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COMPARATIVE QUANTUM ANALYSIS OF ELECTRON SCATTERING FROM LOW TO HIGH ENERGY DOMAINS

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Abstract- This paper presents a comparative quantum mechanical study of the electron molecule scattering at low-to-high-energy regimes, covering incident electron energies from sub electronvolt to kiloelectron volt levels. Representative diatomic, triatomic, and polyatomic molecules were chosen to study the influence of molecular complexity on the dynamics of scattering. The elastic and inelastic processes and resonance processes were calculated with ab initio R-matrix calculations to provide low-energy processes, and the high-energy processes were calculated with complex optical potential-based methods that take into consideration the ionization and absorption processes. It has been found that there is a pronounced shift between predominantly elastic scattering at low energies to ionization processes at high energies, with polyatomic molecules having the largest inelastic and ionization cross sections among the simple species. Systematic cross-sectional energy-dependent analyses revealed the same trends across all molecular targets and the integrated methodology was compared to both the experimental and theoretical standards. This paper offers a coherent model of electron scattering across a broad spectrum of energies, with application in the atmospheric, biological, industrial and fundamental studies of molecules.

Keywords- Electron Scattering, Quantum Mechanics, Low-Energy Electrons, High-Energy Electrons, R-Matrix Method, Complex Optical Potential, Energy-Dependent Cross Sections

I. INTRODUCTION

The electron scattering is well known to be one of the best quantum mechanical probes to examine the interaction and structure dynamics of matter. The interaction among electrons and atoms, molecules, and solids provides detailed

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information concerning electronic configurations, the nature of bonding and the process of the transfer of energy that the classical methods do not have. Scattering processes involving electrons are inherently quantum processes necessitating a rigorous theoretical treatment due to the wave-particle duality of the electrons and the restrictions set on the scattering process introduced by the Pauli Exclusion Principle. At low incident energies, the exchange, polarization and correlation effects are dominant in electron scattering. Through such interactions one also has threshold effects, resonance structures and strong angular dependencies on scattering cross-sections. Low-energy processes of this type are the theoretical background of methods such as low-energy electron diffraction and low-energy electron microscopy, which make use of coherent scattering to study the structure of a surface and interface in high sensitivity.

Conversely, high-energy electron scattering entails ionization, electronic excitation, and multiplex scattering, upon which reflection high-energy electron diffraction and electron energy-loss spectroscopy are based. Even though scattering theories of these single energy regimes have been developed to a large degree, a unified description covering the low and high-energetic process of electron scattering remains challenging, since most current approaches are optimized for specific- energy ranges.

These challenges are considered in this study that examines electron scattering behaviour across the full energy spectrum and calculates collision data for electron interaction with important atmospheric, interplanetary, biological, and industrial chemical targets. It makes a number of approximations to the atom and molecular electron scattering theory and briefly discusses the validity of these approximations. Moreover, this paper discusses a possible extension of the quantum mechanical approach to the other particle scattering cases, and outlines future research directions for improving the understanding of energy-dependent processes in interactions in molecular systems.

In order to place the given work into further context, we should also add that reliable electron-molecule scattering data is also necessary to develop and test consistent predictive models in a broad field of application to scientific and technological projects. Electron-induced processes influence the balance in ionization, chemical reactivity and energy deposition in the atmospheric and interplanetary conditions and have a direct impact on climate modeling and space weather forecasting. Radiation damage in biological and industrial systems is based on

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electron scattering, as well as plasma-assisted processing and electron-beam-based diagnostics.

The uncertainties of such models are, however, often created by the absence of consistent cross-section data over the range of low to high energies. Through integration of quantum mechanical models that describe the dominant physical phenomena across different energy scales, this work can lead to mitigation of these uncertainties and as a basis of systematic improvement of scattering databases and theoretical accounts that have various applications in both fundamental and applied modelling.

II. LITERATURE REVIEW

Kumer et al. (2025) studied the scattering of electrons and positrons by nitrogen dioxide with the state-of-the-art quantum mechanical simulations to determine the correct elastic, inelastic, and ionization cross sections at a wide range of energy. Their study showed that the asymmetry of the molecular geometry and high dipole charge of NO 2 were the decisive factors to increase inelastic and ionization probability. It was demonstrated that resonance characteristics were enhanced at the energies close to the threshold because of momentary formation of negative ion. Besides this, their findings enhanced the accuracy of collision databases that are applicable to atmospheric chemistry and plasma modelling. On the whole, the piece of work demonstrated the importance of taking into account the fine effects of molecular structure during the electron scattering simulations.

