CHAPTER 7 SUMMARY AND FUTURE PROSPECTS

"In this chapter, we accomplish the present research with a summary of the work reported here. We derive significant insights about the present theoretical frameworks employed in this investigation, concerning their significance from an application standpoint. Additionally, we engage in a discussion about the future prospects of the ongoing research, underscoring their importance from an applied perspective".

7.1 Summary of the present work

This thesis starting from the chapter 1 to chapter 6 we have shown various electron collision processes and their relevance applications along with theoretical calculation involving various CSs and of electron induced scattering. The theoretical investigation carried out under the electron collision range starting from threshold to 5000 eV.

The purpose of this research was to establish reliable theoretical methods for computing a wide range of electron collision CSs. In order to quantify the different collision processes in terms of CSs, we made use of different methodology: Spherical complex optical potential (SCOP), Complex scattering potential using ionization contribution (CSP-ic) and recently develop 2 parameter semi-empirical formalism (2P-SEM). To estimate elastic and inelastic CSs, SCOP formalism is applied for intermediate to high energy regime, staring above the IP of the target molecules. The CSP-ic is combined with a spherical complex optical potential formalism to compute ionization CSs alongside the co-produced electronic excitation CSs.

Electron is the fundamental particles, interact with a molecular system which impacting numerous scientific fields. Studying electron scattering from biomolecules plays a crucial role in understanding DNA damage caused by intermediate energy electrons. This thesis focuses on analogous of DNA constituents biomolecules, 3-hydroxy-tetrahydrofuran and α-tetrahydrofurfuryl alcohol, nucleotides (Adenine, Guanine, Thymine, Uracil, and Cytosine), essential components of life. Among various electron-molecule interactions, ionization holds particular significance in plasmas and various industrial applications. Fluoronitriles (C_3F_5N and C_4F_7N) are plasma-relevant molecules have the potential to replace environmentally harmful SF_6 in plasma applications while maintaining their eco-friendly nature. Beyond plasmas and industrial applications, this study extends to furfural and para-benzoquinone - biomaterials with significant roles in green chemistry. These molecules hold promise for applications like energy storage devices and harvesting systems. This research goes beyond isolated DNA components to consider their interactions with electrons in an aqueous phase. Since living cells surround DNA with water molecules, this approach provides a more realistic picture of electron-induced damage. To achieve this, we employed a modified SCOP formalism to compute various cross section for DNA damage assessment.

This thesis involves various calculations for a variety of analogous of DNA/RNA nucleobases (chapter 3), industrial relevance, environment friendly and plasma molecules (chapter 4), DNA constituents in aqueous phase (chapter 5) and Interstellar molecule (chapter 6).

Table 7.1 Summary of the present thesis

Target molecules	Investigation	Chapter
3-hydroxy tetrahydrofuran and α-tetrahydro furfuryl alcohol	• Total, Elastic, Inelastic, Ionization, and electronic Excitations • Correlation study, leading to prediction of polarizability of molecules	3
Furfural and para-Benzoquinone Fluoronitriles (C_3F_5N and C_4F_7N)	• Total, Elastic, Inelastic, Ionization, and electronic Excitations • Dependency of target properties on cross-section values	4
Aqueous DNA constituents: Adenine, Guanine, Cytosine, Uracil, Thymine	• Elastic, Inelastic, Ionisation, electronic Excitations, and Total • Prediction of polarizability and dielectric constant from various correlations	5
N_2	• Ionization, Elastic, Inelastic, electronic Excitation and Total	6

7.2 Advantages and Limitations of the present methodologies

Present methodologies are based on the principles of quantum mechanics to explore the general behaviour of atoms and molecules as they transition from bound (discrete) to unbound (continuous) states. The SCOP formalism offers to estimate various total CSs. Compared to other investigates i.e. R-matrix is computationally efficient, reliable, trustworthy and applicable to a broad spectrum of target systems under study. A key advancement within SCOP is the development of CSP-ic. This initial attempt successfully isolated the ionization (Q_{ion}) CSs from the inelastic (Q_{inel}) CSs, enabling the calculation of five distinct CSs: Q_T, Q_{el}, Q_{inel}, Q_{ion}, and summed Q_{exc}.

The results obtained using SCOP and CSP-ic often shows excellent agreement (within 10% uncertainty) with existing theoretical and experimental findings. However, it is important to acknowledge limitations: The spherical approximation in SCOP might not be ideal for all molecular geometries. Both SCOP and CSP-ic are primarily applied for intermediate to high-energy electron collisions, making them less effective for low-energy interactions. CSP-ic offers a semi-empirical approach to extract Q_{ion}.

7.3 Future prospects

- Our aim to investigate various electron-molecule interaction including differential cross sections, partial ionization, dissociate ionizations as well as dissociative electron attachment.
- We plan to modify our theoretical model potential to study electron interactions with molecules in condensed or solid phases, moving beyond isolated molecules.
- In addition to electron interactions, we intend to explore collisions involving positron with complex molecules.
- Modifications to the model potentials will be explored to enable the calculation of Q_{rot} (rotational) and Q_{vib} (vibrational excitation) CSs.
- We wish to explore R-matrix calculations for complex and larger molecules.
- With the discovery of novel molecules in cometary and planetary environments, we aim to explore their interactions with electrons. This research holds significant potential for applications in astrochemistry.
- Moving beyond isolated molecules, we will explore electron interactions with molecules in condensed phases, such as the ices found on various planets and comets. This research can provide valuable insights into these environments.
- To understand various phenomena related to industrially relevant and modern technological molecules like carbon nanotubes and graphene, we will investigate their interactions with electrons.