XX International Workshop on
Low-Energy Positron and Positronium Physics

XXI International Symposium on
Electron-Molecule Collisions and Swarms

V Workshop on Non-Equilibrium Processes

18-21 July 2019, Belgrade, Serbia

POSMOL 2019

BOOK OF ABSTRACTS

XX Међународна радионица о физици
ниско енергијских позитрона и позитронијума

XXI Међународни симпозијум о
електрон-молекулским сударима и ројевима

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Editors

David Cassidy, Michael J. Brunger,
Zoran Lj. Petrović, Saša Dujko, Bratislav P. Marinković,
Dragana Marić and Sanja Tošić

Serbian Academy
of Sciences and Arts

Institute of Physics Belgrade
University of Belgrade

Belgrade, 2019

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PREFACE

With great pleasure, we would like to welcome the participants and guests to POSMOL 2019, the XX International Workshop on Low-Energy Positron and Positronium Physics, and the XXI International Symposium on Electron-Molecule Collisions and Swarms. The conference takes place in Belgrade, Serbia, at the Serbian Academy of Sciences and Arts, between July 18th and 21st, 2019, with a welcome reception taking place in the afternoon of July 17th. POSMOL 2019 is a satellite meeting of the International Conference on Photonic, Electronic, and Atomic Collisions (ICPEAC), that will be held in Deauville, France, during July 24-30, 2019.

POSMOL 2019 provides an opportunity for collision physicists from both the matter and antimatter communities to meet and share ideas and techniques. Topics in the positron sessions include the latest findings in the fields of positron and positronium physics, antiproton interactions with atoms, molecules and solid surfaces, and additional hot topics. The other sessions will focus on electron interactions with molecules in both gaseous and condensed phases as well as electron swarms. Finally, there will be sessions which discuss the complementary studies of electron and positron interactions with biomolecules, electron induced surface chemistry and studies of collisional plasmas. This combination of topics continues to represent the themes from the three ICPEAC satelites which have merged to form POSMOL. The *International Swarm Seminar* and *Symposium on Electron-Molecule Collisions* merged in 1999 following several joint conferences. The *International Workshop on Low Energy Positron and Positronium Physics* joined the other two in 2005. While POSMOL meetings have been held biannually since 2005, this is the first time that the meeting takes place in Eastern Europe.

POSMOL 2019 brings together over 120 scientists from more than 20 countries and 5 different continents who will attend 5 plenary talks, 36 invited talks, 8 hot topic talks, and more than 100 poster presentations. We are grateful to all the invited speakers and participants for making major efforts to attend the meeting, prepare talks and, in advance, for submitting their manuscripts to the Topical Issue of The Eurepean Physical Journal D: Low-Energy Positron and Positronium Physics and Electron-Molecule Collisions and Swarms.

POSMOL 2019 is augmented by one day Workshop on Non-Equilibrium Processes in honor of the retirement of Professor Zoran Lj. Petrović. This will be a special occasion for his friends to meet and review the progress in the field, specifically his contributions, present new results and look forward to new discoveries. The program includes 10 invited talks, but of equal importance, there will be ample opportunity for sharing memories, many stories and jokes from the past throughout the day and at the celebratory dinner.

We would like to express our gratitude to all members of the Local Organizing Committee, in particular to Dragana Marić (Conference Manager) and Sanja Tošić (Conference Secretary), and the staff of PanaComp, who worked very hard to make this meeting a success. We would also like to thank all the members of the Positron and Electron Advisory Committees, and in particular to David Cassidy and Michael Brunger, for their valuable advice, suggestions and help with the organization of POSMOL 2019.

We gratefully acknowledge the financial support of this meeting, by the Serbian Academy of Sciences and Arts, Ministry of Education, Science and Technological Development of the Republic of Serbia and The European Physical Journal D (EPJ D).

On behalf of the Local Organizing Committee, we wish you a successful meeting and a pleasant stay in Belgrade.

Zoran Lj. Petrović
Saša Dujko
Bratislav Marinković
POSMOL 2019 LOC Chairs
Belgrade, July 2019

ACKNOWLEDGEMENT

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POSMOL 2019

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New Physics with Positron Traps and Trap-Based Beams

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The development of novel positron traps and beams has enabled new investigations of anti-matter. This talk will discuss highlights of recent successes and the critical tools that enabled them. It will conclude with a brief discussion of prospects for further technological progress and the new physics that it might enable.

Studies of antimatter are of interest for a range of scientific and technological applications, including fundamental tests of gravity and tests of symmetries predicted by field theories (e.g., CPT), understanding astrophysical processes, and the characterization of materials. Many applica-tions benefit greatly from tailoring collections of the antiparticles to optimize them for a specific use. Unlike electrons, which are copious in our world of matter, positrons are scarce (e.g., currents of picoamps instead of amps). The need to keep positrons isolated from ordinary matter has motivated the development of methods to manipulate them in vacuum in the form of single-component gases and plasmas.

More than three decades of positron trap and beam development have enabled specially de-signed electromagnetic traps for long-term (e.g., weeks or more) antimatter confinement, cryogeni-cally cooled antiparticle gases and plasmas, high-density plasmas, finely focused beams, and meth-ods to deliver very large bursts and/or short temporal bursts of antiparticles and to create guided positronium (Ps) atom beams [1, 2].

Scientific and technological progress in several areas will be reviewed. It includes the creation and study of antihydrogen atoms and gravity tests [3, 4, 5, 6]; the formation of the positronium molecule (i.e., Ps2, the first many-electron, many-positron state, e+e-e+e-) [7]; and understanding Feshbach-resonances in positron annihilation and the nature of the resulting positron-molecule bound states [8]. Outstanding goals in these areas and the challenges associated with them will be discussed. One challenging goal, for example, is study of many-body physics in the electron-positron system [9]. Prospects and progress on this topic will be discussed in both the classical and quantum regimes, a positronium-atom Bose-Einstein condensed gas (BEC) [10], and the creation of a classical "pair" (i.e., e+ - e-) plasma [11]..

* Supported by the U. S. NSF, grant PHY 17-02230 and DOE DE-SC0019271.

† Recent work involving UCSD was done in collaboration with J. R. Danielson, N. C. Hurst, S. Ghosh, E. V. Stenson, C. Hugenschmidt, and the APEX collaboration.

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Electron Collisions with Molecules and Molecular Clusters

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Electron scattering data requirements in a variety of fields (astrophysics, plasma modelling, medical physics, etc.) have provided significant impetus to the study of electron-molecule collision over the last couple of decades. A case in point is the need to understand how low energy electrons generated by ionizing radiation in a biological medium cause damage to cell constituents [1]. This stimulus has led to the further development of theoretical approaches to treat electron-molecule scattering as well as the reengineering of many of their software implementations. Some of these developments have wider application, as the need to model correlated multielectronic effects that involve the continuum in molecules is also present in the study of molecular photoionization, strong-field process, etc. [2].

The work carried has allowed the accurate computation of cross sections and the investigation of resonance formation [3] for larger targets than ever before as well as high quality calculations for smaller targets. These larger targets include small molecular clusters [4]: their study aims at bridging the gap between the pure gas phase and the actual condensed environment in which many of the collisions of applied relevance take place. Developments have also contributed to improving our fundamental understanding of electron scattering from molecules.

In my talk, I will discuss the present successes and future challenges of studying low energy electron scattering computationally, focussing on the application of the R-matrix method [5, 6] to isolated molecules and small molecular clusters.

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Electron Interactions with Helium Nanodroplets

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Pickup of atoms and molecules into superfluid He nanodroplets (HNDs) is a powerful technique to form clusters and nanoparticles at low (0.37 K) temperatures. The resulting dopant complexes are often analyzed utilizing mass spectrometry after electron ionization [1, 2]. The most abundant ions observed in the mass spectra are free of He. This is a surprising result, given the fact that cations are strongly heliophilic and droplets containing about 2 million He atoms require more than 1 keV of energy to be vaporized.

The typical log-normal size distribution of the neutral HNDs and the Poissonian pickup statistics lead to a substantial size spread of the dopant clusters. Here we report on a novel approach that reduces the size distribution of the HNDs, simply by intense ionization of the HNDs prior to the pickup. Helium droplets containing between 10^5 and 10^{10} He atoms [3] were formed and subjected to electron beams of defined energy and current [2]. Mass per charge distributions were determined by electrostatic energy analyzers for positively and negatively charged droplets [4]. Utilizing two ion sources, each followed by a spherical sector field analyzer, it was possible to unambiguously determine the charge state as well as the mass of charged He droplets. Charge states higher than 65+ as well as 5- could be assigned and neutralization as well as increasing of the charge state could be achieved by the second ion source. Perfect fractional numbers of the mass per charge ratios of product ions with respect to the charged precursor droplets indicate that fragmentation exclusively happens via very asymmetric Coulomb explosion and additional evaporation of a few He atoms. These low-mass ions have been investigated by mass spectrometer systems so far [2]. Coulomb repulsion between charges of same polarity in highly-charged He droplets will lead to minimum energy configurations in the form of Coulomb crystals. Dopants are polarized and attracted by the charge centers, which thereby act as seeds for homogeneous cluster growth. Dopant cluster ions can be liberated from the large highly-charged droplets via multiple collisions with gaseous helium in a RF-ion guide. Depending on the He pressure, dopant cluster ions can be formed with any number of He atoms attached. Tagging of ions with He atoms is currently a hot topic in ion spectroscopy. This is typically achieved in cryogenic ion traps [5-7], however, with much lower efficiency than pickup of dopants into highly-charged HNDs.

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Positron Attachment, Annihilation and Binding in Molecules

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This talk will review the progress in our understanding of positron annihilation in polyatomic molecules. It has been known since the pioneering positronium experiments by Deutsch in the early 1950s, that positron annihilation rates in polyatomic molecules are strongly enhanced compared with the Dirac annihilation rate for an electron gas of the equivalent number density. Besides a strong dependence on the molecular size [1-3], experimental data for room-temperature positrons revealed a remarkable chemical sensitivity of the annihilation rates [4]. In spite of some remarkable insights and first estimates of positron binding energies based on thermal annihilation rates [3], the overall picture remained unclear for nearly half a century.

A concerted effort of theory and experiment over the past 20 years has changed the situation dramatically. Theoretical predictions of positron binding to neutral atoms made in mid-1990s indicated that most polyatomic molecules should be capable of binding the positron. Positron capture into such bound states, accompanied by a vibrational excitation of the molecule, gives rise to vibrational Feshbach resonances (VFR), which enhance the annihilation probability greatly. A theoretical understanding of the direct and resonant annihilation mechanisms and scaling of the positron annihilation rates with the binding energy [5,6] was quickly followed by observations of VFR in the annihilation rates with a trap-based positron beam [7]. In most cases, these resonances correspond to excitations of particular vibrational modes, allowing measurements of the positron binding energy. At present, these have been determined for over 70 molecules [8]. In turn, the strongly enhanced annihilation rates are due to the mode-based VFRs serving as doorways into dense spectra of multimode vibrational states [9]. Long-range dipole coupling between the positron and infrared-active modes allows to explain the resonant annihilation rates for small polyatomic molecules [10], and we have a good overall picture now [11]. However, the role of nondipole interactions [12] and the details of vibrational mode coupling [13] require more experimental and theoretical efforts, while calculations of positron binding are difficult [14], and for nonpolar molecules (e.g., alkanes), have just begun [15].

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Non-Equilibrium in Ionized Gases Determined by Charged Particle Collisions with Molecules

Zoran Lj. Petrović,
with: Saša Dujko, Dragana Marić, Gordana Malović, Nevena Puač, Danko Bošnjaković,
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In their recent, excellent, review Taccogna and DiLecce [1] have tried to systematize the types and to some degree the origins of non-equilibrium in low temperature plasmas. Above all, that paper made a point (perhaps not intentionally) that the intellectual underpinning of the non-equilibrium physics is in explaining how all these different manifestations come about and how those may be explained. We have been trying to make a similar point for many years in a number of review lectures and even some of the papers albeit indirectly in attempts to show how swarm physics brings non-equilibrium into the plasma models [2-5]. The basic idea was that, while thermal equilibrium (TE) is able to provide us with laws that are universally applicable the model of thermal equilibrium is hardly ever applicable in its true and full meaning. At the same time non-equilibrium plasmas with their diversity cannot be explained in terms of formulae but their fundamental description is based on three pillars:
1) elementary data (for a variety of existing particles including the data for their reactions);
2) procedures to model (equations, transport equations, continuity etc…) and
3) inclusion of the boundaries.
In that respect the common, universal rules are provided in the realm of experience rather than the universal, prescribed thruths (formulae). Please note that Local Thermodynamic equilibrioum (LTE) is just the simplest model of non-equilibrium. The main systematics should include splitting phenomena observed in the ionized gases (which also includes positrons in gas filled traps and in the local atmosphere) into two groups:
a) Local field equilibrium (when properties may be stable in space and/or time but processes are not balanced as expected for TE).
b) Non-local, non-hydrodynamic phenomena.
Under the latter group one may label different situation when balances of one or more of the main conserved quantities are not met (number due to non-conservative collisions or local losses, energy and momentum). The relaxation time for these processes may be determined from the elementary processes and the available data and were used as the basis for correcting for non-local phenomena in fluid models. Different combinations of non-equilibrium in different situations produce a large number of the so called ‘kinetic phenomena’ that may not be easily explained based on the elementary data and where one needs kinetic modelling to reproduce the phenomenon.

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New Bounds from Positronium Decays on Massless Mirror Dark Photons

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In this talk, we will present the results of a search for a hidden mirror sector in positronium decays with a sensitivity comparable with the bounds set by the prediction of the primordial 4He abundance from Big Bang Nucleosynthesis. No excess of events compatible with decays into the dark sector is observed resulting in an upper limit for the branching ratio of this process of 4.0 x 10^{-5} (90% C.L.). This is an order of magnitude more stringent than the current existing laboratory bounds and it constraints the mixing strength of ordinary photons to dark mirror photons at a level of epsilon < 5.8 x 10^{-8}. The future prospects to reach a sensitivity on epsilon of the order of 10^{-9} - 10^{-10}, which is of great interest both theoretically and phenomenologically, will also be discussed.

Electron Transport in Molecular Gases: a Modelling Procedure to Evaluate Cross Section Data Sets

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Modelling electron transport is a powerful tool for important applications of radiation [1] to medicine and industry. Even in the case of not using electrons as primary radiation source but photons, protons, positrons or heavy ions, electrons appear as secondary particles which can be generated even at very low energies [2]. For this reason, electron transport needs to be incorporated into accurate radiation models and this requires a complete set of electron scattering cross-section data over a broad energy range [3]. In this lecture we propose a method to evaluate the reliability of these cross-sectional data by comparing the observed energy and angular distributions of electrons transmitted through a magnetically confined beam-gas apparatus [4] with those predicted by a Monte Carlo simulation using our LEPS code [1]. Input data for this simulation are critically derived from a compilation of experimental and theoretical cross-section values obtained through a wide international collaboration [5].

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Dissociative Electron Attachment to Polyatomic Molecules: *Ab initio* Calculation of Attachment Amplitudes and Nonadiabatic Dissociation Dynamics

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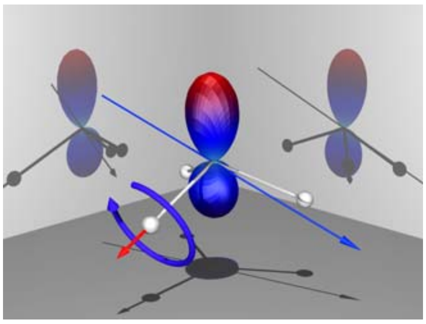

Fig. 1 Entrance amplitude for the $^2A_1$ Feshbach resonance in NH_3

Although dissociative electron attachment (DEA) through metastable anion resonances has been studied experimentally and theoretically since the 1960s [1], it can be said that the field has undergone a renaissance since the introduction of the techniques of momentum imaging [2] and velocity-slice imaging in DEA experiments [3,4]. These experiments provide a degree of insight into the dissociative attachment process not previously accessible. However, without the observation of the final momenta of at least two fragments (the anion and a neutral fragment), it is not possible to directly connect these measurements to the body frame dynamics of DEA. For that reason a combination of the theoretical calculation of attachment amplitudes (Fig. 1) and the experimental measurement of the angular dependence of the anion fragment, has been necessary for the detailed interpretation of this new generation of experiments.

We will discuss the calculation of attachment amplitudes that give the probability for resonant electron attachment to the neutral molecule as a function of the incident electron momentum in the body frame. Thus far, the determination of attachment amplitudes has only been possible in full electron-scattering scattering calculations. The attachment amplitude is not enough to identify the dynamical pathway of dissociation in many cases. Conical intersections between anion potential surfaces are more the rule than the exception, and they can also have features that negate direct dissociation consistent with "axial recoil" dynamics. We will illustrate these phenomena with a complete analysis of DEA to ammonia via the $^2A_1$ Feshbach resonance at 5.5 eV, which produces anion products exclusively via nonadiabatic nuclear dynamics, and with preliminary results on DEA to formic acid, which may be more complicated still.

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Positron and Positronium Physics Around GBAR

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In order to make a direct observation of the effect of gravitation on antimatter, the GBAR [1] experiment aims at measuring the influence of Earth's gravity in the trajectory of antihydrogen atoms. The first step of the experiment is the production of antihydrogen ions and involves two consecutive three- and four-body charge exchange reactions involving positronium atoms and low energy antiprotons. One of the biggest challenges faced by GBAR is to find the best experimental and physical conditions (positronium state, antiproton energy etc...) for enhancing the antihydrogen ion production rate. In this context we present two recent works devoted to the cross-sections computation for the two reactions.

In [2] a new *ab-initio* method is developed to solve Faddeev-Merkuriev equations using Lagrange-mesh techniques to describe collisions of the Coulombic three-body systems. This method has been applied to study $(\bar{p}, e^+, e^-)$ system in the energy range between $e^- + \bar{H}(n=2)$ and $e^- + \bar{H}(n=3)$ thresholds. A special focus is made on the role played by Feshbach resonances and Gailitis-Damburg oscillations appearing in the vicinity of the different reaction thresholds. Our results are in very good agreement with previous works while giving more detailed cross sections [3, 4].

In a second work [5] we explore the possibility to increase the antihydrogen positive ion production rate by assisting the capture processes involved in the two reactions using a laser field having standard specifications (e.g. ion or excimer lasers). By using a formalism adapted from [6-8], we present an extensive study of the influence of the laser parameters (laser field strength and photon energy) on the charge exchange cross sections in the energy range of interest for the GBAR's experiment. Under special irradiation conditions antihydrogen' atom and ion formation cross sections may be significantly increased by the presence of the laser field.

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Injection and Trapping of Positrons in a Magnetic Dipole Trap: Toward Magnetic Confinement of Positron-Electron Plasma

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The APEX collaboration aims to produce the first magnetically confined, long Debye length, positron-electron plasma. Because mass symmetry leads to theoretical simplicity, Per Helander dubs such a system, “the hydrogen atom of plasma physics” and predicts that it should be linearly stable in large parts of parameter space [1]. The APEX approach is to use a levitated dipole to realize magnetically confined positron-electron plasma. Preliminary experiments have used a reactor-based positron source and a dipole magnetic field produced by a permanent rare-earth magnet. Those experiments have demonstrated nearly lossless injection of low-energy (5 eV) positrons into the dipole field [2], and persistence of positron orbits for times in excess of one second [3]. This talk will present a summary of those results as well as an update on development of 1) a buffer gas trap to accumulate positrons, 2) a levitated superconducting dipole trap that will confine plasma of arbitrary non-neutrality, and 3) diagnostics for positron-electron plasma.

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Low Energy Positrons in the Galactic ISM

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In the Milky Way galaxy, positrons, which are responsible for the diffuse 511 keV gamma ray emission observed by space-based gamma ray observatories, are thought to annihilate predominantly through charge exchange interactions with neutral hydrogen. These charge exchange interactions can only take place if positrons have energies greater than 6.8 eV, the minimum energy required to liberate the electron bound to the hydrogen atom and then form positronium, a short-lived bound state composed of a positron-electron pair. I will explain the importance of positron interactions with neutral alkali metals in the warm interstellar medium (ISM). Positrons may undergo charge exchange with these atoms at any energy. In particular, including positron interactions with sodium at solar abundance in the warm ISM can significantly reduce the annihilation timescale of positrons with energies below 6.8 eV by at least an order of magnitude. Including these interactions in our understanding of positron annihilation in the Milky Way rules out the idea that the number of positrons in the Galactic ISM could be maintained in steady state by injection events occurring at a typical periodicity >Myr [1].

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BASE: Ultra-High Precision Measurements of Proton and Antiproton Fundamental Properties

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The BASE collaboration situated at CERN's Antiproton Decelerator facility uses Penning traps to test the Charge-Parity-Time (CPT) symmetry by measuring the fundamental properties of protons and antiprotons to ultra-high precision [1]. One of the properties measured is the dimensionless g-factor which expresses the magnetic moment in units of the nuclear magneton μ_N=q_(p,p¯) ℏ/2m_(p,p¯). The antiproton g-factor is determined by taking the ratio of the Larmor frequency, ω_L, and the free-cyclotron frequency, ω_C, which the BASE collaboration recently measured to 1.5 ppb. This result is consistent with the 0.3 ppb measurement of the proton g-factor, also measured by the BASE collaboration [2]. This measurement improved upon the precision of previous best measurements by a factor of >3000 and was achieved with a completely new measurement scheme utilising two measurement antiprotons and three traps [3].

Another fundamental property which can be measured is the proton-to-antiproton charge-to-mass ratio, $(q/m_{\mathrm{p}})/(q/m_{\bar{\mathrm{p}}})$. Here the free-cyclotron frequency, $\omega_c = qB_0/m_{\bar{\mathrm{p}},\,\mathrm{H}^-}$, of both $\bar{\mathrm{p}}$ and H^- are compared – with the H^- serving as a proxy for the proton. The BASE collaboration has previously measured this quantity to a precision of 69 ppt [4].

In both property measurements, ω_c is determined by measuring the three eigen-frequencies, $\omega_{+,-,z}$ of the trapped particle and applying an invariance theorem; $\omega_c^2 = \omega_+^2 + \omega_-^2 + \omega_z^2$. The individual eigen-frequencies are accessed by means of non-destructive image currents measurements, using tuned superconducting RCL circuits. A number of technical and methodological improvements have recently been made. The implementation of a new superconducting modified-cyclotron frequency detection system allows direct measurements of ω_+, for both $\bar{\mathrm{p}}$ and H^-. This is in contrast to previous measurements where ω_+ is measured indirectly by coupling axial and modified-cyclotron modes [4]. The addition of a resonance-frequency tunable circuit to the axial detection system, in conjunction with significant improvement to the magnetic field homogeneity, has completely eliminated the principal systematic error of the previous 69 ppt result [4]. Finally, the cryogenic standing time and mechanical stability of the apparatus has been greatly improved. These combined improvements have increased the cyclotron frequency stability, when compared to the previous charge-to-mass ratio measurement, by more than a factor of 5.

An overview of the BASE experiment, measurement principles, and an update on the studies with this considerably improved instrument will be presented.

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Positron Interactions with Hydrocarbon Molecules

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According to Helander and Ward [1], tokamaks could be the largest repositories of positrons made by man. A large number of runaway positrons are produced in tokamak fusion plasma including in JET and JT-60U [1], due to pair production caused by the runaway electrons and background plasma ions and electrons. These positrons will further collide with other molecules present in the system creating a pool of new species. In the present work we have chosen those targets having numerous applications in the field of plasma physics and astrophysics. For example, carbon is one the major element present in the plasma-facing material of almost all modern operating fusion devices. Hence, the chemical erosion caused by plasma-wall interactions produces a wide spectrum of hydrocarbons (from simple to complex) which contaminate the hydrogenic plasma [2,3]. The study of these hydrocarbons helps in plasma diagnostics in the diverter region of magnetically confined high-temperature hydrogen plasma [4]. Moreover, these hydrocarbons are also present in the planetary and cometary atmosphere making these targets important in the field of astrophysics as well [5].

Positron scattering from hydrocarbons namely methane, ethane, ethene, ethyne, propane, propene, propyne and isomers of pentane (n-, iso-, and neo-) are studied in the incident energies from low (~1 eV) to high energies (~5 keV). Various cross sections are calculated under the modified spherical complex optical potential framework [6] and complex scattering potential-ionization contribution method [6]. The cross sections reported are total, elastic, inelastic, positronium formation (Ps), ionization, and total ionization cross section. In some cases, we have also reported momentum transfer cross section. These cross section data constitute one of the fundamental parts of simulation dynamics such as Monte Carlo and EPOTRAN. EPOTRAN simulation deals with the study of positron transport in solids or in biological media [7].

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The ASACUSA-Cusp Experiment - Progress Towards an Antihydrogen Beam

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The ASACUSA Cusp experiment aims to perform spectroscopy of the hyperfine structure of ground state antihydrogen in a field-free region. This will allow comparisons with hydrogen which would provide a test of CPT symmetry. To achieve this, spectroscopy apparatus has been developed to use a Rabi type beam method. This apparatus has been successfully tested with hydrogen [1]. Therefore, the present goal of the experiment is to produce a cold spin polarised beam of ground state antihydrogen.

The beam is produced by mixing antiprotons and positrons contained within a multi-ringed electrode trap. The trap is housed within the cold bore of a superconducting magnet which has a cusped field configuration. If the antihydrogen is produced with a low enough velocity, low field seeking states will be preferentially focused on the beam axis by the magnetic field.

In 2012, antihydrogen atoms were observed 2.7 m from the production region [2] however the rate was too low to perform spectroscopy. Subsequent measurements of the distribution of the principle quantum number (n) showed that the bulk of antihydrogen atoms emerging from the trap were in high $n>14$ states. Hence, the requirements for performing spectroscopy are clear, a beam must be produced with higher intensity and lower n.

In this presentation, I will briefly review the previous results from the experiment and give an overview of methods. I will then discuss changes taking place during the period 2019-2020 when there is no proton physics at CERN. Work is underway to both increase the beam intensity and the number of ground state antihydrogen atoms, theoretical and experimental results will be shown and discussed where available.

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Positron Interactions with Targets of Fundamental Interest

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Despite a large body of relatively recent work, both experimental and theoretical (see, for instance, [1, 2]), on low energy positron scattering processes, there are a number of interesting interactions that have not been investigated. This talk will explore recent work at the Australian National University, on positron scattering from neon and ethane.

Measurements are made using a Surko trap and beam system, which produces a pulsed positron beam with an energy spread of approximately 50 meV [3]. The energy of the beam can be tuned between 0 and 200eV, and is magnetically confined using a 500 gauss axial magnetic field. Using techniques developed at the University of California, San Diego [4], we can take advantage of the magnetic confinement to measure a wide range of scattering processes.

While there have been many measurements of total cross sections for positron scattering from noble gas targets, there are relatively few differential cross section (DCS) measurements. In particular, there is only one measurement of DCS for positron scattering from neon [5], and these are not absolute and over a restricted energy range. In this talk, we will present recent measurements of the positron-neon elastic DCS, at energies from 1eV to 40 eV, and discuss the comparison to the most recent theoretical calculations. Despite generally good agreement at the TCS level, there remain discrepancies between the experimental and theoretical DCS. We will also present the first measurements of state selective excitation for the neon electronic states.

In addition to the noble gases, there is significant interest in the low energy interactions of positrons with molecules. In particular, there has been a wide range of measurements of positron annihilation which demonstrate the presence of vibrational feschbach resonances (VFR) [6]. In the second part of this talk, we will outline recent work aimed at exploring the interaction of these resonances with the excitation of vibrational modes of these molecules. The ultimate aim is to shed further light on the formation and decay mechanisms of the VFRs.

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Partial-wave analysis for Positronium–Xenon collisions

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We have proposed a new method to convert measured *ortho*-positronium (*o*-Ps) annihilation rates in gaseous Xe into total and momentum cross sections of Ps–Xe collisions in an ultra-low-energy region where their experimental determinations as functions of Ps energy are extremely difficult [1]. Our method makes it possible to determine not only the *s*-wave parameters, *i.e.*, the scattering length and effective range, but also the *p*- and *d*-wave parameters owing to a selection rule that *ortho-para* Ps spin-conversion is forbidden in *s*-wave scatterings. We have found a small positive scattering length, $A_0 = (2.06 \pm 0.10) \cdot a_0$, which is similar to the Xe atomic radius of $2.04\,a_0$ and is considerably smaller than Xe van der Waals radius of $4.16\,a_0$.

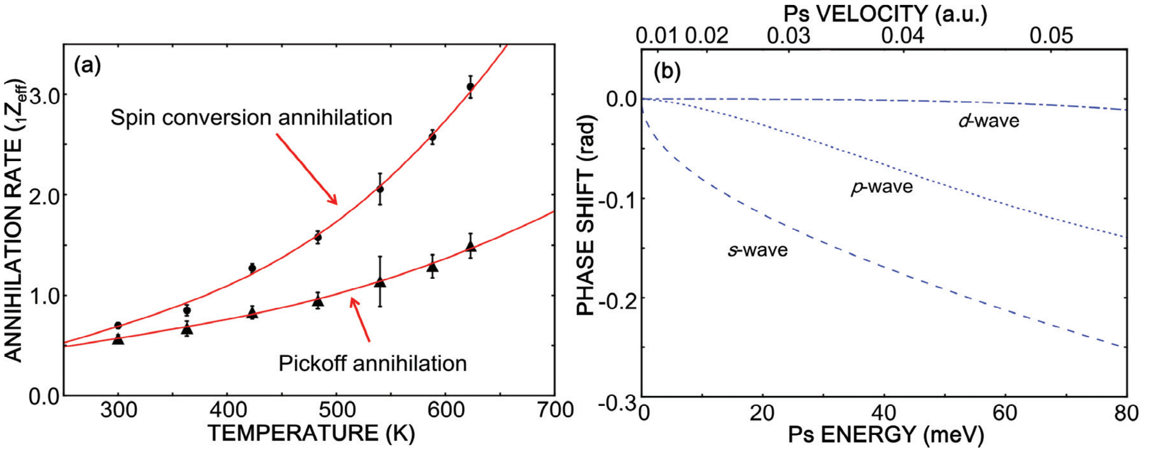
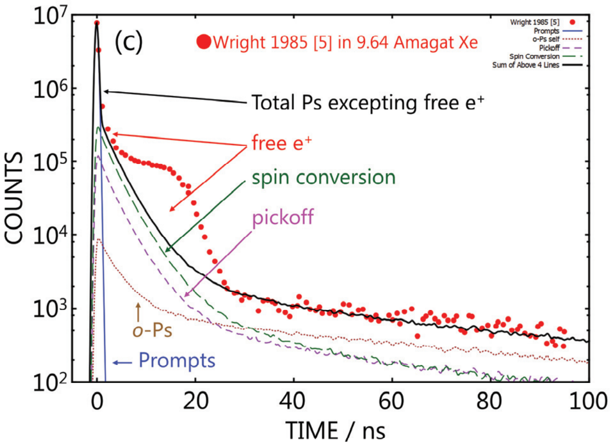


Figure (a) shows the normalized *o*-Ps annihilation rates ($^1Z_{\text{eff}}$) for two paths; the pickoff annihilation and the self-annihilation via *ortho-para* Ps spin-conversion due to the spin-orbit interaction [1,2,3,4]. The measured points [4] are well explained by summing up the partial-wave contributions whose phase shifts (δ_L) are shown in Fig. (b).

We apply the parameters to analyse a positron lifetime spectrum in Xe by Wright et al. [5] where the positronium fraction has been estimated to be 3%. The cross sections for the pickoff annihilation and spin-conversion annihilation are described using δ_L above as $\sigma^{\text{po}} = \pi K^{-2} \sum_{L=0}^{\infty} (2L+1)\left[1 - |S_L(K)|^2\right]$ and $\sigma^{\text{sc}} = \pi K^{-2} \sum_{L=1}^{\infty} (2L+1)|1 - S_L(K)|^2$, where $S_L(K) = \exp[2i\delta_L(K)]$ is the *S*-matrix. We obtain the total counts of 92.1M: 20.6M Ps, 19.2M free positrons, and 50.7M other annihilations within the source and wall. The breakdown of Ps annihilation is 4.9M for *p*-Ps self-annihilation, 0.9M for *o*-Ps self-annihilation, 4.4M for the pickoff annihilation, and 10.4M for the spin conversion annihilation as shown in Fig. (c).



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Cold Muonium Beam for Atomic Physics and Gravity Experiments

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We are investigating methods to create a novel muonium (Mu) source, based on $\mu+ \rightarrow$ Mu conversion in superfluid helium (SFHe), which has the potential of providing high brightness Mu beams for next generation laser spectroscopy experiments. We are also investigating the feasibility of using such sources for measuring the gravitational interaction of Mu.

The positive muon ($\mu+$) which is dominating the Mu mass is not only an elementary antiparticle, but a second-generation lepton too. This makes a gravity experiment highly motivated [1], and complementary to gravitational studies of antihydrogen [2, 3, 4] and positronium [5].

State-of-the-art Mu sources (like silica aerogel, mesoporous SiO_2) emit Mu atoms with a large (thermal) energy distribution, and wide (~ cos θ) angular distribution. Cooling of these porous samples below 100 K results in rapidly declining numbers of vacuum-emitted muonium due to decreased mobility, and atoms sticking to the pore walls [6].

Our proposed method relies on stopping $\mu+$ in a thin layer of SFHe, and forming Mu by capturing an electron from the ionization trail. A fraction of the Mu diffuses to the SFHe surface within their lifetime, where emission into vacuum occurs. The velocity of the emitted Mu (~ 6 mm/μs) is given by their large chemical potential (E/kB ~ 270 K) in SFHe, while the low temperature of the liquid ($T < 0.3$ K) determines their transverse momentum [7].

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Precision Microwave Spectroscopy of the *n*=2 Positronium Fine Structure

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As a purely leptonic system, positronium (Ps) is an ideal system for performing QED tests [1]. QED corrections to Ps energy levels have been calculated up to order $m\alpha^6$, and the theoretical calculations [2] are currently more precise than experimental measurements. The first measurement of the $n = 2$ fine structure was of the $2^3S_1 - 2^3P_2$ transition, conducted in 1975 by Mills, Berko and Canter [3]. This measurement was improved upon by Hatamian, Conti and Rich, in 1987 [4], and then by Hagena and co-workers in 1993 [5]. However, these experiments all relied on generation of Ps atoms in the 2^3S_1 state via positron bombardment into metal targets [6], which is intrinsically inefficient and necessarily results in Ps with energies of several eV. The last fine structure precision measurements are now over 25 years old, with uncertainties of approximately 200 ppm [5]. Here we present the results of a new Ps $n = 2$ fine structure measurement (2^3S_1-2^3P_2) in which 2^3S_1 atoms were produced via laser excitation [7]. This methodology is more efficient and results in the production of much slower atoms, significantly reducing systematic errors.

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Experiments and Perspectives with Metastable 2^3S Positronium Beams

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Positronium (Ps), the short-lived bound state of an electron and a positron, is one of the few candidate systems (with antihydrogen and muonium) being considered for probing experimentally the gravitational interaction with a neutral antimatter system [1]. Several experimental schemes relying on laser excitation to longer-lived excited states (such as the Rydberg levels) have been proposed [2] [3] [4] to extend its otherwise to short lifetime and to allow the atoms to free-fall for a measurable distance.

One very promising canditate is the 2^3S excited state, optically metastable and having 8 times longer lifetime than the ground state and low sensitivity to external field gradients. Producing a pulsed long-lived beam of 2^3S Ps through laser excitation of the 1^3S-3^3P transition and consequent spontaneous decay along 3^3P-2^3S was a novel production scheme recently explored within the AEgIS collaboration [5], on its way of performing the first gravitational measurements on neutral antimatter [6]. This scheme allows the initial Ps atoms to be selected in velocity both in the axial direction, through the precise timing at which the excitation laser is sent, and in the transverse direction, through Doppler selection by the laser bandwidth [7]. Furthermore, it allows the efficiency in producing the 2^3S atoms to be increasing by actively driving the 3^3P-2^3S transition by means of a second laser pulse [8]. The development of this scheme opened the possibility to perform the first experimental explorations towards producing a pulsed collimated beam of 2^3S Ps compatible with deflectometry/interferometry measurements.

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Positronium Emission from Materials for Li-ion Batteries

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A positron and an electron annihilate into gamma-ray photons but before this annihilation, the positron and an electron can bind together to form a positronium (Ps). Mono-energetic positron beams can be used to bombard materials and to probe their atomistic properties. In particular, the implanted positron can diffuse back to the surface of a solid and be emitted as Ps with a range of kinetic energies that provides key information regarding the energy levels of the electrons in the material. These energies can be measured by time of flight (TOF) experiments, but the Ps lifetime before annihilation has been too short for precise measurements. Recently, Jones et al. [1], by exciting the emitted Ps with a laser to greatly increase its lifetime, obtained TOF measurements with an ultimate precision of the order of 5 meV that will allow materials simulations in systems pertinent for Li-ion batteries cathodes [2,3].