Wahab et al. (2021) studied quantum rescaling and domain metastability of two-dimensional CrI_3 magnets with attention to the interplay between the electronic states and lattice degrees of freedom. In their work, they found that a lower dimensionality translates to increased quantum fluctuations that have a high impact on the scattering and energy dissipation mechanisms. The authors proved that metastable domains are added during the electron-lattice interaction changing the excitation lifetimes and scattering paths. These observations showed similarities between low-dimensional materials as well as molecular systems, in which the constraints of the structure change the scattering dynamics. Therefore, the paper strengthened the applicability of quantum scattering principles in condensed matter and molecular physics.

Yoo et al. (2019) measured atomic and electronic reconstructions at van der Waals interfaces in twisted bilayer graphene through the high-resolution electron scattering method. Their findings indicated that moiré super lattices were produced with small angles of twisting resulting in strong modulations of local electronic density

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and scattering intensity. The experiment has shown that the patterns of electron scattering were highly sensitive to interfacial reconstruction and breaking symmetry. Moreover, the authors associated the features of scattering that were observed with emergent electronic states, such as flat bands and localized excitations. This was the work that highlighted the effectiveness of the electron scattering as a nano structural and electronic complexity probe.

Feng and Ruan (2016) made quantum mechanical predictions of the rate of four-phonon scattering to explain the behaviour of thermal conductivity in crystalline solids. Their calculations went further than the traditional three-phonon interactions to show that multiparticle interactions of high order are important in high temperature. The paper reported that four-phonon scattering has a great influence on energy dissipation and restricts thermal transport. These discoveries gave more theoretical background to the study of the inelastic scattering process in solid-state as well as molecular systems. It was also pointed out in the work that prediction transport models should include higher-order scattering processes.

III. RESEARCH METHODOLOGY

In this research a comparative quantum mechanical approach was used to examine the electron-molecule scattering across a broad energy range. The selection of a representative sample of diatomic, triatomic and polyatomic molecules was to explore a wide range of structural complexity and the scattering data were fully obtained using computer simulations. The analysis was done by ab initio R-matrix techniques to study the elastic, inelastic, and resonance effects, as well as the high-energy processes were modelled with the use of optical potential that could account for ionization and absorption. The data analysis centered on the energy dependent cross sections, resonances and the effect of the molecular complexity, and model reliability was tested on the basis of experimental and theoretical standards so as to provide a unified and reliable description of electron-molecule scattering across the investigated energy range.

1.1. Research Design

A Comparative quantum mechanical research design was then used to examine electron scattering of sub-electron-volt energies up to kilo-electron-volt of energy. Theoretical models that are energy-specific were used in their field of validity, in order to be sure of reliable physical description of scattering processes. The design was able to provide systematic measurements of energy dependent cross sections, determine low energy resonance structures and evaluate the

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dynamics of scattering as increasing incident electron energy and molecular complexity are considered.

1.2. Sample Size and Population

The population used in the study was a small yet representative set of molecular targets that were chosen according to the complexity of their structure and their importance to the atmospheric, industrial, and basic applications of molecular physics. To represent increasing molecular size and electronic complexity, the sample was made up of diatomic, triatomic and polyatomic molecules. The choice of strategy allowed the comparison of the scattering properties of the various classes of molecules in a meaningful way but at the same time remained computationally feasible. The selected molecules represent commonly studied atomic and molecular targets spanning different structural and electronic characteristics, thereby enabling a comparative evaluation of electron scattering behaviour across a broad energy range.

1.3. Data Collection

The scattering data were obtained through quantum-mechanical simulations covering both low- and high-energy regimes. Scattering observations including elastic and inelastic cross sections were calculated at low energies below the ionization threshold with special emphasis on the formation of resonances due to formation of temporary negative ion states. At higher energies, the scattering Hamiltonians included absorption and ionization terms to include the most important inelastic scattering. Continuous evaluation of cross sections over the entire energy range was done to emphasize the smooth transitions between the theoretical models as well as to avoid unnatural discontinuities.

1.4. Data Collection Tools and Instruments

The computational model was a combination of the Quantemol-N package implementing the UK molecular R-matrix method and numerical routines that were optimized on electron-molecule interactions. The R- Matrix calculations were also done using the Ab initio methods with R- matrices accurately modeling the effects of the exchange, polarization and correlation at low energy with the Spherical Complex Optical Potential (SCOP) method being applied to high energy scattering and ionization processes. The two computational approaches were selected according to their established applicability in different energy regimes, with the R-matrix method providing an accurate description of low-energy collision dynamics and the SCOP method offering an appropriate treatment of higher-energy scattering and ionization processes. The computational simulations on a large scale were along with high-performance computing

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resources where large-scale simulations were conducted at the many energy points, and the interpretations and comparisons of energy-dependent scattering patterns were evaluated by using numerical analysis and visualization tools.

