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# **The Computational Study of Electron Scattering with Molecules (Elastic and Non-Elastic)**

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صدق الله العلي العظيم

سورة طه: من الآية 114

# *Certification*

I certify that this dissertation, which is entitled **The Computational Study of Electron Scattering with Molecules (Elastic and Non-Elastic)** presented by *Ahlam Khudhair Yassir*, was prepared under my supervision at the Department of Physics, College of Science, University of Basrah as a partial requirement for the degree " doctor of philosophy" in Physics.

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Date: / / 2023

## **Dedication**

I dedicate this dissertation with love and appreciation to my dear ones who mean everything to me in this life. To my beloved parents, whom I have lost and departed, I ask Allah to grant them his infinite mercy and to place them in the highest ranks of paradise. To my dear husband, who is my companion and loyal friend, I thank you for your continuous support and encouragement that has given me the strength and confidence to complete this academic journey.

I also dedicate this dissertation to my dear children and their spouses, who are the source of my happiness and pride. You are my hope, happiness, and the driving force behind my success. I thank you for standing by my side and for your constant support in all areas.

Lastly, I dedicate this dissertation to my precious daughter, who represents the greatest love to me and is the source of my utmost pride and happiness. You are my strength and inspiration, and I hope you are as proud of me as I am of you.

**Ahlam**

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I would like to express my deep gratitude and appreciation for the valuable help and guidance you provided me while preparing my dissertation. It has been a valuable and fruitful experience thanks to your effective support and guidance.

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I look forward to continuing to work with you in the future and benefiting from your valuable experience and knowledge. Thank you again for everything, and I wish you success and prosperity in your academic and professional career.

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I extend my thanks and appreciation (PH.D) graduate students for their assistance throughout the study period sincerely

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## Abstract

This dissertation presents a comprehensive exploration of electron-molecule collisions, including both elastic and inelastic scattering processes, as well as the study of electron stopping power and range within selected molecules. I examine the collision dynamics of electrons with molecules such as [ Ammonia ( $\text{NH}_3$ ), Phosphine ( $\text{PH}_3$ ), Arsine ( $\text{AsH}_3$ ), Stilbene ( $\text{SbH}_3$ )]; [ Water ( $\text{H}_2\text{O}$ ), Hydrogen Sulfide ( $\text{H}_2\text{S}$ ), Hydrogen Telluride ( $\text{H}_2\text{Te}$ ), Hydrogen Selenide ( $\text{H}_2\text{Se}$ ) ]; [Carbon Monoxide ( $\text{CO}$ ), Carbon Dioxide ( $\text{CO}_2$ ) ]. In the first section of the study, with an emphasis on elastic scattering. We calculate the differential and total cross sections theoretically. The second part allocated to the inelastic scattering, specifically the excitation of molecules to higher energy states. The collision of electrons with  $\text{NH}_3$  and  $\text{CH}_4$ , exploring rotational excitation processes. By calculating the total and differential cross sections of these inelastic interactions, we were able to investigate the effects of electron-induced rotational excitation on molecular dynamics. The last section of this dissertation is allocated to the study of electron stopping power and range within selected molecules. We investigate the ability of molecules to stopping the motion of incident electrons and quantized the distance over which electrons lose energy within the molecular medium. This analysis contributes to our understanding of energy deposition and dissipation processes during electron-molecule collisions.

This dissertation provides a comprehensive investigation of electron-molecule collisions, extending elastic and inelastic scattering, rotational excitation, and electron stopping power and range. The findings contribute to our understanding of fundamental collision processes and have

implications for various applications in the fields materials science, radiation physics, and molecular spectroscopy.

## **Abbreviations**

DCS	Differential cross sections
CS	Cross-Sections
HF	Hartree -Fock Approximation
SCE	Semi –Classical Exchange
FEG	Free –Electron -Gas
PO	Polarized Orbital
FN	Fixed-nuclear geometry
BOA	Born-oppenheimer approximation
COM	Center of molecules
DWA	Distorted-wave approximation.
DW	Distorted- Wave
TCS	Total Cross –Sections
MTCS	Momentum Transfer Cross- Section
SEP	Slater Exchange Potential
HFEG	Hara of Free- Electron- Gas
POM	Polarized Orbital Method
TFD	Thomas –Fermi – Dirac
DHF	Dirac –Hartree -Fock
ELSEPA	Elastic Scattering of Electrons and Positrons by Atoms
OEM	One-electron model
SOC	Spin – orbital coupling
ICS'S	Integrated cross - Section
$S_{coll}$	Collisions electronic stopping
$S_{rad}$	Radiation Nuclear Stopping
$S_t$	total stopping power
MOT	Molecular orbital theory
ANR	adiabatic nuclei rotation approximation

	method
$R(E)$	Range of particle
$\alpha d$	Dipole polarizability
$\sigma^m$	Momentum transfer cross section
$V_L^{(nr)}$	Non-relativistic local electron
$F(\theta)$	Spin conserving contribution velocity
$g(\theta)$	Spin –flip contribution velocity
$P_l(\cos \theta)$	Legendre Polynomials
$H$	Hamiltonian
$H_e(r)$	Kinetic energy
$V_{st}(r)$	Electrostatic interaction potential
$V_{ex}(r)$	Exchange potential
$Z$	Atomic number
$V_{cp}(r)$	Correlation-polarization potential
$W_{abs}(r)$	Magnitude of the imaginary absorption potential
$v_L$	Relativistic local electron velocity
$E_L$	Local electron energy
$\rho_e(r)$	Local electron density
(SF)	Space-fixed