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Calculation of Positron Binding Energies Using the Generalized any Particle Propagator Theory

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We recently extended the electron propagator theory to any type of quantum species based in the framework of the Any-Particle Molecular Orbital (APMO) approach [1-3]. This generalized APMO propagator theory (APMO/PT) was applied to calculate positron binding energies (PBEs) of anions and some diatomic molecules using the second order, third order, and renormalized third order quasiparticle APMO/PT approaches and compared our results with those previously calculated employing configuration interaction (CI), explicitly correlated and quantum Montecarlo methodologies. We found that renormalized APMO/PT methods can achieve accuracies of ~0.35 eV for anionic systems, compared to Full-CI results, and provide a quantitative description of positron binding to anionic and highly polar species.

We have employed thermodynamic cycles to relate calculated APMO/PT PBEs with the stability of homo- and heteronuclear $e^+[X^-Y^-]$ compounds formed by two halide anions (X^-,Y^- = F^-,Cl^-,Br^-) and one positron. Our results indicate the formation of energetically stable positron molecules in which the formation of positron covalent bonds underlie the stabilization of the otherwise repelling dihalides, similar to the bond observed in the $e^+[H_2^{2-}]$ complex [4]. Surprisingly, several aspects of the positronic dihalides are similar to those of the purely electronic analogs, $e^-[A^+B^+]$, molecular cations with isoelectronic atomic cores ($A^+,B^+ = Na^+$, K^+, Rb^+) bound by one electron.

Third order APMO/PT approaches display a considerable potential for studying positron binding and positron bonds in large molecules as they provide a reasonable compromise between computational effort and accuracy in view of the well-known difficulties to account for electron-positron correlation.

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Precision Spectroscopy of Trapped Antihydrogen

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The ALPHA collaboration has recently reported on the highest-precision measurement of any pure antimatter system to date by performing a direct measurement of the 1S-2S transition of trapped antihydrogen atoms with a relative precision of approximately 2 parts per trillion [1]. We have also started mapping out the n=2 manifold with initial measurements of the 1S – 2P transition using a pulsed Lyman-α laser [2]. The details of these measurements will be presented, along with the future prospects for optical measurements with antihydrogen place as well as our long term plans for new measurements of this antimatter system.

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Many-Body Theory for Ps-Atom Scattering and Pickoff Annihilation

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A many-body theory for positronium (Ps) interaction with many-electron atoms has been developed to calculate Ps-atom scattering cross sections and pick-off annihilation rates [1]. It takes into account virtual excitations of both objects during the collision. In our approach, we confine the Ps-atom system within a hard-wall spherical cavity [2]. We use a B-spline basis to solve the Dyson equations $(H_0^{\pm}+\Sigma^{\pm})\psi^{\pm}=\varepsilon^{\pm}\psi^{\pm}$ for the electron ($-$) and positron (+) in the field of the target atom. Here, $H_0^{\pm}$ is the Hamiltonian of the electron or positron in the static (Hartree-Fock) field of the atom, and $\Sigma^{\pm}$ is the many-body correlation potential. The Ps eigenstates are constructed from the electron and positron states $\psi^{\pm}$ as $\Psi=\sum_{\mu,\nu}C_{\mu\nu}\,\psi_{\mu}^{-}\psi_{\nu}^{+}$ and found from $H\Psi=E\Psi$, where $H=H_0^{-}+\Sigma^{-}+H_0^{+}+\Sigma^{+}+V+\delta V$, V being the Coulomb interaction and δV the screening correction due to polarization of the atomic electrons. The boundary condition at the wall allows us to find the scattering phase shifts. From these we obtain the scattering cross section, which we compare with recent experimental data [3]. Figure 1 shows the cross section for Ar in the frozen-target approximation (i.e., without $\Sigma^{\pm}$ and δV) and with many-body-theory treatment. The origin of the disagreement with the experiment [3] is unclear, as our calculations are expected to give the cross sections with $\leq 20\%$ uncertainty.

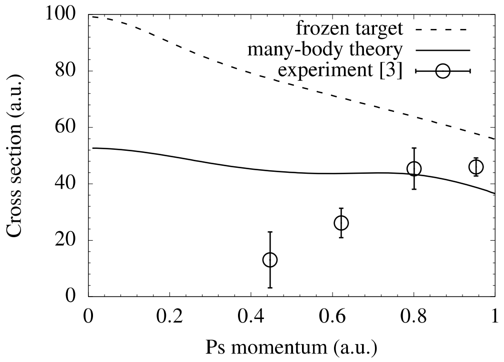

Figure 1: Cross section for elastic scattering of Ps on Ar.

The Ps wave function is also used to calculate ${}^{1}Z_{\mathrm{eff}}$, which determines the *pickoff* annihilation rate $\lambda=4\pi r_o^2 cn\,{}^{1}Z_{\mathrm{eff}}$, where r_o is the classical electron radius, c is the speed of light, and n is the gas density. Previous calculations of ${}^{1}Z_{\mathrm{eff}}$ for noble gases [4] underestimated the experimental data [5] by a factor of 2–5. By accounting for many-body corrections to the annihilation vertex, we obtain values of ${}^{1}Z_{\mathrm{eff}}$ in near-perfect agreement with experiment for He and Ne [1], and within 20% for Ar, Kr, and Xe.

* This work was performed in collaboration with A. R. Swann and G. F. Gribakin [1].

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Positron Interactions with Nitrogen and Oxygen and Pyridine Molecules: Elastic, Inelastic and Total Cross Sections

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Positrons are difficult to handle experimentally, yet their collisional cross sections are necessary for particle track models of medical techniques such as positron emission tomography and in situ ion therapy dose calculation. The use of relatively simple approximations, many built from the first Born approximation [1], has been shown to provide accurate cross-sectional collision data for electron and positron collisions down to collision energies below 100 eV. The available experimental data [2] are always used to benchmark these calculations, and any changes to an approximation are subject to scrutiny.

Improvements to the IAM-SCAR calculation procedure [3], [4], a theoretical approach based on the optical potential method and the geometry of a molecule, have increased its accuracy well below this limit. When applied to electron-molecule scattering, improvements were seen for the cross-sections of collisions with simple molecules when compared with higher levels of theory. The improvements include the screened interference of the scattering wave due to the multiple scattering from the atoms in the molecule, and are now included for both the electron and positron scattering formulations of the IAM-SCAR+I code.

The changes to positron-molecule scattering are explored here on the N_2, O_2 and pyridine [5] molecules. The effects on the cross section are pronounced in the collisional energy range below 100 eV, and the accuracy of the IAM-SCAR method above 100 eV is maintained. The new calculations are compared to other recent calculations and experimental data.

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Experiments with Positronium and Cold Atoms

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Recent progress in manipulating the positronium atom has resulted in accurate state control including excitation to long-lived Rydberg states [1]. The charge exchange reaction between excited positronium and antiprotons is of relevance to antihydrogen production, with two collaborations actively pursuing this mechanism in their experimental programme at CERN [2,3]. Numerical work indicates that the cross-section can be large for excited states of positronium [4], but that the behaviour is not simple [5].

We have recently proposed that cold neutral species could be produced from cold trapped ions via the charge conjugate reaction with an ion [6]. Low temperatures become possible by laser cooling the trapped ions before scattering with positronium, which does not impart significant recoil energy, and thus sufficiently massive neutrals remain essentially as cold as the ions were originally. Species that cannot be laser cooled directly can be sympathetically cooed in the ion trap. By charge exchange with positronium, both charge neutrality and low temperature, which are often desired in precision measurements, could in principle be achieved even in complex species. By a simple scaling of results in [4] the reaction cross section would be sufficiently large to produce a sufficiently dense sample of neutrals for experiments in novel collisions or fundamental tests of symmetry.

The experimental realisation of this proposal will in the first instance allow exploring positronium-ion scattering at low, controllable kinetic energy with species that can be laser cooled directly, with a first goal of understanding the scattering process. Realising this proposal entails combining positronium production and laser excitation with confining and laser cooling ions in an RF-trap. Here, I will present an overview of the proposal and our progress in this project to date.

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Recent Advances in the Theory of Dissociative Electron Attachment

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Dissociative electron attachment (DEA) to polyatomic molecules is a complicated process involving couplings between electron and nuclear motion. Completely *ab initio* calculations are presently possible only for diatomics, and model approaches should be developed for more complex targets, particularly if nonlocal effects, leading to vibrational Feshbach resonances (VFR) and threshold cusps, are important [1-3]. In the last few years we have been working on several problems related to DEA to polyatomic molecules:

• Extension of the nonlocal theory to two and more degrees of freedom. The properties of the Green's operator describing the evolution of the resonant state play the crucial role in the nonlocal effects. Quantum-mechanical and semiclassical methods of its calculation have been developed. They can be incorporated in the equivalent resonant R-matrix theory which is more convenient for model calculations. The general theory has been applied to the CF_3Cl compound. DEA to this molecule was studied in the past by one-dimensional nonlocal theory and two-dimensional local theory incorporating symmetric stretch and umbrella vibrations. The present version combines both nonlocal and two-dimensional effects.

• Application of the effective range theory to description of VFRs and threshold cusps in polyatomics. This theory was applied recently to description of cusp structure in DEA to $Fe(CO)_5$ [4], the molecule important for the development of the Free-Electron-Beam Induced Deposition technique, and to a series of 5-membered heterocyclic rings [5].

• Investigation of the role of the water cluster environment in DEA to polyatomics, particularly to biological-relevant molecules like thymine. There are two effects in this process, one leading to the enhancement of the DEA cross section due to the increased lifetime of the intermediate negative-ion state [6], and the other leading to the decrease of the yield of the anionic fragments due to the hydrogen bonding between the nucleobase and the solvent [7].

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Indirect Dissociative Recombination of Small Ions

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Dissociative recombination (DR) is a process is which a free electron with a positive kinetic energy is captured by a molecular ion while breaking one or several chemical bonds,

$$e^- + AB^+ \rightarrow A + B\,.$$

This is a very efficient chemical process, but is rarely described in chemical textbooks. It is considered to be the most complex of gas-phase reactions leading to the production of neutral atoms and molecules [1].

Historically, we distinguish two different mechanisms for the DR process. In the direct mechanism the reaction is mediated by an electronic resonant state $\boldsymbol{AB}^*$(shape or core-excited resonance), while in the indirect mechanism no such electronic state exists in the Frank-Condon region and the $\boldsymbol{AB}^*$ state is formed by an internal rovibrational excitation (rovibrational Feshbach resonance). For most of the molecular systems both mechanisms interfere resulting in a complicated structures of the DR rates. However, for a number of molecular cations (LiH+, LiHe+, HeH+, . . .) the indirect process dominates in the dissociation.

Although the theoretical models [2, 3] describing the indirect DR with multichannel quantum defect theory (MQDT) have been successfully used [4] for several decades, the recent experimental advances [5] put the accuracy of these models to a test. In this paper we show how the theory helps to setup the experiment and we also report on our progress in development of accurate indirect DR theory and its application to several molecular targets.

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Electron Impact Ionisation and Fragmentation of Biofuels

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Experimental and theoretical studies on electron impact ionisation and fragmentation of the biofuels methanol, ethanol, 1-propanol and 1-butanol, have been performed in this work. The experimental measurements of the cations created in electron impact ionization and fragmentation of these alcohols were observed using a Hiden Analytical quadrupole mass spectrometer (EPIC 300), with a mass resolution of 1 amu. The mass spectrum recorded at an incident electron energy of 70 eV, reveals the probability of forming different cations by either direct ionization or dissociative ionization. Individual partial ionization cross sections (PICS) for the main cationic fragments observed of each alcohol were also registered at electron energies in the range of 10-100 eV. Total Ionization Cross Sections (TICS) were obtained from the sum of the measured PICS, for nearly all cations measured, and are compared to relevant data reported in the literature. In addition, theoretical TICS were calculated using the Binary-encounter Bethe (BEB) and independent atom model with the screening corrected additivity rule (IAM -SCAR) methods. Good agreement between current measured and calculated TICSs and corresponding earlier results was typically found, as it is shown in figure 1. Also, appearance energies (AEs) and Wannier exponents for the most intense cations formed in electron collisions with the studied alcohols were obtained. Where possible, those results are compared to those from an earlier investigation [1].

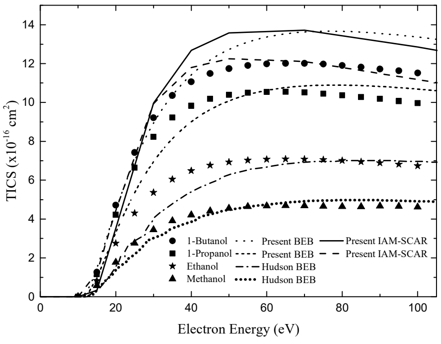

Fig 1: The comparison of the absolute total ionization cross of methanol, ethanol, 1- propanol, 1-butanol in 10-100 eV impact electron energy range.

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Coupled Electronic and Nuclear Dynamics of Dissociative Electron Attachment Revealed by Anion Fragment Momentum Imaging

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Anion fragment momentum imaging experiments employing reaction microscopes [1] or velocity-slice imaging spectrometers [2-3], enable the highly differential, momentum imaging of multiple fragment ions over large collection angles up to 4π steradians. These capabilities allow precise measurements of dissociative electron attachment (DEA) cross sections and the analysis of fragment ion kinetic energy and angular distributions for polyatomic targets. Thus, information on the dissociation dynamics with respect to the incident electron momentum relative to the stationary target (i.e. the laboratory frame) is captured by momentum imaging. *Ab initio* electron scattering calculations provide the crucial added capability to predict the angular dependence of the electron attachment probability, connecting the laboratory frame measurements to the molecular body frame. This combination of momentum imaging and electron scattering theory reveals the dynamics of the dissociating anion formed by electron attachment.

We present recent results on the dynamics of DEA to small polyatomic molecules, addressing the chemistry of transient anions formed by electron attachment. For systems where several negative ion resonances exist, there may be only one bound anion state of an atomic or molecular fragment. So how can two or more resonances produce the same anion and neutral products in the same states? Anion fragment momentum imaging reveals details about intramolecular charge transfer or conical intersections that are implicated in these phenomena. In other systems we observe that one anion resonance can produce two product channels, indicating nonadiabatic transitions between excited electronic states of the transient anion. Preliminary results for formic acid will be reported, where two resonances result in site-selective hydride loss, and key aspects of the dissociation dynamics are revealed.

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Transport Coefficients of Higher-Order for Electrons and Positrons in Neutral Gases and Nonpolar Liquids

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Transport coefficients of third and higher order have been systematically ignored in the traditional interpretations of the swarm experiments, as these experiments are usually performed under conditions in which the contribution of these transport coefficients is not significant. However, it has been shown that the third order transport coefficients (TOTC) are necessary for the conversion of hydrodynamic transport coefficients into transport data which are measured in the steady state Townsend and arrival time spectra experiments. In addition, the TOTC are required for a better representation of the spatial distribution of the swarm, as they describe the asymmetric deviation of the profiles of the number density of charged particles from a perfect Gaussian. Furthermore, if TOTC could be measured and calculated with a sufficient accuracy, this would enable the improvement of the swarm procedure for determining the complete sets of cross sections, as an additional transport coefficient could be included in this procedure.

We have investigated the third order transport coefficients for electrons and positrons in rare gases, as well as for electrons in homogenous atomic liquids. The structure of the third order transport coefficient tensor has been determined by employing the group projector technique, for all configurations of electric and magnetic fields [1]. In addition, the physical interpretation of the third order transport coefficients has been carefully analyzed.

Calculations of the TOTC and transport coefficients of lower order (e.g., drift velocity and diffusion tensor) have been performed in a wide range of the reduced electric fields (E/n_0) by employing Monte Carlo simulations and a multi term method for solving the Boltzmann equation. Both computer codes which are used in this study have been thoroughly tested [2,3]. Among many important points a strong correlation has been found between the E/n_0 profiles of the longitudinal component of the TOTC tensor and longitudinal diffusion. In addition, the TOTC for electrons and positrons in molecular gases have been compared. It has been found that the difference between the TOTC for electrons and positrons can be attributed to the corresponding differences in the rate coefficients for the inelastic collisions. In our study of the electron transport in atomic liquids, the structure induced negative differential conductivity has been thoroughly investigated by analyzing spatially resolved transport data and electron energy distribution functions [4]. Moreover, the influence of various representations of the inelastic energy losses in the liquid phase on the calculated values of the transport coefficients and the first Townsend coefficient has been studied [4].

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Irradiation of Biomolecules by Low Energy Electrons

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Electron impact processes with molecules, including those which result in molecular dissociation, drive plenty of the important processes in many fundamental areas of technology, chemical engineering, the environment, the atmosphere, life and radiation sciences.

It is by now well known that low energy electrons (LEEs), the secondary species in the interaction of ionizing radiation with matter, efficiently produce structural and chemical modifications of many biostructures. These secondary electrons with a kinetic energy distribution up to 20 eV [1] are created in numbers of $5x10^4$ per MeV of deposited energy [2] that makes them the most abundant radiolytic species.

Recent years have witnessed a remarkable growth in the scientific interest in studying the low energy electron interactions with biologically relevant molecules. Among them, a wealth of experimental and theoretical data have been devoted to nucleic acids and their sub-units [3,4] in order to unravel the molecular mechanism how LEEs damage macromolecules.

In this talk I shall present experimental gas phase studies on dissociative electron attachment to heterocyclic organic compounds consisting either of a six-membered ring or a six-membered ring that is fused with imidazole ring. Such chemical compounds are frequently used to mimic the behavior of nucleobases and their metabolic products under reductive conditions. In particular, emphasis will be placed on the description of the formation of the transient negative ions and the comparison of the fragmentation patterns for a series of biologically relevant compounds.

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Electron Swarm and Photon Interactions with Biomolecules and Atmospheric Gases

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In this talk we present recent measurements and, in some cases, accompanying calculations on the interaction of electrons with molecules of biological interest such as THF (Tetrahydrofuran), THFA (Tetrahydrofurfuril Alcohol), and N_2O, the latter molecule of interest in atmospheric and industrial applications. In all cases the pulsed Townsend method has been used [1]. The measurement of the electron drift velocity, W, and the effective ionisation coefficient, α_{eff}, in THF has been used to improve/validate a previous set of electron collision cross sections [2,3]. Measurements on pure THFA have thus far been precluded because of its very low saturation vapour pressure (0.2 Torr at 20 ºC); however, measurements in mixtures of this gas with N_2 and Ar have been made, and a special setup is being built to perform measurements in pure THFA. Using a simulation code [4,5] which, apart from charge transport motion and electron attachment, collisional detachment from negative ions is considered, has led us to determine detachment coefficients at low E/N (up to 8 Td). It appears that electron detachment proceeds readily with fairly large values of the density-normalised ionisation coefficient, in the order of 10^{-15} cm^2.

The second part of the talk will be dedicated to present recent measurements on the photodetachment of negative ions in oxygen and N_2O. Briefly, we have used a standard technique for producing an electron avalanche followed by its slow ionic component. After some delay, a laser pulse (532 nm or 1,064 nm) is aimed at the avalanche at right angles. The photodetachment signals and results dealing with the photodetachment yield will be presented.

While performing the photodetachment measurements we observed that even in the absence of the UV laser light that produces the initial photoelectrons from the cathode, electron avalanches formed due to the ionisation of the gas from the strong photodetachment laser pulse (355 nm and 266 nm), which is an indication of multiphoton ionisation in the realm of the gas, even without focusing the 6 mm diameter laser beam. To substantiate these findings even further, measurements of W and α_{eff} in oxygen were found compatible with those published. Implications of this effect for laser assisted plasma diagnostics and special electron or ion sources will be discussed.

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The Gas-Liquid Interface: Kinetic and Fluid Modelling of Charged Particle Transport

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Modelling of electron transport in the vicinity of the plasma-liquid requires an accurate treatment of electron transport in the gaseous and soft-condensed phases, together with an understanding of the electron transport across the gas-liquid interface. In this presentation, we present simulations which have informed the design of a new experiment which adapts an existing electron-gas phase scattering experiment (e2e) to consider electron scattering from a liquid micro-jet. The results highlight that electron-scattering information (effective cross-sections) can be obtained from the experiment for both the bulk liquid and from the interface. In addition, we present progress on an ab-initio formalism for electron transport in liquids through appropriate generalisations of Boltzmann's equation and associated higher order fluid models to account for spatio-temporal scattering correlations, screening of the electron potential and the effects of (self-) trapping. Application is considered for various atomic liquids as a starting benchmark to consider more complex polar liquids [1] as well as the non-local nature of electron transport in liquids and gas-liquid interfaces [2,3]. Propagation of ionization fronts between the gas and liquid phases are considered.

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Experimental Studies on Low-Energy Electron Collisions with Radiosensitizers

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Various nitroimidazolic molecules have been considered as potential radiosensitizers for hypoxic tumors which are characterized by a lack of oxygen [1]. The desired benefit of radiosensitizers may also partially be ascribed to the action of low-energy secondary electrons. This species is generated in abundant amounts during the irradiation of biological tissue. The kinetic energy distribution of secondary electrons formed finds its maximum below 10 eV. Low-energy electrons may attach to molecules which leads to the formation of transient negative ions. Those states may lead to long-lived anions or they may decay by molecular dissociation or spontaneous electron emission.

In order to develop novel nitroimidazolic compounds for radiation therapy, it is important to investigate the electron attachment properties in dependence of the molecular structure. In this contribution, I will review our previous electron attachment studies with nitromidazolic compounds in the gas phase. The setup used for these studies was a high resolution electron monochromator combined with a quadrupole mass spectrometer. Measurements were also carried with a two-sector field mass spectrometer, which enabled higher electron currents than the monochromator, albeit with lower energy resolution.

The resulting negative ion mass spectra as well as anion efficiency curves showed distinct differences between the studied compounds. Hydrogen loss was observed as the most abundant reaction for the building block imidazole [1]. The DEA experiments demonstrated that the attachment of a single electron may induce the loss of all four hydrogens from imidazole. For nitroimidazoles, the presence of the NO_2 group leads to significant change of the fragmentation pattern [2,3]. For these compounds, DEA reactions are dominated by the loss of small neutral radicals like OH and NO. Finally, for larger nitromidazolic compounds like nimorazole, molecular dissociation plays a minor role and the formation of the parent radical anion is dominant [4]. This observation may point out the mechanism of radiosensitization by nitroimidazolic compounds. The results will be also compared with other DEA studies of radiosensitizers like modified pyrimidines [5].

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Electron Interactions with Biomolecular Models of Increasing Complexity

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We experimentally probed interaction of low energy electrons (<10eV) with biomolecular models in gas phase and clusters. These experiments enable us to explore the effects of molecular as well as environmental complexity on the dissociative electron attachment (DEA).

An important motive in DNA bases is HNCO, which we studied isolated in the gas phase.[1] We demonstrated importance of the σ^*-π^* mixing in the DEA process, as well as the importance of the intramolecular energy transfer during the dissociation.

In DNA bases, the HNCO component undergoes effective hydrogen loss via DEA forming typical $(M\text{-}H)^-$ DNA base radical anions. In our study [2], we demonstrated closing of this dissociation channel by the water environment. Such closing is caused by caging of the dissociation products and intermolecular energy transfer as demonstrated in our work [3].

In more complex biomolecules such as the nucleotides, electron transfer can influence the dissociation.[4] In our study of DEA to dCMP, we demonstrated that in water environment hydrogenation of the transient negative anion may dramatically change the fragmentation and final charge redistribution over the molecule [5].

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Thermalisation in Water Nano-droplets

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The evaporation of a water molecule occurs through the breaking of one or several hydrogen bonds. These hydrogen bonds are responsible for many remarkable features of water. At the macroscopic scale, water is known for its exceptional ability to thermalize a system, while at the microscopic level, a high-speed transfer of vibrational energy via hydrogen bonds is observed. What happens for only a small number of water molecules?

In the experiment carried out with the device DIAM at IPN Lyon, the relaxation of protonated water nanodroplets is observed after electronic excitation of one of its molecules [1-6]. The implementation of a velocity map-imaging (VMI) method associated with the Correlated Ion and Neutral Time-Of-Flight (COINTOF) technique allowed us to measure the velocity distributions of molecules evaporated from mass- and energy-selected protonated water nanodroplets [3, 4]. The behaviour of the measured velocity distributions shows that even for extremely small water nanodroplets, a complete energy redistribution before evaporation prevails and the velocity distributions of these events are close to those expected for macroscopic droplets from around ten water molecules. However, these measurements of the velocity distributions also feature a distinct high-velocity contribution corresponding to the evaporation of a molecule before complete redistribution of energy [1,5]. The measured velocity distributions for heavy water nanodroplets show a proportion of these non-ergodic events more important than for normal water. The measurements carried out with different target atoms show that the proportion of non-ergodic events decreases with decreasing the energy deposited in the droplet.

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Challenges in Obtaining Cross Sections from Electron Swarm Data

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Inferring scattering cross sections from electron swarm experiments through the repeated solution of Boltzmann's equation began in the 1960s with the work of Phelps and collaborators [1]. Since then, different approaches have been explored to automate this process, including the use of optimisation algorithms and artificial neural networks [2,3].

Essential to automating the solution of this "inverse swarm problem" is the ability to solve Boltzmann's equation quickly and robustly. With this in mind, we consider the two-term approximation and solve Boltzmann's equation by integrating inward from high energies; a technique known as backward prolongation [4].

We present a technique for determining bulk transport coefficients efficiently by applying the principle of linear superposition. To demonstrate, we find and compare bulk transport coefficients for electrons and positrons in magnesium and beryllium metal vapours [5,6].

Finally, nonlinear least-squares fitting of argon's elastic cross section is attempted and the ill-posed nature of the inverse problem is highlighted.

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Functional Group Dependence and Site Selectivity in Dissociative Attachment

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It is well known that dissociative electron attachment (DEA) plays an important role in electron induced chemistry. Several experiments have shown that selective fragmentation through DEA enables chemical control. It has been found that this selectivity emerges from two aspects. The first one is purely based on threshold energy and arises from the differences in the electron affinity of the fragments and the bond dissociation energies [1, 2]. The second one originates from functional group dependence [3, 4]. This is mostly seen in core or valence excited resonances. Here, the selectivity is more versatile in that it is independent of the threshold energy and has a broader energy range in which the selectivity is displayed. The optical absorption bands shown by these molecules have common features, characteristic to the functional groups present. It appears that these very features are displayed in the formation of core excited resonances, giving rise to the observed selectivity in braking the O-H, C-H or N-H bonds in molecules through DEA. Such selectivity has been observed in alcohols, carboxylic acids and amines [3, 4]. The site/bond selectivity observed in bigger molecules like Thymine [5] and higher alcohols [6] can also be interpreted based on the functional groups.

We have been continuing the investigation of the functional group dependence in organic molecules on a wider scale, including aromatics, in terms of the mass spectra, ion yield curves, absolute cross sections and momentum distributions. In this talk I would briefly review the role of functional group dependence in DEA and summarize our new findings.

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Chirality Sensitive Effects in Electron Collisions against Halocamphors

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Chirality sensitive effects in electron collisions are often referred to as electron circular dichroism (ECD) and amount to the preferential scattering of spin-polarized beams from pure enantiomer samples. Kessler and co-worker performed a series of gas-phase experiments with halocamphors and other target molecules [1], expressing the ECD effects in terms of electron scattering asymmetries. Those experiments were at least partly motivated by the Vester-Ulbrich (VU) hypothesis for biological homochirality [2], which claims that parity-violating interactions might have selected optical isomers in the early stages of life in our planet. While the VU conjecture is not broadly accepted as an explanation for the chiral selection of biomolecules, Dreiling and Gay (DG) recently reported on the chirality sensitive dissociation of halocamphor molecules [3]. These experiments are fascinating in a number of ways. They are consistent with the principle underlying the VU hypothesis; they are the first account of chiral effects on dissociation electron attachment (DEA) reactions; the reported DEA asymmetries magnitudes sometimes largely exceed those of the scattering asymmetries; and the DEA asymmetries do not correlate with the atomic number of the halogen substituents, as expected from theory.

While theories of scattering asymmetries have long been proposed [4], with emphasis on the basic mechanisms and symmetry properties, little is known about the dynamics of electron-halocamphor collisions. We report fixed-nuclei scattering simulations for 3-Br-camphor, 3-I-camphor and 10-I-camphor molecules, paying special attention to the resonances lying within the energy range addressed in the DG experiments, which are expected to initiate the DEA reactions of interest. We also generalized the usual Feshbach projection operator approach to DEA processes [5] to account for the Coulomb and spin-orbit interactions. We thus obtained expressions for the DEA symmetries that might be of help to understand the DG data.

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High-Resolution Measurements of Total Cross Section for Very-Low-Energy Electron Collisions with Molecules

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Accurate absolute cross section data for electron scattering from atoms and molecules provide important information not only for the fundamental physics of electron collisions but also for many fields such as electron-driven processes in the Earth and planetary phenomena, gaseous discharges, radiation chemistry and plasmas physics. Consequences of several interesting scattering phenomena such as Ramsauer-Townsend effect, shape resonances, vibrational Feshbach resonances, and threshold structure due to a virtual state, appear in the scattering cross section curves especially at very-low collision energies.

Beam experiments with hot-filament electron sources under the single collision condition have provided accurate cross-sections in a wide energy region, even in the energy range below a few hundred meV [1,2], where producing an electron beam at this very-low-energy region was a formidable task using the conventional technique. An alternative method which makes use of photoelectrons produced with the photoionization of atoms using Synchrotron Radiation (SR) source realized the measurements of electron scattering cross sections at very-low energies down to below 10 meV [3] in the single collision condition.

In the present report, results of our recent high-resolution measurements of absolute total cross sections for electron scattering from some small molecules obtained with a technique employing the threshold-photoelectron-source combined with SR [4] are presented. Onsets for some of the vibrational excitation thresholds showed up in the measured total cross section for CO_2, N_2O and CH_4. Integral vibrational excitation cross sections for CH_4 determined from the obtained total cross section were compared with the ones estimated from the swarm experiments [5] which showed reasonable agreements. The total cross section for CO_2 obtained at very-low-energies in the present study agree with those reported by Field et al [6], which showed larger cross section compared to the results of TOF measurements employing a hot-filament [7,8] at around 100 meV. We also note that although the results of Jones et al. showed significant discrepancy from the other earlier works [9] the present total cross section for NH_3 agreed well with those reported by Jones et al. down to the very-low-energies below 30 meV.

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Electron-Impact Vibrational Excitation of Molecular Hydrogen

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Electron-impact vibrational excitation of molecular hydrogen in the ground electronic state is one of the most fundamental processes in electron-molecule scattering. The production of vibrationally-excited H2 is of importance in modelling hydrogenic plasmas, as the cross sections for electronic excitation and dissociative processes have a strong dependence on the initial vibrational level [1,2].

Above the threshold for excitation of the electronic singlet manifold, the dominant mechanism for exciting vibrational levels in the ground electronic state is electronic excitation followed by radiative cascade. Calculations of these processes require a fully vibrationally resolved description of the scattering problem, with an accurate account of electronic channel coupling over a large range of internuclear separations. Previous calculations are limited to those performed using the semi-classical impact-parameter method [3], which is known to yield cross sections up to two times larger than convergent close-coupling (CCC) results for electronic excitation [4]. Using a spheroidal-coordinate formulation of the molecular CCC method, we have performed fully quantum-mechanical calculations of excitation-radiative decay (ERD) leading to vibrational excitation of H2, over the range of energies from 10 to 300 eV.

At lower energies, direct vibrational excitation is the only mechanism for producing vibrationally excited H_2. There has been a long-standing interest in theoretical calculations of the $v = 0 - 1$ excitation due to the disagreement between the two principle experimental methods (crossed beam and swarm analysis). In the energy region of interest, the assumptions of the often-used adiabatic approximation for separating the nuclear and electronic degrees of freedom become invalid, and it is necessary to properly account for the coupling between vibrational levels. Vibrational close-coupling (VCC) calculations have been previously performed [5] with the use of polarisation potentials to allow for an approximate treatment of the coupling to electronic excitations. In this talk we will review the existing calculations and experimental results, discuss the more accurate account of target polarisation possible with the CCC method, and present new VCC results for the direct vibrational excitation of H_2 by low-energy electrons.

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Electronic Excitation of Atoms by Positron Impact Using the Scaling Born Positron Approach

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We will discuss our recent studies for electronic excitation of atoms by positron impact using the scaling Born positron (SBP) approach [1-4]. This scaling method provided not only a simple way to calculate excitation cross sections of many atoms, but also to molecules. The aim of this work was to provide reliable cross sections of atoms using the SBP approach comparable to accurate experimental data as well as to more sophisticated theories. The SBP approach convert the first Born approximation (FBA) excitations cross sections into reliable cross sections comparable to the most accurate theoretical methods. Numerical examples of integral cross sections of H, He, Hg, and Mg are presented to illustrate the applicability of the improved SBP model.

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LEPPP 2

New Calculations on e^+ N_2 Ionization

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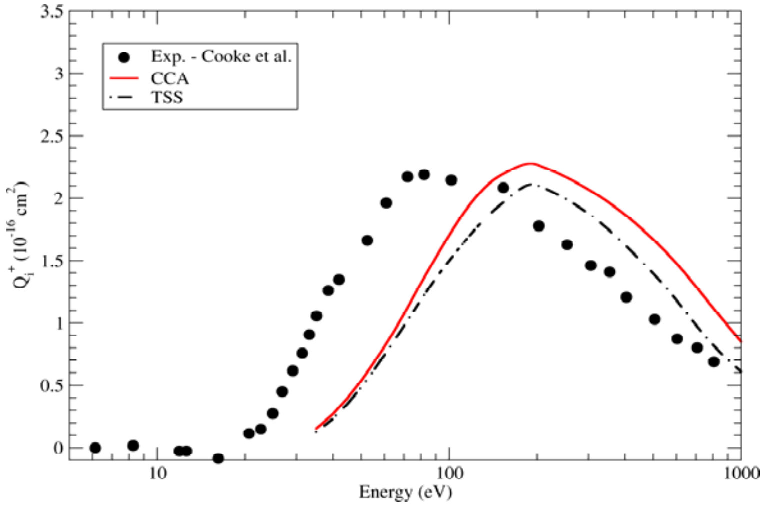
The new experimental total non-dissociative ionization cross sections of Cooke *et al* [1] are about 50-60% lower than the older experimental results of Bluhme *et al* [2]. Our previous theoretical calculations [3] agree with the cross sections of Bluhme *et al*. These calculations were based on the CPE approximation which assumes that if the scattered positron is faster than the ejected electron the positron moves in the field of the neutral molecule, while the ejected electron moves in the field of the positive molecular ion.

In this paper we employ theoretical models based on the CCA approximation, which assumes that both the scattered positron and the ejected electron move in the field of the positive molecular ion. The CCA model was shown to produce ionization cross sections significantly lower than the CPE model [4].



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The above figure shows that our CCA model produces results which agree with the size of the experimental cross sections of Cooke *et al* but our peak appears at an impact energy significantly higher than in the experimental case.

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LEPPP 3

Positron and Electron Impact Ionization of Ne and Ar

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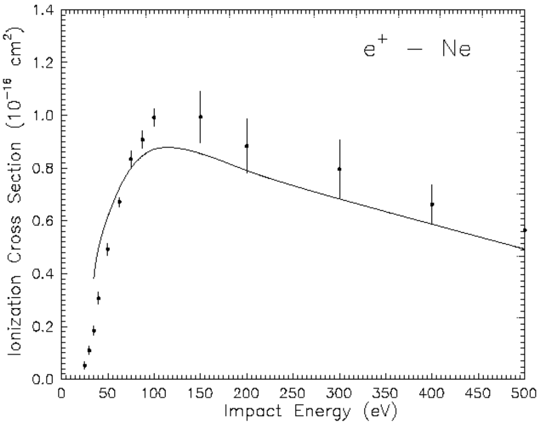
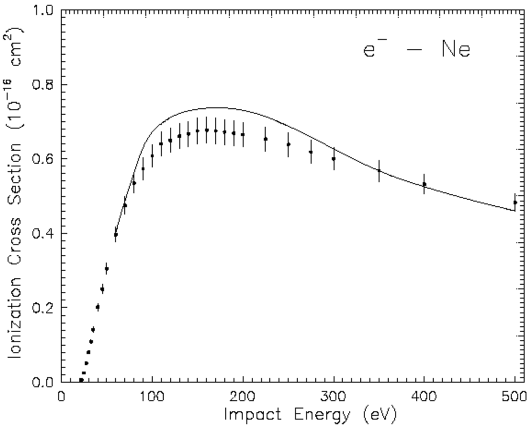
The experimental results for electron impact total ionization cross sections of noble gases are well established [1], while for positron impact ionization Knudsen *et al* [2] provided experimental data for neon and argon. On the theory side work is still needed for atoms heavier than helium.