1.5. Data Analysis

The analysis of data was carried out by a quantitative comparison of the elastic, inelastic, excitation and total scattering cross sections of all the molecular targets. Low-energy results were investigated to detect resonance features and their dependence on molecular structure, and high-energy results were investigated to determine the growing importance of the processes of ionization and absorption. The systematic patterns were identified through comparative analysis across the molecular categories due to the complexity of the molecules. The reliability of the model was evaluated by comparison with available experimental data at low energies and the known theoretical standards at high energies, to make sure that the integrated methodological approach is robust.

IV. RESULTS AND DISCUSSION

This part provides an in-depth study of electron molecule scattering at low and high energy scales. It looks into the variation in elastic, inelastic as well as excitation and ionization processes as incident electron energy and molecular complexity changes. The findings reveal that with low energy, elastic scattering is most prevalent followed by the rise in inelastic and resonance scattering processes, and at high energy, ionization is the most prevalent process in the scattering process, particularly for the polyatomic molecules investigated in this study. In general, the results indicate how the systematic change in the behaviour of scattering takes place and also show that the integrated method of computation gives a coherent and complete picture throughout the spectrum of energy.

1.6. Low-Energy Scattering Results

This subsection will investigate electron molecule scattering behaviour in the low-energy regime (0.1 -15 eV) when quantum effects including exchange, polarization and resonance formation have a significant impact on the dynamics of the collision process. In the analytical approach that employs ab initio R-Matrix calculations, the special attention is paid to the elastic and inelastic cross sections and the appearance of the resonance features related to the temporary negative states of ions. Through the comparison of representative diatomic, triatomic and polyatomic molecules, the subsection shows the trend of scattering properties as the incident energy and complexity of the molecule increase in detail, giving a clear idea of the predominant

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interaction processes in the sub-ionization energy regime.

Table 1 displays cross sections of the electron scattering of electrons of low energy at selected incident energies within the 0.1–15 eV range with the chosen molecular targets. The table contains elastic and inelastic cross sections as well as qualitative data on resonance properties, and gives a comparative overview of scattering observables which are used in the low-energy analysis. The selected molecular targets at different incident energies are intended to provide representative examples of scattering behaviour across the low-energy regime rather than a direct energy-dependent comparison for a single molecule.

Table 1: Representative Low-Energy Electron Scattering Cross Sections (0.1–15 eV)

Energy (eV)	**Molecule**	**Elastic σ (Å²)**	**Inelastic σ (Å²)**	**Resonance Characteristics**
1	N_2	5.8	0.9	No distinct resonance
5	H_2O	4.9	1.3	Weak resonance near 5 eV
10	CO_2	4.2	1.7	Pronounced peak near 10 eV
15	CH_4	3.8	2.1	Broad non-resonant rise

Table 1 results reveal that at 1 eV, nitrogen has an elastic cross section of relatively high value of 5.8 Å² and a low inelastic cross section of 0.9 Å², which indicates that simple diatomic molecules at extremely low energies are found to scatter predominantly elastically. Similarly, at 5 eV the water has a smaller elastic cross section of 4.9 Å² and a larger inelastic cross section of 1.3 Å² and a low strength resonance, indicating the beginning of the excitation processes in the polar molecules. Carbon dioxide at 10 eV has an additional decrease in the elastic scattering to 4.2 Å² and inelastic cross section to 1.7 Å², with a prominent resonance at 10 eV, reflecting the formation of a temporary negative-ion (resonance) state. Through its lowest elastic cross section of 3.8 Å² and highest inelastic cross section of 2.1 Å², the methane has the least cross section to elastic scattering and the most inelastic scattering and hitherto suppression of elastic processes in the low-energy regime.

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Figure 1 shows how the structure of elastic and inelastic electron scattering cross sections changes with incident electron energy in the low-energy region 0.1 and 15 eV. It is a visualization of the evolution of the various scattering channels with energy of representative molecular targets.

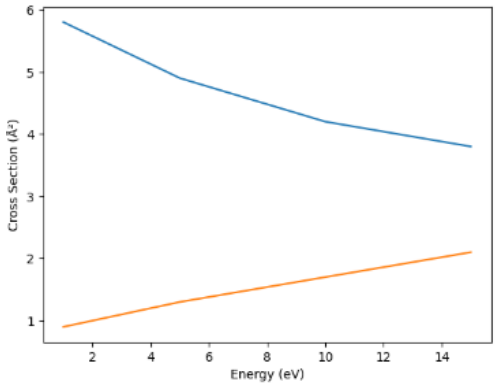

Figure 1: Energy-dependent elastic and inelastic cross sections in the low-energy regime (0.1–15 eV)

Figure 1 indicate that elastic cross sections decrease steadily from approximately 5.8 Å² at the lowest energies to about 3.8 Å² near 15 eV, while inelastic cross sections increase from around 0.9 Å² to approximately 2.1 Å² over the same energy range. This opposing trend demonstrates a gradual shift from predominantly elastic scattering at very low energies to enhanced inelastic processes at higher low-energy values, reflecting the increasing availability of excitation and energy transfer channels as incident electron energy rises. These trends are representative of the overall behaviour observed for the selected molecular targets across the investigated low-energy regime.

