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Marwa H. Handhal & Alaa A. Khalaf

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RESEARCH ARTICLE



Differential and integral elastic cross sections for electrons and positrons collisions with carbon dioxide molecules

Marwa H. Handhal and Alaa A. Khalaf

Department of Physics, University of Basrah, Basra, Iraq

ABSTRACT

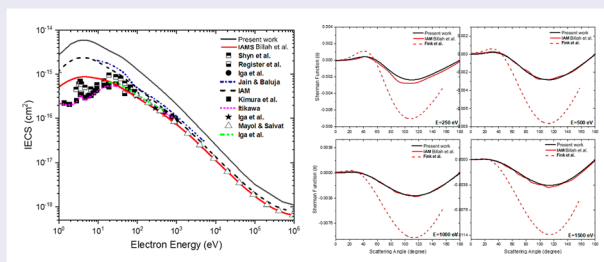
This study investigates the elastic scattering of electrons and positrons by carbon dioxide (CO_2) molecules over a wide energy range from 1 eV to 1 KeV. We have computed differential and integral elastic cross-sections (DCS and ICS) using partial wave analysis and compared the theoretical results with available experimental data. Our findings show a strong correlation with experimental results, particularly at mid to high-energy ranges, validating the employed theoretical frameworks. Additionally, the Sherman function was examined to explore spin polarisation effects during scattering events. This research provides crucial insights for applications in atmospheric physics, materials science, and molecular scattering processes, demonstrating its direct relevance to real-world problems and paving the way for further investigation into particle-molecule interactions.

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KEYWORDS

Electron and positron scattering; molecular scattering; carbon dioxide scattering; cross-section



Introduction

Coinciding electrons and positrons with molecules is a fundamental physical phenomenon that is crucial in various scientific disciplines, including physics, chemistry, and biology. Understanding how these particles interact with molecules provides insights into the behaviour of matter at the atomic and molecular levels [1–3]. Collisions between particles and molecules are essential in understanding the quantum universe. The collision of positrons with carbon dioxide (CO_2) molecules is a unique event that reveals complex interactions beyond traditional models, allowing us to explore new aspects of matter and energy [4,5].

This article highlights the impact of positron collisions with CO_2 molecules and provides an in-depth analysis of differential and integral cross-sections [6]. We examine how these collisions can affect the physical properties of the molecules and offer a new understanding of particle interactions occurring in CO_2 environments

[7]. The process of electron and positron collisions with molecules has aroused great interest in recent times because it explains transport phenomena and the interaction processes of nuclei within the target [8,9]. Electron/positron collisions with molecule cross-section data play a significant role in gas electronics, discharge switches, gas lasers, space science, and radiation research [10]. Since Carl Anderson discovered the positron in 1932, it has been used in many basic scientific experiments, leading to the first production of tapping [11]. The exchange potential is essential for electron scattering, which is absent in positron scattering [12]. A cross-sectional study on CO_2 can provide valuable insights into the distribution, prevalence, and potential risk factors associated with CO_2 levels in a particular population or environment. While CO_2 is a natural greenhouse gas essential for life on Earth; elevated levels of CO_2 in specific contexts can adversely affect human health, the environment, and climate change [13]. The study also

underscores the scientific value of understanding these collisions, as carbon dioxide is a critical molecule in many environmental and industrial processes. By analysing the Sherman function, we uncover the theoretical foundations that govern the orientation of particle collision, aiding in accurate predictions of particle interactions under various conditions. In this work, we investigate the Sherman function $S(\theta)$, integral cross-section (ICS), and differential cross-section (DCS) results for both positron and electron scattering. Carbon dioxide molecules have been the subject of numerous prior studies. In 1999, Satyendra Pal [14] did research on the partial double-differential cross-section (PDDCS) and partial single-differential cross-sections (PSDCS) of the CO_2 molecule using electron collisions at 100 and 500 eV. The collision mechanisms of total scattering, elastic scattering, momentum transfer, excitations of vibrational and electronic states, ionisation, electron attachment, and radiation emission were all examined by Yukikazu Itikawa in 2002 [15]. R. S. Wilde, H. B. Ambalampitiya, and I. I. Fabrikant calculated elastic and positronium (Ps) breakup cross-sections for collisions of positrons with O_2 and CO_2 molecules in the fixed-nuclei approximation in 2021 [16]. In past years specifically in 2022, Billah et. al. [6] and Ana I. Lozano et. al. [17] presented a theoretical investigation of the differential, integrated, elastic, inelastic, total, momentum-transfer, and viscosity cross-sections, along with the total ionisation cross-section, for elastically scattered electrons and positrons from a carbon dioxide (CO_2) molecule in the incident energy range of 1 eV to 1 MeV. In 2024, Ahlam K. Yassir and A.A. Khalaf [18] focused on a theoretical analysis of low-energy electron scattering by polyatomic CH_4 molecules, they study rotationally elastic and inelastic cross-sectional data for CH_4 , which they compare to existing experimental and theoretical findings Display.

Theory

We used an ELSEPA programme for our calculation with no approximations for electron/positron elastic scattering with carbon dioxide in the study state. In partial-wave analysis, the Dirac relativistic equation was solved using a complex optical potential [18],

$$[\hat{c}\hat{\alpha} \cdot \hat{p} + \beta m_0 c^2 + V(r)]\psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (1)$$

$E = \gamma m_0 c^2 = E_i + m_0 c^2$ the total energy, $\gamma = (1 - v^2/c^2)^{-1/2}$, c , is the velocity of light in a vacuum, α & β are Dirac matrices.

