Chapter 6

SUMMARY, CONCLUSION AND FUTURE PROSPECTS

In this chapter, we summarise the work that has been completed and presented in this thesis, as well as draw crucial conclusions about the strengths and limits of the theoretical techniques used in this investigation. We also discuss the future scopes of the present research and their significance from an application standpoint.

6.1 Summary Of The Current Work

We theoretically examined electron interaction processes with numerous compounds and radicals based on their applications in this thesis. We investigated ideas for computing electron collision cross sections in high energy regimes (up to 5000 eV).

The purpose of this research was to create reliable theoretical techniques for determining various electron collision total cross sections. In this thesis, we provided estimations for a number of plasma-relevant and environmentally friendly targets. The current theoretical technique has been successfully extended to hydrated DNA and industrially important compounds.

A simple and practical approach was used to compute the total and ionization cross-sections for electron scattering from atoms and molecules.

The spherical Complex Optical Potential (SCOP) technique was used for the investigation above the ionization threshold. Within the given energy ranges, the current results agree well with previous experimental and theoretical data. (See also Chapters 3, 4, and 5).

Total ionization cross sections have been determined from total inelastic cross sections using the SCOP formalism and the Complex Scattering Potential-ionization contribution (CSP-ic) formalism developed by our research team.

We additionally found elastic and total cross sections utilizing a 2P SEM formalism by our research group.

Table 6.1 provides a brief overview of this study's findings. The table below displays the numerous molecular quantities and categories that were researched, organized by chapter of the thesis.

Table 6.1 Summary of the present work

Sr. No.	Molecules	Investigated quantities	Category of molecules	Chapter
1	CF_2O	Q_{inel}, Q_{ion}, Q_{el}, Q_T, ΣQ_{exc} Relationship between Qion (max) and Polarizability	Plasma relevant molecules	3
2	C_2F_4O			
3	C_3F_6O			
4	C_4F_8O			
5	$C_5F_{10}O$			
6	$C_6F_{12}O$			
7	Adenine	Q_{inel}, Q_{ion}, Q_{el}, Q_T, ΣQ_{exc} Prediction of Polarizability and Dielectric constant	Bio-molecules (DNA)	4
8	Guanine			
9	Cytosine			
10	Thymine			
11	Uracil			
12	Furfural		Industrial relevance	4
13	Parabenzoquinone			
14	Pentafluoropropionic Acid			
15	Pentafluoropropionitrile	Q_{inel}, Q_{ion}, Q_{el}, Q_T, ΣQ_{exc} Estimation of Polarizability and Dielectric constant	Environment friendly and Plasma molecues	5
16	Heptafluorobutyronitrile			

6.2 Conclusion

Here, we have reviewed the advantages and limitations of the current theoretical techniques.

6.2.1 Advantage of present investigation

- Reliable in producing cross-sections for a wide range of targets including atoms, radicals, and molecules.
- To find Q_{ion} from Q_{inel}, our group created and applied a semi-empirical CSP-ic approach utilising the ratio function $R(E_i)$. This method was created since there was no direct or accurate way to find the Q_{ion} from Q_{inel}. Using the SCOP approach, we designed a CSP-ic method for obtaining Q_{ion} from Q_{inel}. This is the first attempt.
- The main benefit of this approach is that it can compute all cross sections (Q_{el}, Q_{inel}, Q_T, Q_{ion}, and ΣQ_{exc}) using an approach similar to SCOP and CSP-ic.
- When compared to other theoretical approaches such as R-matrix, this method is simple, fast, and dependable.

6.2.2 Limitations of present Theory

- The SCOP approach is mostly an approximation based on quantum mechanics. This strategy only works for the spherical scattering problem. As a result, the goal potential should be spherical. Total Cross Sections to the average angular dependency are justified by this approximation.
- SCOP and CSP-ic cannot be used to compute low-energy electron scattering since they are designed for intermediate to high-energy approaches.
- The CSP-ic method is a semi-empirical for determining Q_{ion}.

6.3 Future Prospects

- We wish to use R-matrix computations to investigate low energy electron atoms and molecules scattering.
- Differential cross sections, partial and dissociative ionization of the molecules will be investigated.
- The interactions of electrons with other Bio-molecules, proteins, and pharmaceutical molecules will be investigated.
- We will study diverse phenomena of electron interactions with modern technological compounds and industrially significant chemicals.
- The interactions of positron and photon with atoms and molecules will be investigated.

- To investigate a variety of atmospheric molecules.
- Electron interactions with molecules in condensed phase would be explored, that is, Ices on various planets.
- We would like to explore the electron interactions with newly detected molecules found in various cometary and planetary environments. As a result, application in Astro chemistry field would be explored.