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**Chapter one**

**Introduction**

## 1.1. INTRODUCTION

The collision between an electron and a molecule is of great significance as it can profoundly affect the structure and behavior of the molecule. In this section, we provide a concise overview of the electron-molecule collision process and its wide-ranging applications[1, 2]. Over the past two decades, there has been extensive investigation of electron-molecule collisions by both experimentalists and theoreticians. This surge in research can be attributed to two primary factors:

- (i) Advances in computer technology have made more powerful computers available, enabling researchers to investigate complex targets and collision processes with greater precision. In addition, there have been significant advances in experimental instrumentation, including enhanced electron spectroscopy, the availability of intense sources of polarized electrons, and the development of position-sensitive detectors[3].
- (ii) These developments have substantially helped to the enhanced knowledge and research of diverse collision mechanisms [3]. Electrons are crucial in atomic and molecular physics due to their light mass and superior mobility compared to nuclei. Data pertaining to collision processes involving electrons, ions, and neutral atoms and molecules is of utmost importance for the progress of several fields of physics, such as gas lasers, laboratory plasmas, ionospheres, auroras, stellar atmospheres, interstellar gases, and more recently. Atomic and molecular collisions are a captivating subject due to their crucial role in the advancement of quantum theory [4].

The following factors make it far more challenging to examine electron-molecule collisions than electron-atom collisions;

- 1 - Molecules possess varying degrees of freedom for both rotational and vibrational motion. These can be triggered by small amount of energy compared to electrical excitations. Below the electronic excitation

threshold of the target molecule, energy loss mostly happens through rotational and vibrational excitations [5].

- 2- Due to the presence of several nuclei, the interaction between electrons and molecules at short distances is characterised by a multi-centred and non-spherical nature[6]. Due to variations in the permanent electric multipole moments of various molecules, the interaction between them is generally strong and influenced by their relative orientations, even when they are separated by large distances. The polarisation force exhibits anisotropy, and its magnitude is determined by the polarizability of the target molecule [7].
- 3- When an electron collides with a molecular target, the target might dissociate [8].

## **1.2. Electron-molecules collision processes**

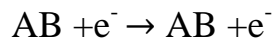
Electron-molecule collisions are a crucial feature of numerous domains of contemporary research [9-11] . Involving a wide variety of paths for dispersion. There is a wide range of scales where these collisions occur, including fields as varied as plasma physics, discharges, and others.

Electron-molecule collisions, on the other hand, are common in hotter parts of the interstellar medium in shocks[12] , and in weakly ionised interstellar mediums[13, 14] . They participate in atmospheric physics at intermediate scales [15]. Influencing the formation of phenomena like terrestrial auroras. Plasma etching and thin film deposition are two examples of the kinds of technologies that rely heavily on electron-molecule collisions, which play an important role in contemporary industries. These impacts are also vital to the laser processes that start in a variety of fusion reactors and discharges. The spark plugs in internal combustion engines, electric lights, and gaseous high voltage switches are just a few examples of where they play a critical role. There is

consensus outside of plasma physics and discharges that these collisions are the primary mechanism by which radiation damages cells [16]. The prevalence of electron-molecule collisions has prompted intensive study of the underlying scattering pathways. Both theoretical and experimental studies [17]. In addition to laboratory studies [18]. Have been done to clarify the nuances of these accidents.

### 1.2.1 Elastic Scattering

In scenarios when the intrinsic condition of the subject and the amount of energy possessed by the incoming electron remain unaltered.



The study of elastic scattering of e<sup>-</sup> - molecules has played a fundamental role in our understanding of molecular structure, intermolecular interactions, and the behavior of matter at the molecular level [19]. Elastic scattering refers to the process in which electrons molecule collides with a target molecule and transfers kinetic energy without undergoing any internal energy changes. This phenomenon has been a subject of scientific inquiry for several decades, leading to significant advancements in both theoretical and experimental techniques [20].

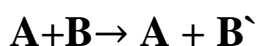
"The investigation of elastic scattering has its origins in the early 20th century when researchers studied the interaction of electrons with atoms and molecules. In 1914, British physicist James Chadwick's discovery of the neutron proved to be a crucial tool in elastic scattering experiments, given its neutral charge. The development of theoretical frameworks like the Born-Oppenheimer approximation and quantum mechanics played a vital role in advancing the understanding of the elastic scattering process.[21].

