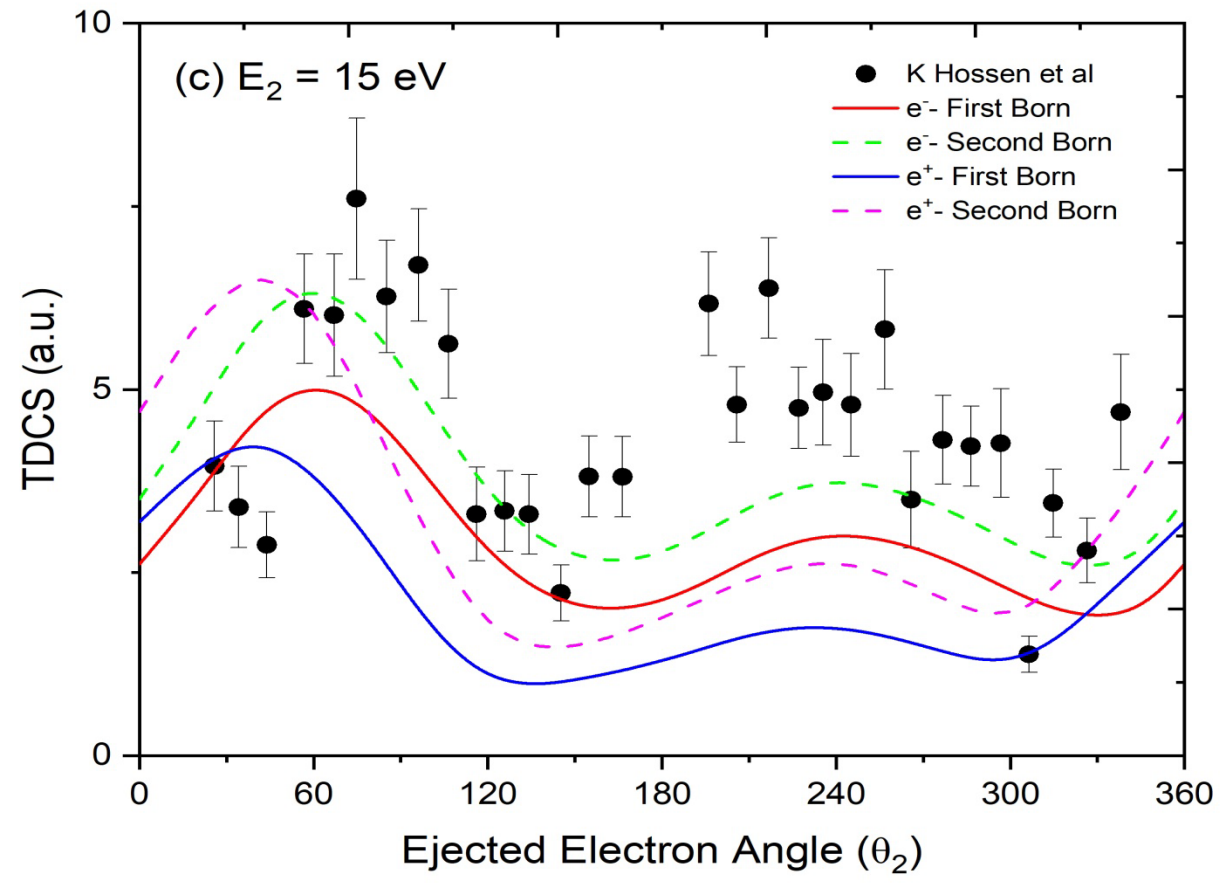
Exp. – Hossen et al.J. Phys. B: At., Mol. and Opt. Phy. 51(21), 215201 (2018)

Results – Electron and positron impact TDCS for CO_2 molecules at 100 eV



Exp. – Hossen et al.J. Phys. B: At., Mol. and Opt. Phy. 51(21), 215201 (2018)

Results – Electron and positron impact TDCS for CO_2 molecules at 100 eV



Exp. – Hossen et al.J. Phys. B: At., Mol. and Opt. Phy. 51(21), 215201 (2018)

Conclusions

Ar (3p) – electron and positron impact

* Present attempt helps to probe the antiparticle – matter and particle-matter interactions and it is observed that the DBWA is able to produce the differences in the trends of TDCS which are projectile charge dependent.
* The binary electron emission is increased for positron impact and the recoil emission is decreased, however in case of measurements both the binary and recoil emission increases for positron impact which may be of interest for further investigation.
* Systematic shift of peaks, shifting away from the momentum transfer direction for positron impact and shifting towards each other for electron impact, is observed with increasing momentum transfer.
* The post collision interaction and target polarization has not been found significant, further theoretical efforts with accurate treatment for electron exchange may be important to understand the disagreement with the experiments.