Equation (1) is solved numerically by using a complex optical potential [19,20],

$$V(r) = V_{\text{real}}(r) - iW_{\text{abs}}(r)$$

$$= V_{\text{st}}(r) + V_{\text{ex}}(r) + V_{\text{cp}}(r) - iW_{\text{abs}}(r) \quad (2)$$

$V_{\text{st}}(r)$, $V_{\text{ex}}(r)$, $V_{\text{cp}}(r)$ represent the static, exchange, and correlation-polarisation potentials. $W_{\text{abs}}(r)$ represents the magnitude of the absorption potential.

The energy of an electron at a distance (r) from its nucleus is,

$$V_{\text{st}}(r) = Z_0 e \varphi(r) = Z_0 e [\varphi_n(r) + \varphi_e(r)] \quad (3)$$

$Z_0 e$: charge of the electron or positron ($Z_0 = -1$ for e^- & $+1$ for e^+). $\varphi(r)$: The sum of the nucleus and electron cloud contributions in a molecule.

$$\varphi_n(r) = e \left(\frac{1}{r} \int_0^r \rho_n(r') 4\pi r'^2 dr' + \int_r^\infty \rho_n(r') 4\pi r' dr' \right)$$

and

$$\varphi_e(r) = -e \left(\frac{1}{r} \int_0^r \rho_e(r') 4\pi r'^2 dr' + \int_r^\infty \rho_e(r') 4\pi r' dr' \right) \quad (4)$$

Where $\rho(r)$ is the electronic charge density of the target molecule.

We must consider that collisions cause rearrangement of the target, which the electron exchange places with a molecule electron. The best method to deal with electron-exchange effects is to replace the non-local exchange interaction with an approximate local potential. The exchange potential was modelled using the method of (Furness & McCarthy) [21] which provides a reliable approximation for this interaction, that is derived directly from the equation by using a WKB (Wentzel-Kramers-Brillouin) like approximation for the wave functions:

$$V_{\text{ex}}^{(-)}(\bar{r}) = \frac{1}{2} [E_i - V_{\text{st}}(\bar{r})] - \frac{1}{2} \{ [E_i - V_{\text{st}}(\bar{r})]^2 + 4\pi a_0 e^4 \rho(r) \}^{1/2} \quad (5)$$

The slow electrons polarise the target molecule's charge cloud, resulting in a dipole moment induced on the electron itself. A (Buckingham) potential, applied to the electron backward, can approximate the polarisation potential energy when the electron is far from the target.

$$V_{\text{pol}}(\bar{r}) = - \frac{\alpha_p e^2}{2(r^2 + d^2)} \quad (6)$$

α_p : Polarizability of the molecule, d : a cutoff parameter, in which polarisation potentials at $r = 0$ do not diverge. Following Mittleman and Watson [22], we write

$$d^4 = \frac{1}{2} \alpha_p \alpha_0 Z^{-1/3} b_{\text{pol}}^2 \quad (7)$$

b_{pol} : adjustable energy-dependent parameter, $b_{pol}^2 = \max\left[\frac{E-50\text{eV}}{16\text{eV}}, 1\right]$, Z ; atomic number.

Perdew and Zunger's parameterisation of electron correlation potentials [23] is adopted,

$$V_{co}^{(-)}(r) = -\frac{e^2}{a_0}(0.0311 \ln r_s - 0.0584 + 0.00133r_s \ln r_s - 0.0084r_s) \quad \text{for } r_s < 1 \quad (8)$$

$$V_{co}^{(-)}(r) = -\frac{e^2}{a_0}\beta_0 \frac{1 + (7/6)\beta_1 r_s^{1/2} + (4/3)\beta_2 r_s}{(1 + \beta_1 r_s^{1/2} + \beta_2 r_s)^2} \quad \text{for } r_s \geq 1 \quad (9)$$

where $\beta_0 = 0.1423$, $\beta_1 = 1.0529$ and $\beta_2 = 0.3334$. $r_s \equiv \frac{1}{a_0} \left[\frac{3}{4\pi \rho_e(r)} \right]^{1/3}$, is the radius of the sphere that contains one electron of the gas in units of the Bohr radius a_0 .

The positron correlation potential [24], is give by the equation

$$V_{co}^{(+)}(r) = \frac{e^2}{a_0} \left[0.5835 + 0.91r_s^{-\frac{1}{2}} + [0.00255 \ln(r_s) - 0.0575] \ln(r_s) \right] \quad \text{for } r_s < 0.302, \quad (10)$$

$$V_{co}^{(+)}(r) = \frac{e^2}{a_0} [0.461525 - 0.04549r_s^{-2}] \quad \text{or } 0.302 \leq r_s < 0.56, \quad (11)$$

$$V_{co}^{(+)}(r) = \frac{e^2}{a_0} \left[-\frac{4.3637}{(r_s + 2.5)^3} + \frac{-6.5755 + 0.4776r_s}{(r_s + 2.5)^2} + \frac{1.43275}{r_s + 2.5} - 0.3149 \right] \quad \text{for } 0.56 \leq r_s < 8, \quad (12)$$

$$V_{co}^{(+)}(r) = \frac{e^2}{a_0} [-15375.8679r_s^{-6} + 44.5047r_s^{-3} - 0.262] \quad \text{for } r_s \geq 8. \quad (13)$$

