Chapter 7

Summary and future prospects

This chapter summarizes the present research work that has been undertaken. We also pointed out the advantages and drawbacks of the present methodologies employed here. The potential reach of the current work and its significance from an application standpoint have been also discussed in this chapter.

7.1 Summary of the present investigation

In this thesis, the focus was placed on electron scattering that have a wide variety of potential applications. The key objective of this investigation is to quantify the electron collision processes in terms of cross sections. In order to calculate the cross section, we made use of two different formalisms: R-matrix method and the spherical complex optical potential (SCOP) approach. The latter method has been used successfully for quite some time and is applicable to scattering at both intermediate and high energies. In the low energy zone, physics gets more intricate, and as a result, a sophisticated approach is necessary. The former technique, viz., R-matrix is able to fulfil this need because it is advanced and sophisticated method.

The R-matrix formalism, an ab-initio formalism is used for low collision energies (below the molecular ionisation threshold), while the SCOP formalism is used for higher energies, generally above the ionisation energies of the molecules. It has been discovered that the transition between the two formalisms takes place seamlessly somewhere in the energy range of 15-20 eV for all of the targets that have been investigated till now.

Complex scattering potential-ionisation contribution method in conjunction with the spherical complex optical potential formalism is used to calculate the ionisation cross sections along with the byproduct- electronic excitation cross-sections. In addition to cross sections, the

inelastic mean free path, mass stopping power, and absorbed dose calculation for aqueous target systems are all taken into consideration during the course of this research endeavour.

Electrons are ubiquitous particles, and their interactions with plasma molecules, astro compounds, biomolecules, interstellar molecular systems, and other pertinent species find significant applications in their respective domains. For instance, the scattering of electrons from biomolecules is an essential part of the research process for determining the DNA damage induced by electrons of low and intermediate energies. Nucleotides, viz., Adenine, Guanine, Cytosine, Uracil, Thymine and nucleosides viz., Adenosine, Guanosine, Cytidine, Uridine and Thymidine, are essential component of living organisms, are the subject of investigation in this thesis. Additionally, among various inelastic processes, the ionization process is particularly significant in plasma and several industrial activities. In light of the significance of the topic, we have selected a group of compounds that can be used in plasma as well as in industrial settings. Fluoronitriles (C_3F_5N and C_4F_7N), the plasma-relevant compounds are being investigated in this article. These molecules have the potential to replace SF_6 in plasma applications while maintaining their environmentally favourable characteristics. There was a dearth of electron collision study of these targets, and thus the present work will add to that body of knowledge. Other than these compounds, a group of deuterated molecules, viz., HD, D_2, D_2O, SiD_x (x=1-3), CD_x (x=2-4) and ND_x (x=1-3), which finds various and wide range of applications in the fields of industries, planetary sciences, semiconductor industries and so on, is also investigated here. The biomaterials furfural and para-benzoquinone, which play important role in the green chemistry, are also studied here. They have significant uses in the fabrication of energy storage devices, plasma fields, energy harvesting systems etc.

Apart from this, electron interactions with the aqueous phase DNA constituents are also attempted here. Since, DNA molecules always found covered with the water molecules in the living systems, considering their aqua phase leads us to more realistic picture. Major essential tools for the DNA damage assessment, viz., cross-sections, inelastic mean free path, stopping power are computed for mainly five DNA constituents (Adenine, Guanine, Cytosine, Uracil, Thymine) by successfully employing modifying SCOP approach.

Additionally, we use the R-matrix technique on fluoromethanes, to investigate the low energy interaction of electrons with this molecule. In addition to computing cross sections in low energy regime, we have also used the SCOP to estimate throughout a wide energy spectrum.