In the 1940, pioneering work by A. K. Kazanskii and I. I. Fabrikant significantly [22]. Advanced our understanding of elastic scattering with

electrons and diatomic molecules. Provided insights into scattering cross-sections and molecular parameter dependence. Subsequent decades saw remarkable growth with technological advancements and theoretical breakthroughs, elevating the study of elastic scattering to new levels[23]. Advancements in computational methods and quantum simulations revolutionized the theoretical understanding of elastic scattering. Sophisticated models and algorithms described scattering processes at different energy regimes, revealing intricate molecular interactions and offering predictions for experimental validation [24].

Currently, elastic scattering remains an active and dynamic field of research, making valuable contributions to various scientific disciplines including atmospheric science, chemical physics, and materials science. Understanding the mechanisms underlying elastic collisions provides crucial insights into molecular structure, dynamics, and the behavior of intricate systems.

### **1.2.2. Non-elastic Scattering**



There are three main processes that this channel focuses on:

Firstly, Molecular excitation which plays a crucial role in various scientific fields, including chemistry, physics, and spectroscopy. Understanding how molecules absorb and emit energy is fundamental to our understanding of chemical reactions, spectroscopic techniques, and the behavior of matter at the molecular level [3].

Secondly when an excited atom, ion, or molecule accumulates enough energy to remove one or more of its electrons, the outcome is ionisation of the molecule. Ionization occurs when an electron jumps from a lower-energy bound state (orbit) to an unbound, higher-energy state [25].

In the third place, we have dissociation, which is a chemical process that involves the breaking apart of a molecule into its component parts. Usually, this happens when a molecule takes in enough energy, usually in the form of heat, light, or collisions with other particles, to overcome the forces keeping its component atoms or groups together [26].

The link between rotational, vibrational, and electronic motion of excited particles is a basic feature of molecular dynamics and spectroscopy. These modes of motion, and the energy exchanges and transitions between them that occur while molecules are in the excited state, have a significant impact on the molecules' characteristics and reactivity. Energy transfer, chemical reactions, and spectroscopic phenomena are just some of the many processes that may be better understood by looking at the interplay of rotational, vibrational, and electronic excitations, see figure (1-1) [1] .

### **1.3. Excitation processes**

Promoting an electron or particle to a higher energy level, or excited state, is a fundamental phenomenon in physics and chemistry. These processes serve a significant role in understanding the behaviour of atoms, molecules, and other quantum systems. Absorption of photons, collision with other particles, and contact with external fields are only a few of the mechanisms that can lead to excitation[27].

It is standard practice in the field of atomic and molecular physics to use spectroscopic methods to investigate excitation processes because of the unique information they give about the energy levels and electronic structures of atoms and molecules[28]. When an electron is excited from one energy level to another, it can either emit or absorb light of a certain wavelength[29]. Other forms of stimulation besides electrical ones include:



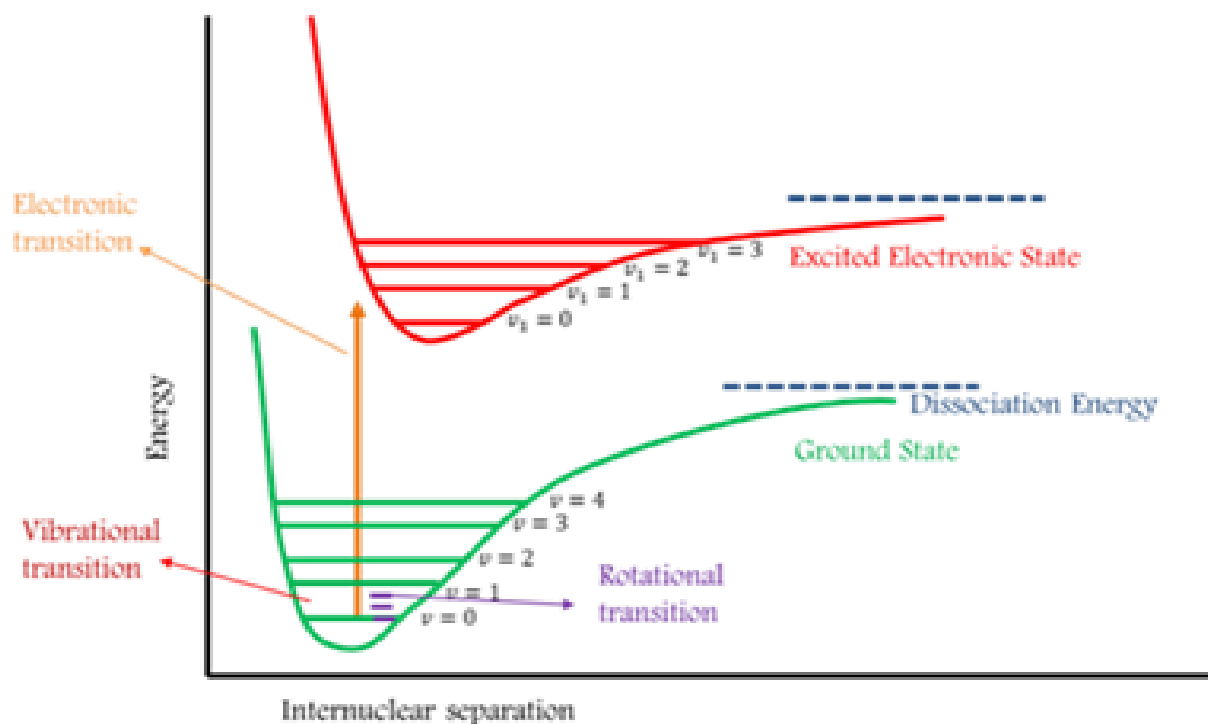


Figure (1-1) depicts the mobility of the molecule as a result of its rotational, vibrational, and electronic energy levels.[1]