In our article, we use partial wave analysis (PWA), which requires that the potential is spherically symmetric or central. The scattering amplitude admits the following partial-wave expansions,

$$f(\theta) = \frac{1}{2ik} \sum_{\ell=0}^{\infty} \{(\ell+1)[\exp(2i\delta_{\kappa=-\ell-1}) - 1] + \ell[\exp(2i\delta_{\kappa=\ell}) - 1]\} P_{\ell}(\cos\theta)$$

and

$$g(\theta) = \frac{1}{2ik} \sum_{\ell=0}^{\infty} [\exp(2i\delta_{\kappa=\ell})]$$

$$- \exp(2i\delta_{\kappa=-\ell-1})] P_{\ell}^1(\cos\theta) \quad (14)$$

k is the relativistic wave number of the projectile that is related to the momentum p and the kinetic energy E by, $\hbar k = p$, $(\hbar k)^2 = E(E + 2m_e c^2)$.

c is the velocity of light in a vacuum, $P_{\ell}(\cos\theta)$, $P_{\ell}^1(\cos\theta)$ are Legendre polynomials and associated Legendre functions, respectively.

The phase shifts $\delta\kappa$ represent the large- r behaviour of the Dirac spherical waves. These are solutions of the Dirac equation of the form,

$$\psi_{E\kappa m}(\mathbf{r}) = \frac{1}{r} \begin{pmatrix} P_{E\kappa}(r)\Omega_{\kappa,m}(\hat{\mathbf{r}}) \\ iQ_{E\kappa}(r)\Omega_{-\kappa,m}(\hat{\mathbf{r}}) \end{pmatrix} \quad (15)$$

$\Omega_{\kappa,m}(\hat{\mathbf{r}})$ the spherical spinors and the radial functions. $P_{E\kappa}(r)$, $Q_{E\kappa}(r)$ satisfy the coupled system of differential equations.

$$\begin{aligned} \frac{dP_{E\kappa}}{dr} &= -\frac{\kappa}{r}P_{E\kappa} + \frac{E - V + 2m_e c^2}{\hbar}Q_{E\kappa} \\ \frac{dQ_{E\kappa}}{dr} &= -\frac{E - V}{\hbar}P_{E\kappa} + \frac{\kappa}{r}Q_{E\kappa}. \end{aligned} \quad (16)$$

The relativistic quantum number κ is defined as $\kappa = (\ell - j)(2j + 1)$ where j and ℓ are the total and orbital angular momentum quantum numbers that are both determined by the value of κ ; $j = |\kappa| - 1/2$, $\ell = j + \kappa/(2|\kappa|)$. We shall normalise the spherical waves so that the upper-component radial function $P_{E\kappa}$ oscillates asymptotically with unit amplitude. For finite-range fields and $r \rightarrow \infty$, we then have,

$$P_{E\kappa}(r) \simeq \sin\left(kr - \ell\frac{\pi}{2} + \delta_{\kappa}\right) \quad (17)$$

As in the non-relativistic situation, attractive (repulsive) potentials result in positive (negative) phase shifts. It is important to note that the theory here applies to both electrons and positrons; the primary distinction between the two particles is the sign of their charges, i.e. the electrostatic interaction with atoms and positive ions is attractive for electrons but repulsive for positrons.

DCS per unit solid angle for spin unpolarised electrons or positrons. This DCS is given by,

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 + |g(\theta)|^2 \quad (18)$$

The total elastic cross-section,

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{\pi} \frac{d\sigma}{d\Omega} 2\pi \sin\theta d\theta \quad (19)$$

The physical manifestation of spin one-half systems can take many forms, the most exciting of which is the free electron, which has intrinsic angular momentum. The

study of electron spin polarisation focuses on electron assemblies in which one of two potential states is preferentially occupied.

Knowledge of spin polarisation or the Sherman function $S(\theta)$ is essential for projectile–molecule scattering, as it can furnish details of the scattering process.

When the calculation of the partial-wave series is feasible, it also provides tables of the scattering amplitudes

(2–29) and the Sherman function.

$$S(\theta) \equiv i \frac{f(\theta)g^*(\theta) - f^*(\theta)g(\theta)}{|f(\theta)|^2 + |g(\theta)|^2} \quad (20)$$

Hence, the scattering amplitudes $f(\theta)$ and $g(\theta)$ describe (Equation 14) entirely the elementary scattering process.