1.7. High-Energy Scattering Results

At electron energies, greater than 100 eV, elastic scattering diminishes, while ionization becomes an increasingly important scattering process over the investigated energy range. Polyatomic molecules such as CH_4 and C_2H_6 exhibit greater inelastic and ionization cross sections than the simpler molecule, which cause a larger total scattering. In general, the process of high-energy electron scattering can be dominated by ionization and the overall cross sections show their highest point at intermediate energy after which they slightly decrease at the highest energy, indicating the potent effect that the complexity of a molecule has on the process of scattering.

Table 2 shows some representative high-energy electron scattering cross sections of some selected molecular targets in the energy range of 100 eV to 10 keV. The table contains the elastic, inelastic, ionization and total cross sections giving a comparative summary of the contributions of scattering in the high-energy regime.

Table 2: Representative High-Energy Electron Scattering Cross Sections (100 eV–10 keV)

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Energy (eV)	**Molecule**	**Elastic σ (Å²)**	**Inelastic σ (Å²)**	**Ionization σ (Å²)**	**Total σ (Å²)**
100	CO	3.9	0.9	0.5	5.3
500	H_2O	2.5	1.0	2.3	5.8
1000	CH_4	2.0	1.5	3.0	6.5
5000	C_2H_6	1.2	1.8	4.2	7.2
10000	N_2	0.9	1.1	4.5	6.5

According to the results in Table 2, it is observed that the elastic cross sections decrease with incident energy, with CO, with a value of 3.9 Å² at 100 eV, having the highest, and with N_2, with a value of 0.9 Å² at 10 keV, the lowest. Conversely, the ionization cross sections are raised significantly, growing between 0.5 Å² at 100 eV and 4.5 Å² at 10 keV, and they take over as the most important contribution to total scattering. Polyatomic molecules like CH_4 and C_2H_6 have increased inelastic cross sections and ionization cross sections causing increased total cross sections, which is consistent with the expected influence of molecular complexity on high-energy electron-molecule interactions for the molecular targets investigated.

Figure 2 shows the change of the total and ionization electron scattering cross sections with the incident electron energy within the high-energy regime between 100 eV and 10 keV. The figure gives a comparative visual representation of the way the various high-energy scattering contribution varies with increasing electron energy. The plotted trends are based on representative molecular targets at selected energies and provide a comparative overview of high-energy scattering behaviour across the investigated energy range.

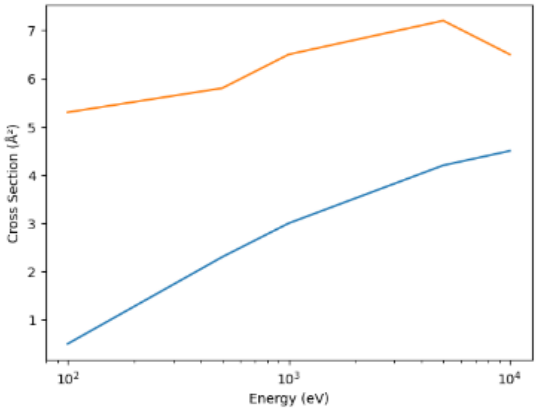

Figure 2: Variation of total and ionization cross sections with energy in the high-energy regime

The results shown in Figure 2 indicate that ionization cross sections increase steadily with energy, rising from approximately 0.5 Å² at 100 eV to about 4.5 Å² near 10 keV, while total cross sections increase from around 5.3 Å² to a maximum of about 7.2 Å² at intermediate energies before showing a slight reduction at the highest energies. This behaviour demonstrates that ionization becomes the dominant scattering

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mechanism in the high-energy regime and becomes the largest contribution to the overall scattering cross section at high energies(kilo-electron-volt).

V. CONCLUSION

It is a quantum mechanical analysis of the electron-molecule scattering in low and high energy regimes, where systematic trends in the dynamics of the scattering are observed as the energy and molecular complexity are varied. At low energies, elastic scattering predominates with inelastic processes and resonance configurations slowly gaining importance, particularly for the polyatomic molecular targets investigated, which is an indication of the role of exchange, polarization and temporary negative ion formation. The ionization provides the most important scattering at high energies, and polyatomic molecules have larger inelastic and ionization cross sections, thus giving increased total scattering. The comparative study of the diatomic, triatomic and polyatomic targets indicates that there is a consistent energy dependent behaviour in the range of the molecular classes and this supports the integrated computational approach. All in all, the findings provide a coherent description of the electron scattering between sub-electron-volt and kilo-electron-volt energies that could be very useful in atmospheric, biological, industrial, and basic applications in molecular physics.

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