

# Applications of Atomic Collision and Electron Scattering: A New Perspective

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*Abstract* : Electrons are omnipresent and electron-induced processes drive many of the most important processes of life, such as photosynthesis (Roach and Krieger-Liszkay 2014). In this paper, some of the varied applications of electron scattering, and the electron collision cross-sections that are required to model and understand such processes, and have mentioned specific data needs where relevant are discussed.

There are many other situations where knowledge of electron scattering processes is required. These include the design of lighting; the development of plasma sources for surgery and dentistry, covered by Fridman and Friedman (2013); the design of hypersonic spacecraft capable of re-entry, as discussed by Celiberto et al. (2014); and in combustion processes, where the removal of electrons by electronegative gases provides a means to extinguish a fire without withdrawing oxygen and is thus used in aircraft to extinguish cabin fires. The study of electron scattering from atoms and molecules has grown rapidly since the Frank and Hertz experiment in 1914 and the first quantum mechanical treatments in the 1930s.

The wide range of applications ensures that the study of such processes will be important in times to come. Much of the data required for such applications will necessarily be generated by theoretical methods, as explained in this paper, with benchmarks being provided by a few definitive experiments. In conclusion, we look back and wonder at the long conceptual journey from hydrogen to complex atoms, from the small and the common to large and exotic molecular systems, which include fascinating radicals and metastable species. Larger targets such as biomolecules offer challenges as well as opportunities. Collisions and scattering that we dealt with in the first five chapters are essentially micro-level phenomena but micro rules the macro, and that was the guiding principle behind the discourses of this concluding chapter. For, it is the basic knowledge that opens possibilities of potential application in diverse fields of technology today.

## I. Introduction

In this paper, I aim to highlight various applications of such electron scattering data from different atomic–molecular targets. Electrons are almost everywhere in the universe and provide one of the simplest probes for exploring matter in its different forms. Electron collisions with atoms, molecules, and ions are dominant in many of the naturally occurring phenomena including the Earth's atmosphere and the atmospheres of other planets and their satellites, in comets and in far-off molecular clouds of the interstellar medium, where they may play a key role in producing the molecular precursors of life. Primarily the ionosphere of the Earth and other planets is formed by ionization produced by solar UV and X-rays, with some of the photoelectrons produced being energetic enough to cause further ionization along with excitation, leading to the magnificent phenomena of the aurora. The solar wind contains not only electrons (average energy ~12 eV) but protons and other charged particles which produce secondary electrons upon interaction with our upper atmosphere. Furthermore, relativistic electrons, though in lower concentrations, are continuously arriving on the Earth as a part of cosmic rays coming from far-off galaxies, etc. Thus, the upper atmospheres of the Earth and planets are a veritable electron collision laboratory in nature. Cross-sections for interaction processes of electrons are therefore necessary inputs into the models for understanding Physico-chemical and dynamic properties of atmospheres/ionospheres of the Earth and other planets as discussed by Haider et al. (2010, 2012) and others. Energy degradation of electrons resulting from ionization and other inelastic processes in specific atmospheres can be investigated by employing Monte Carlo models as demonstrated in Bhardwaj and Mukundan (2015), and references therein. Electron scattering discussed in the previous chapters is a microscopic, i.e. an atomic–molecular phenomenon, while

in applications macroscopic or bulk effects are also important. Therefore, this chapter examines bulk parameters that exhibit dependence on various total cross-sections, to describe electron scattering in other phases of matter. One of the most rapidly developing applications of electron scattering is related to radiation damage in biomolecular systems and the response of biological cells to ionizing radiation (Garcia et al. 2015) and therefore a special section is reserved for this topic.

## II. Various applications of collisions and scattering

Few of the applications of atomic collisions and scattering are mentioned in this section.