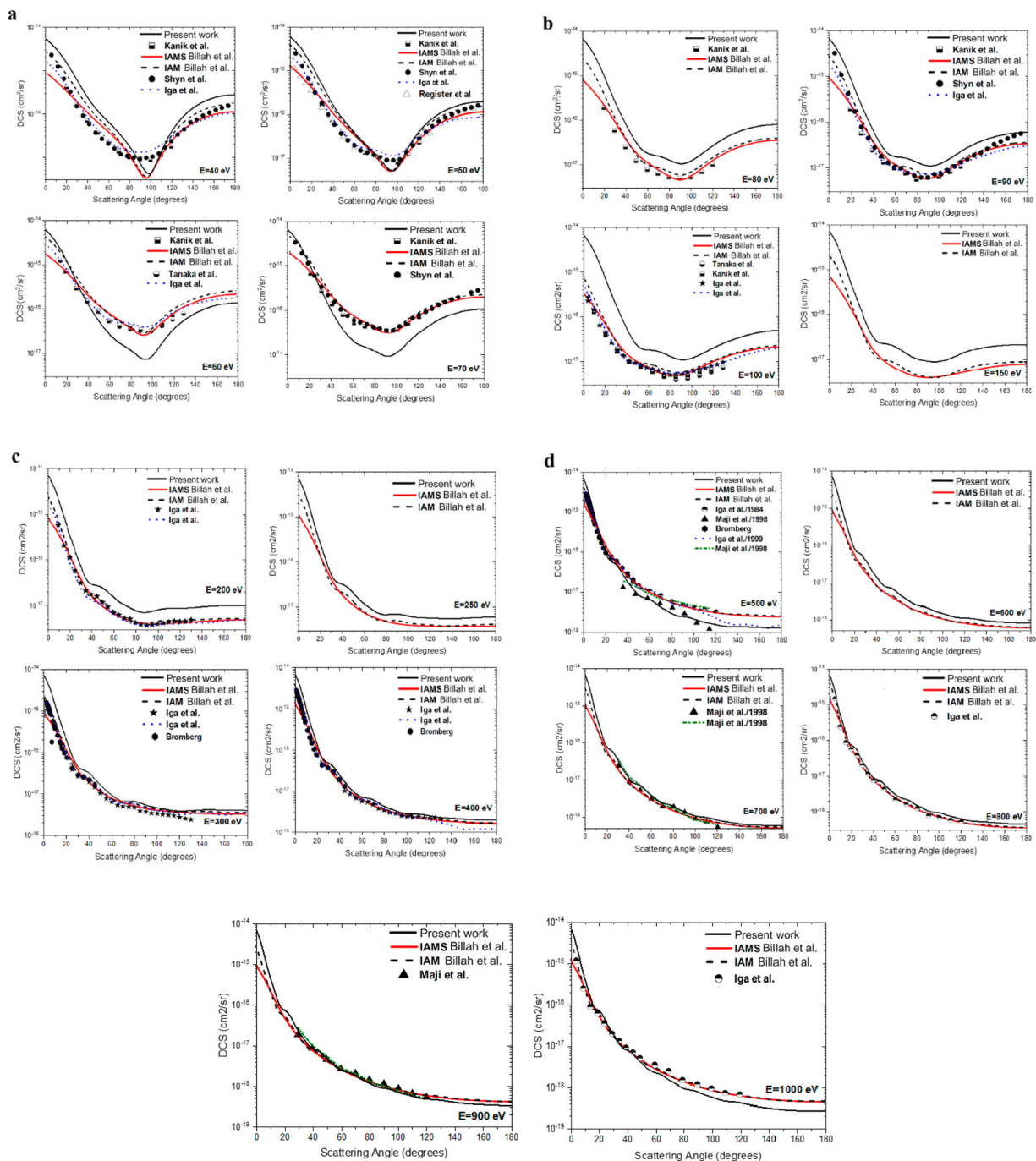


Figure 1. The elastic differential cross section of electrons collision with carbon dioxide molecules at energies of (40–1000) eV. My work is a theoretical black line. Theoretical: Billah et al. IAM, IAMS [6], and Iga et al. [25]. Experimental: Tanaka et al. [26], Shyn et al. [27], Register et al. [28], and Kanik et al. [29], Bromberg [30], Maji et al. [31].

Results and discussion

The current study computed numerous observable variables for the scattering system spanning the energy spectrum of 40 eV–1 KeV using the Elastic Scattering of electrons/positrons by molecules.

The target's characteristics and coordinate geometry concepts compute observable quantities and molecular polarizability. Hartree atomic units, where the values of \hbar , h , and e equal 1, were used for the computations. The Sherman functions, integrated cross sections (ICS), and computed differential cross sections (DCSs) are usually accurate when partial wave analysis is feasible. This estimate of inaccuracy relates only to the accuracy of the calculation and is based on the supposition that the selected central potential faithfully captures the interaction. The calculated DCS, TCS, and $S(\theta)$ results for electron and positron scattering are discussed in the following subsections.

The computed outcomes of the DCSs for the electron and positron scattering are presented in Figures 1 and 2. DCSs for electron impact are computed within the energy range of 40 eV to 1 KeV. In contrast, the DCSs for positron impact are calculated within the energy range of 10 eV to 1.5 KeV. Figure 1 Observing that the DCS values at small scattering angles, such as angle 0, are at their maximum value, we can assume that the interference of quantum waves can explain the differential cross-section behaviour. Since an electron can act as both a particle and a wave, the interference between these waves results in distinct patterns of propagation: At small angles (near 0°), the waves resulting from scattering are constructive, increasing the differential cross-section, at large angles (near 180°), the waves interfere destructively, reducing the differential cross section. A differential elastic cross-section was calculated for many energies for the elastic collision of electrons with CO_2 , and compared our results with the theoretical data of Billah et al. IAM,

