Atomic–Molecular Ionization by Electron Scattering

For analyzing the physical aspects of electron collisions with atoms and molecules, an understanding of cross sections, especially of the ionization cross sections, for the impacting electrons is necessary. Providing a detailed and up-to-date discussion to the theory and applications of electron scattering, this text equips readers with the basic concepts of quantum scattering theories, including complex scattering potential method, cross section results for atoms including those of inert gases, atomic oxygen, nitrogen, and carbon, and also for the less explored atomic systems.

Study of electron scattering phenomena for diatomic and common molecules, polyatomic molecules, and radicals including hydrocarbons, fluorocarbons, and other larger molecules, together with relevant radical species, is discussed in detail. This book discusses applications of electron impact ionization and excitation in gaseous or plasma and condensed matter. Recent advances in the field of electron molecule scattering and ionization for polyatomic molecules are covered extensively.

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Atomic–Molecular Ionization by Electron Scattering

Theory and Applications

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To our teachers and students …

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FOREWORD I

Electron collisions with atoms and molecules are commonplace. In the natural world they occur in lightning strikes, aurorae, and the Earth's ionosphere in general; outside our planet they are important for similar processes in other planets. The glow of Jupiter's aurora can clearly be seen using telescopes from the Earth. Electron collisions also form a primary process in cometary tails that are bathed in the solar wind, and in many other astrophysical processes. Plasma is the fourth state of matter which involves partial ionization of the atomic and molecular components. Plasmas occur naturally in flames, stars, and elsewhere. Humankind has increasingly harnessed the power of electron collisions in many ways: to start cars with spark plugs, in the traditional light bulb, and in many lasers. Much of modern industry is driven by the use of electron collisions to create plasmas which etch silicon and other materials into ever more complex structures or to provide surface coatings to alter, enhance, or protect the properties of materials. The quest to harness the Sun's power on Earth via fusion involves making a vast hot plasma with a wealth of electron collision processes requiring detailed study. In the current century it has also been realized that the damage experienced by bio-systems as a consequence of all types of high energy particles and radiation is predominantly caused by collisions involving secondary electrons. These electrons are created by the ionizing effect of the original high-energy collision particle independent of the nature of the colliding species. In medical applications these collisions can be harmful, causing double strand breaks of DNA, or beneficial as in radiation therapy, which is widely used to exorcize malignant tumours.

Electrons colliding with atoms and particularly molecules can initiate a variety of processes. Probably the most important of these is the creation of ions (charged species) either through impact ionization or by electron attachment leading to positively and negatively charged ions respectively. These ionized species are chemically active and act as initiators of many of the processes mentioned above.

Understanding, controlling, and utilizing the full power of the collisions of electrons with atoms and molecules has thus become a major objective of many physical scientists but with benefits and applications well beyond the field of physical science. However, electron collisions with atoms and molecules are governed by the laws of quantum mechanics. This means that the collisions do not obey the everyday laws of collisions such as those found on the billiard table but instead behave in subtle ways which require understanding of the physics at the atomic level. It is just over a hundred years since Franck and Hertz famously demonstrated that the energy levels of the mercury atom were quantized (i.e. discrete), by studying the effects of electron collisions. Since then our understanding of such processes and our ability to control and harness them has made huge progress. This progress has been achieved through the combined application of greatly improved measurement techniques and enhanced theoretical methods, fortified by the power of modern computers. Of course electron collisions also provide fundamental insights into the nature of the collision partner. There is thus now a wealth of knowledge on the processes that follow electron collisions with atoms and molecules as captured both in data sets that can form the input to detailed models of electron collisions and through general principles of what drives these processes.

I therefore welcome this book. It is written by two physicists who have studied electron collision physics over many decades, gaining important insights into ionization and other processes through applications of novel theoretical and experimental methods. The book places their years of experience in a single volume in an easy and accessible manner for the education and enjoyment of the reader.

Jonathan Tennyson

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FOREWORD II

To study any system, an interaction with the system is essential. For microscopic objects and systems, which cannot be seen by the naked eye, usually the electron (or photon) beam, with known characteristics, acts as the probe. At a micro-distance, the projectile particles interact/collide with the object and subsequently they are scattered in all possible directions. The scattered particles, electrons in our case, carry the signature of interaction with the object (target). Hence, the measurement of the differential cross sections, I(θ, Ø) over all possible directions, yields the total collisional cross section σ(Ei) as a function of the incident energy Ei of the electrons. For the atomic targets, the collisions are elastic as well as inelastic, including ionization. For the molecules, the additional processes like dissociation and the dissociative ionization, etc., are also possible. Besides, the dissociative components may be in the excited state. Myriad phenomena arising out of electron scattering make the study very interesting from the manifold view-points of theory, experiment, as well as applications.