Table 7.1 Present electron collision study for various molecules

Target molecules	Investigation	Reference
HD, D_2, D_2O, SiD_x (x=1-3), CD_x (x=2-4) and ND_x (x=1-3)	• Total inelastic, ionisation, and electronic excitations • Correlation study, leading to prediction of polarisability of molecules	(Parikh, Smruti; Vinodkumar, Mianxi; Limbachiya, 2023)
H_2SO_4	• Total inelastic, ionisation, and electronic excitations • Dependency of target properties on cross-section values	(Parikh et al., 2022)
Adenosine, Guanosine, Cytidine, Uridine and Thymidine	• Elastic, inelastic, ionisation, electronic excitations, and Total	(Parikh, Smruti; Limbachiya, 2023)
Furfural and para-Benzoquinone	• Elastic, inelastic, ionisation, electronic excitations, and Total • Various correlations study	Communicated
Fluoronitriles (C_3F_5N and C_4F_7N)		
Aqueous DNA constituents (Adenine, Guanine, Cytosine, Uracil, Thymine)	• Elastic, inelastic, ionisation, electronic excitations, and Total • Inelastic mean free path, mass stopping power, absorbed dose. • Prediction of polarisability and dielectric constant from various correlations	
Difluoromethane (CH_2F_2)	• Elastic (differential and integral), momentum transfer, inelastic, ionisation, electronic excitations, and Total (0.1 to 5000 eV)	

7.1.1 Advantages and Limitations of the present methodologies

A. R-matrix formalism

It is an ab-initio technique. The concept that underpins the partitioning of the configuration space makes it possible to find a solution to the problem. The R-matrix approaches tackle the extremely complicated physics that arise in the inner area. Understanding low-energy electron atom/molecule scattering can be accomplished with the use of R-matrix methods, which are among the most common and frequently utilised approaches. Due to the fact that R-matrix deals with intricate physics, a variety of rigorous mathematical models have been incorporated here. Calculation is made more challenging as a result; hence, a greater level of computation is necessary. The R-matrix approach is time consuming and can only be used with relatively lower incident energies.

B. SCOP and CSP-ic

It is based on the principles of quantum mechanics and investigates the general pattern of atomic and molecular systems as they go from discrete to continuous states. Under a single formalism, one can derive a number of different total cross sections. In comparison to other theoretical methods, such as the R-matrix, this one is straightforward, quick, and trustworthy. It can do calculations for a wide range of target systems that are the focus of the study. This first attempt at isolating Q_{ion} from Q_{inel}, known as CSP-ic, yielded five different cross-sections: Q_T, Q_{el}, Q_{inel}, Q_{ion}, and Q_{exc}. When compared to other experimental and theoretical data, the results achieved and published here using SCOP and CSP-ic often lie within 10% uncertainty.

While the spherical approximation utilised in SCOP is generally sound, it does not always make sense for molecules with particular geometries. Neither SCOP nor CSP-ic can be used to compute low-energy electron collision data because they are formalisms for intermediate to high energies. Using CSP-ic, one can find Q_{ion} in a semi-empirical manner.

7.2 Future prospects

The importance of the present research work is underscored by the fact that large amounts of data are needed to create the "virtual laboratories" that are essential for studying atmospheric

science, radiation physics, technical plasmas, and astrophysics. Experiments on particular target systems, such as those that are not available in the gas phase, or any radioactive or toxic molecular compounds, can be challenging or perhaps impossible to carry out. If it is conceivable, then the experimental errors can be anywhere from 15% to 25% or even higher. In circumstances like these, the approach that we have developed is of great significance to the field of applied physics. Our goal is to expand the scope of our calculation to include larger and complex molecular systems such as dimers, bio compounds, clusters, and so on. We plan to focus in the future on other interaction processes as well, such as neutral and ionic dissociation. In this regard, some of the unsolved difficulties and unexplored potential are connected to the following aspects:

- We are going to investigate the dissociative ionisation, partial ionisation, dissociative electron attachment (DEA), as well as differential cross sections molecules.
- Modifying the theoretical models to study the condensed or solid phase molecular systems.
- Apart from electron interactions, we would like to now focus on positron and positronium collision study.
- We wish to extend the electronic and nuclear charge density that is offered by density functional theory to incorporate it in the SCOP formalism for future work.
- Apart from cross-sections, other essential quantities applicable in various research and applied fields are also into the focus for the future work.
- To account for larger and complex molecules, we want to expand R-matrix calculations.
- To compute the rotational and vibrational excitation cross-sections, modification in the model potentials is aimed.