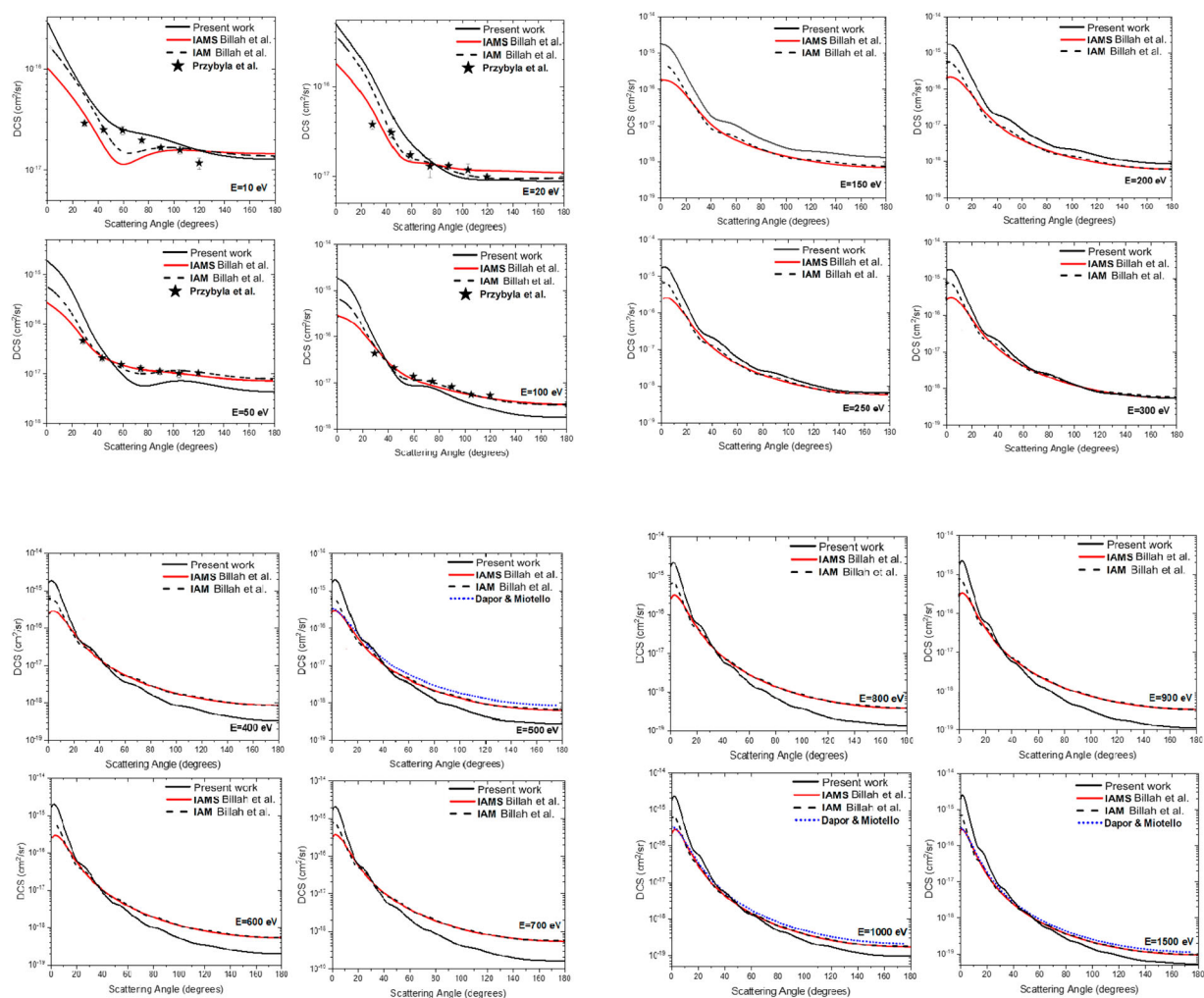


Figure 2. The elastic differential cross section of positrons colliding with carbon dioxide molecules at energies of (10–1500) eV. My work is a theoretical black line. Theoretical: Billah et al. IAM, IAMs [6], and Dapor and Miotello [32]. Experimental: Przybyla et al. [33].