Conclusions

Ar (3p) – Coplanar Asymmetric Ionization at 1 keV

- Second Born approximation is significant at smaller scattering angles – i.e. for the small momentum transfer conditions
- Significant shift observed in the binary peak positions.
- Post Collision Interaction (PCI) and Target Polarization Potential not found to be significant in this energy regime

Ar (3p) – Perpendicular Plane Ionization

- Reasonable agreement with measurements in the 55 eV to 200 eV above IP projectile energy range.
- The DCS at the higher energies evolves into a broad flat structure with the side lobes reducing in magnitude

Conclusions

Xe (5p) – Coplanar to Perpendicular Plane Ionization

- Reasonable agreement with measurements with certain disagreement in the lower scattering angle regime
- The trends of TDCS seems to depend on kinematics rather than target

Conclusions

W and W^+

* Present distorted wave TICS results show nearly same magnitude as obtained by semi-relativistic distorted wave results obtained earlier for the W atoms.
* The distorted wave TICS results for the W^+ ions overestimate the measurements and Coulomb-Born results however the distorted wave TICS calculated with fine-structure mode for W^+ ions show smaller values.
* The TICS results for W and W^+ have been in agreement with the relativistic DWA and TDCC results
* The differential cross sections for the W atoms and W^+ ions is found to sensitive on the direction of momentum transfer i.e. scattering angle.

Conclusions

N_2 molecule - $3\sigma_g$ orbital

- The trends of TDCS are extracted as a function of momentum transfer through various energy loss values.
- The effect of reversal of the direction of Coulomb field between the projectile and molecular target is studied through the relative intensities of binary lobe for positron and electron impact and the directions of the binary lobes.
- There are points of agreement and disagreement between the theoretical and experimental results with large discrepancies.

Conclusions

N_2 molecule - $3\sigma_g$ orbital

- Both the theory and measurements show enhanced binary emission of electron for positron impact ionization.
- Nearly same recoil intensities for positron and electron impact are observed for the higher momentum transfer both in the theoretical and experimental results.
- There are significant discrepancies in the relative magnitude of binary lobes for electron impact case.
- The binary lobe positions obtained by the theoretical results are shifted towards lower values of ejected electron angles in comparison to the experimental positions

Conclusions

H_2O molecule - $1b_1 + 3a_1$ **orbital**

* In conclusion present DWBA2 results obtained for water molecule are in reasonable agreement with the measurements with certain discrepancies in terms of binary to recoil peak ratios and positions of peaks.

CO_2 molecule

- Two peak structure is observed in the present DWBA calculations as measurements
- Better agreement with measurements observed for higher ejected electron energies
- Second order Born effects found to be significant
- Further investigations underway

Future Plan

* Electron impact cross sections of beryllium hydrides and Boron hydrides
* Electron impact cross sections of W ions, q=2,3…. ….
* Study of electron /positron / ion impact processes on simple to complex molecules of biological importance
* Study of electron impact processes on high Z targets

Research Collaborators

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* Dr. Christophe Champion, University of Bordeaux, France
* Prof. Masahiko Takahashi, Tohoku University, Japan
* Dr. Didier Sebielleu, University of Rennes, France
* Dr. Chuguang Ning, Tsinghua University, Beijing, China
* Prof. L. C. Tribedi, TIFR, Mumbai, India
* Dr. Jiro Itatani, ISSP, Tokyo University, Japan
* Prof. Yasuyuki Nagashima, Tokyo University of Science, Tokyo, Japan
* Prof. Wolfgang Quint, GSI, Germany (new initiative)

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Thanks

ありがとうございました