### 1.3.1. Rotational excitation

The early 20th century marked the start of research into rotating excitations in molecules. Chadwick made the seminal discovery of the neutron, an uncharged subatomic particle with a mass comparable to that of a proton, in 1914. This finding paved the way for the study of electron and charged particle interactions with molecules. Following Chadwick's discovery of the neutron, scientists could explore how particles like electrons and photons interact with particles undergoing spin-excitation. Since then, several developments in experimental and theoretical methodologies have helped us better understand molecular dynamics and spectroscopic features through

the study of spin excitations [30]. The study of rotating excitation in electron collisions plays a crucial role in understanding molecular interactions and energy transfer mechanisms. When molecules experience rotational transitions in the absence of electronic or vibrational alterations, this area of study focuses on the resulting changes in the molecules' dynamics as a result of their interactions with electrons. Temporary excitation without enduring structural changes results from the transmission of reversible energy to the molecule in this process [31].

### **1.3.2. Vibrational Excitation:**

Increased vibrational motion in a molecule is the consequence of a process known as vibrational excitation, which involves the transfer of energy to the molecule. The study of molecular motion and chemical reactions greatly benefits from an appreciation of this phenomenon [32]. Due to low electron energies at low temperatures, rotational excitation may predominate over vibrational excitation by electron impact in interstellar settings. Other astronomical phenomena, such as comets and planetary ionospheres, have shown that it is, in fact, quite important [33]. Vibrational excitation is less difficult to study than rotational excitation, although less is known about it from experimental observations because of its low energy. As most measurements begin with molecules in their vibrational ground state, differentiating between energetically near vibrational modes can be difficult. Theoretical predictions show that when beginning from vibrationally excited states, the results of electron impact vibrational excitation might vary greatly [34].

### **1.3.3. Electronic Excitation**

This kind of excitation entails the elevation of one electron from a lower energy orbital to a higher energy orbital inside the molecule, leading to the molecule assuming an electrically excited state. Electronic excitation plays

a significant role in phenomena such as absorption and fluorescence spectroscopy [5].

## 1.4. Stopping power

The interaction of charged particles with matter is a central occurrence in the fascinating field of atomic and molecular physics, serving as the basis for many physical and chemical processes. The study of the stopping power of electrons in molecules stands out as a particularly important and fruitful area with substantial significance due to its relevance across many fields of study and technology [35].

$S$  represents the "stopping power" of a medium, which in this case is molecules, to prevent the further loss of energy by high-energy charged particles, such as electrons, as they pass through it. Radiation treatment, materials science, astrophysics, and the study of complex chemical systems all place a premium on comprehending the complicated mechanisms of energy deposition and transfer that occur when electrons interact with molecules[36].

### 1.4.1. Collisions electronic stopping ( $S_{coll}$ ):

Electronic stopping power embodies the energy dissipation resulting from interactions between the charged particle and the electrons within the traversed material, prominently driven by electromagnetic forces. Principal mechanisms encompass ionization and excitation of atomic electrons within the material, culminating in the creation of electron-hole pairs and the emission of photons. The magnitude of electronic stopping power hinges upon the velocity (energy) of the charged particle and intrinsic material properties, with particular emphasis on electron density [37].

Electronic stopping power constitutes an indispensable asset in realms such as ion implantation, microelectronics fabrication, and the comprehensive

comprehension of the behavior of charged particles within diverse materials [38].

#### 1.4.2. Radiation Nuclear Stopping ( $S_{rad}$ ):

Nuclear stopping power arises from interactions between the charged particle and the atomic nuclei nestled within the material, with these interactions being predominantly governed by nuclear power. The genesis of nuclear stopping power is traced to the scattering of the charged particle by the atomic nuclei, ushering in alterations in the particle's trajectory. The magnitude of nuclear stopping power is contingent upon the charge and mass attributes of the projectile and target nuclei, alongside the projectile's velocity [39]. Experiments in nuclear physics, the development of particle accelerators, and the methodical investigation of radiation shielding materials all benefit greatly from nuclear stopping power. Beyond these two broad classes, a chimaera called as "total stopping power ( $S_t$ )" arises, deftly incorporating the electronic and nuclear aspects. When used in the real world, total stopping power provides a holistic picture of the total energy loss that charged particles experience when passing through a specific substance[40].