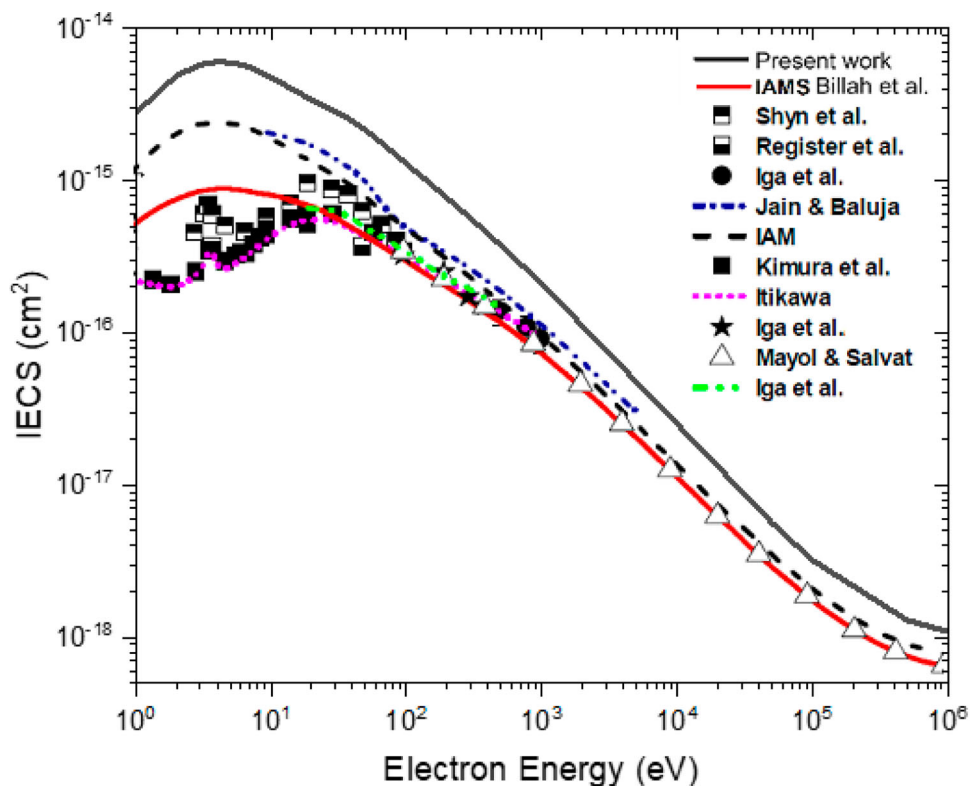


Figure 3. The integral elastic cross section for the scattering of electrons from carbon dioxide. My work is a theoretical black line. Theoretical: IAM, IAMS Billah et al. [6], Iga et al. [25], Jain and Baluja [34], and Itikawa [35]. Experimental: Iga et al. [36], Shyn et al. [27], Register et al. [28], Kimura et al. [5] and Mayol and Salvat [37].

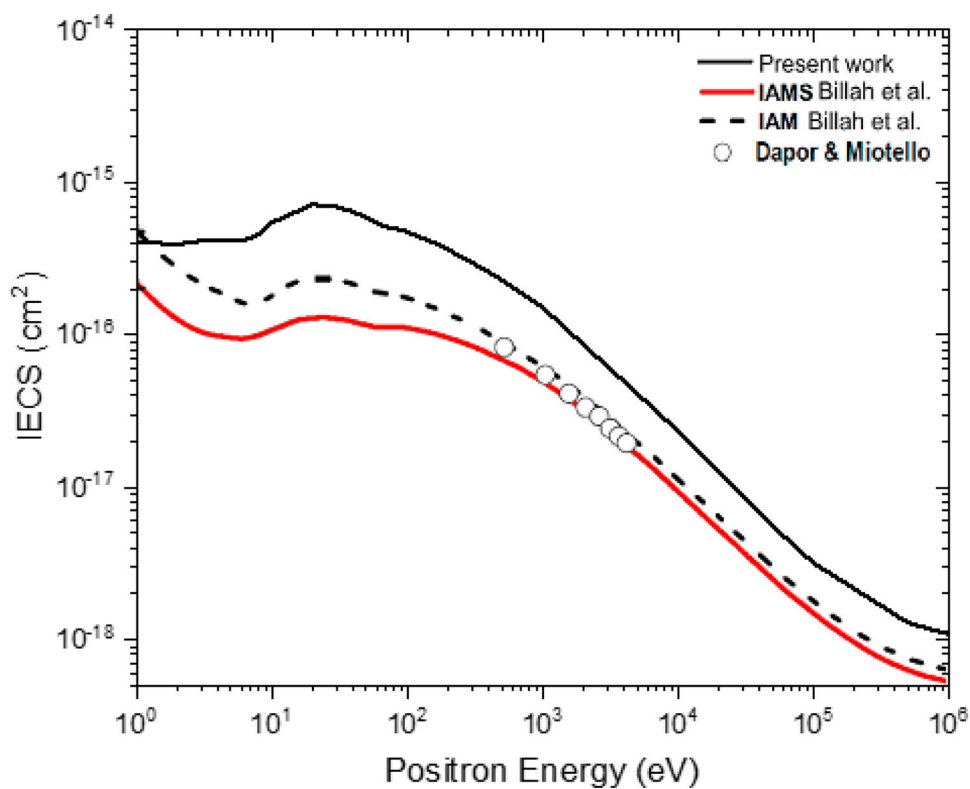


Figure 4. The integral elastic cross section for the scattering of positrons from carbon dioxide. My work is a theoretical black line. Theoretical: IAM, IAMS Billah et al. [6]. Experimental: Dapor and Miotello [32].