For positron impact ionization we found that the CPE model agrees with experimental data for all noble gases [3]. The CPE approximation assumes that if the scattered positron is faster than the ejected electron the positron moves in the field of the neutral atom, while the ejected electron moves in the field of the positive molecular ion.

In this paper we adapted the theoretical model CPE for electron impact ionization of neon and argon. Electron exchange was included in the 'maximum interference' approximation [4]. In the two figures shown below we show the level of agreement between model CPE and the experiments of refs.[1, 2] for the ionization of neon.





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Using Strong Laser Fields to Produce Antihydrogen Ions

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We provide estimates of both cross section and rate for the stimulated attachment of a second positron into the ($1s^2\,{}^1S^e$) state of the $\overline{\mathrm{H}}^+$ ion using Ohmura and Ohmura's (1960 Phys. Rev. 118 154) effective range theory, Reiss's strong field approximation (1980 Phys. Rev. A 22, 1786), and the principle of detailed balancing. Our motivation for producing $\overline{\mathrm{H}}^+$ ion include its potential to be used as an intermediate state in bringing antihydrogen to ultra-cold (sub-mK) temperatures required for a variety of studies, which include both spectroscopy and the probing of the gravitational interaction of the anti-atom. We show that both cross section and rate are increased with the use of a resonant laser field.

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LEPPP 5

Electronic Excitation of H_2O by Positron Impact

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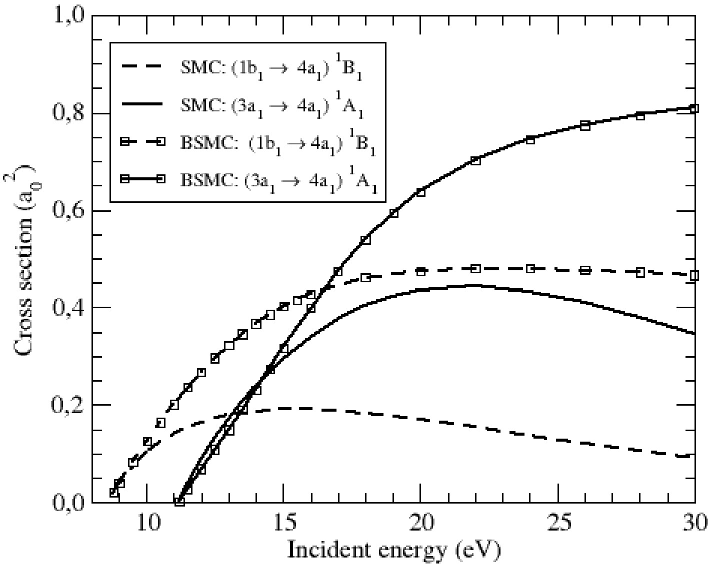
Electronic excitation is a very important mechanism of energy loss when positrons penetrate into liquid-water and also in biological systems [1]. In this work, we present results for the electronic excitation of H_2O by positron impact from threshold to 30 eV. The calculations were performed with the Schwinger Multichannel Method [2] using the same scheme of basis set treatment of [3]. The excited states of the target were described within the Improved Virtual Orbital formulation [4]. From the electronic ground state configuration, we considered the low-lying transitions $(1b_1 \rightarrow 4a_1)^1B_1$ and $(3a_1 \rightarrow 4a_1)^1A_1$ in two and three channels levels of approximations. Results for the transitions considered are given in the figure.



The results labeled SMC and BSMC are obtained, respectively, in the pure SMC and SMC combined with higher partial waves from a first Born calculations. In this last case, the maximum partial wave considered from the SMC amplitude was l=2.

As observed by Gil et al for electron scattering, the cross sections associated to the $(3a_1 \rightarrow 4a_1)^1A_1$ transition have a higher magnitude when compared to the $(1b_1 \rightarrow 4a_1)^1B_1$ one.

Results show that the electronic excitation cross sections show no appreciable changes when the number of excitation channels is varied.

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Rotational Excitation of O_2 by Positron Impact

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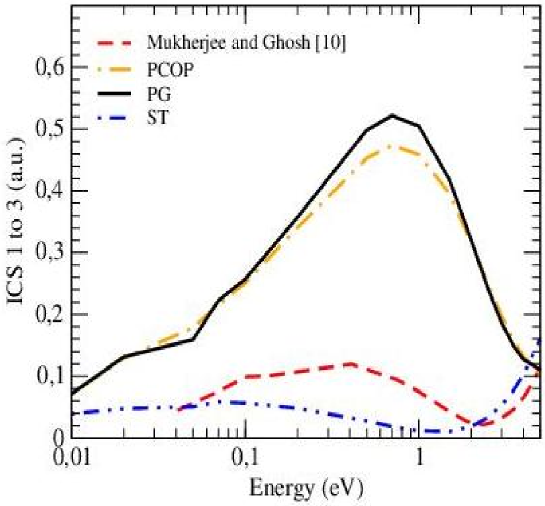
In this work, we calculate the rotational excitation of O_2 molecule by positron impact for energies between 0,01 and 5,0 eV wihinn the adiabatic rotational approximation. Recently, our group performed an investigation about low energy positron scattering by O_2 [1]. More specifically, we calculated the elastic scattering cross section for energies below the positronium formation threshold (~ 5,4 eV) with the Positron Correlation-Polarization Potential (PCOP) [2], studying how the inclusion of higher order polarizability terms in the asymptotic polarization potential affect the elastic cross section. Here we calculate the $J_i = 1 \rightarrow J_f = 3$ rotational transition using as input data the T-matrices of Tenfen et al [1] and compare our results to the previous ones developed by Mukherjee and Ghosh (MG) [3], also performed with the PCOP formulation.



Our results are presented in the figure. The dashed line are the results of MG [3], the dot-dashed and the solid lines are our results obtained with the α_2-PCOP (PCOP) and the γ-PCOP (PG) respectivelly (see table III of Tenfen et al [1] for details). The dot-dashed-dot line represents our results in the static (ST) approximation.

Some insight about the nature of the discrepancies between the rotational cross sections can be obtained if we pay attention to the fact that MG employed the SCF wavefunction of Cade and Wahl [4] for the $^3\Sigma_g^-$ state of O_2, while we used a Hartree-Fock wavefunction constructed from a slightly modified SVP+Rydberg basis of Dunning and Hay [5]. It suggests that different anisotropic electronic densities were considered in each calculation. MG [3] report a cutoff radius of 3,12 a.u. while we report 1,91 a.u., a value substantially different. Since our cutoff radius is smaller, we find that the polarization presents a leading role in the scattering process. It explains why MG results are relatively closer to the ones we have found in the ST approximation.

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Low Energy Positron Scattering by C_2H_2

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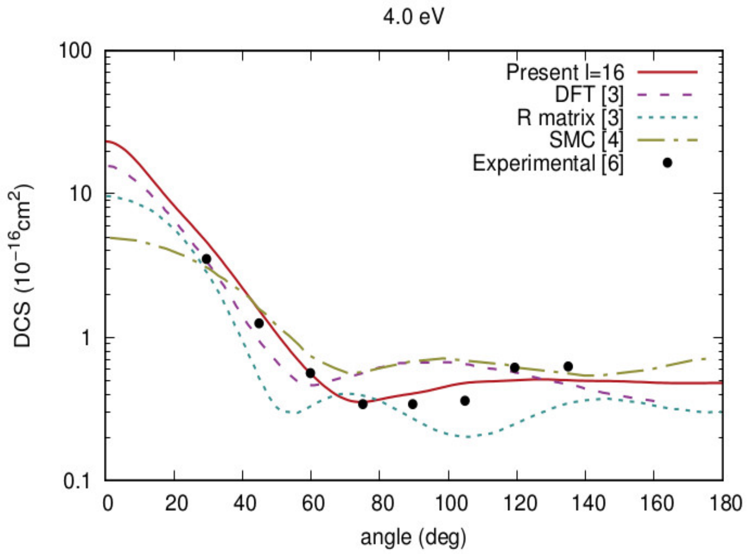
In this work we calculated the differential and integral cross sections for positron scattering by C_2H_2 in the static plus polarization level. We employed the Method of Continued Fractions [1] in order to solve the scattering equations, and the PCOP [2] as the polarization-correlation model. We compare the obtained results with the previous calculations [3, 4, 5] and measurements [6, 7, 8] presented in the literature. In the figure, we compare the obtained 4 eV differential cross sections with the referenced data.



The static cross sections obtained agrees very well with the static results presented in reference [3]. However, since we considered a generously large partial wave expansion (l = 16) and a well defined polarization correlation model we obtained differential cross sections that exhibit better agreement with the respective experimental data. The polarizabilities employed were $\alpha_0 =$ 28,68 a.u. and $\alpha_2 =$ 11,47 a.u.. The obtained integral cross sections are in fair agreement with those reported in reference [3].

We expect that the inclusion of the quadrupolar polarizability and the hyperpolarizabilities will enhance the differential cross sections in the lower angle region which will affect the integral cross sections, particularly in the lower energy range considered (up to 1 eV) as observed in ou previous investigation about positron-O_2 scattering [9]. It is worth to mention that the experimental total cross sections available in the literature are not forward corrected, such that the expected enhancement of the cross sections mentioned above may be desired in order to obtain a better description of the positron scattering with C_2H_2.

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Rovibrational Excitation of Rare-Gas Dimers by Positron Impact

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Positron scattering by the Argon dimer (Ar_2) is studied for very low incident energies using the zero range potential (ZRP) method [1]. We considered, beyond the traditional ZRP, an alternative formulation that accounts the polarization effect of the atom [2], inspired by the modified effective range theory (MERT) [3]. The scattering calculations are reported in three levels of sophistication: the fixed nuclei, the rigid rotor, and the rovibrational approximations.

Our results show how the elastic, rotational, and rovibrational cross sections depend on the positron-atom scattering length and on molecular parameters. An analytical expression for the positron-Ar_2 scattering length is calculated. From fig. 1, we find that the inclusion of atomic polarization affects the elastic and rovibrational (00->nJ, being n the final vibrational state and J the final rotational state) cross sections. From this figure, we also find that a vibrational transition (00->10) is more likely to happen than a rotational one (00->02), due to the magnitude of the transition cross sections.

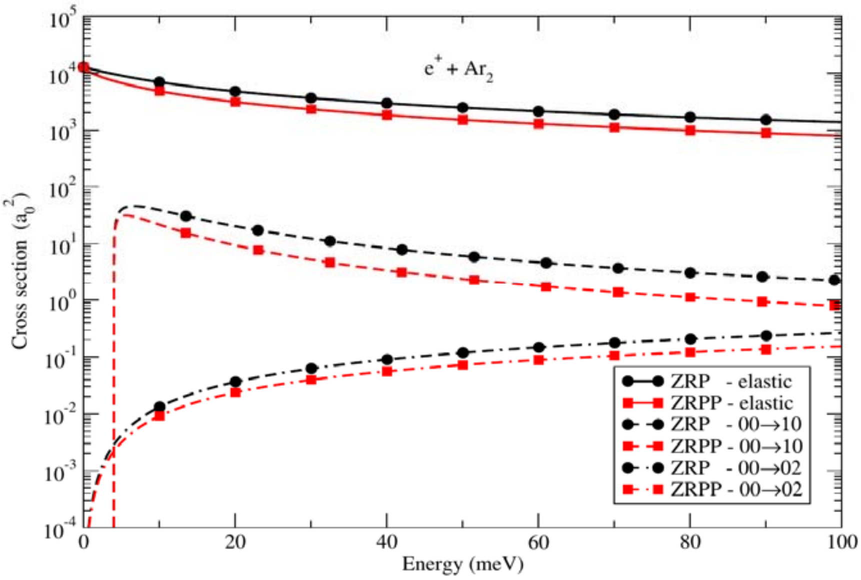

Figure 1: Elastic and rovibrational 00->nJ cross sections. Lines with circles are results provided by the traditional ZRP. Lines with squares are results accounting the polarization effects (ZRPP). Solid lines: elastic cross section. Dashed lines: 00->10 transition cross section. Dashed-dashed-dot: 00->02 transition cross section.

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Rotational Excitation of Tetrahedral Molecules by Positron/Electron Impact

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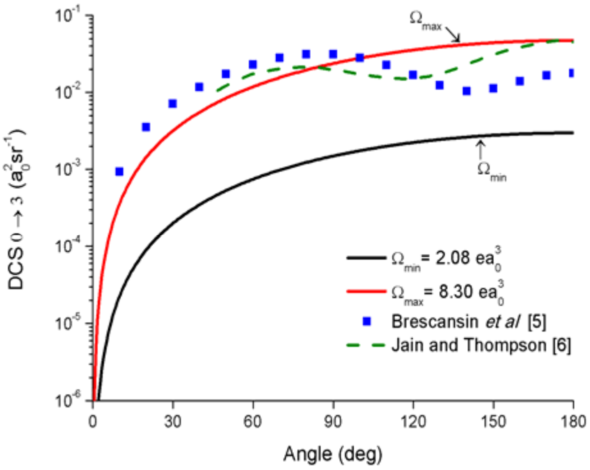
Rotational cross sections of tetrahedral molecules caused by low energy positron/electron impact are the subject of this work. In special, we developed [1] a scattering model based on the Born approximation combined with the asymptotic multipole interaction in order to compute: the rotational cross section; the rotational differential cross section; and the rotational momentum transfer cross section. The above assumptions permitted us to achieve analytical expressions for such cross sections. The reliability of the calculations lies on the fact that the positron density decreases rapidly as it penetrates the molecular field, leading to negligible contributions associated to correlation, moreover, according to symmetry (for Td systems the polarisability is isotropic), the asymptotic polarisation might not affect considerably the rotational scattering amplitude.



Our scattering model exhibits good agreement for positron rotational cross sections when compared to the *ab initio* potential calculation of Jain and Thompson [2], for both octupole $(J_f = J_i \pm 3)$ and hexadecapole $(J_f = J_i \pm 4)$ transitions. A complete analysis is given in a previous work [1]. The present figure compares differential cross sections for octupole rotational excitation of methane by electrons at 3eV. We have considered the lowest [3] (solid line with Ω_{min}) and highest [4] (solid line with Ω_{max}) octupole moments reported in literature.

Our results are compared with the *ab initio* calculation of Brescansin *et al* [5] (squares), where the scattering amplitude is generated by the Schwinger multichannel method, and with the *ab initio* potential calculation of Jain and Thompson [6] (dashed-line). Both computed the rotational transition using the adiabatic-nuclei-rotation approximation (ANR). These sophisticated calculations suggest the existence of a structure above 90 degrees, this effect might come from the short range potentials. However, the comparison exhibits fair agreement with the previous reported calculations especially in the forward scattering region. The inclusion of correlation and exchange potentials combined with a distorted wave approximation are the main elements in the improvement of the model.

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Low Energy Positron Diffusion in Krypton Gas: a Random Walk Approach

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We performed a random walk simulation to study how positrons diffuse in a gaseous media formed by krypton atoms [1]. The positrons are produced by a punctual source, having initial energy of 6.0 eV, a value below the positronium formation threshold ($E_{Ps} \sim 7.20$ eV). The elastic and the annihilation cross sections are provided as input data in order to calculate the probability of direct annihilation. The energy variation of the positron in each collision is calculated considering two models: the Sauder-Thermalization-Model (S-TM) [2], in which the energy variation does no depend on the scattering angle; and the Maxwell-Boltzmann-Thermalization-Model (MB-TM), in which the energy variation is calculated considering the scattering angle. In practice, the MB-TM is closer to a real experiment, once it is able to describe a Maxwellian velocity distribution for the positrons after a thermalization time "t_T". In both models, the scattering angle is randomly chosen.

Figure 1 presents the results considering both thermalization models for 10^5 positrons, considering gas temperature of 300 K and density of 10 amagats. The left panel shows a histogram for the energy in which the positron annihilated "E_{anni}". In the MB-TM, the positrons may annihilate with energies below the thermal energy of the media $<E_{kr}>$, what does not happen in the S-TM. This, however, does not strongly affect the annihilation radius r_{anni} distribution as the right panel suggests.

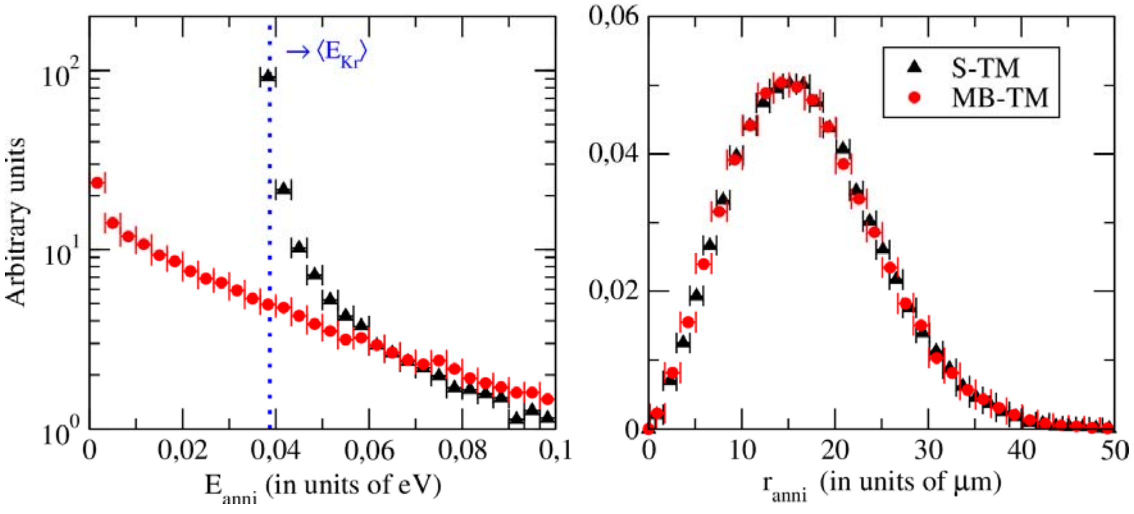

Figure 1: Left panel: histogram of the energy in which the positron annihilated within S-TM and MB-TM. Right panel: histogram of the distance from the origin where the position annihilated.

The following step to bring the simulation even closer to real systems is to consider an anisotropic model for the scattering angle by means of the differential cross sections. Such an improvement is currently being implemented.

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Deep Minima and Vortices for Positronium Formation in Positron-Hydrogen Collisions

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Using the Kohn and inverse Kohn variational methods we find two deep minima in the positronium (Ps) formation differential cross section for positron-hydrogen collisions in the energy range of the Ore gap [1]. The deep minima correspond to exact zeros in the Ps-formation scattering amplitude. We relate these zeros to vortices in the extended velocity field associated with the Ps-formation scattering amplitude. For the extended velocity field, the momentum of the incident positron and the angle of the scattered electron are allowed to vary. Each zero in the Ps-formation scattering amplitude is part of a circular ring of zeros due to azimuthal symmetry. We study the convergence of the position of each zero with respect to partial wave and we compare the position of the second deep minimum that we obtain with earlier results [2, 3].

Previously, vortices in the velocity field associated with the ionization amplitude have provided an explanation of deep minima in the differential cross sections for electron- and positron-ionization [4, 5]. The introduction of the extended velocity field enables us to show that vortices also occur for the atomic process of charge exchange.

Recently, we apply multichannel effective range theory with [6] and without the polarization potential in the Ps-p channel [7], and determine the position of the zeros in the Ps-formation scattering amplitude with each of these theories.

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Deep Minima in the TDCS for Positron-Helium Ionization Computed Using the Coulomb-Born Approximation

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A deep minima in the measurements of the triply differential cross section (TDCS) for electron-helium ionization at an incident energy of 64.6 eV [1,2] was recently interpreted in terms of a vortex in the velocity field associated with the ionization amplitude [3]. Recently, we applied the Coulomb-Born approximation to this process at the same incident energy [4] and obtained a deep minimum. We found that its position agrees reasonably well with the result of a time-dependent close-coupling calculation [5].

We apply the Coulomb-Born approximation to positron-helium ionization and find a deep minimum in the TDCS and a corresponding zero in the transition matrix element. We determine the velocity field associated with this amplitude and discover that the velocity field rotates around the position of the zero, and in the opposite direction to the velocity field for electron ionization from the same target.

S. J. W. is thankful for support from the NSF under Grant No. PHYS-1707792.

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Calculations of the Ps_2 Bound-State

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The Ps-Ps system is a fundamental four-body Coulomb system that comprises of leptons of equal mass. It has been shown that it is feasible to create a Bose-Einstein condensate of Ps [1,2].

We plan to use the inverse Kohn and Kohn variational methods to compute accurately scattering lengths, phase shifts and cross sections for elastic Ps-Ps scattering. These methods with flexible highly correlated trial functions have provided accurate results for elastic Ps-H scattering [3].

We have begun our investigation of the Ps-Ps system by determining the ground-state and binding energies of Ps_2 using the Rayleigh-Ritz variational method with different trial functions. We compare our results of the energies and the expectation values of different interparticle distances with results from other calculations [4, 5].

S. J. W. is thankful for support from the NSF under Grant No. PHYS-1707792.
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Close Coupling Calculation of Positron-N_2 Scattering Cross Sections

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The elastic, rotational, and vibrational cross sections for positron scattering from molecular nitrogen are reported within the close coupling approach [1]. A three dimensional potential energy surface was computed using coupled cluster electronic structure calculations with the finit nuclear mass correction methodology [2]. The elastic cross section shows a good agreement with previous theoretical and experimental reports [3, 4]. The rotational and vibrational cross sections were used to describe a recently reported experiment on positron cooling by a nitrogen gas at 300 K [5]. Our prediction suggest that the positron cooling rates is mainly due to vibrational excitation of the molecular gas, as opposed to a previous model which indicate that the cooling is driven by a rotational excitation mechanism [5].

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Low-Energy Scattering Properties of Ground-State and Excited-State Positronium Collisions

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Ground-state Ps collisions have been extensively studied due to growing interests in the creation of a spin-polarized Ps Bose-Einstein condensate (BEC) [1, 2]. To reach the BEC regime, experimental methods for producing Ps ensembles have been studied to achieve higher densities [3, 4]. One method for extracting information about the densities of atomic ensembles that is of recent interest for the Ps system is through the measurement of the cold-collision (clock-shift) frequency shift. One application where the clock-shift measurement has been successful in determining densities has been in the study of hydrogen ensembles to probe densities both far from and near to the BEC regime [5, 6]. In order for an experiment to probe Ps densities using the same techniques, knowledge of *s*-wave scattering lengths for ground-state excited-state atomic collisions should be well characterized, forming the motivation for this study.

The four-body Hamiltonian investigated in this study considers only the two-body Coulombic interactions between the two electrons and two positrons in the system. The spin-spin, spin-orbit and other relativistic interactions are neglected. This problem is solved using hyperspherical coordinates, which treats all fragmentation pathways on an equal footing, with the primary interest being, but not limited to, Ps bound states. The Hamiltonian is solved in a coupled electron and coupled positron spin basis in order to simplify the construction of the total wavefunction with proper anti-symmeterization requirements. Only states with zero total orbital angular momentum and positive parity are considered in this work in representing *s*-wave collisions.

From adiabatic and diabatic potential curves, *s*-wave scattering properties are investigated in the Ps(1*s*)-Ps(2*s*) elastic and inelastic channels. Spin recoupling is implemented to represent experimentally relevant spin states of each Ps atom in a two-body collision, both in coupled spin states with total spin and uncoupled spin states, specifying spin and spin projection quantum numbers for both Ps atoms. Scattering cross-sections and scattering lengths are provided for experimentally relevant uncoupled spin states. Also, an estimate of the cold-collision frequency shift per unit density for a gas of spin-polarized triplet Ps is determined.

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Positronium Formation in Forward Direction from the Fullerene

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Following the impact of positrons with matter the formation of exotic electron-positron bound-pair, the positronium (Ps), is a vital process in nature. Varieties of target systems from atoms to smaller molecules to condensed matters have been accessed by the Ps-formation spectroscopy. However, clusters and fullerenes in gas-phase have largely been one uncharted target territories, while Ps formation from such targets can yield novel effects, since solid-like delocalized electrons in nanoparticles are contained in atom-like finite spaces. Our recent studies using C_{60} targets predict ubiquitous diffraction resonances in the Ps formation [1,2].

To further motivate applications of this spectroscopy to fullerene targets as well as to access target-level- and Ps-level-differential measurements, we now compute Ps formation cross sections in the forward collision direction within a very narrow angular range of 0 – 10° which is likely measurable by the existing technologies. The electronic structure of a C_{60} molecule is described by the local-density approximation (LDA) with LB94 exchange-correlation functional [3]. The positron impact on C_{60} leading to the Ps formation is treated by the continuum distorted-wave-final-state approximation [4]. Comparisons with the angle-integrated results for the Ps(1*s*) formation following the capture from HOMO and HOMO-1 molecular levels reveal more prominent diffraction resonances in the forward angle signal. Supported by the US National Science Foundation grant PHY-1806206.

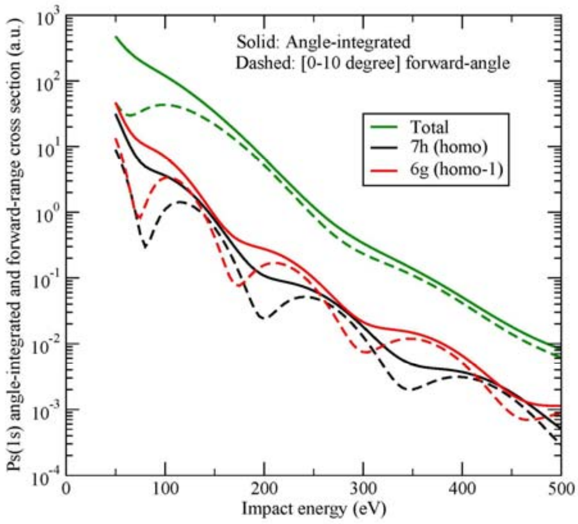

Figure 1. Ps(1*s*) formation cross sections as a function of positron impact energy in angle integrated and in 0 – 10° forward-angle range. The capture has occurred from C_{60} HOMO and HOMO-1 levels.

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Theoretical Study of Proton Transfer Reactions Induced by Positron Attachment

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The positron is the antiparticle of the electron and has the same mass and spin as an electron, but the opposite charge. When a positron collides with an electron, it annihilates with emitting gamma-rays. This unique nature is widely applied to a medical tool which probes cancers in human bodies and to a materials tool detecting voids in samples. Recently, a low-energy positron beam technique developed by Surko's group has revealed the existence of resonances associated with vibrationally excited states of positron-attached molecules. However, its dynamics has not yet been understood at an atomic level.

In this work, we discuss the influence of hydration on positron binding in amino acid, proline, from a computational viewpoint. Proline has the semirigid five-membered ring structure. This is in contrast with the fact that other amino acids generally have a large number of structural conformations. We employed the global reaction route mapping (GRRM) code developed by Maeda and Ohno to explore the low-lying structures of neutral proline·$(H_2O)_n$ (n = 0, 1, and 2) clusters [1-3]. Positron binding energies were then calculated for each low-lying equilibrium structure using the multi-component molecular orbital (MC_MO) method [4-6].

Fig. 1 displays relative energies of the equilibrium structures of proline·$(H_2O)_2$. These structures can be categorized into three groups: structures without intramolecular hydrogen-bond (non-HB), structures with intramolecular hydrogen-bond (HB), and structures with zwitterionic form (ZW), respectively. It was found that the most stable positron-attached structure with zwitterionic motif is energetically more stable than the most stable neutral cluster. This indicates that positron attachment can induce structural change. Fig. 2 shows the potential energy profiles along the intramolecular proton transfer coordinate. The positronic proton transfer process was found to be exothermic since the zwitterionic forms has a high positron affinity due to its large dipole moment [7].

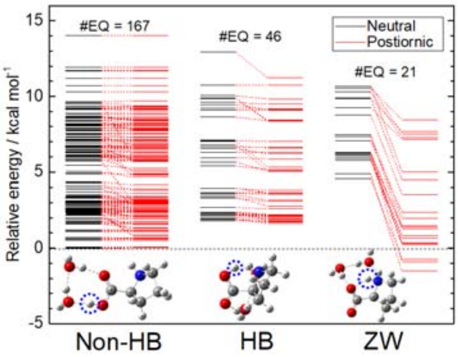

Fig. 1 Relative energy of equilibrium structures

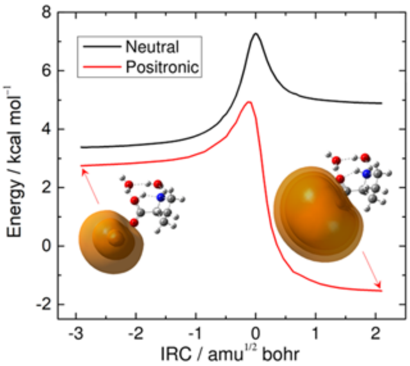

Fig. 2 Potential energy profile for proton transfer

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Positrons as a Diagnostic Tool in Plasmas and the Galaxy

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Positrons have been used for diagnostic purposes in probing material properties, such as porosity and medium composition by exposing a target to a source of positrons, in clinical diagnostics as a radio-tracer for positron emission tomography, and as a tool in the case of galactic observations, to aid understanding of the structure of the universe. While the general trends are understood and can be explained, the finer details are often lacking, and the predictive power of simulations is hindered by this.

We discuss the use of positrons as a diagnostic in two contexts using Monte Carlo transport simulations. In both contexts, we identify the energy loss in a collision as the quantity which the observations are sensitive to and call for more detailed studies of this quantity.

The first context is the use of a positron beam as a probe for properties of a plasma. While existing diagnostics, such as the use of Langmuir probes, can extract detailed information about the electron and ion energy distributions in a plasma, these probes necessarily disturb the plasma. On the other hand, a positron beam would only negligibly influence the plasma, as the number of positrons is small compared with the density of the gas. Our preliminary results have shown that positrons are sensitive to spatial differences in the plasma, and so might be useful as a selective probe of the plasma geometry in a chamber.

The second context [1] is a surrogate model for positron transport in the galaxy. We have proposed a benchmark to capture the essential features of a cross section model, using analytical forms for the cross sections. We vary the energy-sharing ratio in ionisation collisions and observe significant differences in the observables that are relevant to interpretation of astronomical observations.

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Positronium Manipulation for Antihydrogen Production

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The AEgIS collaboration (Antihydrogen Experiment: gravity, Interferometry, Spectroscopy) is aiming at testing the Weak Equivalence Principle (WEP) on neutral antimatter. The WEP states that everything massive falls at the same rate under gravity. A cold beam of pulsed antihydrogen (Hbar) sent through a moiré deflectometer is the scheme considered to measure the free fall of Hbar in the Earth's gravitational field.

In AEgIS, Hbar can be produced in a pulsed way utilizing the charge exchange reaction [1]. The implementation of this scheme involves producing a cloud of positronium atoms (Ps, the bound state of an electron and a positron) by implanting a 20 nanoseconds bunch of positrons into a nanochannel silicon target [2]. The Ps atoms are excited to a Rydberg state (an excited electronic state of high principal quantum number) through a two photon resonant transitions. Two laser pulses are used, one in the UV range to excite Ps atoms from the ground state to n=3 and a second one in the mid infrared to excite the transition between n=3 and the Rydberg state [3-4]. After free flight, the Rydberg Ps atoms reach a plasma of antiprotons kept into a Penning trap made of a 1T magnetic field and circular electrodes. Collisions between Rydberg Ps atoms and antiprotons can lead to the formation of Hbar atoms.

We report on recent progress inside the AEgIS experiment. We will focus on the development of a recent technique for quick diagnostic of Ps excitation and velocimetry using two photon resonant ionization and an MCP for imaging the photopositrons trapped on their cyclotron motion after ionization. This background free technique allows for both spatial and temporal resolution in imaging the Ps cloud properties. This efficient scheme offers the possibility to regularly check the status of Ps production during Hbar production run.

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Polarization in the Production of the Antihydrogen Ion

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We provide estimates of both the cross section and rate coefficient for the stimulated attachment of a second positron to create the ion for which the polarization of the initial state is taken into account. Building on prior work [1,2], we show how to analytically integrate the resulting six-dimensional, three body integrals, which result may be used for Hylleraas final-state wave functions with arbitrary powers, or wave functions composed of explicitly correlated exponentials of the kind introduced by Thakkar and Smith [3], a 200-term version of which we use. We extend Bhatia's [4] polarization results down to the low temperatures required for the GBAR collaboration's studies of the gravitational interaction of the anti-atom [5].

The two-electron polarization [6] cross-term is of intrinsic interest because it has every appearance of being singular at the origin, but non-singular when integrated numerically. We show that conventional approaches [7] lead to a final integral with two singular terms that may be made to cancel in lowest order. But higher-order terms in such approaches defy analytical integration.

We use two Gaussian transforms [8] to bypass this blockage to yield a fully analytic result. Even in this method one avoids the ultimately singular form only by integrating out the radial integrals before solving the second Gaussian integral. The aforementioned defiant integrals are thereby given analytic form.

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Status of the GBAR Experiment at CERN

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The aim of the GBAR experiment is direct measurement of the gravitational acceleration of the simplest anti-atom, the antihydrogen. Free fall of antihydrogen atoms, created by photodetachment from extremely cold positively charged ions will be observed to determine the acceleration. Use of charged ions allows for cooling the atoms to the extremely low temperature needed for precise measurements. The anti-ions are created in two consecutive reactions in a dense positronium cloud, which is generated by an intense positron pulse in a small cavity covered by mesoporous silica. A low energy (9 MeV) linear electron accelerator is used to produce positrons which are then cooled in a buffer gas trap and accumulated in a high field Penning-Malmberg trap. Antiprotons of 100 keV kinetic energy are supplied by the new ELENA facility at the Antiproton Decelerator at CERN. They are further slowed down by a pulsed decelerator. A high field antiproton trap will be added in a later phase of the experiment. A proton source is available to study the matter equivalent of the two key reactions. A laser system has been set up to excite positronium to 3D state in order to increase the production cross section. The positron and antiproton beamlines and the reaction chamber have been recently installed in the experimental area at CERN. The positron beamline is functional and the experiment received antiproton pulses albeit not yet with the expected quality and precision. We present the setup and discuss the performance of the positron line.

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Hyperfine Resonance of Positronium Atoms Using a Static Periodic Magnetic Field

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A positronium (Ps) atom has a ground-state hyperfine structure which is split into singlet and triplet spin states, called para-Ps and ortho-Ps, respectively. The transition energy is 8.4×10^{-4} eV (203 GHz), in the THz frequency domain. Usually the resonance of the hyperfine structure was measured using microwaves.

There is an another type of technique for the measurement of atomic resonances. When an atomic beam passes through a static periodic field, the atoms feel an oscillating field with a frequency $f=v/a$, where a is the period length of the field and v the atomic velocity. If f coincides with the transition frequency, a Motion Induced Resonance (MIR) occurs [1]. This was applied to atomic resonances using a periodic magnetic structure. Such “magnetic” resonance was only observed for the Zeeman sub-levels of Rb atoms at around 100 kHz.

Recently we succeeded in producing an energy-variable ortho-Ps beam from 0.2 to 3.3 keV [2]. We used this Ps beam and the MIR method for the observation of the hyperfine resonance of Ps. This is the first demonstration of this technique for a system including an antiparticle, for a purely leptonic system, and in the THz frequency domain. We developed a multi-layered transmission magnetic grating [3] realizing a strong magnetic field amplitude of around 0.15 T and 10% resolution as shown in Fig. 1(a). Ortho-Ps atoms pass through the periodic magnetic structure and are counted by a detector. At the resonance frequency, ortho-Ps atoms transition to para-Ps atoms which annihilate immediately and, hence, are not detected. Therefore, by counting the number of Ps atoms as a function of the velocity, we may observe the resonance signal. Figure 1(b) shows the preliminary analysis of the experimental results. The details will be presented at the conference.

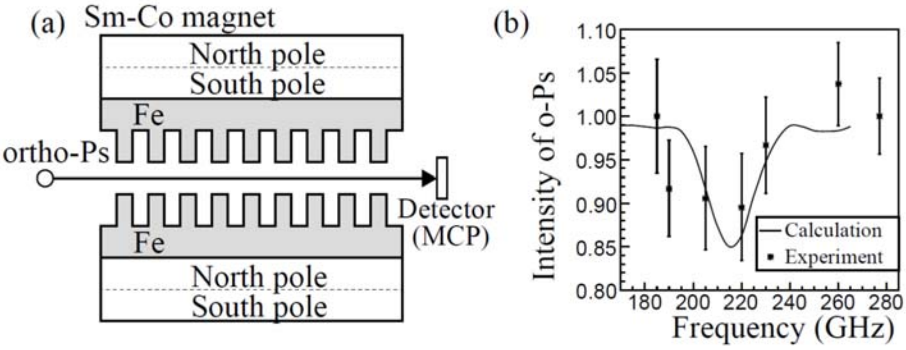

Fig. 1 (a) Conceptual drawing of the grating. (b) Resonance shape.