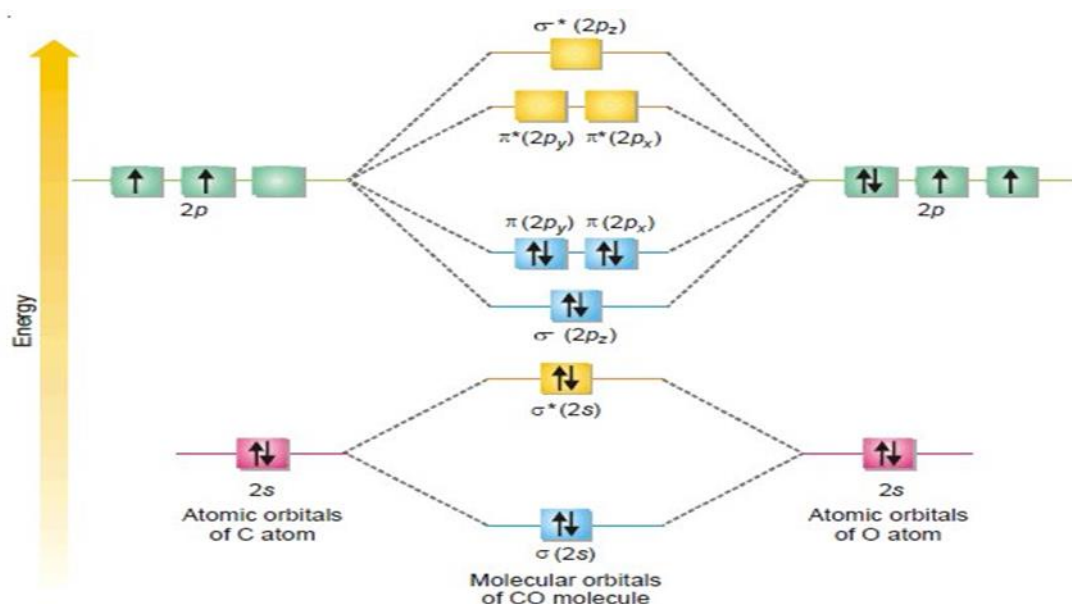
What matters most is the context and energy spectrum of the particles under investigation when deciding between electronic and nuclear stopping power[41].

### 1.5. Molecular orbitals Theory

Quantum chemistry's molecular orbital theory (MOT) is a cornerstone idea because it provides a robust framework for elucidating molecules' electronic structure and characteristics. Using quantum mechanical concepts, it sheds light on molecule bonding, electronic spectra, and chemical reactions [42]. The molecular orbital theory (MOT) is a

fundamental theory that describes the distribution of electrons in molecules by combining the orbitals of the individual atoms in a linear fashion. These molecular orbitals cover the whole molecule and provide quantized space for the electrons. The distribution of electrons in these molecular orbitals dictates the molecule's overall electronic structure and regulates its chemical behaviour[43]. Using MOT, we have come a long way in our comprehension of chemical events. It has shed light on fundamental ideas including bond formation, bond length, and bond energy. MOT can foretell a molecule's stability and reactivity, as well as its electronic spectra; by taking into account the symmetries and energies of the relevant atomic orbitals [44].

The contributions of prominent scientists were crucial to the growth of MOT. Friedrich Hund invented the idea of molecular orbitals and established laws for electron scattering[45] . Orbital interference and hybridization are two major ideas contributed by Robert S. Mullikin conceived the theory and helped develop it further [46] . There is a strong relationship between MOT and intermolecular forces, which John Lennard Jones did much to advance our knowledge [47]. Figure (1-2) shows the orbitals and types of bonds .



**Figure (1-2) shows the theory of molecular orbitals [47].**

( $\sigma$ ) bonds" and ( $\pi$ ) bonds" refer to two different types of covalent bonds that can form between atoms in a molecule.

### 1- Sigma Bond ( $\sigma$ ):

One sort of covalent bond is the sigma bond, which develops when the orbitals of two atoms overlap one another end to end along the bond axis. This direct contact fortifies the link between them. Sigma bonds can arise between s orbitals, s and p orbitals, or two p orbitals in various combinations. The electron density is most dense along the bond axis of sigma bonds, which are most common in single bonds (such as C-C and C-H)[48].

## 2- Pi Bond :( $\pi$ )

When two unpaired p orbitals meet perpendicularly, they produce a pi ( $\pi$ ) bond, a kind of covalent bond. Because of this overlap, pi bonds are often weaker than sigma bonds. Double and triple bonds are common examples of multi-bonding structures that contain pi bonds. One sigma bond ( $\sigma$ ) and one pi bond ( $\pi$ ) are present between carbon atoms in a carbon-carbon double bond (C=C) [49].

## 1.6. Molecular characteristics

Atoms form substance, and chemical bonds bind molecules. Molecular structures, characteristics, and behavior are important in chemistry, biology, and materials research. Studying molecular characteristics can help scientists understand chemical processes, molecule interactions, and the creation of new materials with specialized properties [50].

Molecular properties include molecule shape, electrical structure, and spectroscopic activity. Molecular geometry helps explain a molecule's form, symmetry, and spatial orientation. The energy levels, orbital arrangements, and electron concentrations of a molecule's electrons are its electronic structure. Spectroscopic techniques may reveal molecules' vibrational, rotational, and electronic changes by studying their electromagnetic radiation interactions [51].