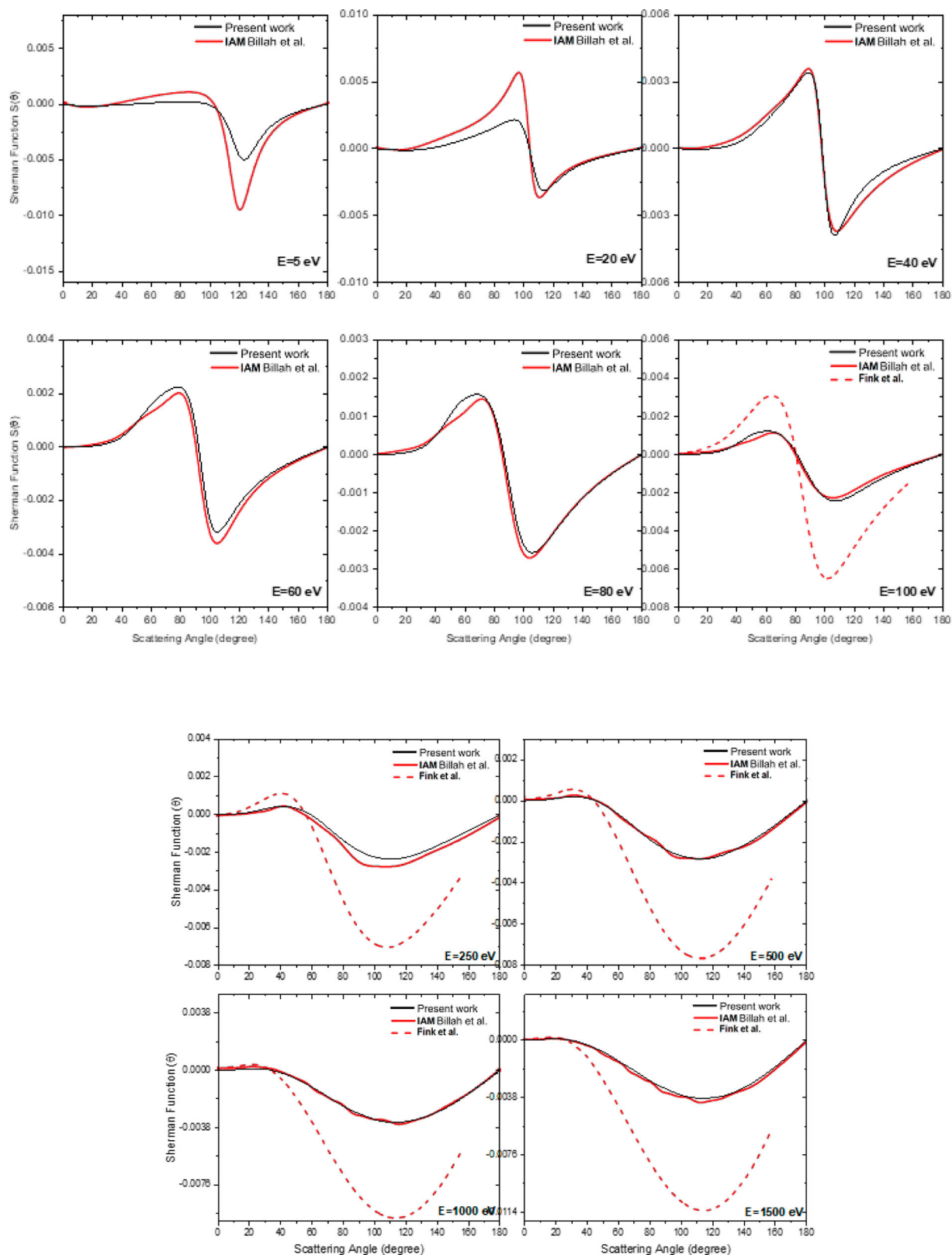


Figure 5. The Sherman function describes the electron collision with carbon dioxide. My work is a theoretical black line. Theoretical: IAM Billah et al. [6], Fink et al. [38].

IAMS [6], and Iga et al. [25] for DCSs at (40–1000) eV, and the experimental data with Tanaka et al. [26], Shyn et al. [27], Register et al. [28], and Kanik et al. [29], Bromberg [30], Maji et al. [31]. The experimental result, however, was consistent with the theoretical data of Differential Cross Sections (DCSs) for low energies. The data showcases the polarisation effect at very low energies, specifically for a specific set of incident electron energies. At higher energies at scattering angles less than 80° , the DCS behaviour takes maximum values because incident electrons approach straight or obtuse angles. Values exceeding 100° are also caused by backscattering.

In Figure 2, a differential elastic cross-section was calculated for many energies for the elastic collision of positrons with CO_2 . We will also compare our results with the theoretical data of Billah et al. IAM, IAMS [6], and Dapor and Miotello [32]. Experimental: Przybyla et al. [33].

In Figure 3 an integral elastic cross section was calculated for a collision of electrons with CO_2 . At a range of energies from (1 eV to 1 MeV). We compared our results

with theoretical data from IAM, IAMS, Billah et al. [6], Iga et al. [25], Jain and Baluja [34], and Itikawa [35]. Experimental: Iga et al. [36], Shyn et al. [27], Register et al. [28], Iga et al. [36], Kimura et al. [5] and Mayol and Salvat [37].

In Figure 4, an integral elastic cross section was calculated for a collision of positrons with CO_2 . Also, at a range of energies from (1 eV to 1 MeV). We compared our results with theoretical data from IAM, IAMS, Billah et al. [6]. Experimental: Dapor and Miotello [32].

Figure 5 demonstrates the computation of the Sherman function for electron collision at low energies (5, 20, 40, 60, 80, 100) eV and compares it with the theoretical outcome of IAMS Billah. [6]. In addition, we compared high energy levels (250, 500, 1000, 1500) eV and contrasted it with the theoretical findings of IAMS Billah. [6] and Fink [38] (Figure 6).

Figure 5 demonstrates the computation of the Sherman function for positron collision at low energies (10, 20, 50, 100) eV and compares it with the theoretical outcome of IAMS Billah. [6].