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Coordinate-Space Method for Calculation of Ps-formation Matrix Elements and its Application to Positron Scattering on Hydrogen Negative Ion

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Positron has been a subject of many studies due to it being an antimatter particle and having various practical applications. One of the main challenges for theoretical studies of positron collisions is calculation of rearrangement (Ps-formation) matrix elements that are computationally expensive. Previous state of the art methods [1, 2] applied to the positron scattering problem were based on momentum-space transformations and involved the Coulomb singularity that required special numerical techniques. As a result, application of the momentum-space based method to more complex and/or charged targets was quite challenging [3].

We have recently developed a new method [4] of calculating Ps-formation matrix elements within the convergent close-coupling (CCC) approach. In this report, we present details of the method, test against previous benchmark calculations and then apply to e^+-H^- scattering to obtain electron-loss, Ps-formation and electron-detachment cross sections. The CCC method has been applied to this scattering problem within the single- and two-center approaches. Figure 1 presents electron-loss (sum of Ps formation and electron detachment) cross section calculated within the single- and two-center methods. Agreement of the two results above the electron-detachment threshold confirms internal consistency of the method.

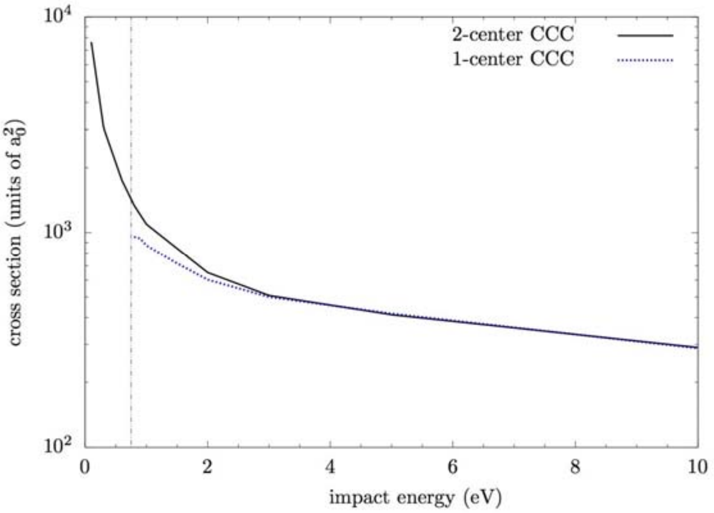

Figure 1. Comparison of single- and two-center results for electron-loss cross sections. The vertical line is the electron-detachment threshold of the H−.

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Coincidence Electron Ionisation Mass Spectrometry: Precursor-Specific Relative Ionisation Cross Sections

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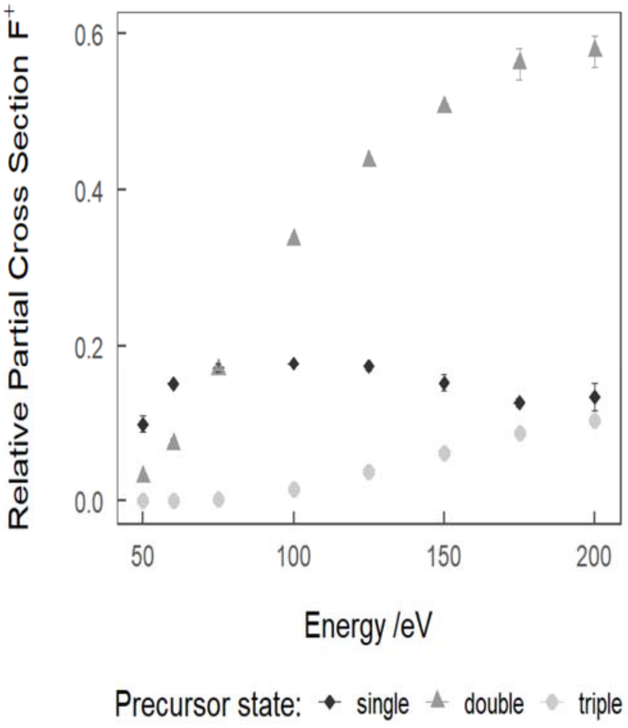
Many electron transport codes include ionisation cross sections, but they often do not account for effects of multiple-ionisation events [1], [2]. Coincidence measurements of cations produced in electron-molecule collisions provide cross-sectional datasets of ionisation cross-sections. These datasets are useful in particle transport modelling [3], nanodosimetry[2], astrochemical modelling[4], and anywhere electrons are expected to encounter free molecules. This submission describes a well-established experimental set-up at the UCL Chemistry Department which can record partial and precursor-specific ionisation cross sections. Representative datasets are reported for the molecules PF3, NH3, and Pyrimidine.



Precursor specific relative ionisation cross sections for the production of F+ from PF3 via single, double, or triple electron ionisation processes.

The apparatus, based on a time-of-flight mass spectrometer, generates relative partial ionisation cross sections, as a function of ionising electron energy, for each product ion (e.g. F+ from PF3) detected following the electron-molecule collision, as for many standard mass spectrometry experiments. However, additionally, our apparatus detects, in coincidence, pairs or triads of ions arising from individual double and triple ionization events. Detecting these ions in coincidence provides the data to generate precursor specific relative ionisation cross sections. These data reveal the contribution to the individual ion yields from single and multiple ionisation. Such cross sections indicate multiple ionisation often contributes significantly to the product ion yield above 50 eV.

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Methods for Reducing the Dimensions of Many-Body Integrals in Calculations of Low-Energy Antihydrogen Rearrangement Collisions

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Methods are devised for eliminating a variable from a three dimensional integral over a cube, in cases when integration with respect to this variable can be carried out analytically. This is done for various variable transformations and is applied to leptonic rearrangement processes, such as formation of Ps and Ps^- in antihydrogen collisions with systems such as He or H_2, which occur in the trapping of low-energy antihydrogen (see, for example, [1]),

With different coordinate systems appropriate for the initial and final stages of the interaction, in calculations where leptonic contributions to collision *S*- or *T*-matrix elements are calculated as volume integrals after detailed wavefunction calculations for the distinct arrangements, these integrals are calculated as dense-mesh brute-force multidimensional (9 for 3 leptons) numerical integrals. The system symmetry may allow 1 or more dimensions to be treated analytically following rearrangement of certain coordinates and the order of integration. This increases the accuracy of the calculation and saves significant computation time, especially important when the integral is calculated in several ways to check accuracy of finite long-distance limits and representation of arrangements in ‘unsympathetic’ coordinates. Initial coordinates could be those of the 3 leptons, or the centre of mass of e^+e^- (for Ps) or of all 3 leptons (for Ps^-) plus either a positron and an electron or 2 electrons.

The leptonic azimuthal angle coordinates are the Cartesian coordinates of the cube. The form and symmetry of the combined functions of these coordinates in the various wavefunctions determine the allowed transformations which can eliminate a variable: we present examples. Integration of various analytic test integrands with respect to the Cartesian coordinates gives rise to expressions involving binomial coefficients (combinations), which can be equated to corresponding results obtained using the transformed sets of 2 variables, producing relations between the combinations. The relations can be proved independently (see, for example, [2]), and give checks on the analytical procedures used to evaluate the integrals by coordinate transformation. Incorporating these test integrands into the full integral programs allows preliminary checks on the numerical procedures and coding used to evaluate the application integrals.

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Inelastic Resonant Scattering of Positronium by (Anti)hydrogen Atom

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Positronium (Ps) scattering by an atomic target has been one of the intriguing subjects in positron physics [1]. Recent development of Ps beam [2] provides strong tools for future precise studies on Ps-atom scattering. Ps scattering by a hydrogen atom (H) involves fundamental aspects of Ps-atom collisions. Besides, a rearrangement scattering of Ps by an antihydrogen atom ($\overline{\mathrm{H}}$), a charge-conjugated system of Ps-H, has been featured recently as a promising scheme to produce antihydrogen positive ion ($\overline{\mathrm{H}}^+$) [3]. The $\overline{\mathrm{H}}^+$ ions are expected to be useful intermediates for preparation of ultra-cold antihydrogen atoms, which can be a good probe of gravity between matter and antimatter.

This work investigates slow inelastic scattering of Ps-H ($\overline{\mathrm{H}}$) via resonance state. Ps excitation occurs when the collision energy between Ps and H, E_{col}, exceeds 5.10 eV, and a rearrangement reaction channel, $\mathrm{Ps} + \mathrm{H} \to \mathrm{H}^- + \mathrm{e}^+$, opens for $E_{\mathrm{col}} > 6.06$ eV. Between these thresholds, it has been predicted that a series of resonance states converging to $\mathrm{H}^- + \mathrm{e}^+$ dissociation threshold appears. These resonance states are considered as Rydberg states between H^- and e^+, and have three decay branches into H + Ps (1s/2s/2p). While their energies and total lifetimes have been calculated by a complex scaling method [4], information on their decay branches is limited.

In order to investigate the partial widths (partial decay rates) of these resonance states, we employ a four-body coupled rearrangement channel method [5] on H + Ps inelastic resonant scattering. In this framework, a total wavefunction Ψ is described as $\Psi = \sum_c \psi_c + \sum_\upsilon a_\upsilon \Phi_\upsilon$, where ψ_c satisfies rigorous boundary conditions of the initial/final scattering states and the latter sum with constants a_υ represents intermediate states of the scattering. The intermediate state Φ_υ describes four-body correlation during the scattering and is written in terms of finite-range functions using a Gaussian expansion method [6]. The 4-body Schrödinger equation, $(H - E)\Psi = 0$, is converted into coupled integro-differential equations, and is solved by a finite difference method. Amplitude of ψ_c at large distance gives S-matrix elements and partial cross sections. Partial widths of resonance states are extracted from the behaviour of partial cross sections around resonance energy.

We report that resonance states decay predominantly into H + Ps (1s) and decay branches into H + Ps (2s/2p) are less probable. Accuracy of our calculation is examined by near-threshold behaviour of the partial cross sections, satisfaction of detailed-balance in S-matrix, and conservation of probability current.

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Progress Towards a Pulsed Positronium Beam

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The Positronium (Ps) atom is the short-lived bound state of an electron and a positron. One way of producing an energy tuneable Ps beams is via charge exchange with atomic or molecular gases, with the positron beams used in the production of Ps beams are typically derived from a radioisotope positron source (β^+ emitter, ^{22}Na) and a rare gas positron moderator [1]. In some systems, a remoderation stage has been used which provides a time tagging mechanism with high temporal resolution [2]. To date, many atomic and molecular gases have been used to produce Ps beams over a range of energies ($3 < E_{Ps} < 500$ eV) [3].

A large body of Ps-atom scattering work has been conducted using typical Ps beams. The most striking result has been the observation that the Ps atom scatters like an equivelocity electron [4], a result which has been explained using the impulse approximation [5]. Ps scattering from molecules has hinted at features corresponding to the excitation of temporary negative ion states of the host molecule [6].

At the Australian National University, we are developing a new Ps beam system based on a Surko-style trap and beam system [7]. This buffer gas trap allows positrons to formed into a pulsed beam, with well defined energy, before being used to produce an atomic Ps beam via charge exchange. One advantage to this scheme is the superior energy resolution provided by the Surko-style buffer gas trap system, compared to a typical moderated positron source. In this talk, we will present the latest progress towards a new, high energy resolution, pulsed Ps beam system for investigation of positronium interactions with a range of atomic and molecular targets.

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Ab Initio Study of the Effect of Molecular Vibrations on the Positron-Binding to Polyatomic Molecules

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The positron, which is the anti-particle of the electron, is now widely used in both scientific and technological areas. The detail mechanism of such processes, however, is still unclear in the molecular level. A positron affinity (PA) value, which is a binding energy of a positron to an atom or molecule, has now been experimentally measured by Surko and co-workers for many molecular species such as acetaldehyde, acetone, and acetonitrile molecules [1], based on the vibrational Feshbach resonance by incident low-energy positrons. Thus, in order to elucidate the mechanism of the positron binding to molecules, the theoretical analysis including the effect of molecular vibrations is indispensable. In this study, we will show the effect of molecular vibrations on PA values, based on ab initio multi-component quantum Monte Carlo (QMC) [2] and molecular orbital (MCMO) [3] methods for the electronic and positronic wave functions simultaneously, and the anharmonic vibrational quantum Monte Carlo (QMC) method [4].

In order to analyze the PA value including the effect of molecular vibrations, we introduced vibrational averaged PA (PA_ν) defined by the following equation:

$$\mathrm{PA}_\nu \equiv \frac{\int \mathrm{PA}^{[X]}(\boldsymbol{Q})|\Psi_\nu(\boldsymbol{Q})|^2 \mathrm{d}\boldsymbol{Q}}{\int |\Psi_\nu(\boldsymbol{Q})|^2 \mathrm{d}\boldsymbol{Q}},$$

where $\boldsymbol{Q}$ is a set of vibrational coordinates and Ψ_ν is the vibrational wave function of the ν-th vibrational excited state. The $\mathrm{PA}^{[X]}(\boldsymbol{Q})$ is the vertical PA value at the molecular geometry $\boldsymbol{Q}$, defined by the total energy difference of the parent molecule (X) and its positron attached system ($[X; \mathrm{e}^+]$) as $\mathrm{PA}^{[X]}(\boldsymbol{Q}) \equiv E^{[X]}(\boldsymbol{Q}) - E^{[X;\mathrm{e}^+]}(\boldsymbol{Q})$. In this study, $E^{[X;\mathrm{e}^+]}(\boldsymbol{Q})$ and $\Psi_\nu(\boldsymbol{Q})$ were calculated with configuration interaction level of MCMO theory [3] and vibrational QMC method [4], respectively.

In the case of formaldehyde (CH_2O) molecule, the vertical PA value at the equilibrium position is predicted as +25(3) meV with QMC calculation. Applying the anharmonic vibrational analysis, the vibrational excitation of the C=O stretching mode enhances the PA value, whereas the excitation of CH_2 rocking mode deenhances it. We confirmed that such PA variations arise from the change in both permanent dipole moment and dipole-polarizability at each vibrational excited state. We will show some results of other larger molecules.

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Vertical Detachment Energies of Solvated Positronium

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Synopsis We report a theoretical study of vertical detachment energies for positronium in water, using classical Monte Carlo statistical mechanics simulations and quantum mechanical calculations with the Any Particle Molecular Orbital (APMO) through a QM/MM methods.

In the last decades the interest in the physics and chemistry of positronic systems has increased. The advance in the techniques of production and manipulation of positrons has allowed important experimental results in the research on positronium (Ps) atoms at low energies [1], and simulations of positron slowing down in water [2, 3] suggests the occurrence of thermalized solvated Ps atoms along the positron tracks..

We developed a force field (FF) for Ps-water interactions, which allows for Monte Carlo (MC) simulations of the solvated Ps at thermodynamical equilibrium, carried out with the DICE code [4]. The FF was built from precise calculations for the dispersion coefficient of the Ps-O interaction [5], and models for determining these coefficients [6]. We also assumed the repulsive part of the FF to be dominated by the electron-oxygen interaction, as usual in models for Ps annihilation in polymers [7].

Stastically uncorrelated Ps-solvent configurations, representative of the NPT ensemble, were generated from the MC simulations. Subsequently, we performed quantum mechanical calculations for the Ps-solvent configurations employing the APMO method implemented in the LOWDIN code [8]. The calculations focused on the energies of the elecronic and positronic singly occupied orbitals, which allow for estimates of the vertical detachment energies of the Ps atoms.

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Positronium Total Cross Sections

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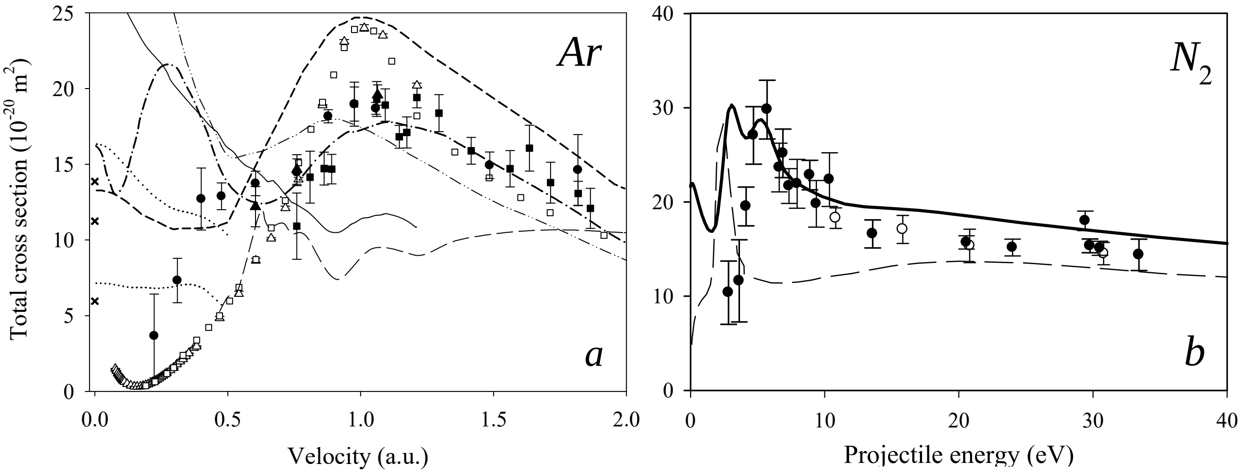
In recent years, investigations of Ps scattering at intermediate velocities have revealed that the Ps atom scatters from atoms and molecules with a similar total cross section to that of a bare electron [1], even near velocities at which resonances and interference effects occur for the electron [2,3,4] (Figure 1). Current investigations have extended measurements for Ps collisions with Ne, Kr and Xe and will be presented at the conference and compared with recent theories [e.g. 5-10]. Analysis based on the hypothesis that Ps is strongly polarised in collision with atoms and molecules will also be discussed [4].



Left, figure 1a: Ar total cross sections. ●,■,▲, Ps; △, □, electrons, as in [2]; —··—, [5]; —·—, [6]; ·····, [8]; - - - -, [9]; other lines, ×, theory as in [2]. Right, figure 1b: example of resonances in N_2 total cross sections. ●,○, Ps; — — —, electron measurements as in, [4]; —, theory [10].

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Absolute Differential Positronium-Formation Cross Sections From The Inert Atoms

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Absolute differential cross sections for ground-state positronium formation near zero degrees have been measured using the positronium beamline at UCL [1] from Ne, Ar, Kr and Xe targets [2], expanding and complementing previous work with Ar, He, H_2 and CO_2 [3]. The ratios of the differential to integral positronium formation cross-sections for each target will also be presented. These provide a measure of the degree of forward collimation of the positronium production process as a function of energy. Examples are shown in figure 1 for Ar. In addition, trends among targets have been observed consistent with the statistical description of inelastic processes [4] and will be discussed at the conference.

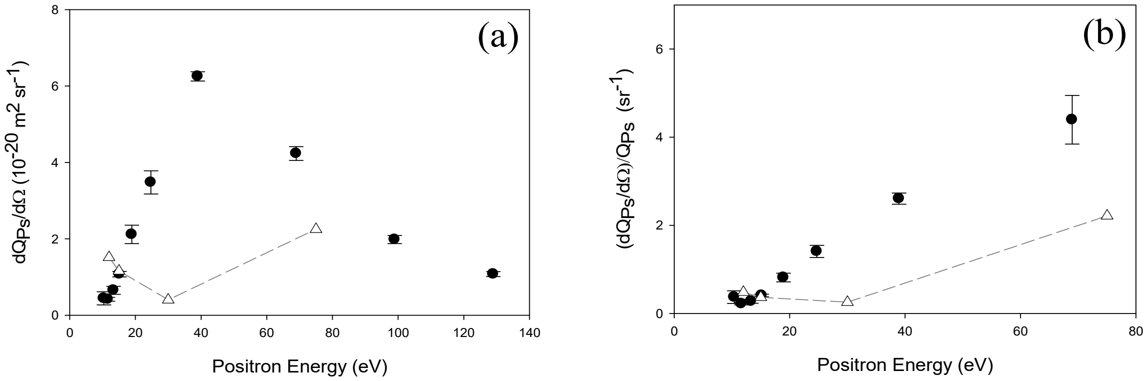

Figure 1. (a) Differential Ps formation cross section and (b) forward collimation for Ar near zero degrees [3]. Also shown are the truncated coupled-static calculation of McAlinden and Walters (triangles) [5] and a dashed line to guide the eye.

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The Role of Different Inelastic Processes in Thermalization of Positrons in Penning-Malmberg-Surko Trap at a Reduced Background Temperature

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In this paper we analyze the role of inelastic processes in positron thermalization, in a standard three stage Penning-Malmberg-Surko trap (buffer gas trap). A Monte Carlo (MC) Model of such a gas filled trap has been developed [1] based on a well-tested MC model for electrons. Previously a MC model was used to follow the thermalization of positrons in different background gases and in the gas filled traps [2, 3]. Natisin et al. have simulated thermalization by using assumed Maxwellian distributions to gas cooled down to the liquid nitrogen temperature [4]. In this paper we focus on sampling of positron energy distribution functions (PEDF) and also on the role of rotational excitation that was shown to be inefficient in case of thermalization to 300 K. Simulations were conducted at constant background gas temperatures of 300 K and 77.2 K throughout the entire period and also with a transition from the room temperature to 77.2 K at the time t_0. It was found that rotational excitation of N_2 contributes little above the room temperature but becomes the dominant process in thermalization to 77.2 K when mean energy drops below 20 meV.

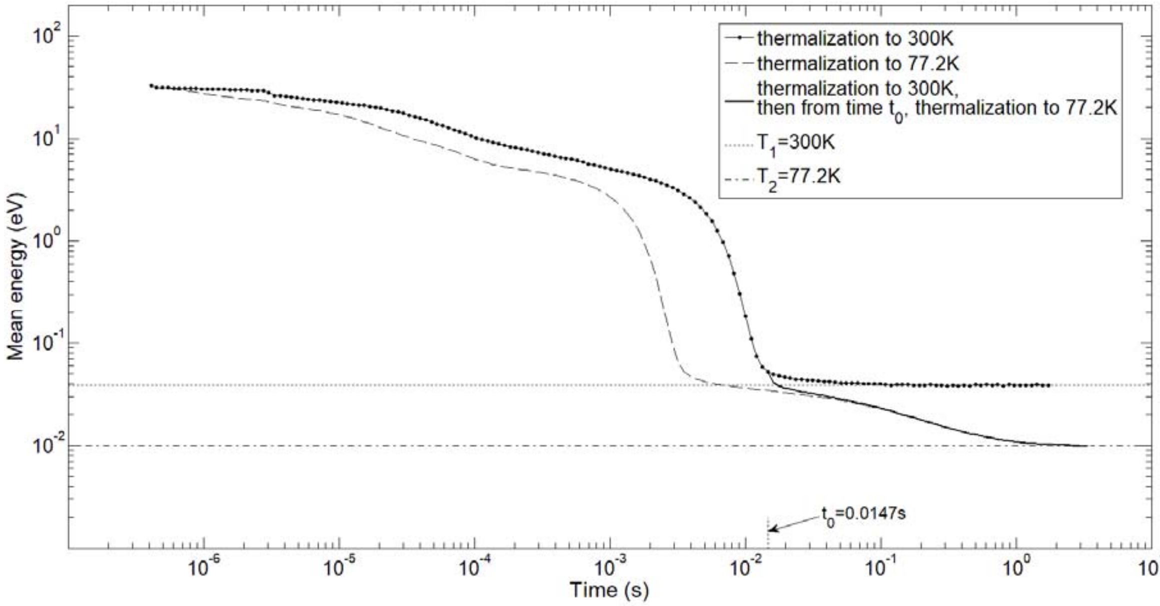

Figure 1. Mean energy in the third segment as a function of time for thermalization to 300 K, 77.2 K, and a stepwise process with transition from 300 K to 77.2 K at the moment t_0. We also show energies corresponding to the two temperatures as the horizontal lines.

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Positron Accelerator for Positronium - Cold Ion Scattering Experiments

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Positron trajectories through an accelerator, designed for positronium (Ps) production via implantation into mesoporous silica (SiO_2), were simulated in preparation for scattering experiments involving Ps and laser cooled ions in an RF-trap[1]. This would allow for high implantation depths into the SiO_2 sample with a low local electric field. The design consists of a single electrode to which an electric potential is applied, while positrons from a two-stage positron accumulator[2] are within the device.

Simulations (run on Simion 8.0.8) used a positron cloud of 10^4 particles with a Gaussian energy distribution of 26.68 eV with standard deviation 0.18 eV and three-dimensional Gaussian spatial distribution corresponding to 11 ns length and 1.5 mm radius to match obtained experimental data. The simulated positron cloud is accelerated by an electrode of length, inner diameter and outer diameter of 130 mm, 26 mm and 28 mm respectively, to which a potential of -2.0 kV is applied with a 20 ns rise time. Characterisation of the simulated particle cloud will be discussed with respect to trigger delay time of accelerator electrode. At optimum efficiency 93.21 ± 0.01 % of positrons were accelerated to 2021.4 ± 0.3 eV with a similar time width to the input (11.18 ± 0.19 ns). Progress towards experimental realisation of the proposal in [1] will be discussed.

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New Measurements of Positron Annihilation on Molecules*

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Experiments have shown that low-energy (sub eV) annihilation spectra of positrons on molecules are typically dominated by relatively sharp features that have been identified as vibrational Feshbach resonances (VFR) involving fundamental modes [1]. Further, in most molecules there is a broad spectrum of enhanced annihilation between the fundamentals, in the region of combination and overtone vibrational modes, where the density of modes is typically too high to identify discrete modes [2]. Ultimately, the experimental resolution of the spectrum is dependent on the energy resolution of the positron beam. Over the last several years, we have made a number of advancements in understanding the factors limiting the energy resolution of trapped based positron beams [3].

Several experiments will be described, including new measurements of positron binding energies for several alkane molecules with chlorine or oxygen substitutions. Also, annihilation spectra are compared for rings vs chains using a room temperature buffer gas trap beam with slightly improved resolution that reveals anomalous broadening of the VFR structure in the ring geometry. We will describe the status of our cryogenic buffer gas trap, which has the capability to enhance the energy resolution by a factor of five [4]. Lastly, we will also discuss the possibility of clarifying the role of combination and overtone modes in the broad background spectrum [5].

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Effects of Magnetic Non-adiabaticity and Measurement of the Energy Distribution of a Solid Neon Moderated Positron Beam*

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High quality, trap-based positron beams typically operate in the regime in which particle transport is adiabatic. In this regime, the quantity ($E_\perp/B$) is a so-called adiabatic invariant (AI), where $E_\perp$ is the energy in cyclotron motion in the direction perpendicular to magnetic field (B). Adiabaticity requires the parameter $\gamma = (2\pi v_{||}/\omega_c)\ (1/B)(dB/dz) < 1$, where ω_c is the cyclotron frequency and $v_{||}$ is the parallel positron velocity [1].

Discussed here is a positron beam from a ^{22}Na source and a cone-shaped solid neon moderator. For all beam transport energies ≤ 100 eV, invariance holds quite well for the beam from the buffer gas trap (BGT) to the test-gas cell [2]. However, upstream of the BGT, breaking of AI is observed for transport energies ≥ 60 eV. This has been identified to be due to the low magnetic field and strong gradients at front end of the beam tube separating the solid-Ne moderator source stage and the BGT. The principle effect of the breaking is that it scrambles the parallel ($E_{||}$) and perpendicular energy ($E_\perp$) beam distributions, leading to broadening of both, while the total particle energy is conserved. Experimental results for a fixed source magnetic field show increases in mean perpendicular energy with increased moderator bias in the range 60 – 80 V, in the regime where $\gamma \geq 1$.

The result of these studies is that the mean total energy of the positrons from the solid neon moderator could be reliably measured with the result that, in the adiabatic regime, mean $E_\perp \sim 0.8$ eV, mean $E_{||} \sim 1.6$ eV (relative to the moderator bias), and parallel energy spread FWHM ~ 2 eV. Measurement of the spatial distribution of positrons from the cone-shaped surface of the neon moderator will also be discussed, as will implications of these observations for BGT-based beam systems.

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Precision Frequency Measurements with Trapped Antihydrogen

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The ALPHA (Antihydrogen Laser Physics Apparatus) Collaboration based at CERN, focuses on the production and spectroscopic investigation of antihydrogen, with the intent of determining if CPT symmetry breaking occurs between the neutral matter and antimatter counterparts. Currently to date, 2019, the lineshape of antihydrogen's 1S-2S transition has been characterised [1], with the resonance frequency measured to within ~5 kHz of the expected 2.5×10^{15} Hz hydrogen transition. This gave us a CPT invariance to a relative precision of 2×10^{-12}. Improvements in this comparison can continue with regards to testing CPT as the hydrogen transition is currently known to a precision of 10.4 Hz [2]. The ALPHA measurement is currently dominated by transition time broadening which can be reduced by cooling the antihydrogen atoms. To move towards laser cooling of antihydrogen, the 1S-2P manifold, which contains a cycling transition, was addressed with a pulsed laser and measured to be 2,466,051.7±0.12 GHz in a 1.033 T field [3]. The pulsed laser allowed the time of flight of antihydrogen atoms to be resolved on the silicon vertex detector. Simulations show that the detected time and axial distributions of the laser-induced annihilation events are sensitive to the radial temperature of the trapped antihydrogen which facilitates the diagnosis of laser cooling attempts. These attempts combined with an upgraded frequency reference which exceeds a fractional precision of 8×10^{-13}, will lead to improvements in the precision of future antihydrogen frequency measurements.

Laser cooling antihydrogen would also have an utility in the new ALPHA-g experiment, which aims at measuring the gravitational acceleration of antihydrogen [4].

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Calculations of Positron Scattering, Binding and Annihilation for Atoms and Molecules Using a Gaussian Basis

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The interaction of positrons with atoms and molecules is characterised by very strong electron-positron correlation effects. For atoms and small (e.g., diatomic or triatomic) molecules, these effects are described successfully using many-body theory [1], explicitly correlated Gaussians [2], convergent close coupling [3,4], quantum Monte Carlo [5] and configuration interaction methods [6]. For larger and particularly, nonpolar molecules, no *ab initio* calculations can reproduce experimental data, e.g., the positron binding energies [7,8]. To obtain understanding and the basic features of this problem, we have recently developed an approach that uses a model correlation potential [9]. This has enabled us to reproduce accurately the positron binding to alkanes for the ground and 2nd positron bound states, and to predict the corresponding annihilation rates [10].

Here we test the method of Ref. [9] for positron scattering, annihilation and binding (where applicable) for atoms (He, Be, Mg and Ar) and make predictions for small molecules (H_2, N_2, Cl_2 and CH_4). The positron-molecule potential is written as $V(\mathbf{r}) = V_{\text{st}}(\mathbf{r}) + V_{\text{cor}}(\mathbf{r})$, where $V_{\text{st}}(\mathbf{r})$ is the electrostatic potential of the target, and $V_{\text{cor}}(\mathbf{r}) = -\sum_A (\alpha_A/2|\mathbf{r}-\mathbf{r}_A|^4)\{1-\exp[-(|\mathbf{r}-\mathbf{r}_A|/\rho_A)^6]\}$ is a model correlation potential, where the sum is over the target's constituent atoms A, with the nucleus at position $\mathbf{r}_A$ and the hybrid polarizability α_A [11]. The cutoff parameters ρ_A are taken from Ref. [12] for Be, Mg, and He; for Ar we choose it to reproduce the accurate s-wave scattering phase shift from many-body-theory calculations [1]; for C and N we use the same value as for H, while for Cl we use the same value as for Ar (due to the similar radii of these atoms). We use Gaussian basis sets to solve the Schrödinger equation for the positron using a modified version of GAMESS [13] to obtain the negative-energy bound states (where they exist). Scattering data (s-wave phase shifts and Z_{eff}) are obtained by correctly normalizing Gaussian-based positive-energy positron pseudostates. Our calculations confirm positron binding for Be and Mg, and predict it for Cl_2 (with the binding energy of ~10 meV). The scattering phase shifts and Z_{eff} are broadly in agreement with accurate calculations (where available) and/or experimental data, including large Z_{eff} values for Be, Cl_2 and CH_4, that are enhanced by weakly bound or virtual positron states.

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Positron Cloud Characterisation

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Low energy positron clouds from a two-stage buffer gas accumulator [1] have been characterised with the aim of implementing resistive cooling. Resistive cooling can be described by a Stokes's viscous drag term, which offers a more correct test of the independent particle compression model [2]. The lifetime, energy distribution, magnetron frequency and axial bounce frequency have all been determined using destructive diagnostic methods. Without the use of rotating wall electric fields, positron clouds have been held in a deep, harmonic potential well within a '3rd stage' Penning-Malmberg trap for more than 100 s.

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Positron Transport in H_2 in Electric and Magnetic Fields Crossed at Arbitrary Angles

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Using a multi term theory for solving the Boltzmann equation [1], we investigate the positron transport in H_2 in electric and magnetic fields crossed at arbitrary angles. The hierarchy resulting from the spherical harmonic decomposition of the Boltzmann equation in the hydrodynamic regime is solved numerically by representing the speed dependence of the phase-space distribution function in terms of an expansion in Sonine polynomials about a Maxwellian weighted function. Values and general trends of positron transport properties over a range of angles and field strengths are reported here. In particular, we explore the existence of two families of transport coefficients, the bulk, and the flux, which results from the explicit influence of Positronium (Ps) formation upon the transport coefficients. We also explore the validity of Tonks' theorem for positrons assuming the most general case of arbitrary field orientations where special attention is placed upon the procedure for accurate determination of momentum transfer collision frequency as a function of positron mean energy.

The second important aspect of this work concerns the validity of cross sections for positron scattering in H_2 [2,3]. For reduced electric fields greater than approximately 100 Td (1 Td = 10^{-21} Vm^2), we have noticed the existence of runaway positrons. The runaway phenomenon is a consequence of decreasing probabilities of positron interactions with neutral molecules for higher electric fields. Under these conditions, positrons gain more energy than they can lose in collisions and hence no steady-state can be reached. This raises a number of questions regarding the accuracy and completeness of the current set of cross sections. Machacek and coworkers [4] have reported the total inelastic cross section that is higher than the one used in our calculations which might be used to explain the low threshold electric field for runaway of positrons. In order to resolve this issue, for the lower energy positrons, we consider the influence of rotational excitations on positron transport. For higher energies of positrons (greater than approximately 10 eV), we investigate the following fundamental issue: What is the nature of missing processes and what are the implications of the fact that Positronium (Ps) formation is dominant over the inelastic processes for energies between 10 and 50 eV. The runaway phenomenon of positrons is investigated by a Monte Carlo simulation technique.

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Calculations of Stark Shift and Ionization Rate for Positronium in Strong Electric Fields

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We calculate the ground state energy and the ionization rate for positronim (Ps) in electric field for different field strengths and compare these quantities with the corresponding values for the hydrogen atom. The Hamiltonian describing the relative motion of such a two-particle system reads $H = p^2/2\mu - 1/r - Fz$ (in atomic units), where F is the field strength and μ is the reduced mass, which for Ps and for hydrogen takes the values 1/2 and 1, respectively. At weak fields the ground state energy E and the ionization rate w are given by the quadratic Stark shift approximation and by the Landau formula [1], which can be written in the form

$$\tilde{E} = -\frac{1}{2} - \frac{9}{4}\tilde{F}^2, \quad \tilde{w} = \frac{4}{\tilde{F}}\exp\left(-\frac{2}{3\tilde{F}}\right),$$

where

$$\tilde{E} = E/\mu, \quad \tilde{w} = w/\mu, \quad \tilde{F} = F/\mu^2$$

are the mass-scaled values for energy, ionization rate and field strength. A comparison with numerical calculations we have done (using the wave-packet propagation method and the complex-rotation method [2]) shows that these formulae fail at stronger fields, but the scaling transformations remain valid (see Figure 1). The latter gives us the ability to get accurate values for E and w for Ps either by direct numerical calculations or by scaling the corresponding numerical data for hydrogen [2].