## 1.7. Molecular symmetry

In physics, molecular symmetry is essential to understanding molecule properties, quantum mechanical processes, solid-state behaviour, and spectroscopy. Its broad usage in physics has improved our knowledge of molecular systems and provided a solid platform for theoretical and

experimental investigation. Researchers can advance materials science, quantum chemistry, and other fields of physics by using molecular symmetry to comprehend molecules' intricate symmetrical groupings and behaviors [52].

By shedding light on the symmetrical shifts that occur during chemical reactions, symmetry considerations contribute in the understanding of molecular dynamics and reaction processes[53]. A symmetry operation is any manipulation that leaves the thing looking the same as before. Think about a water molecule, for instance. A 180-degree rotation along an axis travelling through the oxygen (O) atom in the middle of the molecule, between the two hydrogen (H), will not alter the molecule's overall shape. Similarly, if we reflect the molecule across any of the two mirror planes, as shown in the diagram below, the symmetry of the molecule will be preserved[54].

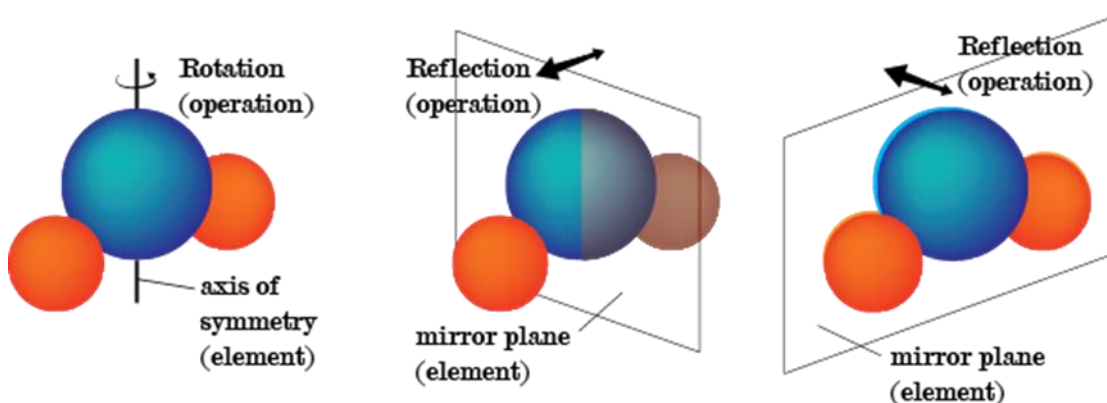


Figure (1-4): A schematic depiction of symmetry operations and their constituent parts [54].

Any given symmetry operation must be performed with respect to some axis, plane, line, or point known as the symmetry element. All points that keep their coordinates after the symmetry transformation are included in this symmetry element. The unchanging points in a rotation create a symmetry axis, whereas in a reflection, the unchanged points form a symmetry plane.



## **1.8. Dipole moment of molecules**

Dipole moment is an important property of molecules that results from their internal charge distribution. It is crucial in many subfields of physics since it elucidates such fundamental questions as what causes molecular polarity, how molecules interact with one another, what causes spectroscopic phenomena, and how molecules respond to the presence of an external electric field. Examining the theoretical foundations, experimental measurement techniques [55].

To relate the molecular structure to the electrical behavior, knowledge of the dipole moment is essential. It helps researchers learn more about the polarity of molecules, which is important for understanding intermolecular forces and interactions. The dipole moment also plays a crucial role in spectroscopic research, allowing for the decoding of molecule spectra and the determination of electronic characteristics[56].

Researchers learn a lot about molecules' characteristics, materials science, and how they react to electric fields by studying their dipole moments. A thorough comprehension of the dipole moment benefits from theoretical underpinnings like quantum mechanical models and computational tools. Accurate estimation of dipole moments is possible using experimental methods including spectroscopy and dielectric measurements [57].

## **1.9. Polarizability of molecules**

Molecules' electric field behavior, intermolecular interactions, and spectroscopic phenomena may all be better understood if one has a firm grasp on their polarizability [58]. This introductory science article will discuss polarizability, including its theoretical underpinnings, experimental measurement methodologies, and scientific importance. is the property of molecules to experience induced polarisation in the presence of an external

electric field. It measures the sensitivity of the molecule to an electric field and provides information on the likelihood of electron displacement and the formation of transient dipoles. The theoretical knowledge of polarizability is anchored on quantum mechanics and electromagnetic theory[59]. For theoretical descriptions and forecasts of molecular polarizability, models like the classical oscillator model and the quantum mechanical dipole response model are useful.

### **1.10. HOMO – LUMO energy gap**

Understanding the electronic structure and characteristics of molecules in great detail is possible thanks to the molecular orbital theory, a central foundation in quantum chemistry. To describe the distribution of electrons delocalized throughout the whole molecule, rather than localised on individual atoms, it goes beyond the usual atomic orbital method. This theory is essential for understanding the intricate workings of chemical bonds and electrical behavior on the molecular scale [60].