### 1. ELECTRON SCATTERING PROCESSES IN NATURE AND TECHNOLOGY

Our understanding of many physical phenomena is strongly coupled to our understanding of the role of electrons in the discrete and continuum excitation of atoms and molecules. Many electron driven processes are observed by the release of energy from an atom or molecule excited by energy transfer from the colliding electrons, energy dissipated in the form of light emitted from the decaying excited state. The most dramatic examples of such electron-induced fluorescence are the aurorae. Aurorae are not confined to the Earth but have been observed on Jupiter and Saturn in our Solar system and are expected to be prominent in many other exoplanetary systems; indeed, such phenomena may be one of the first physical processes we may directly observe in exoplanets. An excellent recent review of electron collisions in atmospheres is that of Campbell and Brunger (2016). The 'extreme' case of electron excitation is ionization and this has been central to the discussion in this book. Ionized media or plasmas are the dominant forms of matter in the universe and therefore electron-induced ionization is, perhaps, the most important electron collision process. Natural examples include planetary ionospheres, stellar atmospheres, and the interstellar medium (ISM). Stellar atmospheres are an example of 'dense plasma' like those found in fusion reactors, whereas the ISM is an example of a 'diffuse plasma'. Plasmas are used in many diverse industrial and technological processes. A recent review has highlighted the need to study electron collisions for plasma reactions with biomass (Brunger 2017). Plasma etching has been at the forefront of the development of micro, and now, nanoscale device fabrication. Plasmas also provide one of the main sources of lighting and are increasingly used in medicine with applications from sterilization to surgery.

Electron-induced dissociation of molecular targets yields fragments that may strongly influence the local chemistry, for example by the production of radicals or 'energy-rich' long-lived (metastable) fragments. Such 'electron-induced chemistry' (Bohler et al. 2013) may be controlled by 'tuning' the incident electron energy to select specific dissociation pathways, this is particularly true when the process is known as Dissociative Electron Attachment (DEA) contributes to the collisional process. DEA is most effective at low energies but recently it has been shown that such chemistry can occur at higher energies where electron impact Dissociative Ionization (DI) is also able to influence the local chemistry (Engmann et al. 2013). DI induced chemistry may be the most important mechanism in Focused Electron Beam Induced Deposition (FEBID) where a high energy (keV) electron beam passes through a beam of precursor gas above a substrate. Electron induced dissociation fragments the FEBID precursor gas to create free metal atoms which subsequently deposit on the surface to build nanostructures. However, DEA and DI cross sections are only available for a few relevant targets and, often only as relative values derived from measured ion yields. Theoretical calculations are currently unable to provide a full description of the branching ratios of DI and DEA.

### 2. ELECTRON SCATTERING IN DIFFERENT PHASES OF MATTER

Throughout this paper, references to atomic or molecular targets have been mainly confined to their gaseous state. However, many-electron scattering processes in industry and technology occur in other forms or phases. In dense gases, the molecular targets may 'cluster' to form dimers or larger systems, for example,

in a humid atmosphere the target molecule AB may cluster with  $n$  water molecules to form  $AB \cdot (H_2O)_n$ . Ionization of such clusters tends to show the product ions  $A^+ / B^+$  or  $A^- / B^-$  solvated with  $m$  water molecules forming  $A^+ (H_2O)_m$  or  $B^- (H_2O)_m$ . Electron scattering from such a cluster may be treated as a multiple scattering problem with scattering from each component treated successively.

To date, this approach has only been developed by a few groups, Bouchiha et al. (2008), Caprasecca et al. (2009), and Fabrikant et al. (2012). More recently, the first full R-matrix calculation of a complex system of two hydrated biomolecules (pyridine and thymine) has been reported by Sieradzka and Gorfinkiel (2017). Experiments investigating electron interactions with clusters have shown that many internal processes (physical and chemical) within the cluster may affect the final products and these are not predicted from simple 'multiple scattering' calculations for example the nucleophilic displacement ( $S_N2$ ) reaction  $F^- + CH_3Cl \rightarrow CH_3F + Cl^-$  may be induced by resonant electron capture in gas phase binary clusters of  $NF_3$  and  $CH_3Cl$  (Langer et al. 2000). Once the target molecules are in bulk or condensed phase the scattering problem becomes a more complex, multidimensional, problem with the energetics of the system is dramatically altered compared to those in the gas phase. For example, in the condensed phase, the excitation (and hence ionization) energies of the molecule are altered due to interactions with its neighbors. Thus in the case of water, the lowest molecular transition is blue-shifted by more than 1 eV (Mason et al. 2006, Hermann and Schwerdtfeger 2011). Furthermore, Rydberg states are suppressed in the condensed phase and maybe quenched entirely. Shifting of electronic state excitation energies, in turn, shifts the position and changes the lifetime of scattering resonances and may significantly alter the magnitude of the cross-section. For a comprehensive review of how low energy electron scattering changes from gaseous to condensed phase see Carsky and Curik (2012). The threshold of ionization processes and their cross-section(s) are also altered in the liquid and condensed phase.