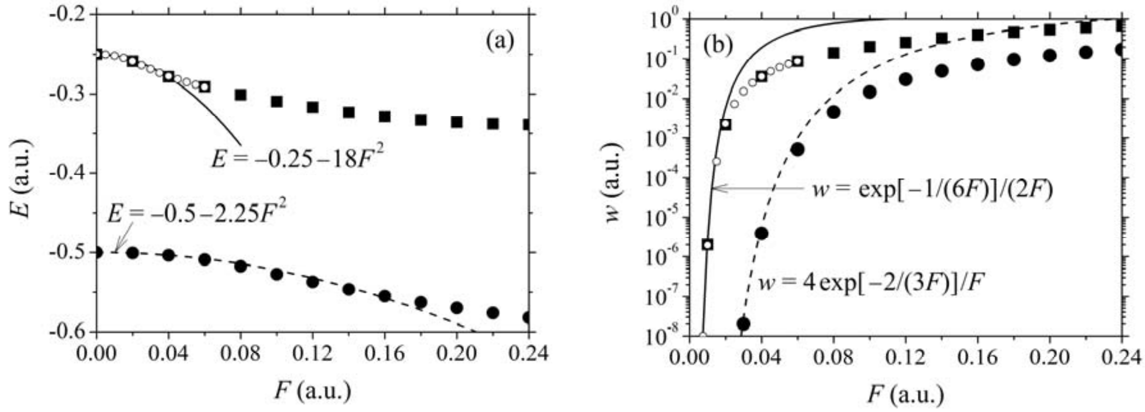

Figure 1. The ground state energy E (a) and the ionization rate w (b) for the hydrogen atom (dashed line, circles) and for positronium (full line, squares) as functions of the strength of external electric field F. The lines and symbols represent analytical (formulae) and numerical results, respectively. Open circles represent the results for Ps obtained by scaling numerical data for hydrogen.

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Dissociative Electron Attachment to MgCN

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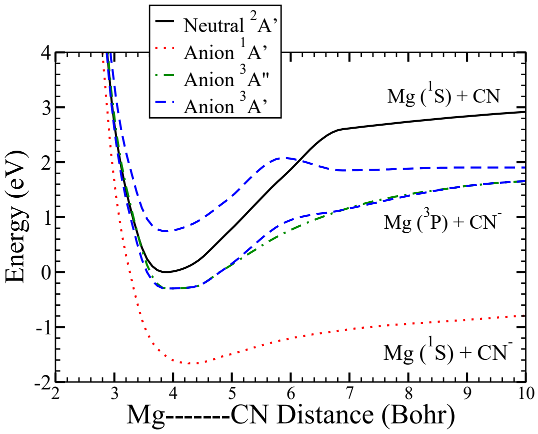
The mechanism for the formation of CN^- in circumstellar envelopes such as IRC +10216 is unclear [1]. It has been proposed that dissociative electron attachment to MgCN or MgNC, the reactions:

$$e^- + MgCN \rightarrow Mg + CN^-$$
$$e^- + MgNC \rightarrow Mg + CN^-$$

could be involved in CN^- production [2]. Both MgCN and MgNC have been observed in IRC+10216[3, 4, 5].

We have carried out a series of structure and electron scattering calculations using the Complex Kohn variational method [6] to study the positions and widths of the electronic resonant states in this system. It was found that the potential of the ground state of the anion lies below the potential of the neutral molecule for all geometries (MgCN and MgNC). There are anion states that cross the neutral, but these dissociate into the excited states of Mg.



The resonance positions and autoionization widths were calculated on a grid of Jacobi coordinates and used as input to a time-dependent treatment of the nuclear dynamics, in one-, two- and three-dimensions. The multidimensional wave equation is solved using the MultiConfiguration Time-Dependent Hartree (MCTDH) approach [7]. The cross sections for dissociative electron attachment were determined. We will discuss the results and their implications for the formation of CN^- in the circumstellar media.

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Site Selectivity In Dissociative Electron Attachment To Acetaldehyde

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Functional group dependent site selectivity in dissociative electron attachment (DEA) has provided a new avenue to control of molecular dissociation [1]. Valence excited resonances, which are highly localized in the molecule are known to be responsible for this selectivity. Such localized resonances have neutral excited states as parent states with localized valance excitations. So far, such resonances were found to result in the formation of H^- from H atoms bonded to the O, N or C atoms. Here we present the first evidence of site selectivity that is caused by the presence of these atoms at the nearest neighbour site.

We have carried out detailed measurements of momentum distribution of the H^- ions generated by DEA to acetaldehyde using velocity slice imaging technique [2]. H^- ion yield shows two peaks at 6.8eV and 9.4eV. The momentum image at the two peaks are shown in Figure 1. Based on the momentum images at various electron energies and a comparison with H^- from acetone [3], we conclude that the observed outer ring in the momentum image around 6.8 eV originates from the C-H site of the aldehyde group. The central anisotropic blob observed in the image and the broader second peak appear to have the same origin. The second peak resembles that observed in acetone and is understood to be from the methyl group present in the molecule.

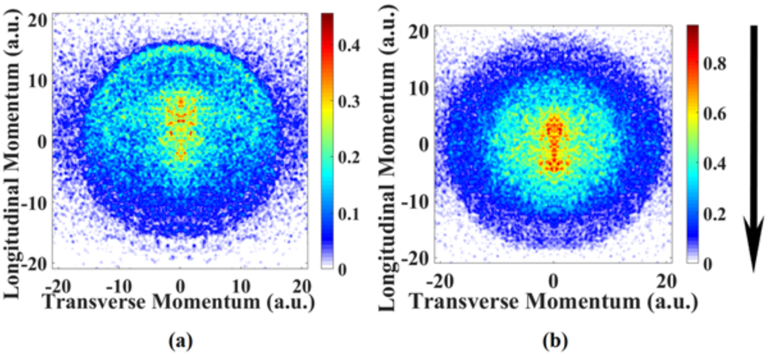

Figure 1: H^- momentum images at (a) 6.8eV and (b) 9.4eV from DEA to acetaldehyde. (Arrow indicates electron beam direction)

The formation of H^- from any organic molecule containing OH group peaks around 6.5 eV, showing O-H site selectivity. This is attributed to the lone pair excitation of the O atom that leads to the O-H bond dissociation. The present observation of H^- peaking at 6.8 eV (outer ring in momentum distribution) commensurates with a two-body break up from the aldehyde group. Similar to OH containing compounds, this dissociation appears to stem from the lone pair excitation of the O atom, which is the nearest neighbour to the aldehyde C-H site. This is the first ever report of the role of nearest neighbour atom in site selectivity of DEA.

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Functional Group Dependence in Dissociative Electron Attachment to Pyrrole

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Dissociative electron attachment (DEA) is the most efficient way to explore the structure and dynamics of excited states of molecular negative ions. More importantly, DEA has been shown to be a tool for chemical control [1, 2]. One crucial aspect of the chemical control using DEA is the functional group dependence present in this process [1, 2]. It has been shown that H^- formation from DEA to aliphatic compounds follows a pattern that depends on the functional group present and roughly mimics that shown by the prototype hydride - e.g. H^- from DEA to alcohols and amines show parallels with that from DEA to water and ammonia, respectively. This functional group dependence of DEA process leads to site selective fragmentation of N-H, C-H and O-H bonds using electron energy as a control parameter. In the case of N-H and O-H bonds, the localization of excitation is understood to be due to lone pair excitation of N or O atom. As noted above, prior studies of functional group dependent site selectivity have been largely restricted to aliphatic compounds [2]. However, in aromatic organic molecules like pyridine, pyrimidine, aniline, benzyl amine, delocalized electrons influence this site selectivity due to mixing of lone pair electrons [3]. Here we present a specific case on the effect of delocalized electrons on DEA patterns observed in pyrrole.

Pyrrole is an interesting six pi-electron heterocyclic aromatic ring molecule in which lone pair electrons of N contributes to the delocalized system of electrons of the ring. H^- from pyrrole is found to have two broad peaks at 5.5eV and at 9.5eV respectively of electron energy. Momentum image of this fragment obtained using Velocity Slice Imaging (VSI) at 5.5eV resembles that from H^- from NH_3 [4] which is consistent with the functional group dependent site selectivity in DEA. This peak is found to be absent in the n-methyl pyrrole. The VSI image at second peak, viz. at 9.5eV is quite intriguing. It has a distinguishing feature unlike that from benzene even though peak energy matches with the resonance from phenyl group [3]. We believe that this distinguishing feature might be a signature of the lone pair electrons of the N atom becoming part of delocalized pi electrons in pyrrole.

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Resonance Electron Interaction with Heterocyclic Compounds: Vibrational Feshbach Resonances and Hydrogen Atom Stripping

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Studies of dissociative electron attachment (DEA) to biologically relevant molecules representing building blocks of living matter allows us to disclose the basic mechanisms of interaction of high energy radiation with living tissues [1-3].

In the present paper we study low-energy (0-15 eV) resonance electron attachment in a series of 5-membered heterocyclic rings (isoxazole, imidazole, pyrazole, pyrrole, 1-methyl- and 2-methylimidazole) under gas-phase conditions by means of electron transmission and DEA spectroscopies.

Sharp features, with fwhm less than 0.1 eV, observed in imidazole, pyrazole and pyrrole close to 0.45 eV, i.e. quite below the energy of their lowest-lying $\pi*$ shape resonances detected at 1.90, 1.87 and 2.33 eV, respectively, are associated with formation of diffuse negative ion states bound by long-range forces. The effective range theory (ERT) calculations support this interpretation. Since the permanent dipole moments of pyrazole and pyrrole are below the supercritical (2.5 D), the polarization interaction plays an important role in formation of these states.

In addition to the general observation of cleavage of the N-H bond at incident electron energy close to 2 eV, elimination of as much as three hydrogen atoms from the molecular negative ions are detected at higher energies with the only exception of methylated imidazoles. This complex process is associated with ring opening and formation of diatomic hydrogen as one of the neutral fragments that is the only way to satisfy the energetic conditions.

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Selective Bond Excision of Nitroimidazoles in Electron Transfer Experiments

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Nitroimidazoles and derivatives have been under investigation especially because of their electron-affinic properties to be used as radiosensitisers in radiation treatments, namely in solid tumours growing in a hypoxic environment [1], and recently two new fluorine-18 labelled 2-nitroimidazole derivatives were successfully prepared to be used as potential PET radioligands for tumour imaging [2]. However, the molecular mechanisms related to the reactions involving nitroimidazoles after irradiation are not fully understood yet. Thus, its understanding means a key step for the development of new radiotherapeutic drugs and treatments.

Here we present a comprehensive investigation on charge transfer experiments yielding negative ion formation in collisions of fast neutral potassium atoms with nitroimidazole and methylated derivative molecules. The anionic fragmentation pattern shows that the decomposition of the precursor parent anion leads to single and multiple bond cleavages of the molecules, and it is slightly different when compared with DEA studies [3,4]. Selective excision of hydrogen atoms from the N_1 position in 4-nitroimidazole (4NI) is completely blocked upon methylation in 1-methyl-4-nitroimidazole (1m4NI) and 1-methyl-5-nitroimidazole (1m5NI). Additionally, only (4NI) and 2-nitroimidazole (2NI) are efficient in selectively producing neutral $OH^\bullet$ and $NO^\bullet$ radicals in contrast to (1m4NI) and (1m5NI) [5]. The present work contributes to the current need of pinpointing a class of charge transfer collisions that exhibit selective reactivity of the kind demonstrated here, extending to tailored chemical control for different applications such as tumour radiation therapy through nitroimidazole based radiosensitisation.

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High-Resolution ($e^- + H_2O$) Scattering near 0°

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A fully electrostatic beam [1] characterised by a high angular discrimination (≈ 0.7°) has been used to measure the total cross section (σ_T) of electron scattering from water vapour in the energy range (3 - 100) eV. Measurements for σ_T have previously been carried out on the same equipment for $e^+ + H_2O$ [2].

Although measurements for electron systems have been investigated since the early 20th century, discrepancies had remained among experimental and theoretical results at low energies until now e.g. [3, 4]. The new results for σ_T are presented in figure 1, together with previous experimental and theoretical determinations. The effect of forward scattering has also been probed in the angular range 0° – 3.5° and measures of the average (rotationally and vibrationally summed) differential elastic cross sections for energies ≤ 12 eV have been obtained at a scattering angle ≈ 1°. These measurements provide the first test of theoretical predictions in an angular region experimentally unexplored until now.

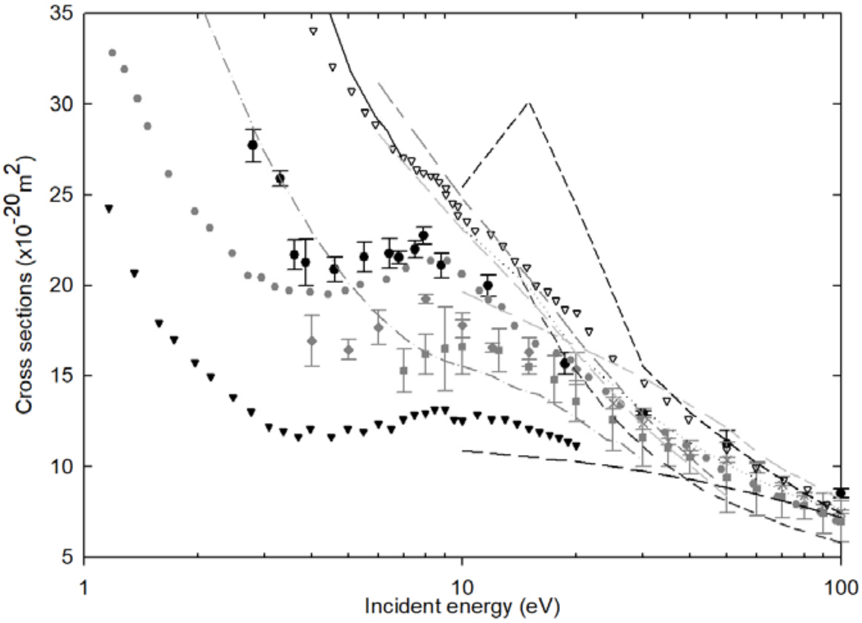

Figure 1. Cross sections for electron scattering from H_2O. Solid symbols denote direct measurements, hollow symbols denote measurements corrected for forward angle elastic scattering and lines denote theories [5].

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Collisions of Low-Energy Electrons with Halogenated Benzenes: Shape Resonances and Differential Cross Sections

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Since the pioneer work of Boudaïffa *et al*. [1] indicating that single and double strand breaks in DNA can be induced by low-energy electrons (LEEs) and, some later works showing that the dissociation process can by mediated by the formation of a resonance in specific sites of the DNA chains [2], many theoretical and experimental groups have been working on electrons interactions with molecules of biological relevance and their precursors. In particular, the characterization of resonances and their role in the dissociation processes. More recently, halogenated DNA and RNA [3] as well their precursors [4] have also gained attention because their sensitizing effect in cancer treatment by radiotherapy.

Here we will present integral, momentum transfer and differential cross sections for elastic scattering of low-energy electrons with halogenated benzenes. This is a extension of our recent work where we presented theoretical and experimental cross sections for low-energy electron interactions with chlorobenzene [5]. The halogenated benzene molecules are simple systems that can be seen as prototypes for radiosensitizers and, also present a peculiar spectrum of temporary anion states. The theoretical integral and differential cross sections were calculated with the Schwinger multichannel method implemented with pseudopotentials (SMCPP) [6] for electron impact energies up to 30 eV. Some additional electronic structure calculations will also be presented in order to properly characterize the shape resonances of halobenzenes. We will also compare the theoretical differential cross sections (DCSs) with experimental data for chlorobenzene. A discussion comparing the present results with theoretical and experimental results for benzene molecule will also be provided.

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Elastic Electron Scattering by Halocarbon Radicals in the Independent Atom Model Approach

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One of the major areas of the application of low temperature discharge physics is the plasma modelling and processing of semiconductor materials [1]. Such technology mostly uses halocarbons in the role of feedstock gases (e.g., CF_x, CF_xCl, x = 1-3) [2,3].

We calculated the differential (DCSs) and integral (ICSs) cross sections for elastic electron scattering by the CF_x (x = 1-3) and CF_2Cl radicals. The DCSs are obtained in the 7-75 eV energy range, while the ICSs are from 1 to 1000 eV. We used the independent atom model (IAM) for DCS calculations, while the simple additivity rule (IAM-AR) is used for the ICSs [4]. The optical potential (OP) method is used to calculate the atomic scattering amplitudes. The real OP for the e^- + C, F, Cl scattering consist of static, local exchange and polarization, scalar-relativistic and spin-orbit coupling potentials (RSEP-approximation) [4]. The equilibrium interatomic distances are calculated by CCSD(T)/aug-cc-pvdz *ab initio* theory.

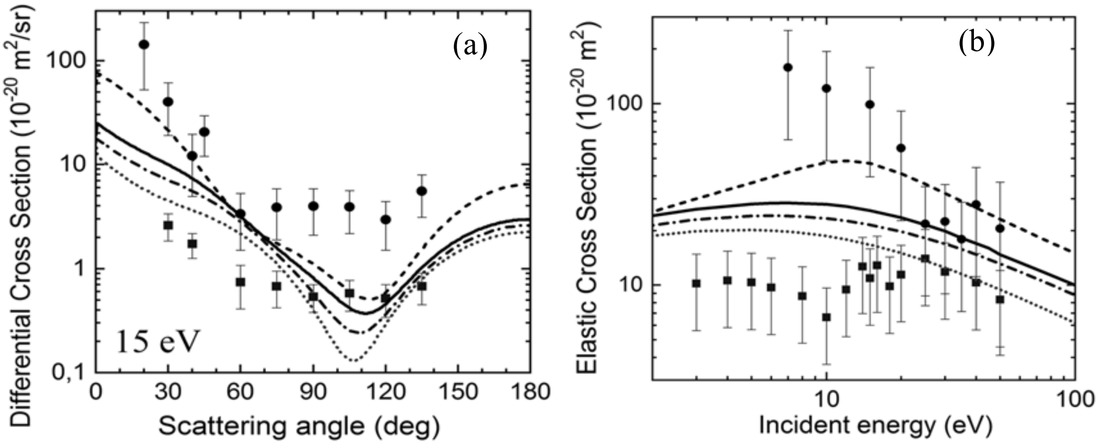

Figure 1. Cross sections of elastic electron scattering by CF_3 (solid), CF_2Cl (dash), CF_2 (dash-dot) and CF (dot) radicals calculated by RSEP theory. (a) – DCS at 15 eV (IAM); (b) – elastic ICS (IAM-AR). Experiments are for e^-+CF_2 [2] (■■■) and e^-+CF_3 [3] (●●●) scattering.

In Fig.1(a) the calculated DCSs are compared with the available experimental data for e^-+CF_2 [2] and e^-+CF_3 [3] scattering (see also [4]). The ICSs are also compared with the measured data (see Fig.1(b)). Our results show a fairly good qualitative agreement with the available experimental cross sections in general. We can see in Fig.1 the essential influence of the chlorine atom for the DCSs and ICSs of e^-+ CF_2Cl scattering as compared with the data on CF_3 and CF_2 target radicals. More detailed results will be presented at the conference.

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Ab Initio Study of Appearance Energies in Electron-Impact Dissociative Ionization Processes of Small Chalcogenide Clusters

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The processes of elastic scattering, excitation and dissociative ionization in binary collisions of low-energy electrons with a broad range of atoms and molecules are intensively studied in recent decades [1]. However, the data about the controlled low-energy electron interaction with sulphur, selenium and tellurium chalcogenide clusters are practically missing in the literature.

In order to calculate the energy characteristics of the reaction products in dissociative ionization processes, i.e. the appearance energy (E_{ap}) or the more general ionization (I) and dissociation energies (D), we performed total energy calculations by the GAMESS software package [2]. The corresponding molecular energy characteristics considered as the reaction enthalpy change, and calculated as the total energy difference of the initial and final products of the reaction [3].

The *ab initio* study of the neutral and ion fragments of S_n, Se_n, and Te_n (n=1–8) clusters was performed by means of DFT and MP2 theories. Large, aug-cc-pv$X$z -type (X=2,3) basis sets were used in the calculations. The doubly-charged positive ion fragments were also considered. A rather good quantitative agreement is found in a comparative analysis of the energy characteristics with the available experimental data from the literature.

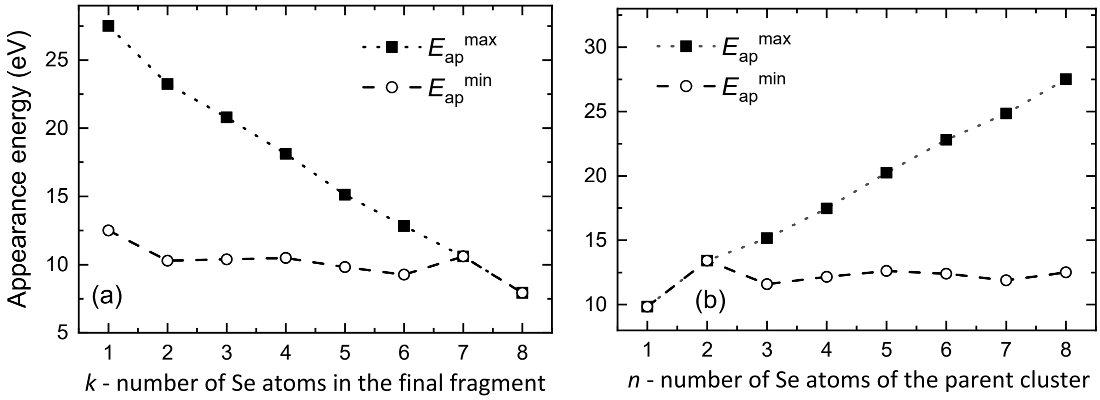

Fig. 1. Calculated minimal and maximal appearance energies of the Se_k^+ $(k \le 8)$ ion fragments from Se_8 (a) and of the Se^+ ions from Se_n parent clusters (b).

In Fig.1(a) the calculated maximal $E_{ap}[Se_k^+ - (8-k)Se/Se_8]$ and minimal $E_{ap}[Se_k^+ - Se_{8-k}/Se_8]$ appearance energies are shown for the different Se_k^+ $(k \le 8)$ fragments. Fig.1(b) shows the maximal $E_{ap}[Se^+ - (n-1)Se/Se_n]$ and minimal $E_{ap}[Se^+ - Se_{n-1}/Se_n]$ appearance energies for the Se^+ ion. At k=8 and n=1 the ionization energies of the Se_8 molecule and Se atom are used.

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Total Electron Scattering Cross Sections from Benzene

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We present total electron scattering cross sections (TCSs) from Benzene (C6H6) molecules in the (1–1000 eV) impact energy range. Experimental TCS values have been obtained with two different systems, a magnetically confined apparatus for low-intermediate impact energies (1-300 eV) and a linear electron beam transmission arrangement for intermediate-high energies (100-1000 eV). Results are compared with our independent atom model and screening corrected additivity rule with interference term (IAM-SCAR+I) theoretical approach [1] (see Figure 1).
The magnetic system [2] used for the lower energies is based on an intense axial magnetic field confinement of the electron beam with the aim of converting every scattering event into a kinetic energy loss in the forward direction. This technique increments the effect of the "missing angles" [2] and therefore measured TCSs tend to be lower than the "actual" cross section values. The magnitude of this effect has been calculated with the help of our theoretical data. The experimental set up for intermediate-high energies used an extremely good angular resolution ($<10^{-5}$sr) and enough energy resolution (<500 meV) to accurately measure (±5%) the attenuation of the electron beam even at such relatively high energies [3].

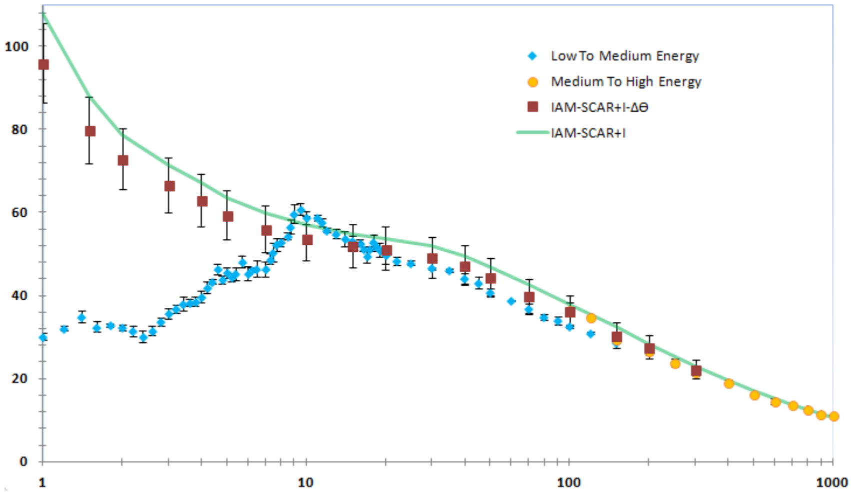

Figure 1. Present theoretical (IAM-SCAR+I) and experimental results . Calculations excluding the "missing angles" are also presented as IAM-SCAR+I-Δθ.

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Electron Induced Vibrational Excitation Cross Section and 2D Electron Energy Loss Spectra of Methyl Formate

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Studies of electron interaction with methyl formate have applications in astrochemistry because methyl formate is detected in interstellar medium such as molecular clouds, molecular comets or cores [1, 2]. Large number of secondary electrons (electrons with energy <20 eV) produced in interstellar medium due to interaction of high energy radiation with interstellar icy grains. Therefore, the understanding of secondary electron reaction with methyl formate might contribute to the development of astrochemistry. In the current work we used electron energy loss spectroscopy [3] to probe the resonances in methyl formate and identifying which vibrations have crucial role in DEA to methyl formate. The resonances in methyl formate and its decay into different vibrational modes are visualized by constructing 2D electron energy loss spectra [4] from many electron energy loss spectra recorded at different incident electron energies. The vibrational excitation cross section data of methyl formate recorded in the energy range 0 to 6 eV shows threshold effect due to long range electron-molecule interaction and π^* shape resonance centered around 2.1 eV. This π^* shape resonance is partly responsible for electron attachment dissociation of methyl formate and formation of $HCOO^-$, $COOCH_3^-$ and OCH_3^- [5].

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Symmetry Control of DEA in Pyrrole Revealed by Absolute Cross Sections and 2D Electron Energy Loss Spectroscopy

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We present the energy dependent absolute cross section for elastic scattering and vibrational excitation of pyrrole in the incident electron energy range 0 to 10 eV. Pyrrole is an aromatic organic compound having heterocyclic five membered ring structure with chemical formula C_4H_4NH. The heterocyclic five membered ring structure is common in basic building block of many biologically important molecules like DNA, RNA, proteins etc. Therefore, pyrrole can be considered as a prototype molecule to study how low energy electrons interacting with biological systems.

Electron energy loss spectra of pyrrole are recorded to identify its different molecular vibrations. Absolute cross sections for each observed molecular vibrations are measured at scattering angle of 135^0. Additionally, we constructed 2D electron energy loss spectra of pyrrole by measuring many electron energy loss spectra at different incident electron energies. 2d electron energy loss spectra [1] is very informative way of visualizing resonances and its decay into different vibrational modes. The vibrational excitation cross section data shows resonant structures at 2.5 and 3.5 eV and pronounced vibrational Feshbach resonances below 1 eV. Electron energy loss spectra and vibrational excitation cross section data are used to explain dissociative electron attachment (DEA) to pyrrole, which shows abduction of H from breaking the N-H bond. Electron energy loss spectra at resonant energy of 2.5 eV and MO analysis of N-H and C-H out of plane bending vibrational mode indicates that C-H and N-H out of plane bending vibrations have crucial role in DEA to pyrrole.

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Fragmentation of Glutamine Molecule by Low-Energy Electron-Impact

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The new data on the fragmentation of the glutamine ($C_5H_{10}N_2O_3$) molecule belonging to the essential amino acids related to the formation of the ionized products due to the low-energy (<100 eV) electron impact are presented. Both experimental and theoretical techniques used in this work were described in detail in our previous papers (see, e.g. [1]). The glutamine molecule mass-spectrum measured by us (see Fig. 1) is generally close to that for the electron-impact ionization quoted in the NIST database [2]. The fragments produced were identified by a mass-spectrometric method using the magnetic mass-spectrometer combined with an extensive DFT-theory approach.

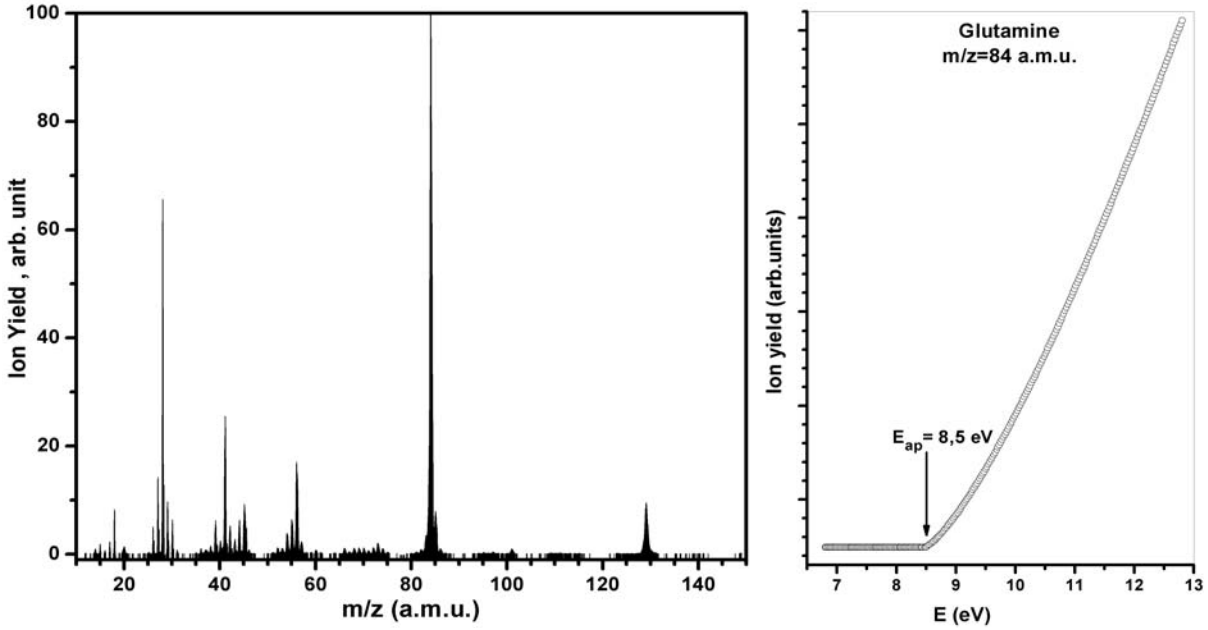

Fig. 1. The glutamine molecule mass spectrum measured at the 70 eV electron energy(left) and the threshold area of the yield function for the $C_4H_8N_2^+$ a.m.u. fragment ion (right).

We have also determined the appearance energies E_{ap} for the following fragment ions: $C_4H_8N_2^+$ (*m/z* = 56 a.m.u.) – 8.5±0.1 eV (see Fig. 1), $C_2H_4NO^+$(*m/z* = 56 a.m.u.) – 13.3±0.1 eV, $C_2H_3N^+$ (*m/z* = 41 a.m.u.) – 12.2±0.1 eV and CH_2N^+ (*m/z* = 28 a.m.u.) – 13.9±0.1 eV. The analysis of the mass-spectrometric data on the glutamine molecule electron-impact fragmentation accompanied by theoretical calculations allowed the main dissociation mechanisms of the above molecule under the low-energy electron impact to be determined.

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Electron-Impact Vibrationally-Resolved Electronic Excitation and Dissociation of Molecular Hydrogen

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Molecular hydrogen and its isotopologues are present in a range of vibrationally excited states in fusion, atmospheric, and interstellar plasmas. Electron-impact excitation cross sections resolved in both final and initial vibrational levels of the target are required for modelling the properties and dynamics, and controlling the conditions of many low- temperature plasmas [1]. Measurements of excitations in H2 by electron impact are typically limited to scattering on the ground vibrational state, and hence there is significant demand for accurate theoretical calculations of scattering on excited states. The majority of the available data have been obtained using the adiabatic-nuclei (AN) impact parameter (IP) method [2], and are resolved in the initial, but not final, vibrational levels. At low to intermediate energies, the IP results are up to a factor of two higher than the available experimental data for scattering on the ground vibrational state, and are likely to be similarly inaccurate for scattering on excited levels. To our knowledge, there have been no previous efforts towards compiling a database of electronimpact electronic excitation cross sections for H2 resolved in both the initial and final vibrational levels.

Recently, the convergent close-coupling (CCC) method has been utilized in the fixed-nuclei (FN) approximation to provide a comprehensive set of accurate cross sections for electrons scattering on H2 in the ground (electronic and vibrational) state [3]. The CCC method has also been applied in the AN approximation to study collisions with the H2+ and H2 molecules in the ground vibrational state [4,5,6], yielding good agreement with experiment in each case. Here we extend the CCC method to generate a complete set of cross sections resolved in all initial and final vibrational levels for electronic excitations from the ground electronic state to a number of low-lying singlet and triplet states.

The vibrationally-resolved description of the e-H2 scattering problem has also allowed for an analysis of electron-impact dissociation of H2. We have calculated cross sections for dissociation of H2 into neutral fragments over a wide range of incident energies, accounting for dissociative excitation, predissociation, and radiative-decay dissociation. We expect that the present calculations will be of considerable interest for modelling fusion plasmas, where H2 and its isotopologues are present in a range of excited vibrational states.

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Low Energy Electron Scattering by Uracil[H_2O]$_n$ Clusters

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Solvent effects on physical and chemical properties are essential when dealing with molecular processes of biological interests. In this study we introduce a new methodology for incorporating the environment effects on the low-energy electron scattering by uracil using microsolvation modeling. The formation of low-energy (0eV ~ 4eV) resonant states are related to dissociative dynamics of transient anions [1-2], and can be used to infer radiosensitizer qualities for uracil-related systems, such as halogenated uracils [3].

In the present work we addressed the electron scattering problem using uracil[H_2O]n as the target, and we have combined classical Monte Carlo (MC) simulations and Schwinger Multichannel (SMC) methods for both approaching the geometries/configurations selection and performing quantum scattering calculations, respectively. MC simulations were performed in the NPT ensemble with standard conditions of temperature and pressure, and SMC method has been implemented using pseudopotentials in the fixed nuclei approximation.

When comparing to those obtained for isolated uracil with the same method [4], we conclude a systematic stabilization on the energies (about -0.1eV ~ -0.5eV) and widths of the first two π^* resonances from the integral cross sections signatures of different clusters. The stabilization is pointed as a consequence of the water influence on the electronic structure of the neutral species (solute) and also as a manifestation of features involving solute-solvent hydrogen bonds [5]. Correlations between electronic properties in solution and the influence of the solvent on the electron attachment properties have been reported and they allow one to use the presented methodology for predicting solvent effects from the statistical point of view.

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Total Cross Section for Electron Scattering from $SnCl_4$ Molecules

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Experiments on total cross section (TCS) measurements for electron scattering from molecules of tetrahedral symmetry have been conducted in our laboratory from many years [1-6]. In the present research TCS for electron collisions with $SnCl_4$ molecules have been measured in energy range from 0.6 to 300 eV in linear electron-transmission mode using the 127° electrostatic electron spectrometer [7].

Preliminary TCS data are shown in figure 1. TCS function is characterized by several distinct enhancements. These structures may be related to the resonant scattering, i.e. a temporary capture of an incoming electron into an unoccupied orbital of $SnCl_4$ molecule. The influence of the central atom in molecule on the TCS energy dependence was also examined, by comparing the results for XCl_4 compounds, where X = C, Si, Ge and Sn respectively. TCS functions for these molecules have similar shape: two dominant maxima of energies near 1-2 eV and 9 eV, separated by deep minimum. Detailed discussion will be presented on the Conference.

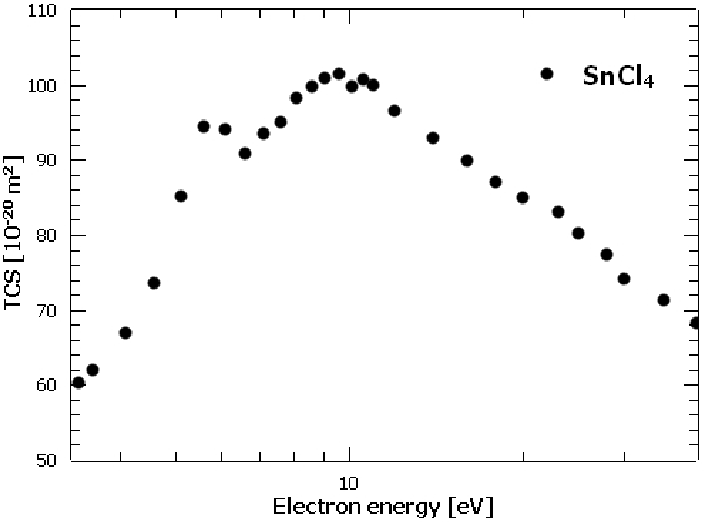

Fig. 1. Preliminary experimental data on TCS for electron scattering from $SnCl_4$ molecules.