The theory of molecular orbitals emphasises the importance of the combining of atomic orbitals to produce molecule orbitals. The molecular orbitals sigma ( $\sigma$ ) and pi ( $\pi$ ) are particularly significant. Two s orbitals constructively overlap to make a  $\sigma$  orbital, and two p orbitals side by side to produce a  $\pi$  orbital. When it comes to bonding and establishing the electrical characteristics of molecules, these orbitals play a pivotal role [61].

Also of relevance is the energy dispersion between the lowest unoccupied molecular orbital (LUMO) and the highest occupied molecular orbital (HOMO). Understanding molecular reactivity and electronic characteristics relies heavily on these orbitals [62].

Recognising the electrical behaviour, stability, and bonding in molecular systems requires knowledge of the energy distribution of the HOMO and

LUMO orbitals and the alterations to these distributions owing to intermolecular interactions. It's useful for understanding how to create optoelectronic devices, organic semiconductors, and molecular sensors that have precisely customised electrical characteristics[63].

### **1.11. Background and Historical review**

Since around 1930–1940, scientists have been studying the results of electron–molecule collisions. In the 1930s and 1940s, scientists learned a lot about what happens when electrons and molecules collide. Here's a historical backdrop along with descriptions of significant theoretical and experimental work throughout this period, in 1930 saw the development of quantum mechanics as a basic framework for explaining particle interactions. Understanding quantum-level collision events relied on the theoretical work of giants like Werner Heisenberg and Erwin Schrödinger. (1925)[64].

Max Born and Robert Oppenheimer advanced our theoretical knowledge of electron and molecular elastic scattering processes. Their research paved the way for a more complete description of the energy-conserving interactions between electrons and molecules resulted in the identification of the positron, an experimental confirmation of particle-antiparticle annihilation through inelastic collisions [65].

The collision theory of Born and Oppenheimer was employed in order to investigate the many events that occur on the influence of the electron with molecules [20]. In 1936, a scientist studied the scattering of electrons off of corners by molecules of hydrogen across an angular range of  $5^\circ$  to  $150^\circ$  and a range of incident electron energies [66].

Cloud chamber experiments were one of the unique methods created in the early 1940s by scientists like C. F. Powell, C. C. Butler, and E. H. S. Burhop to examine the elastic scattering of charged particles. Their work

helped us better comprehend electron-molecule interactions. Theoretically, quantum mechanics plays a pivotal role due to its fast development from its start in the early 20th century. In the preceding decades, pioneering physicists like Max Born, Werner Heisenberg, and Erwin Schrödinger had created the framework for quantum mechanics. Their theories laid the groundwork for figuring out how electrons and particles collide [67].

The application of sophisticated computational tools continued to develop theory throughout the 1950s. John C. Slater, among others, made substantial contributions, leading to the invention of the Hartree-Fock technique. This computer method improved our ability to anticipate the consequences of electron-particle collisions and shed light on the underlying quantum mechanical principles at play in these collisions [68]. Experimentalists also made tremendous breakthroughs during this time. F. Powell, C. C. Butler, and E. H. S. Burhop were among the first to develop innovative experimental methods employing cloud chamber technology in the 1940s. The elastic scattering of electrons and molecules was the focus of these investigations. They helped us grasp these interactions much better by thoroughly analyzing angular distributions and scattering cross-sections [69].

Experiments with high-energy electrons performed by Robert Hofstadter in the late 1950s were a major step forward in deciphering nuclear structure and electron scattering. We owe a great deal to his ground-breaking research on electron scattering and nuclear form factors, which expanded our understanding of elastic scattering processes [70, 71].

The researcher examined the use of the Born approximation in the context of electron collisions with neutral hydrogen molecules in 1954. Calculations of the cross sections for collisions with accompanying vibration and rotation [72].

It wasn't until 1966 that researchers were able to determine the differential and integral cross-sections for the elastic scattering of a slow electron by a hydrogen molecule. We generalise the short-range electrostatic interaction using spherical harmonics. There are also triple interactions and long-range polarization [73].

In 1985 made major theoretical advances to understanding electron-molecule elastic scattering. Their research laid the groundwork for understanding how electrons and molecules interact with one another [74, 75].

In 2000[76, 77] . In this investigation, focused on the role that unbound or scattering states play in molecule electronic structure computations in the field of computational chemistry .The paper presents a method for dealing with collisions between electrons and molecules and emphasises how well it scales across parallel computing settings ranging from massively parallel supercomputers to clusters of individual workstations. Improved performance and the ability to study collisions involving bigger polyatomic molecules are the goals of this modification [78].

In 2012 study uses both an experimental and theoretical technique to examine electron scattering from acetone ( $\text{CH}_3\text{COCH}_3$ ) [79]. In 2016, researchers examined the electron scattering cross sections of compounds of astronomical significance. It gave us new information on how electrons and other particles interact in space, including how elastic collisions and spin excitation processes work [80].

In 2020, this research proposes a hybrid experimental/theoretical investigation. It comprises differential, total, and momentum transfer cross-sections, offering information on the scattering dynamics and electron-molecule interactions in nitrobenzene[81].