In the present book, written by Professors K. N. Joshipura and Nigel Mason, collisions of electrons with atoms are briefly discussed initially. In the greater part of the book, molecules are considered as targets. The study is extended to the radicals and the metastable molecules, while a few molecules of biological interest are also considered. The applications of various scattering cross sections to diverse fields like astrophysics, astrochemistry, nanotechnology, etc., are described in the last chapter.

Both the authors are experienced players in the field of electron–atom–molecule collisions. They have a good number of publications to their credit. From the theory as well as application point of view the present book should be quite useful.

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PREFACE

Electrons are ubiquitous in nature and throughout modern industry, and therefore there are varieties of situations in which electrons interact with atoms and molecules producing diverse physical and chemical phenomena. Extensive studies, both experimental and theoretical, have been carried out on the interactions of electrons with different atomic and molecular targets; indeed the last few decades have witnessed rapid developments in the techniques and methodology for exploring electron–atom/molecule scattering. The wider recognition of the role of fundamental electron interactions in natural phenomena (for example, the observation of aurorae on other planets and the contribution of electron interactions in astrochemistry), in underpinning novel technologies such as Focussed Electron Beam Induced Deposition (FEBID), and as a major source of radiation damage by ionizing radiation has led to an increase in the size of the international community studying electron collisions in all phases of matter.

In this book, our aim is to provide an overview of the field with a focus on theoretical methods used to describe the collisions of intermediate to high energy (exceeding about 15 eV) electrons. The book has six chapters and begins with a discussion of the subject by outlining the necessary textbook background on atoms, molecules, and quantum scattering theories. Attention has been devoted (in Chapter 1) to atomic sizes or 'radii' – something that is normally missing in most books and reviews of this kind. A brief survey of atomic radii, running across the periodic table of elements, is outlined.

The major part of this monograph provides an up-to-date review of electron scattering from atoms and molecules, summarizing recent publications. Although the title of the present book mentions ionization specifically, the contents are comprehensive in that we highlight several important inelastic processes ocurring in the background of elastic scattering. For many atoms and a large number of molecules, recent theoretical results are discussed along with experimental and other data, and wherever possible recommended data are presented to provide the user with data sets for models and simulations of processes in which electron interactions play a significant role.

The book also provides a summary of basic and most used electron scattering theories and, in particular, discusses an approximate theoretical formalism, called 'Complex Scattering Potential – ionization contribution' method, developed by the authors to derive ionization cross sections for a large variety of atomic and molecular systems typically from the first ionization energy onwards, up to 2000 eV or so.

Results for common/atmospheric atoms and molecules are presented in Chapters 2 to 4, while results for polyatomic and/or exotic molecules, including hydrocarbons, fluorocarbons, and biomolecules, etc., are presented in Chapter 5. Of particular interest are the reactive radicals and long-lived metastable species for which experiments are scarce or non-existent and hence the theoretical cross section data hold more significance to the user community. Attempts have also been made, separately for atoms and molecules, to correlate the dynamic quantities, i.e., total cross sections, with some of the static properties of a variety of atomic and molecular systems.

The final chapter, Chapter 6, discusses many fields of science and technology where electron interactions with atoms and molecules play a prominant role. Nature provides large veritable laboratories in the form of the atmospheres of Earth, Mars, Venus, Jupiter, Saturn, etc., and their satellites to explore the role of electron interactions with atoms and molecules whilst their importance has also been revealed recently in comets and other astronomical systems, including the atmospheres of exoplanets.

Electron scattering is a dominant process in many technological fields such as gaseous electronics and electrical discharges, mass spectrometry, lasers and plasma systems, etc. Indeed many of the plasma and related nano-fabrication techniques such as the emerging FEBID and EUV lithography are governed by electron induced processing and scattering. We briefly discuss the role of electron scattering in regulating plasma confinement in fusion plasmas. We also briefly discuss the interaction of electrons with larger biomolecular systems, since it is now recognized that secondary electron emission, and subsequent electron regulated damage to cellular DNA, is a determining factor in radiation damage and, if controlled, may provide new treatment processes in clinical radiotherapy.

For completeness we also discuss electron scattering in the condensed phase of matter and consider scattering by the electron anti-particle, the positron. Scattering of positrons with several atomic and molecular targets is reviewed, mainly in the spirit of providing a comparison with electron scattering.

Thus, in essence, our plan in this work is to place before the scientific community an updated overview of the status of electron interactions with atoms and molecules and the current theoretical methods for exploring such effects. Whilst we emphasize high energy theoretical research, we provide the reader with a comprehensive set of references from which they can explore the field further. We have also demonstrated the wide range of applications of electron scattering from atoms and molecules and hope the data compilation will be of use to these communities whilst providing them with a description of the underlying physics. We recognize that we may have missed some results and as new data are being published all the time this book will need updating. Suggestions and comments are most welcome in this regard.

June 2018 Kamalnayan N. Joshipura

Nigel Mason