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Anomalous Diffusion in Radio-Frequency Electric Field in CO_2

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A Monte Carlo simulation has been employed in order to determine the temporal behavior of diffusion coefficients in the RF electric field in the CO_2 gas within one period of time-dependent radio-frequency (RF) electric field. Behaviour of diffusion coefficients, within one period of 100 MHz electric field oscillation (E/N=200Td), have been the topic of interest of our study, where an interesting effect was revealed. At these parameters, we noticed that longitudinal diffusion coefficients exceed transversal ones and reach its maximum while the electric field passes zero value. The effect is well known as anomalous time dependence of the longitudinal diffusion coefficient.

The effect was first observed by White and et al. [1], by Maeda et al [2] and by Petrović et al [3]. These authors gave detailed physical explanation, together with the conditions needed for its arising. Namely, when the electric field changes sign, momentum relaxation redirects velocities of electrons, but the energy relaxation of electrons is very small, so increasing of longitudinal diffusion coefficient is happened. At that time point, fast electrons from EEDF continue to keep the direction of their moving, but slower electrons are redirected and accelerated in the new direction of the field. These changes electron motion make longitudinal diffusion coefficients exceed the transversal ones.

The effect was first observed for the Reid ramp model gas, but also for the real gases, for SiH_2 and Si_2H_6 by Shimada et al. [4], for N_2 by Popović et al. [5] and for CO by Aoneas et al. [6]. It can be noticed that the anomalous time dependence of the longitudinal diffusion coefficients in the case of CO_2 is found at low frequencies and at small values of electric field, which is very similar to results for N_2 and CO.

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DEA and DI Measurements of Potential FEBID Precursor $Ru(CO)_4I_2$

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Interactions of precursors with low-energy electrons (LEEs) are important in focused electron beam induced deposition (FEBID) [1,2]. The LEEs are secondary electrons, emitted from the surface, both inside and outside the electron beam radius, and as such they may contribute to impurities and broadening of the deposit [3]. Precursors interacting with LEEs can dissociate through two channels, dissociative electron attachment (DEA), and dissociative ionization (DI). In order to identify the best precursors, it is important to determine how these LEE interact with the precursors, both in the gas phase and on the surface, and identify trends across different types of molecules.

Here we present the results of experimental measurements of DEA and DI of the potential FEBID precursor molecule $Ru(CO)_4I_2$ and investigations of the dissociation pathways. We find that DEA to $Ru(CO)_4I_2$ proceeds mainly through sequential carbonyl loss, with the loss of two carbonyl molecules dominating the spectrum. Furthermore, loss of iodine is observed.

DI leads to more dissociation, with Ru, I, I_2, RuI, and RuI_2 dominating the mass spectrum. In DI sequential carbonyl loss is also observed, but at lower intensity. We measure an upper limit on average carbonyl loss of 2.04 for DEA and 2.88 for DI.

These gas phase results are compared to XPS surface studies to evaluate the compound for use as a FEBID precursor. Good agreement in dissociation patterns are found between the methods.

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Atomic and Molecular Suite of R-matrix Codes for Ultrafast Dynamics in Strong Laser Fields and Electron/Positron Scattering

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We describe and illustrate developments of the atomic and molecular ab initio R-matrix suites for time-independent calculations of electron scattering and photoionization and time-dependent calculations of ultrafast laser-induced dynamics. In the field of electron/positron-molecule collisions, the study of more complex targets has required improvements in software. The time-dependent atomic and molecular codes address the new set of challenges presented by attosecond science, to describe dynamics of matter in strong femtosecond lasers: recent moves to study complex multi-electron systems make the need for a matching ab initio theoretical description even more pressing.

Our R-matrix code suites [1, 2] have undergone a major upgrade and are available to the community on Zenodo [3]. For molecules, a major development has led to the release of UKRmol+, based on the UKRmol code developed for electron/positron- molecule scattering. The extended suite includes B-spline representation of the continuum via the new GBTOlib integral library as well as photoionization calculations. Significant performance improvements include a new parallel Hamiltonian build algorithm, memory optimization and a parallelized R-matrix propagator. This work enabled calculations for molecular clusters, higher scattering energies and improved quality description of smaller targets. The second layer of the R-matrix suite comprises R-matrix with time (RMT) [4] codes, which can now propagate both atomic and (with fixed nuclei) molecular wavefunctions in time. Recent work allows arbitrary polarized light and interfacing with the atomic RMATRXI suite, enabling studies of spin orbit dynamics in ultrafast laser fields.

We illustrate all these developments with recent results from both suites, including photoionization of water (RMT) and inelastic electron scattering from thiophene (UKRmol+).

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Calculation of Cross Section for Li^- Production in Dissociative Electron Attachment to LiH Molecule

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We present the description of the dissociative electron attachment to the LiH molecule within the discrete-state-in-continuum model [1]. Our attention has been primarily focused on the production of Li^- ions occurring via the $A^2\Sigma^+$ shape resonance mechanism.

The LiH molecule is interesting from the point of view of astrophysics since it participated in chemical processes in the early Universe [2]. From the theoretical viewpoint its description is challenging due to a large dipole moment and strong correlation of electronic and nuclear motions [3]. We describe the process in terms of the discrete state, which represents the $A^2\Sigma^+$ state of LiH^-, interacting with the e^- + LiH continuum. The model is based on potential energy curves of LiH and LiH^- from MRCI calculations, together with eigenphase sums of e^- + LiH scattering obtained by the *R*-matrix method. Several models, which reproduce the ab-initio data very well, were constructed with a qualitatively different threshold behaviour of the decay width.

The cross section of the Li^- production is about four orders of magnitude larger than in the case of the H^- production in the dissociative electron attachment to the H_2 molecule. The mutual relative difference among the models is about 20 %.

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Ion-Pair Formation in Neutral Potassium-Neutral Pyrimidine Collisions: Electron Transfer Experiments

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Here we present a comprehensive investigation of the decomposition mechanisms of pyrimidine molecules in collisions with hyperthermal neutral potassium atoms in the (30-800 eV) impact energy range using a crossed molecular beam setup [1]. Negative ions formed by electron transfer from the neutral potassium atom to the target molecule have been time-of-flight mass analysed and the energy loss spectrum of K^+ ions in the forward direction at 111eV have been measured. In addition, the experimental results are supported by theoretical calculations of the lowest unoccupied molecular orbitals (LUMOs) accessed in the collision process.

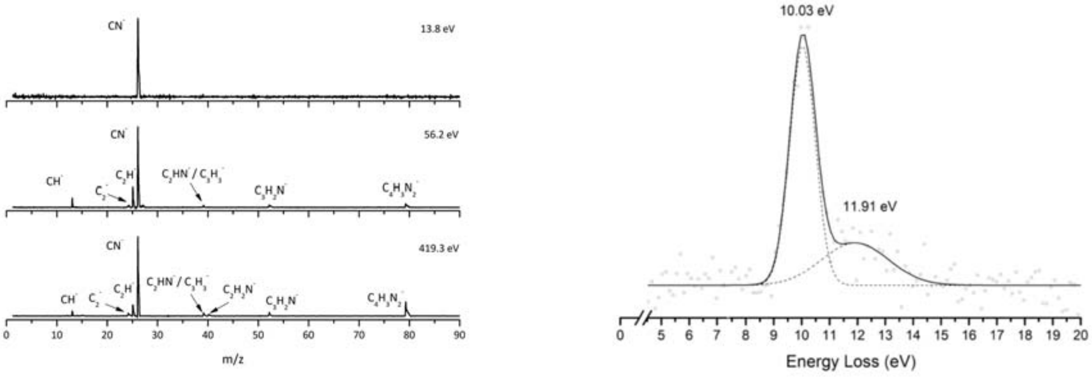

Figure 1. Time-of-flight negative ion mass spectra in potassium-pyrimidine collisions at 30, 100, and 700 eV lab frame energy and K^+ energy loss spectrum in the forward direction at 111 eV lab frame.

The most abundant product anions have been assigned to CN^- and C_2H^- and a vertical electron affinity of (-5.69 ± 0.20) eV was obtained and may be assigned to a π_3^* (b_1) state that leads to CN^- formation. Particular importance is also given to the efficient loss of integrity of the pyrimidine ring in the presence of an extra electron, which is in contrast to dissociative electron attachment experiments [2, 3].

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Total electron Scattering Cross Sections with Molecules of Biological Interest as Measured with a Magnetically Confined Electron Beam System

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Recently, the international community has paid considerable attention to the study of low-energy electron interactions with molecules of biological interest. It is now well-established that those electrons play an important role inducing damage to biological systems, especially to DNA/RNA [1]. One of the main goals of these studies is to create accurate data bases containing all the processes, elastic and inelastic, that may take place during the slowing down of electrons by successive collisions with the molecular targets of interest. Within this framework, the total electron scattering cross section (TCS) is a key parameter since it represents the sum of the contribution of all possible processes at a given energy; thereby, they can be used as reference values to check the consistency of the available integral cross section either calculated or experimental.

Novel experimental TCS results for molecular targets of biological interest (*para*-benzoquinone, pyridine, sevoflurane, and thiophene) in the (1-300 eV) impact energy range [2,3,4,5] are presented in this study. A *state-of-the-art* magnetically confined electron transmission apparatus has been optimized and validated to obtain the present measurements [6,7]. The present experimental results have been compared, wherever possible, with previous data available in the literature, and with the results of a calculation carried out for the present study within the IAM-SCAR+I and R-matrix formalisms [8]. As a consequence of this comparison, resonances due to electron attachment processes have been identified for the lower impact energies (1-10 eV).

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Vibrational Excitation and Dissociative Electron Attachment Cross Sections in Cyanoacetylene HC_3N

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Cyanoacetylene, HC_3N, has been attracting attention due to its abundance in a number of extraterrestrial environments, such as molecular clouds or Titan's atmoshere. It is believed, that the chemical transormation in such environments is to a large degree driven by an electron impact. At the same time, there is very little data on the electron collisions with HC_3N available, we are aware only of one experimental quantitative DEA study. [1]

We have used three electron collision setups: an electrostatic spectrometer with hemispherical analyzers, quantitative DEA spectrometer with time-of-flight analyzer, and high-resolution DEA spectrometer with quadrupole analyzer. With the first one, we probed the elastic and vibrationally inelastic cross sections at 135° scattering angle, combining the two later ones, we determined the partial DEA cross sections.

The vibrational excitation cross sections reveal presence of four shape resonances. The first one gives rise to a pronounced boomerang structure which overlaps with the threshold peak originating from the electron-dipole excitation, and thus creates and interesting patterm. This resonance is visible in all the vibrations. The other resonances are much more selective, especially the two σ^* states are prominent only in the excitation of the CH and CN stretch modes. The DEA cross sections are in an excellent qualitative agreement with the data of Gilmore and Field [1], however, the present absolute data are approximately by a factor of two lower. The comparison with the vibrational excitation data allows for assignment of the DEA bands.

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Resonances, Vibrational Excitation and Dissociative Attachment in HNCO

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Many unsaturated and/or strongly polar molecules show very high dissociative electron attachment (DEA) cross sections for production of the dehydrogenated closed-shell anions (M-H)$^{-}$. Two effects can contribute to this. First, target molecules with double or triple bonds possess low-lying unoccupied orbitals which can give rise to π* resonances with long lifetime. Second, in the case of molecules with sufficiently strong dipole moment or high polarizability, their long-range interaction dramatically enhances the dissociative cross section even for the broad σ* resonances, due to their interaction with long-range-supported bound or virtual states.

HNCO, the simplest molecule containing the four basic elements of life, has a bent equilibrium structure (HNC angle of 124°) and thus a priori mixes the two mechanisms. We have experimentally measured cross sections for vibrational excitation of its individual vibrational modes by electron impact and the DEA cross section for the production of NCO^{-} fragment. The VE cross sections reveal effects both due to long-range interaction (sharp cusp at the opening of the N-H stretch overtone vibration) and due to formation of π* resonances. The DEA cross section shows a sharp onset and fine structures near the threshold. We have constructed a nonlocal resonance model for the involved resonant state. It combines the effects of nonzero electron angular momentum and dipole-supported states. This leads to unusual behavior of its width at various geometries. Because the potential energy gradient of the autoionizing state points in the direction of the N-H bond, nuclear dynamics is essentially one-dimensional. The results agree with the experiment both quantitatively and qualitatively. [1]

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Theoretical Cross Sections for the Ionisation of Molecules by Single Electron Impact

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We propose a theoretical approach to calculate the cross sections for the electron impact ionisation of molecules. It is based on the First Born Approximation using a distorted wave function to describe the behaviour of the ejected electron. The molecular wave functions are computed using Gaussian, as single-center wave functions. To take into account the random orientation of the ionised molecule, we calculate the cross sections for an average molecular orientation with the proper average method. Using this approach, the computing challenges are reduced without compromising the validity of the theory. This makes it particularly interesting for complex biological targets. Our previous work [1-3] shows that the cross sections calculated with this method are in good agreement with the measured cross sections for different molecules. In the figure below, we show the calculated triple differential cross sections (TDCS) for the ionisation of pyrimidine, a structural unit of DNA bases thymine and cytosine. Our approach provides more realistic cross sections in comparison with another existing method [4].

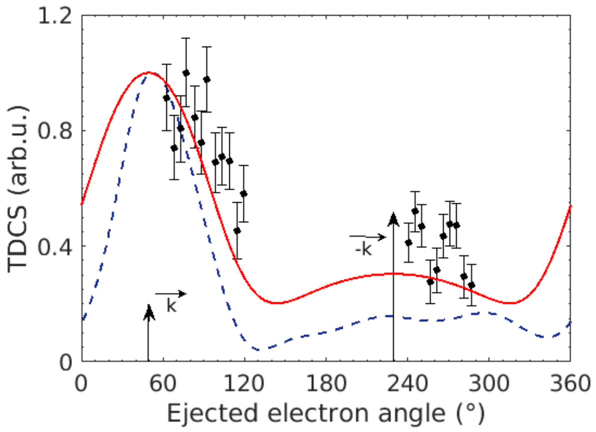

Figure 1. Summed TDCS from the highest and next-highest occupied molecular orbitals of pyrimidine by single electron impact. Our results (solid line) are compared to experimental data (squares) and theoretical M3DW cross sections from [4].

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Dissociative Electron Attachment in HNCO

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Dissociative electron attachment (DEA) plays an important role in a number of environments with a high abundance of slow electrons [1]. DEA has been successfully studied using the nonlocal resonance model [2] in numerous molecular systems [3]. However, the use of the nonlocal model was so far limited to one-dimensional problems. We present the results of DEA in isocyanic acid HNCO using a one-dimensional model and our ongoing efforts to extend calculations to two dimensions.

DEA in the HNCO molecule was investigated in a combined experimental and theoretical study [4]. Nuclear dynamics included one nuclear degree of freedom along the H-N bond, with an HNC angle fixed in equilibrium geometry. The theoretical model reproduced all the fine features of the experimental spectrum, with calculations yielding cross section about 30% higher than the experimental one.

HNCO is a suitable candidate for extension of nonlocal resonance model to two dimensions as the NCO part of the molecule is nearly linear and the molecule can be approximated as an atom - linear rigid rotor system. This model allows us to describe vibrational excitation of HNC bend motion and H-N stretch in addition to DEA.

The first step in extending the calculations to the additional dimension is a proper characterization of involved potential energy surfaces of neutral molecule and anion. Ab initio data computed using coupled cluster approach (CCSD-T) was fitted using 2D splines. Vibrational states and energy levels of neutral molecule were calculated using the DVR method. Energy differences of lowest energy levels are in agreement with spectroscopically obtained values.

The second step is to parametrize the electron-molecule scattering data using the discrite-state-in-continuum model. For this purpose we performed the fixed-nuclei R-matrix calculations using the UK molecular R-matrix suite of codes [5] for large number of NH-bond lengths and HNC bond angles. After suitable parameterization of these data is available we perform the scattering calculation for the full nonlocal dynamics for these two degrees using the coupled partial-wave expansion.

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Laser-Induced Thermal Desorption for the Production of Intact Nucleoside Targets for Electron Collision Experiments

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DEA is known to play a significant role in radiation damage to DNA [1] but understanding of the specific pathways remains incomplete. Gas-phase experiments on relatively small components of DNA enable the most direct comparisons with high-level calculations and hence provide valuable insights. Such experiments generally apply low electron beam currents and / or probe channels with low cross sections and thus depend on high target densities of intact molecules. This can be achieved for nucleobases using standard oven systems (although a number of experimentalists have reported difficulties with guanine [2]). However, the study of larger DNA components in the gas phase is hampered by their increased thermal lability and even the *single step* in complexity to nucleosides is associated with significant propensity for thermal decomposition [3]. In response, Greenwood and co-workers [4] have developed *laser induced thermal desorption* (LTD) whereby a CW laser is used to heat stainless steel foil with a layer of molecules condensed on the other side (closely related to *laser-induced acoustic desorption* – LIAD, using a pulsed laser beam). We have recently built a similar LTD source at the OU [5] and have carried out a multi-photon ionization (MPI) study of uridine to test the dependence of fragment ion branching ratios on heating laser power. These experiments have been supported by thermochemical calculations to predict the products of thermal decomposition. The results showed that intense targets of uridine can be produced by LTD without any thermal decomposition, highlighting the value of the method in this complexity regime. The experiments have also revealed evidence for changes in fragment ion production from different multi-photon ionized isomers of uridine, most likely due to isomer-dependent neutral excited state dynamics [6] in between the absorption of the first and second photons.

A new experiment has been developed at the OU specifically to study DEA to molecular targets produced by LTD. We are planning to test the new experimental system on uridine in the near future and are hoping to obtain the first results in time for presentation at POSMOL 2019.

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Electron Collisions with N_2H Molecules and Electron Detachment

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Low energy electron collisions with the N_2H radical are investigated using the R-matrix method [1,2]. Potential energy curves for the N_2H radical and corresponding anion N_2H^-, are obtained for perpendicular, colinear and bent geometry within a complete-active-space self-consistent-field (CAS) configuration interaction (CI) approximation [3].

Cross-sections for elastic scattering are calculated as a function of electron collision energy where the N_2-H bond length is stretched in each of the different molecular configurations. The resonance energies E_r and auto-ionization widths Γ found near threshold in the elastic scattering cross sections (for each geometry) are determined using the time-delay method [4]. The resonance energies and widths are both calculated a function of the N_2-H bond length, with the N_2 molecule held fixed at its equilibrium position, for the three different molecular arrangements. The results from our electron-molecule scattering calculations are then used in dynamical studies of low energy electron detachment cross sections within a local complex potential approximation and compared with previous experimental studies [5].

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Crude Potential Model for Mobility of Polyatomic Molecular Ions in Nitrogen and Oxygen Gases Using the MOBCAL

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Ion mobility spectrometry (IMS) has been widely used to analyse and identify chemical species of ionized molecules based on their mobility in a gas [1]. Recently, the IMS is applied for the detection of environmental pollutions, chemical warfare agents, illicit drugs, and explosives because the IMS devices work under atmospheric pressure and detect agents very quickly.

To understand the ion mobilities measured in the IMS theoretically, the MOBCAL program is widely used in physical chemistry. The original MOBCAL program has been developed by Martin Jarrold group in 1996 for the theoretical calculation of ion mobility in “helium” buffer gas [2, 3]. In the MOBCAL program, the potentials between a molecular ion and a gas are approximated as a sum of the potential between atoms. Each potential between atoms is given by a Lennard-Jones type function which has only two parameters.

We found the manuscript on the modification of the MOBCAL to calculate ion mobility in N_2 gas [4], but it seemed that that no one reported on the application for the mobility in another gas. Then, we have estimated and proposed potential parameters for calculation of ion mobility in air with introduction of virtual uni-atomic molecular gas named “AIR” because the most important application of IMS is the measurement in the atmosphere [5].

In this work, we have determined the potential parameters for calculation of ion mobility in N_2 and O_2 gases using only established date of van der Waals radii for each neutral atom [6] and Lennard-Jones potential parameters for several uni-atomic and diatomic molecules in literature [7].

Using the new potential parameters, we have calculated the mobilities of several ions in N_2 and O_2, respectively, and estimated the mobilities in atmospheric air as weighted averages of mobilities in pure gases using Blanc’s law [8]. For H_3O^+-attached normal saturated hydrocarbons, the calculated mobilities in “AIR”, the averaged values, and experimental data [9] show excellent agreements.

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Dynamics of OH^- Production in Dissociative Electron Attachment to Water

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As all the living tissue in its natural environment is always solvated in water it is important to study the effect of low-energy electron collisions with water, especially from the point of view of the radiation damage. Although there exist several experimental and theoretical studies [1-5] on dissociative electron attachment (DEA) to water, some phenomena are still controversial like the formation of OH^-. Theoretical calculations [2] rule out the presence of OH^- due to DEA. Some experiments confirmed its presence [3] while other attributed the OH^- formation due to ion-molecule collisions [4].

We have recently modified a DEA setup with trochoidal electron monochromator to incorporate a velocity map (VMI) detector, which enables us to measure the kinetic energy and angular distribution of the produced anions along with absolute DEA cross-sections. The setup can produce pulsed electron beam with 250 meV resolution and can record velocity map images of the anions separated by 1 amu simultaneously.

We have studied DEA to H_2O and D_2O molecules using the VMI spectrometer. In this report we confirm that the formation of OH^- and OD^- is due to DEA and not due to ion-molecule collisions. We are also presenting the velocity map images of O^- and OD^- separately for the first time.

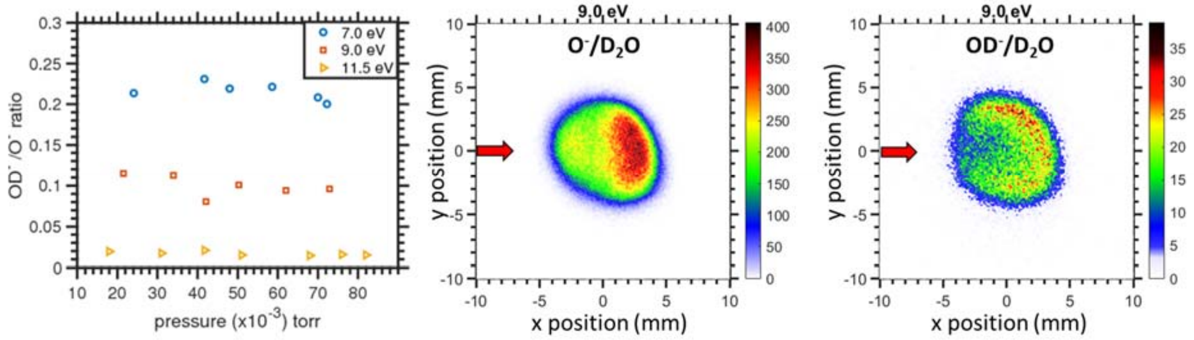

Fig:1 (a) The OD^-/O^- formation ratio at different gas pressures. (b) Velocity map image of O^- and (c) OD^- ions formed via DEA to D_2O at 9 eV incident electron energy.

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Electron-Induced Excitation and Dissociation Dynamics of NCCN

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We report experimental data on the low energy electron collision with cyanogen, NCCN. The complete vibrational excitation and dissociation dynamics of NCCN has been probed between 0-10 eV incident electron energy range. Only a few reports [1-2] on electron collision studies with NCCN molecule is available in literature.

In low-energy electron attachment, the incoming electron gets attached with the parent molecule forming a temporary negative ion (resonant state), which can either autodetach into the neutral parent molecule in the different vibrational and/or electronically excited state or dissociates into an anionic and neutral fragments – dissociative electron attachment (DEA).

Two different experimental setups have been used to study the formation of resonances in NCCN – an electron energy loss spectrometer (EELS) with double hemispherical electron monochromator and analyzer and a dissociative electron attachment (DEA) spectrometer. The DEA setup, consisting a trochodial electron monochromator, has been modified here to incorporate a velocity map imaging (VMI) detector to be able to measure the kinetic energy and angular distribution of the produced anions along with the absolute DEA cross section. Figure 1 (a) shows the two-dimensional energy loss spectra of the scattered electron recorded at 135° with respect to the incoming electron beam. The 2D spectra is an elegant way to visualize the different vibrational excitations and resonances.

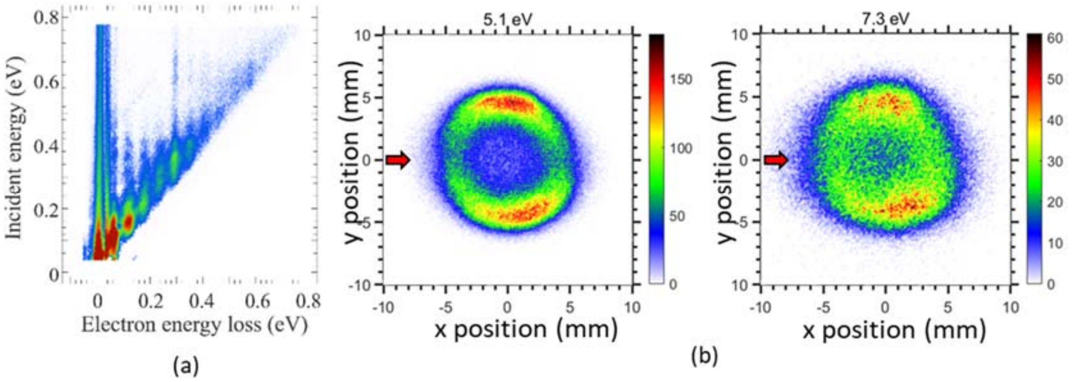

Fig.1 (a) Two-dimensional electron energy loss spectrum of NCCN. (b) Velocity map images of CN^- ions produced due to DEA for two different incident electron energies.

Figure 1(b) shows the time sliced velocity map images (VMI) of the CN^- ions produced via DEA in NCCN for two different electron energies. The absolute DEA cross-section, kinetic energy and angular distribution of the CN^- ions are measured here. In both vibrational excitation and DEA cross-section measurements two prominent resonances were observed around 5 and 7 eV. From the combined vibrational excitation and VMI measurements surprising effect related to the symmetry of the resonant state has been observed [3].

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Low Energy Electron Scattering from H_2O^+

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Molecular ions are important species in cold regions of astrophysical, planetary, cometary and man-made plasmas. In those environments, electron collisions with molecular ions can lead to the production of hot (kinetically rich) species by dissociative recombination (DR) as well as the fragmentation of target through dissociative excitation (DE). While DR has been widely studied both theoretically and experimentally, there are very few studies devoted to DE. This latter process, however, also contributes reactive species to the medium, not only when the target is a cation but also for neutral molecules, and is therefore of relevance in other environments (e.g. irradiated biological matter).

One of the few experimental studies that investigated DE is the ASTRID experiment of Jensen et al [1] on H_2O^+ and HDO^+ that, by measuring the energy deposited by the neutrals into the detector, were able to separate events produced by DR and DE. An accurate modelling of the DE process, even in the lower energy range, requires considering a number of states of the cation as well as the large number of resonances (metastable states of H_2O) that decay into these cationic states and how the nuclear wave packet evolves on all these (coupled) potential energy surfaces. Our initial aim is therefore to provide qualitative insight into the experimental results.

In order to do this, we have carried out R-matrix calculations for electron-H_2O^+ collisions for a number of geometries of the cation using the UKRmol+ suite [2,3]. We have obtained cross sections for excitation into the lowest excited state (A) of H_2O^+ and the predissociating B state. We have also identified and characterized a couple of resonant states of H_2O above the B state that could influence the short-time dynamics on this state and, in this way, modify the DE fragmentation branching ratios.

In addition, we take advantage of the recent studies by Suarez et al [4, 5] on the fragmentation of the B sate of H_2O^+ to shed some light on the interpretation of the experimental results at lower scattering energies.

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Ionization Coefficients in Low-Pressure DC Discharge in Vapours of Alcohols

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Non-equilibrium discharges in alcohols gain more attention of researchers due to a very broad field of application, from nanoscience, biomedicine, food and cosmetic industry to environmental remediation. However, despite the rapid development of various applications, there is still a lack of data on elementary processes in these discharges. Therefore, it is very important to conduct systematic measurements in well controlled conditions that can provide correct data and accurate phenomenology. The basic processes are, in quantitative terms, best studied in simple geometry and for this reason, our measurements were performed in a non-equilibrium plate-parallel DC discharge in the vapours of several selected alcohols: methanol, ethanol, isopropanol and n-butanol.

In our experiment, the breakdown voltages and ionization coefficients are measured between 3.1 cm separated copper cathode and quartz anode deposited with the transparent, conductive platinum film [1]. The ionization coefficients for alcohol vapours are obtained from steady-state Townsend discharge by using axial emission profiles and Paschen curves [2]. This is justified by the fact that swarm-like conditions can apply for breakdown itself and for the discharges operating in the low current limit (zero space charge effect) [3, 4], where the emission profiles reflect the multiplication of electrons between electrodes. Accordingly, the slope corresponds to the ionization coefficient once equilibrium with the local field is reached [2, 5]. However, spatial emission profiles of discharges in alcohol vapours at moderate (close to Paschen minimum) and high (left-hand branch of Paschen) reduced electric fields (E/N) have the dominant part of emission due to excitation by heavy-particles – by ions and fast neutrals. These processes can mask the emission from electron induced excitation, so the determination of effective ionization coefficient (α/N) from discharge emission profiles is limited to the range of conditions where dominant emission is induced by electrons from 1 kTd to 9 kTd. Our results (copper cathode) are compared with the results by Hasegawa and Date [6], gained with a quartz plate and a gold thin-film plating embedded in the middle of the cathode. The results show a good agreement in the part where the ranges of the reduced electric field overlap ($E/N > 1$ kTd). Additionally, we used experimentally attained ionization coefficients for the calculation of the secondary electron yields for alcohol vapours discharges.

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QEC – Quantemol Electron Collisions Software

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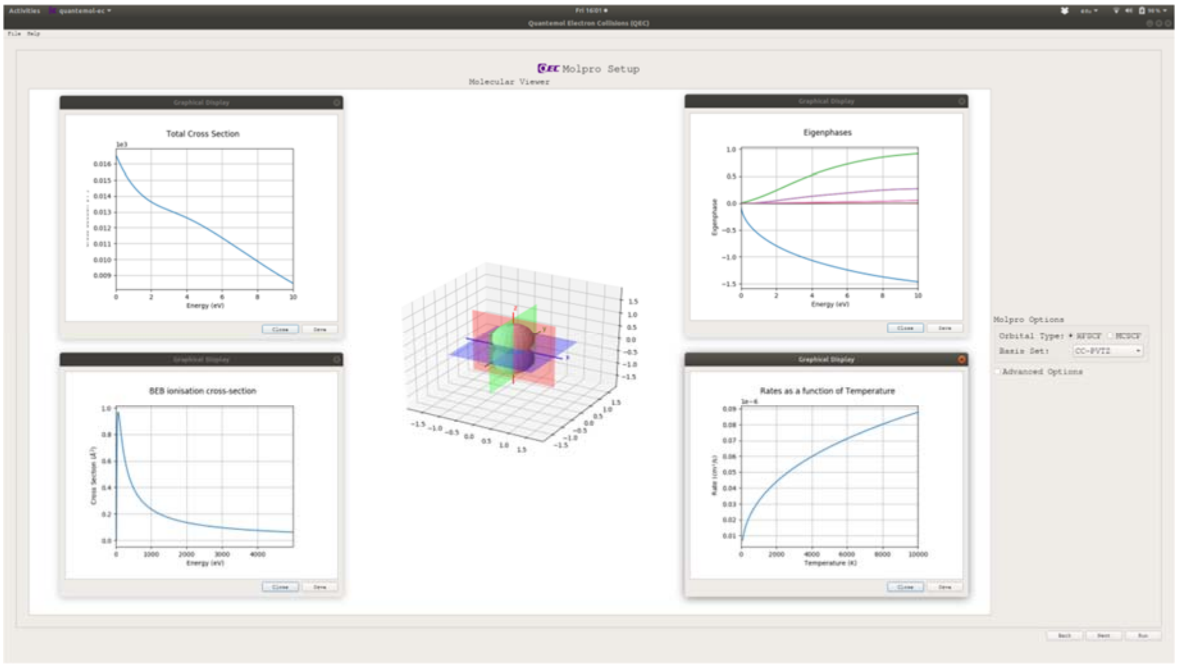

Molpro Options
Orbital Type: ● HFSCF ○ MCSCF
Basis Set: CC-PVTZ
☐ Advanced Options

Collisions of low energy electrons with molecules are important for understanding many aspects of the environment and technologies. Understanding more about the processes that occur in these types of collisions can give insights into plasma etching processes, edge effects in fusion plasmas, radiation damage to biological tissues and more. Quantemol has radically updated it's previous software, QN [1] for calculating observables relevant to these processes in the new Quantemol Electron Collision (QEC), simplifying the user experience, improving reliability as well as implenting new features. The QEC GUI interfaces the Molpro [2] quantum chemistry package for molecular target setups to the sophisticated UKRMOL+ [3] codes to generate accurate and reliable cross-sections. These include elastic cross-sections, super elastic cross-sections between excited states, electron impact dissociation, scattering reaction rates, dissociative electron attachment, differential cross-sections, momentum transfer cross-sections and high energy electron scattering cross-sections. With this new interface we will be implementing dissociative recombination estimations, branching ratio estimations, vibrational excitations for neutrals and ions, and effective core potentials in the near future. Come visit my poster for a demonstration!

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„Recommended” Cross Sections for Electron Collisions with Molecules

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Closer and closer deadlines for the peaceful use of thermonuclear energy [1] and recent discoveries in astrochemistry [2] triggered a renewed interest in electron-molecule scattering. A series of papers is under publication by our group, starting from CH_4, C_2H_4, NF_3 to nitrogen oxides (NO, N_2O, NO_2). Differently from earlier works, now the inquiry moves from total cross sections [3] into processes that are responsible for the energy-loss in plasmas, i.e. total and partial ionization, electronic and vibrational excitation, and rotational excitation and de-excitation. Comprehensive comparisons have been done.

The main novelty of our approach is the extensive referring to the theory. The UK R-Matrix code (and the Quantemol package) proved to be the most versatile tool to calculate elastic cross sections both in molecules dominated at low energies by resonances like NF_3 [4] and in polar targets like H_2O [5]. The R-Matrix codes allowed also to evaluate electronic excitation in nitrogen oxides (work in progress). For validation of total ionization cross sections we use with success the Born-Bethe binary encounter model [6]; however, application of this model to partial ionization cross sections [4] still requires some experimental input.

Further consistency of the proposed sets is obtained by comparison of cross sections from beam techniques with data derived from swarm experiments, both for pure and (what is even more stringent) mixed gases [7]. “Recommended” cross sections are prepared possibly for all partial processes, in a wide (0.01-1000 eV) energy range. An extensive discussion of the methodology will be given at the Seminar.

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Water Acting as a Catalyst for Electron-Driven Break-Up in Biochemically Relevant Hydrogen-Bonded Systems

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Electron-impact ionization of atoms and molecules is relevant to understand and interpret a wide range of scientific and technological phenomena including radiation damage in biological tissue [1]. An important role in this respect plays water and hydrated systems which have been the subject of intense studies due to their importance in life and environmental sciences [2].

In the present work, we investigate the electron-collision induced ionization and fragmentation processes in clusters consisting of water and bio-relevant molecules. We use the multi-particle coincidence technique (reaction microscope) in which the momentum vectors of all charged final state charged particles (electrons and ions) are measured in coincidence [3, 4]. The biomolecule employed here is tetrahydrofuran (THF, C_4H_8O) which is often regarded as being the simplest molecular analogue of deoxyribose in DNA. Figure 1 presents the measured fragment ion time-of-fight (TOF) spectra for both THF clusters and hydrated THF clusters induced by electron ionization (E_0 = 65 eV). Compared to the fragmentation of isolated THF molecules in clusters we find a strong and new ring breaking reaction: $C_4H_8O \rightarrow C_2H_4O^+ +$ neutrals. This is manifested by the species $(C_4H_8O)\cdot C_2H_4O^+$ for pure THF clusters and $(H_2O)\cdot C_2H_4O^+$ for hydrated clusters (see encircled assignments in Figure 1). The measured binding energy spectra and ab-initio dynamical calculations show that in the hydrogen-bonded dimers the activation energy for the ring opening channel is significantly reduced. Therefore, we observed that in dimers the water molecule or a second THF molecule act as catalysts for the break-up of the THF ring structure. Detailed results on hydrated THF complex and other biochemically relevant clusters will be presented at the conference.