## **1.12. Aims of dissertation**

The aims of this work is to study the differential cross sections of steady state, excited state, and total momentum of electron collisions with molecules while studying the stopping power of electrons in molecules. Through a computational study of electron scattering with molecules (elastic and inelastic) and comparison with experimental and theoretical results, this work adds to the understanding Electron-particle interactions and their outcomes are better investigated across a number of scientific applications by analyzing cross-sections in both steady-state and dynamic systems.

The purpose of this dissertation is to examine the theoretical use of collisions and identify the physical processes responsible for electron stalling, including inelastic and elastic scattering, and transitions electronic induced collision.

## **1.13. Dissertation Organization**

The outline of the dissertation looks like this:

The first chapter is a comprehensive introduction to electron collisions with molecules. Highlighting the elastic and inelastic scattering of electrons and the stopping power of electrons in molecules.

This includes presenting several types of elastic and inelastic scattering. This thesis focuses on studying the differential, total and total cross sections of the elastic and inelastic collision of a group of molecules in both cases. I give a systematic overview of the relevant theoretical and scientific literature. This literature review provides context for the research by highlighting the latest developments. These results help shed light on the mechanisms behind collision processes by providing quantitative information on the probability of scattering at different angles and energy.

In Chapter 2, we examine the different types of dispersion potentials and the theoretical methods used in the calculations. Studying the theoretical foundations of dispersion analysis modeling. Calculating and predicting dispersion behavior requires the use of theoretical techniques.

In the context of elastic dispersion collisions involving electrons and molecules, the results are examined in Section A of the third chapter of the dissertation. In this chapter, we provide a comprehensive examination of the differential, total, and momentum cross sections for each elastic scattering event, as well as other calculated results. Part B focuses on the rotational excitations that occur in collisions between electrons and molecules.

These cross sections are essential for learning about rotational dynamics and dispersion behavior. Determining the extent and force of stopping the electron in the event of its collision with molecules was the subject of the fourth chapter of the dissertation.

Finally, Chapter Five was devoted to discussion and conclusion

## **Chapter two**

# **The Theoretical part**



## Chapter two

### 2.1. Introduction

When particles collide with a potential field or with one another, basic physics phenomena called scattering. Important areas of study rely on it, including nuclear physics. Subfields within physics include atomic and molecular physics, particle physics, and condensed matter physics. Important information about particle characteristics, interactions, and underlying systems may be derived from scattering experiments and theoretical models [82]. Particles or fields undergo scattering when they collide with one another and cause them to diverge from their initial paths. Particles are scattered throughout the process, which results in the transmission of energy, angular momentum, and momentum. Research into scattering has led to a deeper comprehension of particle properties and movements, interactions, and composition at different scales [83]. Scattering can appear in numerous forms, such as resonant, inelastic, and elastic scattering, each distinguished by specific properties and occurrences. Particles engage in elastic scattering when they maintain a constant total energy during the process of scattering, without exchanging energy or stimulation with one another [84].

This study focuses on examining collision dispersion mechanisms at different energy levels. we gained a comprehensive understanding of fundamental molecular interactions and their structure. Additionally, we refined theoretical models and computational approaches to calculate momentum transfer, differential and total cross sections, and other relevant values.

Next, we will discuss the theory pertaining to the non-excited and excited parts and finally demonstrate the stopping power of electrons.

## 2.2. Elastic Scattering

Physics and chemistry have great benefit from theoretical studies of elastic scattering processes involving molecules and rapidly moving electrons. [85]. This aims to comprehend the fundamental ideas and concepts that underlie these interactions, which have numerous real-world applications. The theoretical foundation for the investigation of electrons' elastic particle scattering is provided in this section. We are initially focusing on the Hamiltonian factor, which is made up of molecules and electrons' kinetic energy, potential energy, and interactions with one another. Dirac's relativistic formula describes the motion of a projectile with rest mass  $m_0$  moving at a speed  $v$  in a central field with potential  $V(r)$  [86].

As follows:

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

When

$$\psi_{Ekm}(r) = \frac{1}{r} \begin{pmatrix} P_{Ek}(r)\Omega_{k,m}(r) \\ iQ_{Ek}(r)\Omega_{-k,m}(r) \end{pmatrix} \quad \text{Dirac spherical waves}$$

$$\varepsilon = \gamma m_0 c^2 = \varepsilon_i + m_0 c^2 \quad \text{is the total energy}$$

$$\gamma = \left(1 - \frac{v^2}{c^2}\right)^{-\frac{1}{2}}$$

Where  $\alpha$  and  $\beta$  are the typical  $4 \times 4$  Dirac matrices,  $c$  is the speed of light in a vacuum, and  $\varepsilon_i$  is the incident particle's kinetic energy.

### 2.2.1. Potential visual complexity

The package of radial subroutines [87]. As well as a complicated optical potential [88]. type are used for solving the Dirac equation numerically

$$V(\mathbf{r}) = V_{\text{real}}(\mathbf{r}) - iW_{\text{abs}}(\mathbf{r}) \quad (2-2)$$