### 3. THE TERRESTRIAL ATMOSPHERE

One of the first applications of our understanding of electron collisions was to model the Earth's ionosphere. The terrestrial ionosphere was first characterized by the development of radar in the 1930s, whereupon the plasma nature of the Earth's upper atmosphere was identified and it was soon proven that aurorae were the result of electron collisional phenomena. Subsequently, the phenomena of day and night glow were also discovered and the role of electron interactions with terrestrial atmospheric atoms and molecules quantified. The structure of the Earth's upper atmosphere and typical electron densities. The ionosphere is formed by the interaction of the terrestrial atmosphere with the solar radiation and solar wind, and its persistence and spatial properties are defined by the terrestrial magnetic field. During a solar storm 'coronal ejections' may send a high-intensity pulse of charged particles (protons and electrons) into the Earth's upper atmosphere which may produce an avalanche of secondary electrons, that collide with nascent oxygen and nitrogen atoms and molecules, which in turn are excited before decaying, yielding the bright color curtains often seen in northern and southern polar regions. These are the famous aurorae. Some of the earliest theoretical estimates of electron scattering cross-sections and in particular ionization cross sections were derived to provide input into models and simulations of the Earth's ionosphere and aurorae, with Mott and Massey reporting in their early papers the cross-sections for electron scattering from oxygen and nitrogen (Mott and Massey 1965). Experiments to measure total scattering cross-sections of molecular oxygen and nitrogen were amongst the first measured (Ramsauer 1921) but studies of electron interactions with atomic oxygen and nitrogen had to wait until the 1960s when beams of O and N atoms could be prepared using microwave discharges (Sunshine et al. 1967, Smith et al. 1962). However, it is still difficult to prepare high-density pure beams of such atomic targets (>25% O and >10% N), so experimental data for such cross-sections remain sparse and models must depend on theoretical derivations. The R-matrix scattering code is now capable of providing highly reliable and accurate (within 10%) cross sections for



electron scattering at low energies (below ionization energy) whilst the semi-empirical methods are valid above the ionization threshold. Ionization cross sections have been reliably calculated for all important atoms and molecules in the terrestrial ionosphere.

#### 4. ELECTRONS, COLLISION, SCATTERING, AND NANOTECHNOLOGY

The nanoscale revolution was one of the major advances in science and technology during the late twentieth century. Our ability to manipulate systems down to nanoscales, build and exploit nanoscale particles and structures is at the forefront of current scientific research. Perhaps the most dramatic example of nanoscaling is the fabrication of electronic devices with nanoscale characteristics. The steady shrinking of the size of the transistor from microns to 10s of nanometres has been central to the increase in computational efficiency and, the operation of the so-called Moore's law stating that the number of transistors on a microprocessor chip will double every two years or so, has been core to the development of the semiconductor industry. However, Moore's law may be coming to an end (Waldrop 2016), requiring new methods for fabricating structures below 10nm, e.g., Focussed Electron Beam Induced Deposition (FEBID) and Extreme Ultraviolet Lithography (EUV). Nevertheless, future production of many of the 'chips' required by the semiconductor industry will continue to rely on plasma processing methods in which electron processes are dominant.

#### 5. POSITRON ATOM/MOLECULE SCATTERING

While this paper is dedicated to the study of electron scattering, a complimentary field is the study of the electron anti-particle, the positron. The study of antimatter is an important aspect of astrophysics since one of the major questions arising from the study of the birth and propagation of our universe is why there is so little antimatter remaining when matter and antimatter were formed in the big bang at the same/ similar rates. Furthermore, by studying antimatter it is possible to gain further insights into many of the fundamental electron-matter collisions such as atomic/ molecular excitation where positron collisions are free of 'exchange' effects while the static and polarization force fields are opposite in the case of the positrons in contrast to electrons.

### III. CONCLUSION

This paper is dedicated to the study of electron scattering, a complimentary field is the study of the electron anti-particle, the positron as well. In this paper, multiple applications of electron scattering and collisions are discussed.

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