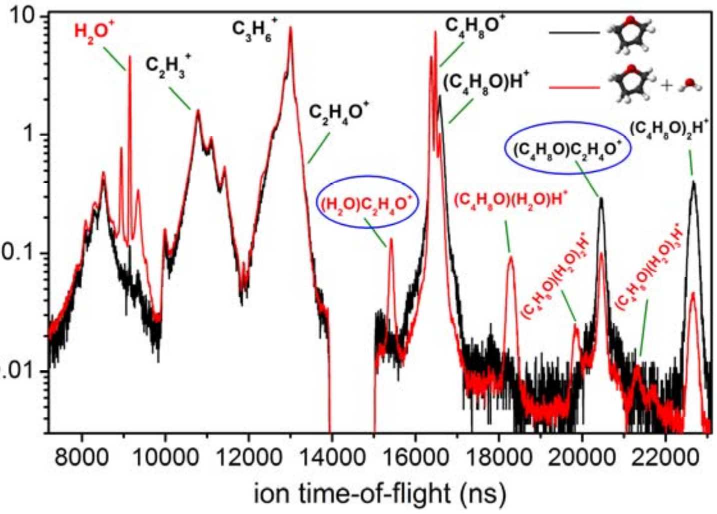

Figure 1. Measured fragment ion time-of-flight spectra of pure THF and hydrated THF clusters. The parent ion $C_2H_4O^+$ is found at 16700 ns.

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Setting New Boundaries for Electron Scattering with Highly Excited States of H_2

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A recent electron-impact excitation experiment conducted by Maseberg *et al.* [1] has provided detailed measurements on the fluorescence resulting from the $d^3\Pi_u \rightarrow a^3\Sigma^+_g$ transition in molecular hydrogen. However, there appear to be discrepancies between the theory and experiment. This presents a demand for accurate, *ab initio*, quantum mechanical calculations to investigate highly-excited electronic states in molecular targets, near and above threshold. Traditionally this causes a problem for most theoretical approaches. We demonstrate a scalable approach for polyatomic systems, using the R-matrix theory.

We are using the brand new UKRMol+ codes [2] which for the first time allow us to use B-spline basis functions to describe the continuum. We are using an R-matrix sphere of radius 100 a_B and a specialised Dunning basis set, t-aug-cc-pVTZ [3] to describe diffuse, excited states. A B-spline only continuum is used to reduce the effect of linear dependence, whilst also providing a better description of the continuum.

We present total and differential cross-sections for electron scattering with H_2 calculated using electronically excited states, up to an including, n=3. We demonstrate good agreement with existing results, both experimental and theoretical (see Fig. 1).

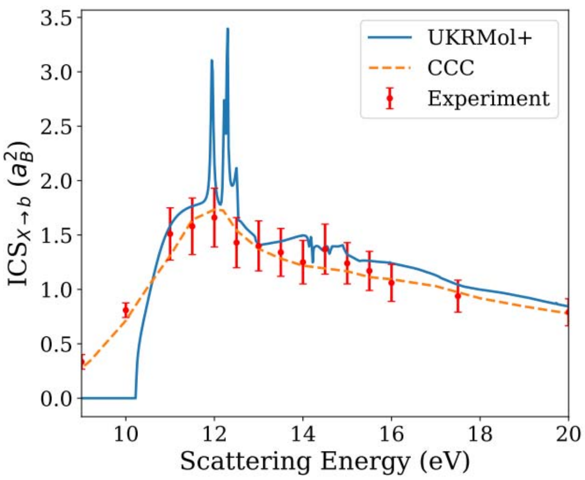

Figure 1. Integrated Cross-Section $X\ ^1\Sigma^+_g \rightarrow b^3\Sigma^+_u$ transition; (solid) UKRMol+ using fixed nuclei approximation, R=1.448 a_B, (dashed) CCC theory using adiabatic nuclei approximation [4] and (dots) experiment [4].

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Tackling Mixed Rydberg and Valence States in Nitric Oxide with the RMPS Method

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We are using the UKRMol+ R-Matrix with Pseudo-states (RMPS) method [1, 2] to investigate electron collisions with a Nitric Oxide (NO) target. This molecule is an open-shell radical, where the unpaired electron occupies a degenerate π-orbital. This presents a challenge for current quantum chemistry methods when attempting to model the target excited states. This is due to two vastly different types of excited state namely, Rydberg and Valence-type states. Several authors have presented solutions to this problem by employing Multi-Reference Configuration Interaction [3] and Density Functional Theory [4]. However, these methods apply to single states only. We require a method that can produce an optimized set of molecular orbitals (MOs) capable of describing all the excited states of interest across the all the geometries required. We find that Multi-Configurational Self-Consistent Field (MSCSF) suffers from severe discontinuities (see Fig. below) as the NO bond-length increases, or if previous geometries are used (not shown) the Rydberg-like states are lost. However, these issues can be alleviated by employing the RMPS method (see Fig. below). We will present preliminary results, using the latest UKRmol+ codes for electron scattering with NO.

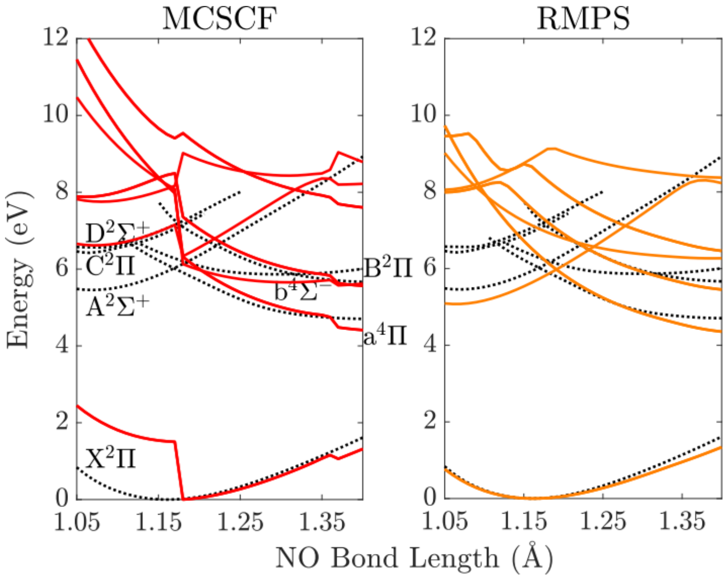

Figure 1. (dashed line) NO PECs from Gilmore [5]. (left-solid) MCSCF calculation using Molpro [6], (right) UKRMol RMPS calculation based on MCSCF calculation.

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Experimental Determination of H_2 Mass Stopping Powers for Low-Energy Electrons

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We present experimental mass stopping powers of electrons in gaseous H_2 obtained with a newly developed electron time-of-flight spectrometer, for the incident electron energy range of 10 eV to 25 eV. In our procedure the average energy loss is derived from our conversion of electron time-of-flight spectra into equivalent electron energy loss spectra so as to obtain the values of mass stopping power using energy loss as the parameter for electron scattering.

The mass stopping power (MSP) - a useful parameter obtained from collision studies - is of fundamental importance in biomedical dosimetry, radiation physics, chemistry, medicine and biology involving neutrons, protons, X-rays and electrons [1].

Although, MSPs are widely used in many fields they are rarely obtained experimentally. This is because in these measurements the complete electron energy loss spectrum should be measured, and the spectrum should be corrected for instrumental transmission effects.

Our measurements were obtained from a recently constructed time-of-flight (TOF) spectrometer, consisting of an intense energy un- selected pulsed electron gun and a TOF analyser [2, 3]. In our studies we collide low-energy electrons with target H_2 gas molecules in a crossed beam configuration, and we measure transmission-free TOF electron scattering spectra. We used these TOF spectra provide experimental MSP of electrons in H_2 in the low electron energy range [4].

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Low-Energy Electron Scattering from Molecular Hydrogen

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The electron-impact excitation of molecular hydrogen counts as being the most significant problem in electron- molecule collisions. Molecular hydrogen is the simplest neutral molecular target and is abundant in astrophysical and planetary environments where electron-molecule excitation collisions play an important role in the production of observed photoemissions. Accurate collision data for molecular hydrogen are important for many applications ranging from astrophysics and fusion research to material science and combustion physics.

The excitation of the $b^3\Sigma_u^+$ repulsive state that decays into H(1^2S) + H(1^2S) ground state atoms is a major contribution to the dissociation cross section and is the most important dissociation pathway to forming atomic hydrogen atoms at low incident electron energies and is of great importance in modelling gaseous environments such as astrophysical and industrial plasmas where molecular hydrogen is a substantial constituent.

We present time-of-flight differential cross-section measurements and convergent close-coupling calculations of differential cross sections for the electron-impact excitation of the $X^1\Sigma_g^+ \rightarrow b^3\Sigma_u^+$ transition in molecular hydrogen [1, 2]. In this work, agreement between theory and experiment is found to be overall excellent, and marks a transition in electron-molecule scattering where differential scattering of excitation is found to be in such precise agreement. We will also present total electron-impact excitation differential cross sections for H_2 for which agreement between theory and experiment is found to be excellent.

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Low Energy Differential Elastic Electron Scattering from Propyne (C_3H_4)

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There has been considerable interest in low-energy electron interactions with gaseous molecular targets especially during the last several decades because of their fundamental importance in the physics, biology, and chemistry of plasmas [1,2]

We present experimental differential elastic scattering cross sections (DCSs) for low energy electron scattering were determined from these DCSs.

Our apparatus consist of a high energy-resolution electron gun/analyser system; both are equipped with double hemispherical energy selectors to provide well-defined electron beam energy profiles and finesse. Typical electron currents ranged around 19-26 nA, with a corresponding energy resolution of between 40 and 55 meV, full width at half maximum. The experimental setup is located in a magnetically shielded vacuum chamber, with a base pressure of 10^{-8} torr.

The measurements of DCSs are obtained using the relative flow method with helium as standard, in a crossed electron-molecular gas beam arrangement. Our measurements are made at incident electron energies in the range of $1 - 30$ eV and scattering angles in the range of 10° -130°. In order to evaluate ICSs and MTCSs for propyne we performed series of measurements of elastic differential cross section (DCS) for a range of scattering angles (10°-130°) and energies (1 eV to 30 eV). ICSs and MTCSs were calculated from the measured DCS by extrapolating the DCS to 0° and 180° and applying standard numerical integration methods. Each DCS set was extrapolated to 0° and 180° by a polynomial curve [3].

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Tracing Fragmentation Channels to Specific Clusters of Nitromethane by Stark Removal Experiments

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Distributions of different clusters within neutral beams can present a major challenge in analysing electron-driven processes and drawing comparisons with theory. Küpper, Meijer, and co-workers have demonstrated that the Stark effect can be exploited to select specific conformers [1] and clusters [2] from rotationally-cold beams produced in pulsed supersonic expansions. Pulsed molecular beams are suitable for action spectroscopy experiments but are much less applicable to studies of collision-induced processes with relatively low cross sections. Here we show that Stark deflection can be used to trace reaction products to distinct irradiated neutral cluster configurations. While the present measurements involve electron impact ionization, our ultimate aim is to carry out DEA experiments on selected clusters.

The contribution focuses on experiments where an argon beam seeded with nitromethane molecules and clusters passed through a 2-wire type Stark deflector. The skimmed centre of the supersonic beam then crossed an ionizing electron beam and we recorded mass spectra as a function of the Stark deflector voltage. Molecules and clusters were progressively Stark removed from the target depending on their effective dipole moment (a function of permanent dipole moment and rotational state) over mass. Simulations using the CMIStark package [3] and a C++ code developed in-house enabled us to compare the experimental results with the predicted Stark removal of different structures as a function of rotational temperature. By analysing the nitromethane+ (NM+) signal, we were able to determine both that the ion came predominantly (but not entirely) from isolated molecules and that their rotational temperature was between 10 and 25 K. Assuming this rotational temperature is representative of the beam as a whole, we found that the experimental Stark removal curves of protonated nitromethane NMH+ and (NM)CH3+ showed good agreement with the simulated Stark removal curve of one of the two NM dimer geometries that we were able to stabilize at M06-2x/aug-cc-pVDZ level. Specifically, the agreement provides evidence that the detected NMH+ and (NM)CH3+ came mainly from ionized side-by-side dimers (SSD, permanent dipole moment 0.55 D) with negligible (if any) contributions from colinear dimers (CD, 8.11 D). Born-Oppenheimer molecular dynamics (BOMD) calculations comprising intramolecular vibrational energy redistribution (IVR) of 10 eV in the cationic ground states of SSD have been carried out in order to better understand the observed reactions

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Absolute Differential Cross Sections for Electron Scattering from Anaesthetic Molecules

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We have investigated elastic electron scattering from anaesthetic molecules, halothane and sevoflurane, in the medium energy range from 50-300 eV [1]. Experiment has been performed on the UGRA apparatus [2] settled at the Institute of Physics Belgrade. The experimental setup, based on a crossed beam technique comprising of an electron gun, a single capillary gas needle and a detection system with a channeltron, was used to measure differential cross sections. The absolute scale for the cross sections is obtained by relative-flow method using argon gas as a reference [3]. Absolute DCSs for elastic electron scattering from sevoflurane at 100 eV are shown in Fig.1.

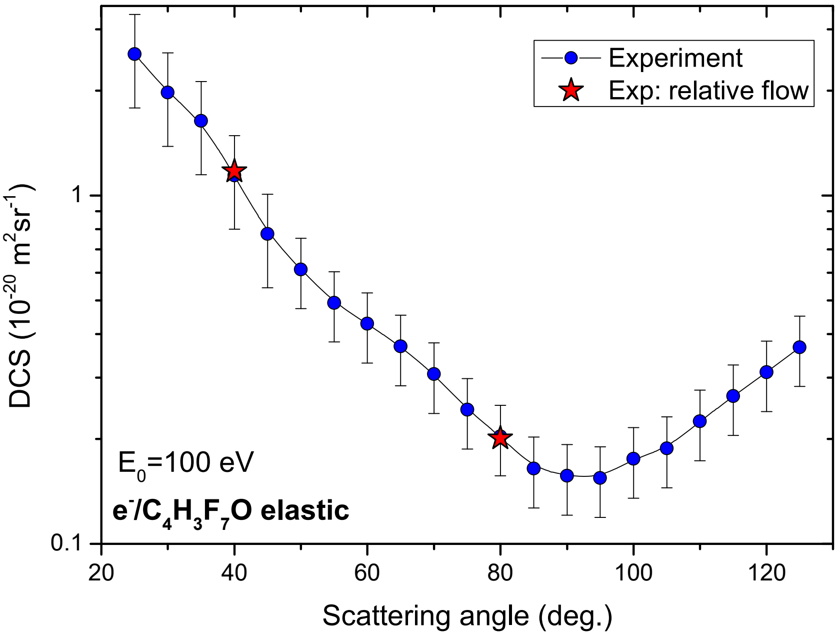

Fig.1. Angular dependence of the DCSs for elastic electron scattering from sevoflurane at 100 eV. Circles represent absolute experimental differential cross sections; stars represent absolute values obtained by relative flow method.

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Cross Sections for Collisional and Radiative Processes: BEAMDB and MOLD Databases

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Many fields in today's science such as plasma physics [1], astrophysics [2, 3], etc. depend on data for atomic and molecular collision and radiative processes. Recently, electron interactions with some of astro chemical compounds have been reviewed [4], while the importance of electrons in understanding of processes inside comas has been recognised in Rosetta Mission [5,6]. For the radiative processes we consider photo-dissociation cross-sections for the individual ro-vibrational states of the diatomic molecular ions such as H_2^+, He_2^+, HeH^+, LiH^+, NaH^+ and MgH^+ ions [7]. We also consider processes of collisional ionisation (chemi-ionization) and collisional excitation and de-excitation [8]. A collection of new data for electron interactions with molecules as well as radiative data for photo-dissociation will be presented.

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Monte Carlo Studies of Electron Transport in Crossed Electric and Magnetic DC and RF Fields in C_2H_6O and C_2H_6O/Ar Mixtures

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We present the results for electron transport in C_2H_6O (dimethyl ether-DME) and C_2H_6O/Ar mixtures under the influence of crossed electric and magnetic constant (dc) and time varying (rf) fields. Electron kinetic data for DME and DME based gas mixtures are of interest for modelling of particle detectors, especially the Microstrip Gas Chambers (MSGC) [1]. These mixtures are candidates for the use in detectors for LHC and HERA-B [2].

We have used an exact and well tested Monte Carlo (MC) simulation technique that has been described elsewhere [3, 4]. The set of cross sections for electron-DME interaction obtained in our previous study was used as the basis for simulations [5]. We calculated transport parameters (e.g. mean energy, drift velocity and diffusion coefficients) for electrons in pure DME in dc **ExB** for $50 \leq E/N \leq 2000$ and $0 \leq B/N \leq 2000$ Hx (1 Td = 10^{-21} Vm^2, 1 Hx = 10^{-27} Tm^3). In the case of time varying **ExB** orthogonal configuration fields, we have separately studied the influence of the magnitude and frequency of the fields on the transport coefficients for electrons in DME/Ar mixtures. At first we considered the influence of the magnitude of B/N ($0 \leq B/N \leq 2000$ Hx), for E/N = 100Td, f = 100 MHz, and then the effect of the electric field frequency for two different values of B/N (B/N = 0, 1000 Hx). Several expected effects were observed, like anisotropy of diffusion and anomalous longitudinal diffusion. All of the observed kinetic phenomena are dictated by the shape of the cross sections involved.

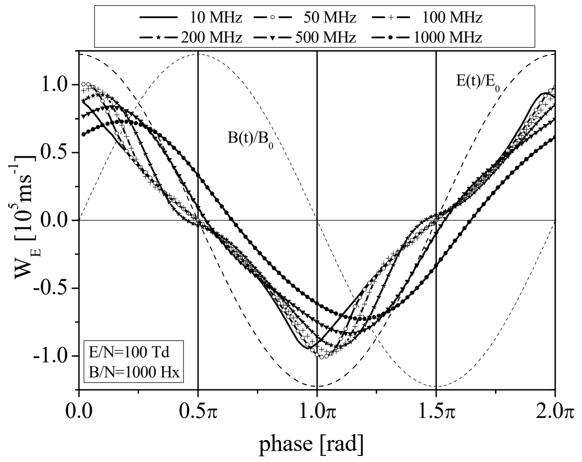

Fig.1. Temporal profiles of the drift velocity as a function of the field frequency

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Dissociative Ionization Dynamics of Dielectric gas C_3F_7CN

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Due to a very high global warming potential (GWP) of 23500, a widely used insulation gas SF_6 will no longer be applicable in high-voltage equipment, such as switchgears and other high power energy distributing circuits. A big effort has been invested in finding a suitable alternative that is environmentally friendly and has good dielectric strength. One of very promising candidates that meets those criteria is heptafluoroisobutyronitrile (C_3F_7CN). While a few companies are already supplying their switchgear products with this insulating gas, the majority of equipment around the world is still using SF_6.

The electron collisions are elementary mechanism which governs the discharge chemistry and physics in an insulating medium under high-voltage switching conditions. In order to better understand discharge reactions in this gas, it is important to know its fundamental physical properties. Being quite a new replacement gas in the industry, C_3F_7CN is not well studied and there is a lack of cross sections data in the literature. Apart from one experimental study done by Li et al [1], there are only a few theoretical studies, where Xiong et al. [2] reported calculated cross sections.

In this work, we present the experimental absolute partial ionization cross sections in the range (0-100) eV and electron impact ionization mass spectra of C_3F_7CN [3]. A reflectron time-of-flight (RTOF) experimental setup was used to record the mass spectra. Second experimental setup based on trochoidal electron monochromator and equipped with time of flight ion detection was originally designed for dissociative electron attachment experiments. We modified it in order to be able to measure absolute total ionization cross sections. We show that ionization proceeds mainly through one dominant channel leading to a complete dissociation of molecule. Our computational non-adiabatic treatment is able to reproduce experimental findings with a good agreement.

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Cross Section Set for O_2H^+ Ions in Water Vapor

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The cross section set for scattering of O_2H^+ ions on H_2O is obtained by using Denpoh-Nanbu model (DNM) [1] appropriate for polar targets [2] (Fig.1). Gas phase formation enthalpies for all reactants and products given in [3] were used for calculation of thermodynamic thresholds. In oxygen rich plasmas, the O_2H^+ ion can be easily formed from metastable O_2^+ ion [4] that is usually present in the discharges. There is no information neither for association reaction [formation of $(O_2H^+)\cdot H_2O$ ion] nor for exothermic reactions related to the resulting ion. List of all possible endothermic reaction products and their thermodynamic thresholds used in DNM calculation are shown in Table 1.

Table 1. List of reactions and the corresponding thermodynamic thresholds energies for $O_2H^+ + H_2O$.

No	Reaction products	Threshold [eV]
P1	$O_2H^+ + H_2O$ (EL)	0.0000
P2	$O_2H^+ + H_2 + O$	5.0589
P3	$O_2H^+ + OH + H$	5.1128
P4	$H_3O_2^+ + O$	0.9910
P5	$H_2O^+ + O_2H$	1.2315
P6	$H_2O^+ + O_2 + H$	3.3312
P7	$H_2O^+ + OH + O$	4.0733
P8	$O_2^+ + H + H_2O$	2.8273
P9	$OH+ + O + H_2O$	4.4918
P10	$OH^+ + H_2O_2$	3.0379
P11	$OH^+ + 2OH$	5.1812
P12	$O^+ + OH + H_2O$	5.1095
P13	$H^+ + H_2O + O_2$	4.3477
P14	$H_3^+ + O_3$	3.9427
P15	$H_3^+ + O_2 + O$	5.0433
P16	$H_3O^+ + 2O$	2.3404
P17	$H_2O_2^+ + OH$	1.0067
P18	$H_2O_2^+ + O + H$	5.4301
P19	$H_2O_3^+ + H$	2.1277

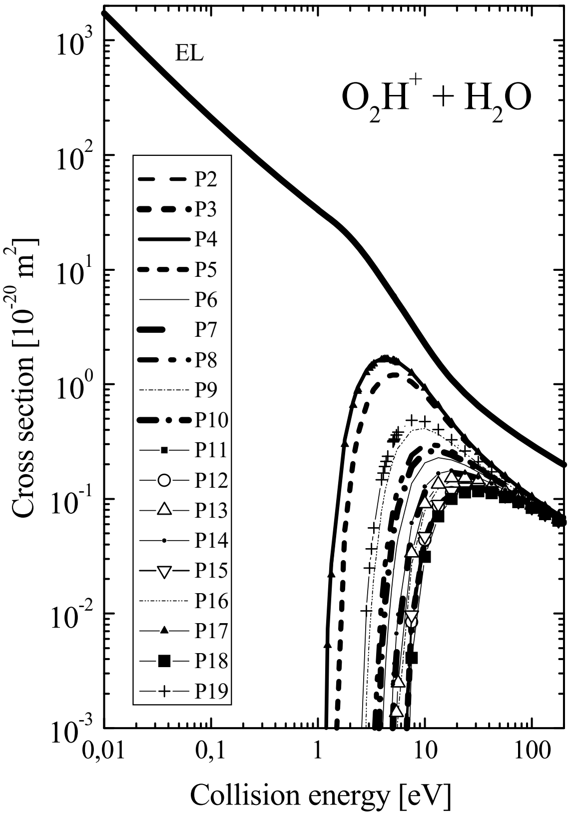

Figure 1. Cross section set for O_2H^++ H_2O.

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A Gas Phase Study on Low Energy Electron-Induced Decomposition of Potential Gold Containing Precursors for FEBID Technique

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Gold nanostructures have been known as key enabling structures in plasmonic devices, for biosensors with immobilized antibodies and as electrical contacts. There are different fabrication techniques for building these kind of structures such as photolithography, metal layer deposition, etc. However, these techniques are restricted by pre and/or post treatments, multi steps nature, and the need of photoresist materials. Focused Electron Beam Induced Deposition (FEBID) is a new single-step, direct-write nanofabrication technique which is capable of writing 3D nanostructures on different substrates. In this technique, a focused high-energy electron beam is applied to a substrate under continuous feed of gaseous, molecular precursors that typically constitute organometallic compounds. These compounds decompose through electron molecule interaction leaving a non-volatile deposit while volatile fragments are pumped away. However, there are still some challenges in this technique such as low metal purity and broadening effects of the deposit which stem from incomplete precursor decomposition and co-deposition of background gas. These effects are largely attributed to the interaction of the precursor molecules with backscattered and low energy secondary electrons, which are unavoidably generated when high-energy irradiation impinges on surfaces [1, 2].

Classic examples of FEBID precursors have been already used to fabricate gold nanostructures are Au(III) and Au(I) based precursors such as Au(acac)Me_2 and ClAuCO. The Au(acac)Me_2 precursor has acceptable volatility and stability in room temperature, however it suffers from low deposit purity. In contrast, the ClAuCO precursor shows high deposit purity, but it is unstable at room temperature and so it is difficult to handle. In the current study, we are systematically comparing the low energy induced dissociation of different Au(I) precursors for FEBID technique [3, 4].

Here we present preliminary results of the thermal stability and the gas phase decomposition of such novel gold(I) complexes, provided by the group of Lisa McElwee-White at the University of Florida. Specifically, we focus on the decomposition of these compounds through dissociative electron attachment, dissociative ionization and dipolar dissociation in the electron incident energy range from about 0-70 eV.

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Promoting Reaction Channels in Dissociative Electron Attachment to Improve the Cross-Linking Efficiency of SAMs for the Production of Carbon Nano-Membranes

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In recent years, the Gölzhäuser group (University of Bielefeld) has developed a universal scheme for the fabrication of carbon nano-membranes (CNMs) by electron induced cross-linking of aromatic Self-Assembled Monolayers (SAMs) [1], a process where the cross-linking is mainly attributed to electron induced C-H bond rupture in the monomers through dissociative ionization [2].

Considering the different nature of low energy electron induced processes [3] and in particular the bond rupture selectivity and efficacy of dissociative electron attachment (DEA), we hypothesize it is possible to control the cross-linking and functionalization of CNMs. First experiments in this direction were recently conducted on the halogenated biphenyls: 2-iodo-biphenyl, 2-bromo-biphenyl and 2-chloro-biphenyl, showing significantly enhanced cross-linking efficiency for 2-iodo-biphenyl - an effect that was attributed to the comparably high efficiency of iodine loss from this compound through DEA at threshold [4].

Inspired by these results we are currently trying to improve the electron induced cross-linking of SAMs, promoting reaction channels in DEA through exothermic formation of HF at 0 eV [5,6]. Neutral HF formation is supported by intramolecular hydrogen bonds. Currently we are investigating the influence of intramolecular -O···H···F, -S···H···F and -N··H···F bonds on DEA to potential SAMs precursors, aiming to enable exothermic HF formation and to investigate this route intermolecularly in the cross-linking process.

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Dissociative Recombination with a Scattering Matrix Approach; HeH+ as a Test Case

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The helium hydride ion (HeH^+), is one of the simplest molecular ions, it has great significance with it being believed to be the first molecule to have existed in the universe (with recombination leading to the production of H_2), and its presence in the interstellar medium and some planetary nebulae such as NGC 7027 (with recent confirmation of detection) [1].

Using a computationally inexpensive approach to obtain the dissociative recombination (DR) cross section [2] and Quantemol's QN software [3] to run R-matrix calculations, calculations could be run at low computational expense with very good correlation between this method and a more full calculation of the diatomic HeH^+ [4] at low energy, with the only outliers being resonances that are accounted for in that previous more rigorous expensive calculation.

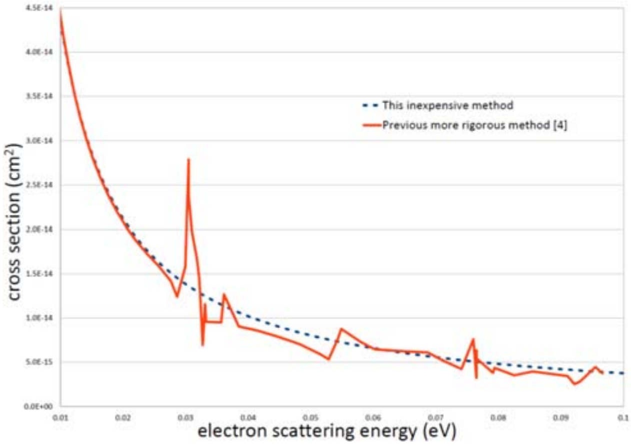

Figure 1: Graph comparing the current inexpensive method of calculating DR cross sections using the equation below (dashed line) and the previous more rigorous method [4] (solid line).

$$< \sigma > = \frac{\pi \hbar^2}{4m\epsilon} \sum_{i=1}^{3N-5} \sum_{ll'\lambda\lambda'} \left| \frac{\partial S_{l\lambda,l'\lambda'}}{\partial q_i} \right|^2$$

In the equation above for this method of calculating the DR cross section, the rotation of the molecular target is neglected, the cross section is averaged over autoionizing resonances, autoionization lifetime is assumed to be much longer than the predissociation lifetime, and the harmonic approximation is used to describe the vibrational states of the core ion. By taking small changes in molecular geometries, for a diatomic you can get an estimate of the cross section by replacing the partial derivative with the change in S-matrix element, $S_{l\lambda,l'\lambda'}$ over the change in geometry, q_i instead. The cross section for each collision energy $\in$, is then a function of the sum over all channels of the change in the S-Matrix element over the change in geometry (i.e. small change in internuclear distance from equilibrium).

The plan is to apply this methodology to polyatomic systems which are yet amenable to a full treatment.

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Comparison of RF Breakdown in Argon and Oxygen – Monte Carlo Simulation

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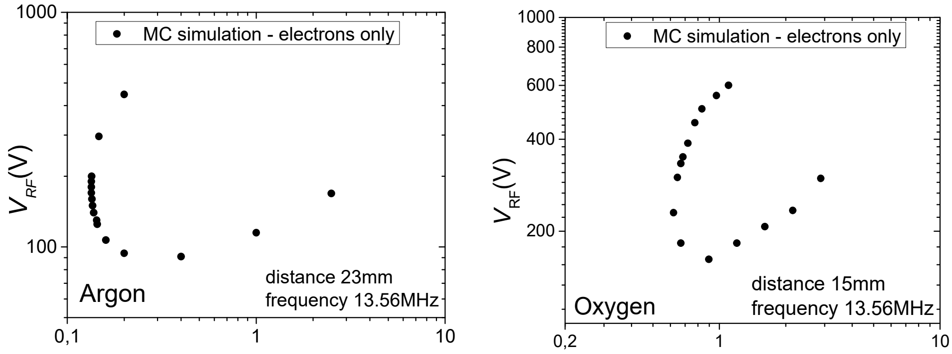
Since 1940s and von Engel's simple theory [1], physical background of radio-frequency (RF) breakdown hasn't been updated to a greater extent. There have been some explanations by experimental scientist Valeriy Lisovskiy [2], but he was basically expanding on the von Engel's theory. In general, breakdown can be described as a movement of charged particles in externally applied electric field, with electrodes representing the boundaries. In case of RF electric field, breakdown can be achieved only with electrons, where alternating field direction pulls electrons back and forth between the two electrodes. That is a feedback mechanism for maintaining the discharge. The best approach to modelling the breakdown is to follow a charged particle swarm by applying a Monte Carlo technique. In our previous work [3] we have examined RF breakdown in argon. As an extension of that work, we will examine how breakdown conditions change for an electronegative gas such as oxygen. In figure 1 are shown breakdown voltage curves for argon and oxygen as background gases. At this point, only electrons are included and there are no effects on electrode surfaces.



a) b)

Figure 1: a) Voltage breakdown curve for argon as a background gas, distance between electrodes is 23 mm and frequency is 13.56 MHz; b) voltage breakdown curve for oxygen as a background gas, distance between electrodes is 15 mm and frequency is 13.56 MHz.

The main difference between argon and oxygen is in electron attachment in oxygen. At low pressures the slope of the oxygen curve is not that different from the argon curve. At these conditions the main loss mechanism is absorption by electrodes. On the other hand, at high pressures, slope of the oxygen curve is significantly steeper compared to the argon curve. This increase of the breakdown voltage is a direct consequence of increased losses in gas volume due to the electron attachment. This process also affects strongly the spatial profile of the electron swarm as compared with that for argon.

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Gas Phase Study of Low Energy Electrons in Dissociation of TFMAA as a Monomer in EUVL Technique

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Photoresist is one of the most important components of EUVL and technological advancement are in progress. The current study aims to establish gas phase branching ratios and cross sections for low energy electron induced fragmentation for monomer units as model compounds for typical EUVL resist materials. One of the fluorine-containing monomers for extreme ultra violet lithography is 2-(Trifluoromethyl)acrylic acid (TFMAA) which has been studied in the gas phase to study the reactions of the molecule with low energy electrons through sublimation in to high vacuum where they are exposed to low energy electrons generated by a trochoidal electron monochromator and the influence of incident electron energy on fragmentation is investigated by means of mass spectroscopy. Fig. 1 shows the positive mass spectra of TFMAA which has been recorded at 70 eV. Also, special emphasis will be on halogenated derivatives to study possible means of activating local radical reactions in such resists materials. The energy range explored will be 0-150 eV with an achievable resolution better than 100 meV. TFMAA shows an intense HF loss which can help us to study and develop the resist materials by controlling the chemistry, changing the solubility and moving from acid driven chemistry to electron induced chemistry (Fig. 2).

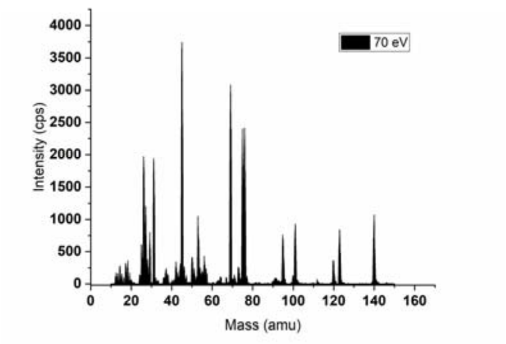

Fig. 1. Positive mass spectra of TFMAA at 70 eV

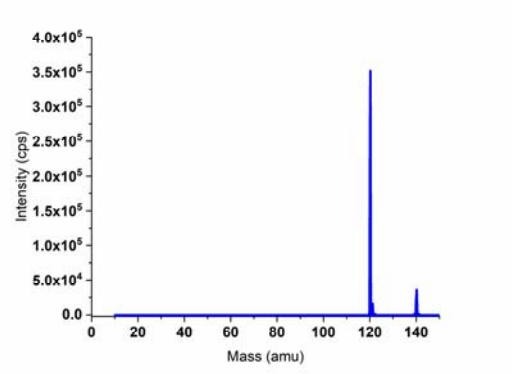

Fig. 2. Negative mass spectra of TFMAA at 0 eV

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Low Energy Electrons (5 -15 eV) Processing of Condensed Methyl Acetate: a Relevant Compound for EUV Lithography

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In semiconductor industry, Poly (Methyl Metacrylate), PMMA, is used as a spin-coated resist film for lithography. The film is a positive resist as the irradiation process induces weaknesses in the film allowing the selective removal of exposed areas by further treatment. In the quest of higher patterning resolution, the use of extreme ultra-violet radiation (EUV) above the ionization threshold generates secondary low energy electrons (LEE). A blur effect results from the uncontrolled chemistry associated to the multiple processes in competition triggered by LEE[1], both side-chain and main-chain scissions being observed [2].

A better knowledge of the LEE induced chemistry in PMMA will help for the improvement of the patterning control. We present here a LEE irradiation study of methyl acetate (CH_3COOCH_3) thin layers. The compound, representative of PMMA side chains, is condensed at 160 K in UHV. It is then irradiated by LEE in the range 5-15 eV. The induced chemistry is probed by electron stimulated desorption (ESD), measuring the neutral fragments released in gas phase during irradiation [3]. Thermally programmed desorption (TPD) of the irradiated films is recorded for the detection of fragments trapped in the layer matrix. A strong fragmentation onset is observed at 8 eV with the release of neutrals of 29, 43, 44 and 59 Dalton. The effective cross-section is as high as to 1.10^{-16} cm^2 for film processing at 10 eV, an energy where enhanced desorption is observed. Possible involved mechanisms will be discussed [4].

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Cross Sections and Rate Coefficients for Electron Impact Dissociation of Hydrogen Molecular Ions

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Collisional processes in laboratory research [1,2] and astrophysical environments [3,4] traditionally attract researchers' attention. Here we consider processes of electron impact dissociation of hydrogen molecular ions. A collection of new data for cross sections and rate coefficients are presented. In order to enable the better and more adequate use of data, we give for the rate coefficients a simple and accurate fitting formula based on a least-square method, which is logarithmic and represented by a second degree polynomial.

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Electron Driven Reactions to Boronic Acids

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Low energy electrons (LEE) has been shown to have a strong potential for driving local chemistry at the molecular level. DNA damage in living systems caused by ionising radiation is strongly related with secondary electrons interactions that attach to the DNA components or to the surrounding water molecules, driving bond dissociation. Pioneering studies of Sanche and co-workers [1,2] showed the effectiveness of LEE, with energies below the ionisation threshold, in inducing single and double strand breaks. The ability of LEE, (either free or bounded) in selectively attacking a specific bond in one molecule is highly effective. [3,4] Therefore, understanding the fragmentation pathways of (bio) molecules due to LEE is critical for molecular manipulation.