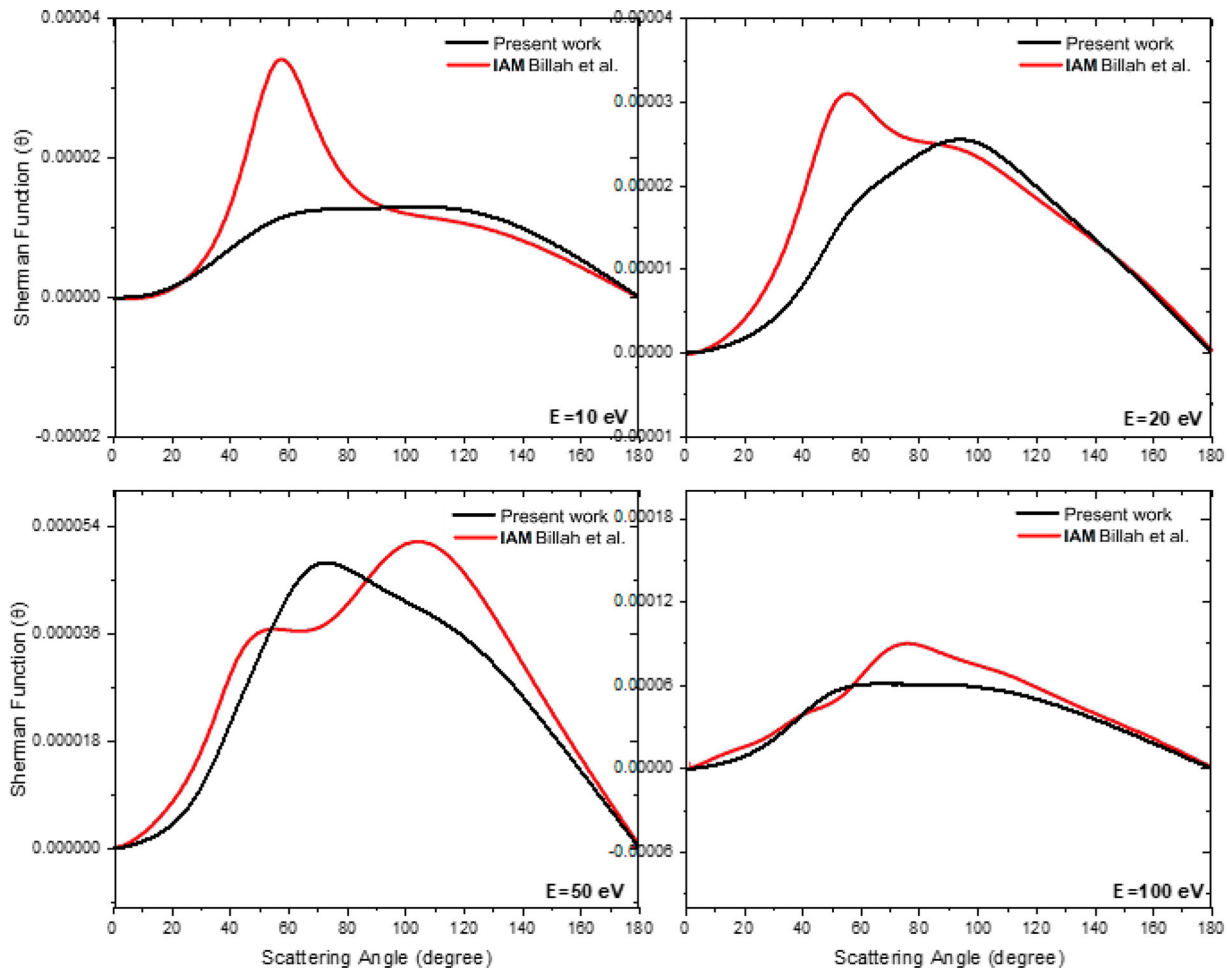


Figure 6. The Sherman function describes the positron collision with carbon dioxide. My work is a theoretical black line. Theoretical: IAM Billah et al. [6].

The scattering angle significantly impacts how the Sherman function behaves. Polarisation asymmetry is often minimal at modest scattering angles (around 0°) because the particles maintain their original polarisation, and the scattering is generally elastic. The asymmetry increases at large scattering angles (around 180°) because of the significant momentum transfer, which causes a considerable change in the spin vectors.

The effects of decay that positrons experience upon collision with a molecule's electrons add another level of complexity. In addition to generating photons, the decay modifies the particles' ultimate polarisation and velocity. As a result of decay and the ensuing asymmetry in polarisation, the positron Sherman function may display distinct patterns at varying energies.

Conclusions

In conclusion, this work explores the elastic scattering of electrons and positrons by Carbon Dioxide (CO_2) molecules, emphasising the computation of integral and differential cross-sections for energies ranging from 40 eV to 1 KeV. The results show a good agreement with the theoretical predictions and the actual data, especially in the medium and high-energy areas, proving the validity of the techniques used, which include the relativistic Dirac equation and partial wave analysis.

This study also investigates the Sherman function, which sheds light on spin polarisation effects during scattering events. Understanding the fundamental dynamics of particle interactions in CO_2 Settings depend on this feature. The findings contribute substantially to the study of molecular scattering and provide insightful information for future research in materials science, atmospheric physics, and related fields. The thoroughness of this analysis highlights how intricate electron and positron interactions are with molecular targets, opening up new avenues for investigation.

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Disclosure statement

No potential conflict of interest was reported by the author(s).

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