Boronic acids are known in literature since 1860. They were originally used as simple boron precursors and as intermediate agents in chemical synthesis.[5] In the last three decades, their potential as biomedical agents was discovered and explored. Now, they are considered powerful drug entities due to their unique properties such as stability, reactivity as mild Lewis acids and ease of handling. [6] Interactions of LEE with boron containing compounds can not only elucidate unknown fragmentation pathways but also design new reaction in drug design.

In the present communication we describe the role of electron transfer in potassium collisions with phenyl and cyclohexyl boronic acids, in order to better understand the dissociation channels, with relevance for medicinal chemistry applied to drug design. Differences in the dissociation channels between both boronic acids as a function of collision energy are discussed, as well as the influence of the boron hybridization in the formation of BO^- and BO_2^- fragments.

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Trajectory Surface Hopping Dynamics for Coupled Resonant Anions

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Low energy electrons can efficiently transfer its energy to molecular nuclear degrees of freedom, through the formation of resonant anions. Theoretical descriptions of the electron induced dynamics usually rely on precomputing multidimensional complex valued potential energy surfaces and propagating the nuclear wavepacket. In view of the considerable computational burden involved, this approach is usually limited to models of reduced dimensionality [1] or to small molecules [2].

Here I will present a new strategy for describing the dynamics of resonant anions. Nuclei are classically propagated, according to energies and nuclear energy gradients computed on-the-fly with bound state methods. Separate scattering calculations provide a model for the widths of the resonances. Finally, non-adiabatic couplings between resonant states and between them and the scattering continuum are accounted for with an adapted version of the fewest switches trajectory surface hopping method [3].

The methodology was employed to investigate dissociative electron attachment to iodoethene. Around 0.5 eV, a σ^* resonance promptly induces the elimination of the ioidide ion. The same fragment is also formed around 1 eV, where the initially formed π^* resonance couples to the dissociative σ^* state. Both mechanisms were found to efficiently lead to dissociation, as the corresponding cross sections are within the same order of magnitude. Comparison to available experimental data [4] is quite encouraging.

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Dissociative Electron Attachment and Chiral Sensitivity of Halocamphors

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Chiral sensitivity in polarized-spin electron scattering is an interesting phenomenon that involves parity violation. Originally motivated by the Vester-Ulbrich hypothesis for biological homochirality [1], experiments of electron scattering by halocamphor species showed a subtle asymmetry effect and appoint several characteristics for a few explanation [2,3].

The investigation of the transmitted polarized electron current indicated that the transmission asymmetry is enhanced by the formation of resonances [2]. More recently, the dissociated fragment current asymmetries for 3-Bromocamphor, 3-Iodocamphor and 10-Iodocamphor were measured by Dreiling *et al.* [3], which have revealed puzzling results. The proposed mechanisms that could explain the asymmetry consists of three spin-orbit interaction effects, although their prediction do not match with the experimental results, pointing out the need for a better understanding of the dissociation mechanics.

A low-energy electron, when interacting with gas phase halocamphor targets, can trigger dissociative electron attachment (DEA). So far, a theory that explains the DEA asymmetry has not been formulated yet, although it is expected that larger DEA cross sections might account for be followed by larger DEA asymmetries.

We present recent DEA dynamics studies for the three above mentioned halocamphors, based on a semi-local pseudo-diatomic model. We also infer the dissociation asymmetries and compare them with the experimental results.

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Total Cross Sections from Chlorobenzene in Electron Transfer Experiments

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Atom-molecule collisions yielding ion-pair formation, in the particular case of diatomic halogenated molecules (e.g. Cl_2, Br_2, I_2, ICl and IBr), have been thoroughly investigated in a wide range of collision energies to explore the role of the target's internal degree of freedom resulting in negative ion formation [1]. Additionally, such broad collision energy range also allows to study the dynamical properties of the temporary negative ions formed prior to dissociation [2].

Here we are particularly interested in probing the role of chlorobenzene's electronic structure, a polyatomic molecule that upon electron transfer in neutral potassium collisions, yields Cl^- only, conferring a pseudo-diatomic like behaviour regarding its fragmentation pattern, i.e. $K_{hyp}^0 + C_6H_5Cl \rightarrow K^+ + (C_6H_5)^\bullet + Cl^-$. Such electron induced bond breaking pertains either to an initial capture of the extra electron into a σ* MO in the C-Cl bond or to C_6H_5Cl ring π* MO followed by an intramolecular electron transfer to σ*. In the latter case this will require a considerable change in geometry to allow such effective process to occur. Additionally, from low-energy Schwinger multichannel method implemented with pseudopotentials, shape resonances characterized as π* at around 0.7 eV, 0.76 eV, and 5.2 eV belonging to the B_1, A_2, and B_1 symmetries, respectively, and a σ* resonance at 2.8 eV in the A_1 symmetry have been reported [3]. We present novel data on neutral potassium – neutral chlorobenzene collisions, where total relative cross sections for Cl^- production have been obtained from threshold up to 1000 eV in a crossed molecular beam setup equipped with a TOF mass spectrometer [4]. The energy dependence shows an enhancement of the cross section at $\sim 1.1\times10^4$ m/s relative velocity due to C–Cl bond-stretching from which we have obtained a H_{12} value of approximately 22 meV for the energy gap between covalent and ionic curves under at a crossing radius of 2.8 Å. Moreover, potassium cation energy loss spectra have been obtained at 110 and 200 eV lab frame collision energy and within this context, we also discuss the role of the accessible electronic states. Further details will be presented during the poster session at the meeting.

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Production and Exploration of Rydberg Highly Charged Ions

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Highly Charged Ions (HCIs) may be considered ideal mini-laboratory in which one can study the physics of matter and light in an environment of high internal electric field that can not be recreated with standard lab equipment. Rydberg Highly Charged Ions (RyHCI) in which a single electron occupies a high principle quantum number state, in particular, provide excellent test beds for precision measurements of fundamental constants, quantum electrodynamics, and precision X-ray wavelength standards. Even though these systems are highly desirable, the formation of such extreme electronic states is not straightforward due to excitation energies that are many orders of magnitude higher than that of ordinary laser accessible transitions. We will create HCI beams of different kinetic energies at the Clemson University Electron Beam Ion Trap (CUEBIT) facility and intersect them with different neutral atoms of a gas jet target. High-resolution and broadband X-ray spectrometers will be used to observe transitions directly to the ground state simultaneously with alternative cascade channels.

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Fluid Modeling of Resistive Plate Chambers: Effects of Collisional Data on the Detector Performance

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Since their introduction in 1980s, Resistive Plate Chambers (RPCs) have become widely used gaseous particle detectors employed for large area timing and triggering purposes in high energy physics experiments [1]. These devices consist of one or several gas gaps sandwiched between the electrodes of high volume resistivity such as glass or bakelite.

Although there were many approaches to modeling of RPCs [2,3], they all rely on accurate input electron collisional and transport data. However, the accuracy of these data and their effect on results was not a subject of due analysis. For example, we found that different cross section sets for $C_2H_2F_4$, the most common component in such devices, used as an input in the microscopic Monte Carlo model of a timing RPC can have a significant effect on the calculated RPC performance [2].

In this work, we employ a 1.5-dimensional classical fluid model to investigate the effect of input data on calculated signal and streamer development in ATLAS triggering RPC [1] which uses a 2 mm gas gap with a gas mixture of 94.7% $C_2H_2F_4$ + 5% iso-C_4H_{10} + 0.3% SF_6. We show that the signals calculated with different $C_2H_2F_4$ cross section sets can differ by several orders of magnitude (Figure 1).

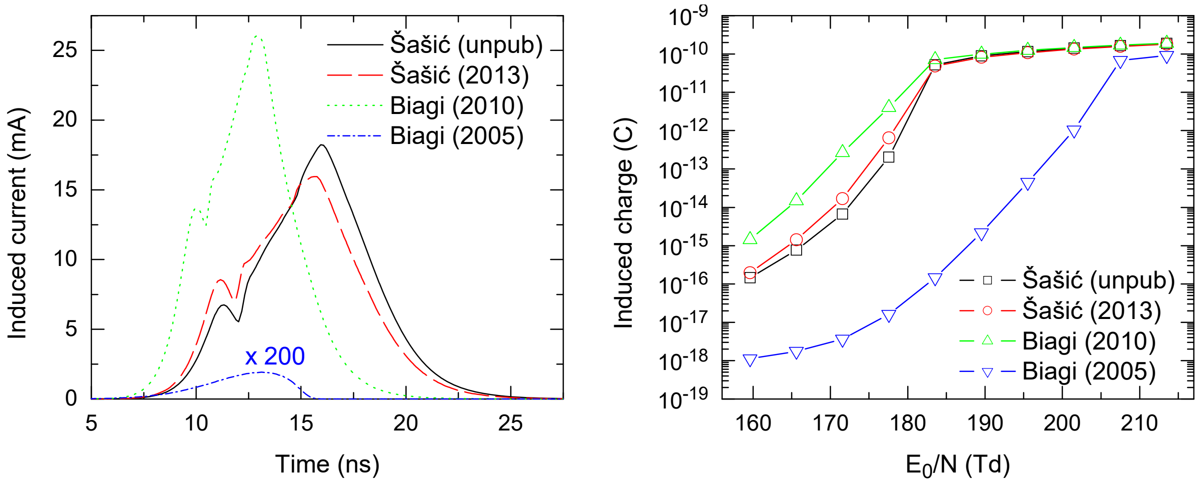

Figure 1. Induced current (left) and induced charge (right) in ATLAS triggering RPC. The induced current is obtained for the external electric field of E_0/N = 196 Td. Results are calculated using four different $C_2H_2F_4$ cross sections sets.

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Electron Transport and Streamers in the Atmosphere of Titan

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Since the era of the Voyager missions in 1980s, the possibility of lightning on Titan has been investigated by theoretical and experimental studies of its complex atmospheric chemistry. Titan is the largest of Saturn's satellites and has a massive atmosphere with surface pressure exceeding that on Earth by approximately 50%. Titan's atmosphere is largely made up of N_2 and CH_4 and trace amounts of H_2 and HCN. The presence of hydrocarbons, including C_2H_2, C_2H_4 and C_2H_6 and various nitriles has also been detected. The modelling studies of Titan's atmospheric chemistry suggest the existence of lightning since the amount of HCN and C_2H_2 in the atmosphere cannot be explained in terms of photo-chemistry models [1].

In this work, we discuss whether streamer discharges, pre-cursors of lightning, exist in Titan's atmosphere [2]. Streamers are thin channels of non-equilibrium plasma whose dynamics is entirely governed by the highly-localized non-linear regions of space charge and steep gradients of the electron number density. We approach the problem at two stages. First, using the cross section sets for electron scattering in N_2 and CH_4 as an input, we solve the non-conservative Boltzmann equation and we run Monte Carlo simulations [3]. We are focused on how the electron transport coefficients are influenced by the amount of CH_4 in the mixture and by the temperature of the background gas. The transport coefficients are then used as an input in a 1.5 dimensional fluid model to simulate the transition from an electron avalanche into a negative streamer and propagation of negative streamer ionization fronts. In particular, we present our recently developed fluid model in which the electron collisional term in the continuity equation is expanded in terms of the electron number density.

In addition to fluid models, using cross section sets for electron scattering in N_2 and CH_4 as an input, we perform Monte Carlo particle in-cell simulations (PIC-MCC) [2,4]. We use a 2.5 dimensional PIC-MCC to simulate the development of electron avalanches from an initial electron-ion patch and their subsequent transition into positive and negative streamers in ambient electric fields between $1.5E_k$ and $3E_k$, where E_k is the critical electric field of a given mixture. We investigate the electron density, the electric field, the front velocities as well as the transition from an electron avalanche into a streamer in various N_2-CH_4 mixtures. Among many important points, it is found that on Titan, a successful streamer inception would require a large electric field of 4.2 MVm^{-1} (approximately $3E_k$).

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EMS 62

Effects of Anisotropic Scattering on Electron Transport in Argon

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Using a Monte Carlo simulation technique [1], in this work we investigate the effects of anisotropic electron scattering on electron transport in argon. Electron transport coefficients and other transport properties are firstly calculated for the isotropic scattering model using the set of cross sections developed at Keio University [2,3]. In an anisotropic model of scattering, for the angular distribution of inelastic collisions we use the cosine distribution.

The effects of anisotropic electron scattering on electron transport are examined for swarms moving under the influence of a DC electric field. Calculations using the isotropic model of scattering are compared with those in which the anisotropic model is assumed, over the range of the applied reduced electric fields *E/N*. It is found that the transport coefficients in the anisotropic model are greater than those calculated under the conditions of isotropic scattering, but only in the limit of the higher electric fields. As an illustrative example, in Figure 1 we show variation of the electron mobility and of the transverse diffusion coefficient with the reduced electric field in both scattering models.

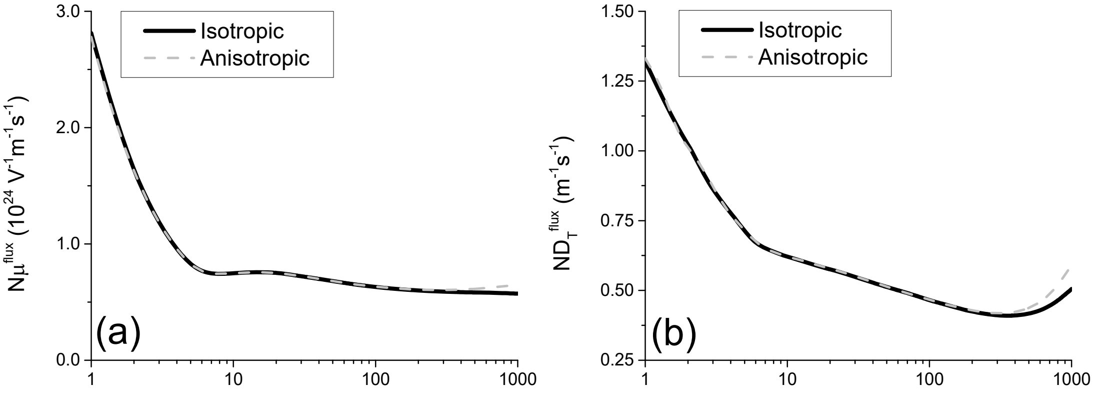

Figure 1. Variations of the electron mobility (a) and transverse diffusion coefficient (b) with E/N for isotropic (full line) and anisotropic (dashed line) models of scattering.

In addition to DC studies, we investigate the effects of anisotropic scattering on electron transport in radio-frequency fields. Temporal profiles of electron transport coefficients as well as the cycle-averaged values of transport coefficients are calculated for both models of scattering over the range of the field amplitudes and field frequencies. In addition, the effects of anisotropic electron scattering on electron velocity distribution function are also studied.

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Cross Sections for Scattering of Electrons on Tetrafluoropropene HFO1234ze Obtained from the Swarm Data

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Tetrafluoropropene (HFO1234ze, $C_3H_2F_4$) is a newly synthesized hydrofluoroolefine gas that due to its favorable properties has been considered for application as a gaseous dielectric and as a coolant. The transport data have been measured by de Urquijo and coworkers and by Franck and coworkers [1]. In both cases pulsed Townsend experiments were used and in both cases, preliminary data for fitting were drift velocities and effective ionisation coefficients (combination of ionization and attachment). We have tried to fit both sets of data for the pure gas and its mixtures with argon and nitrogen as measured by de Urquijo and coworkers. A two-term code has been used for numerous iterations and in the final stage Monte Carlo code [2] has been applied to obtain accurate and well defined transport coefficients.

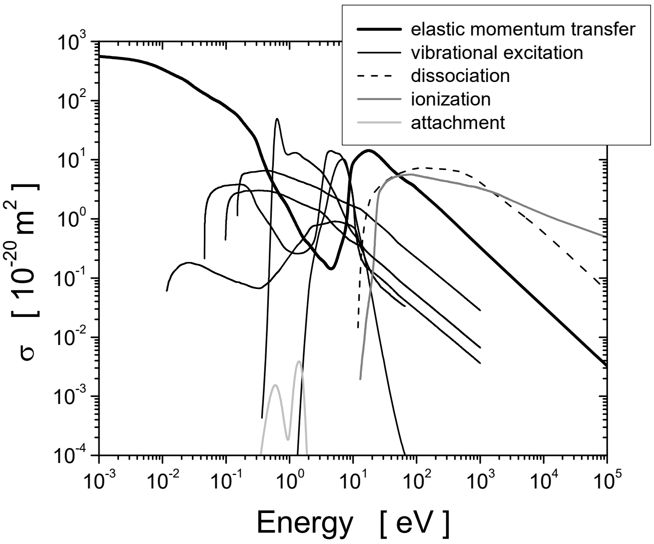

Figure 1. The cross sections for electron scattering on HFO1234ze, including vibrational excitation, one attachment process, dissociative excitation and ionization.

Starting from an initial set of cross sections taken from a similar gas (in this case octafluoropropane [3]) the set of cross sections shown in Figure 1 was achieved. Due to lack of information on the energy losses in the moderate energy range, the inelastic cross sections should be regarded as effective (i.e., each one may represent more than one process, or may bear a contribution from processes other than one effective cross section).

The critical reduced electric field of HFO1234ze is substantially lower than that of SF_6 because of low attachment cross sections. Thus, because of its boiling point of -19°C pressurized gas mixtures with buffer gases such as N_2 or CO_2 may be considered for dielectric application [4].

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Excitation Cross-Section for e-N_2H Scattering

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Low energy electron collision is of fundamental interest for various field of science and technology viz. atmospheric science, plasma physics, study of ultracold gases and electronics. Due to practical difficulty in performing experiments for every molecule in various environment, researchers rely upon theoretical data in many instances. Also, theoretical data is useful for modelling purposes due to its high resolution. The accuracy of any theoretical result depends on the model employed, especially how the target is represented. Hence, the results are very sensitive to the definition of target states and scattering functions constructed. In the present study, R-matrix formalism is employed to calculate electron excitation cross-section for e-N_2H scattering. It helps in the indirect determination of N_2 in molecular clouds. To consider the channel coupling effect we have used 28 scattering channels in configuration interaction approximation with three complete active space (CASCI). N_2H is highly polar. Hence, consideration of distortion of the target charge cloud during the collision event is very important. The polarization effect is considered efficiently using Born approximation. For the present calculation, the CASCI model is implemented through QuantemolN expert system [1]. All the calculations are performed in the ground state equilibrium geometry of N_2H.

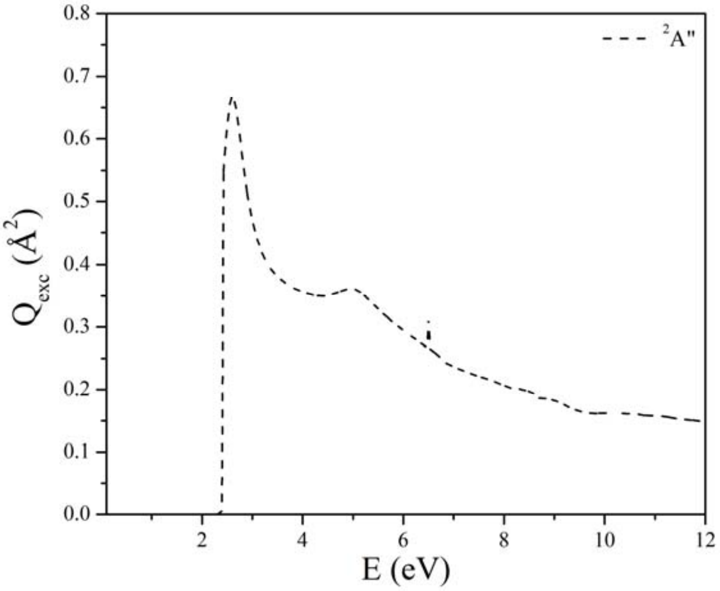

Figure 1: Excitation cross-section for e-N_2H scattering.

Fig.1 illustrates the excitation cross-section of e-N_2H scattering. We observed a sharp rise in excitation cross-section near threshold and peak around 2.6 eV. Another shoulder like feature is observed around 5.5 eV. These features appear due to change in eigen phase corresponding to $^3A''$ and $^1A'$ respectively. Further details will be presented at the meeting.

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Electron-Induced Fragmentation of Peptide Model Molecules

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Dissociative electron attachment (DEA) to biomolecules plays an essential role in radiation damage initiated by high-energy radiation. A variety of biomolecular systems, including DNA, RNA, and proteins constituents have been the focus of a lot of the DEA experimental work over last two decades [1]. These studies showed rich fragmentation patterns formed via resonant electron capture into one of the metastable valence states of a molecule. However, resonance characterization still remains challenging in spite of a number of theoretical and experimental attempts. Therefore, our recent work focuses on targets, such as amides, that can be considered models for larger biologically relevant molecules, that are peptides. The choice of these simpler systems, containing amide bonds, was dictated by a possibility of performing high-level electronic structure calculations and a possibility of studying them in the gas phase.

Here, we present our results of experimental and computational studies of the gas-phase DEA to three prototypical peptide molecules, formamide, N-methylformamide (NMF), and N,N-dimethylformamide (DMF). In addition to careful investigations of all fragments formed via DEA [2], our great focus has been on amide bond rupture (Figure 1). Interestingly, a double-resonant structure was observed at similar energies in the ion yields for all ions resulting from this C-N bond cleavage, such as NH_2^- for formamide, $NHCH_3^-$ for NMF, and $N(CH_3)_2^-$ for DMF. Several of possible mechanisms of electron attachment were considered computationally in order to characterize these peaks. Based on our calculations, these resonances can be assigned to core-excited dipole-supported resonances populated upon DEA [3]. Our results suggest that the formation of "spin-forbidden" dipole-supported resonances can be of a general implication of DEA to larger biological complexes, containing the amide bond.

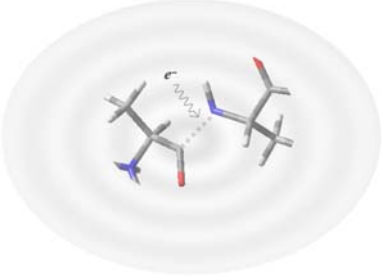

Figure 1. Incoming low-energy electron first attaches and then cleaves the peptide bond.

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WL 1

Metastables as a Probe for Low-Temperature Plasmas
Correlation between N* and n_e in Ar

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Large number of experimental and theoretical studies of neutral metastables in argon have been performed in order to explore and clarify the macroscopic and the microscopic characteristics of low-temperature plasma sources for over three decades. The accumulated set of data comprising number density and temperature of the metastable, N^* and T_g, as well as the electron density n_e in various kinds of low-temperature plasmas over a wide range of external parameters enable the analysis and review of the inner plasma parameter in the form of the relative densities, N^*/N_g and n_e/N_g normalized by the feed gas density N_g, based on a simple theoretical rate equation in real space,

$$\frac{\partial}{\partial t}N^*(t) = k_m n_e N_g - k_{Teq} n_e N^* - k_{mp} N^* N^* - k_{3sq} N^* N_g^2 - k_{imp} N_{imp} N^* - \frac{D_m}{\Lambda^2} N^*$$

Indispensable is the development of the non-invasive diagnostics for metastables, and of the tunable diode laser in a visible-near infrared domain ($\lambda < 1\mu$m). It enabled optical absorption spectroscopy for measurements of N^* and T_g of the metastable in Ar. A reasonable cross-correlation in the above equation,

$$\frac{n_e}{N_g} = -\frac{k_{mp}}{k_{Teq}}\frac{N^*}{N_g} - \frac{k_{mp}}{k_{Teq}}\left(\frac{k_m}{k_{Teq}} + \frac{I_d}{k_{mp}}\right)\left(1 + \frac{k_m}{k_{Teq}}\frac{1}{\left(\frac{N^*}{N_g} - \frac{k_m}{k_{Teq}}\right)}\right)$$

is found between N^*/N_g and n_e/N_g during a steady-state under condition without three-body collision and diffusion, i.e., $I_d = 0$. A strong positive correlation between N^*/N_g and n_e/N_g in the present analysis demonstrates that the metastable density N^* can be an indirect indicator of the plasma density n_e in a low-temperature plasma. It will be noted, in addition, that the high-sensitivity of electrons to the surrounding local field makes it difficult to observe the local density and its distribution in a low-temperature plasma even though there exist several traditional methods to measure n_e. The details of the present result are published as the review article [1].

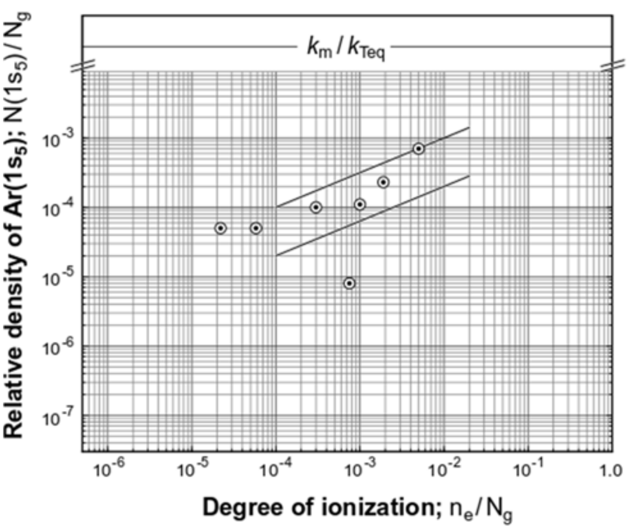

Figure: Example in micro hollow-cathode discharge under various external parameters.

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Dancing with the Stars: Laboratory Astrophysics with Highly Charged Ions

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The abrupt end of the dance of two neutron stars was recorded as the first detection of a gravitational wave and heralded in the new era of multi-messenger astronomy. The subsequent measurements across the electromagnetic spectrum holds great promise for a deeper understanding of the physics in these extreme environments. Of particular interest is a deeper understanding of the heavy-element nucleosynthesis expected to occur in the ejecta from this neutron-rich environment, the so-called r-process. The laboratory spectroscopic data on the vast range of heavy elements (Rb-U), including the lanthanides and actinides, are so severely limited at present that emission models are only in qualitative agreement with the observed spectra.

To partially alleviate this situation, a computational/experimental laboratory astrophysics collaboration between Auburn University, Clemson University, the University of Georgia, and Queen's University Belfast has been formed to generate reliable line lists for a range of r-process elements from neutral to triply charged. I will mainly discuss the experimental effort which will be undertaken at the Clemson University EBIT (CUEBIT). The CUEBIT has recently gone on-line and is now producing up to fully stripped ions from low to medium Z targets. The trap is connected to a beam line which was designed to extract and focus decelerated (down to 100's q eV) beams of single charge state ions and deliver them to modular back-end apparatus.

Time permitting, I will discuss additional experimental progress in measuring charge exchange-induced X-ray and extreme ultraviolet emission from systems relevant to both solar and extrasolar sources. Extensive observations are expected from near-term x-ray telescopes missions (e.g. XRISM) and complementary laboratory investigations of these processes aid in the understanding of observed astrophysical spectra and are extremely useful to help scientists make judicious choices of spectral ranges for future observations.

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Foundations and Interpretations of the Pulsed-Townsend Swarm Experiment and the use of Machine Learning for Self-Consistent Cross-Section Sets

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The pulsed-Townsend (PT) experiment is a common swarm technique which is routinely used to (i) provide transport coefficients for plasma discharge modelling, and (ii) assess the accuracy and self-consistency of cross-section sets of electron/ion interactions with gaseous systems. The Townsend coefficient, drift velocity and diffusion coefficient for electrons and ions drifting and diffusing in background gases. In this work, the governing equation used to analyse the PT experiment is analysed when non-conservative processes are operative. It highlights, the transport properties derived from PT experiments are not directly comparable to the standard transport coefficients. We highlight, however, how the reaction rate and bulk drift velocity can be better approximated from these PT transport properties, although proper comparison with the bulk transport coefficients requires a slight reanalysis of the PT experiment current transients. Estimates of the errors originating from the incorrect governing equation and subsequent analysis are presented for various atomic and molecular gases as a guide for uncertainties in the previous data. Further, in this presentation we will highlight the use of machine learning techniques to develop self-consistent cross-section sets for electron-neutral interactions in both gaseous and liquid systems.

All That You Never Wanted to Know About Breakdown

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This talk represents an overview of Prof. Zoran Lj. Petrović's impact on the studies of electrical gas breakdown. The starting point will be his work with late Art V. Phelps and co-workers, which is a key reference in the field. Papers, such as [1-4], represent a comprehensive revision of Townsends' theory of breakdown and low-current low-pressure discharges. These papers show how atomic physics, swarm physics, surface interaction, and discharge physics are connected through the phenomenology of gas breakdown. More importantly, these early studies unlocked an entire field that is still very active, proving that the ground principles laid in [1-4] are valid even in a wider range of conditions than initially assumed. Laboratory for Gaseous Electronics at the Institute of Physics Belgrade continued the work along these lines to this day.

The work initiated in ref. [5] has shown that recommendations and predictions made by Petrović, Phelps *et al.* [1-4] are valid, not only in the near-breakdown conditions, where spatially constant electric field and absence of space charge allow swarm modeling, but also under the highly non-local conditions, where kinetics is considerably changed. Following papers, such as [6], pushed the story a step further, by including kinetics of ions and fast neutrals at high reduced electric fields. A comprehensive review of ionization coefficients in pure gases and gas mixtures, based on [4] was presented in [7], and extended to the analysis of secondary electron yields in [8]. The same principles scaled down to micrometer dimensions in [9]. The significant advance in the field was made by reducing the time scale in [10], where we were able to follow early stages of the breakdown and development of higher current discharges and make a final step in understanding instabilities, such as oscillations and constrictions of the non-equilibrium discharges.

The most recent work in this field is directed to studies of a breakdown in liquids of interest for a wide range of interesting applications [11], which will require significant adjustments in the description of the electron; ion, fast neutral - molecule collisions.

This work is supported by MESTD, projects OI 171037 and III 41011.

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It's all About Monte Carlo

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Kinetic Monte Carlo (KMC) algorithms have been effectively used in recent years to study atomic recombination and molecule formation on surfaces [1-3]. KMC simulations are exact, in the sense that they follow the time-evolution of one element of the statistical ensemble, simulated without any subjacent approximation. They provide the answers to the questions 'when, where and what', determining the dynamics of the surface. In short, it is considered that the system may undergo k transition events, $\{e_1,\ldots,e_k\}$, characterised by transition rates $\{r_1,\ldots,r_k\}$, and that the number of particles capable of experiencing a given event are $\{n_1,\ldots,n_k\}$. Upon the successful choice of 'what' (which event) and 'where' (on each position on the surface), time is advanced by randomly selecting an increment τ from an exponential distribution with parameter $\lambda=\Sigma_i n_i r_i$, namely $\tau = (1/\lambda)\ln(1/r)$, where r is a random number drawn from the uniform distribution in the unit interval, as initially proposed in [4].

Despite the success of KMC algorithms in describing relatively complex surface kinetics [1-3], the coupling with gas phase chemistry remains tenuous. The large differences in the characteristic timescales, which can vary over several orders of magnitude, makes the situation even worse regarding a full MC description including the electron kinetics as well. This work points out how to achieve a common formulation of KMC algorithms capable of addressing simultaneously, in a fully coupled way, the surface, chemical and electron kinetics. It focuses on the recent progress made in the KMC description of surface kinetics [1-3] and reviews the current state of KMC algorithms for gas phase chemistry [5], using oxygen discharges as a test case. In addition, a new KMC method to study the electron kinetics is outlined. The new approach is suited to study the coupled kinetics in nanosecond discharges [6], where the high values of the reduced electric fields limit the accuracy of the calculation of the electron energy distribution function using a 2-term Boltzmann solver and where the influence of collisions with different excited states and of the atomic kinetics can be significant.

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The Multi-Phase Game: Liquid Wets Gas, Gas Dilutes Plasma, Plasma Surrounds Liquid and all Together They Produce Solid Nanorocks

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The modern low temperature and atmospheric pressure non-equilibrium plasma has made tremendous advances in a relatively short time with respect to providing added value across a broad range of important applications. However, the complexity of the plasma and its interaction with environments and surfaces resists detailed experimental exploration. Distances and timescales for important reactions are often on the nanoscale and measurements are often beyond our meagre resources. A typical plasma-liquid setup has thin interface regions above and below the nominal interface boundary. Apart from charged, atomic and molecular species, these regions also inevitably contain macroscopic objects such as liquid droplets and possibly plasma-filled bubbles. In certain experiments, they can also contain solid nanoscale and microscale particles. Between the macroscopic and the molecular, we also have clusters. This is a truly complex problem in multiphase systems and to date we have tended to minimize the importance of these "extra" phases. Of course, when these objects are large enough, they can be considered as traditional surfaces but on the microscale or lower, these solid/liquid objects can be totally surrounded by plasma, exchanging charge, energy and mass. The plasma-filled bubble is similarly surrounded. We consider the question as to whether it is valuable, or even possible, in this context to study the plasma interaction with individual objects at microscale or lower. In our recent work, we attempt to study such interactions with individual liquid microdroplets, with nanoparticle ensembles and with nanoparticles inside droplets and in this talk, the focus will be on microdroplet studies.

The plasma-microdroplet can act as an individual laboratory experiment enabling a range of conditions that cannot otherwise be achieved. For example, precise control of the gas environment becomes a new parameter while flow and convective forces onto the liquid surface can be minimised or even eliminated. The spherical symmetry enhances the computational capabilities as does the reduced geometric dimensions. The liquid surface is irradiated by ultra-low energy electrons and at these energies the interaction of electrons with liquid is thought to be one of the primary reasons that plasma – liquid interactions are so advantageous, able to locally create high densities of active species that can treat cancer cells, destroy antibiotic resistant microbes, encourage seed germination in agriculture and synthesise novel chemicals and nanomaterials. On the gas side, an evaporation shell layer may contain a cocktail of positively and negatively charged clusters along with a very high localised vapour density. We can speculate that this may lead to amplified non-equilibrium gas-phase chemistry, the products of which may be sequestered by the droplet boundary. By controlling the plasma exposure time of the droplets to the sub-millisecond range, which is not possible with any other steady-state system, we may gain insight into the transport and mass accommodation of radical species before the onset of Henry's Law. The disadvantage is of course the very small droplet volumes and their velocity.

We will report current microdroplet results and highlight new directions via Plasma-XPS where we hope to study the plasma induced chemistry of liquid droplets and solids on a monolayer scale via instantaneous freezing. We also aim to explore optical and tunable infrared absorption (1um – 12um) of droplets and their surrounding vapour layer, in flight.

Collisions and Impacts in Semiconductor Device

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In this talk, the review of collaboration work with Prof. Zoran Petrovic and the developmental research related to collision and impacts in semiconductor devices are presented. In 1994, a first collaborative paper with Prof. Zoran Petrovic entitled "The Radical Transport in the Narrow-Gap-Reactive-Ion Etcher in SF_6 by the Relaxation Continuum Model" to Japanese Journal of Applied Physics as a result of work in Keio University are published [1]. In this paper, neutral radical transport in narrow gap reactive ion etcher using SF_6 gas was discussed. Following that a paper to Physical Review E entitled "The Radical Transport in the Narrow-Gap-Reactive-Ion Etcher in SF_6 by the Relaxation Continuum Model" are published [2]. After the simulation and modeling research of non-equilibrium plasma, my research field is shifted to semiconductor device simulation and circuit design not the semiconductor processes.

Current research fields include compound semiconductor device simulations such as GaN and SiC. Two examples of collisions and impacts in semiconductor devices are shown. With the development of power electronics in recent years, next generation power semiconductor devices are needed. Gallium nitride is a promising material for high frequency, high power, and low loss devices because it has a wider band gap, higher breakdown voltage, and higher saturation velocity. Heat generation is a serious problem because power devices operate in high current and high voltage regions. Therefore, in order to analyze non-stationary electrical and thermal phenomena in nanoscale devices, a self-consistent Monte Carlo simulation method that can simulate electron transport and phonon transport microscopically and simultaneously is used.

In second, SiC Impact Ionization Coefficients evaluation work is introduced as a recent work. To know the impact ionization coefficient in SiC semiconductor device is very important work because of SiC is key power device in near future. The device breakdown caused by impact ionization is an issue to avoid for the reliable operation. However, the measurement of impact ionization coefficient is not easy issue due to lack of direct measurement in the device itself. Therefore, we use the device simulation method to overcome this issue, and the simulated results is compared with experimental results of the measurement of break down voltage in the devices.

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Double Layers & Striations in Spherical Plasmas

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The observations of and research on double layers and striations in gas discharges has a long history. The study of plasma double layers underwent a resurgence of interest in the 1970s by, notably, Noah Hershkowitz and his collaborators. Most of the research over the decades has involved collisionless gases $p << 1$ mTorr in, typically, Ar or He. In 1997 the Russian group of Nerushev, *et al.* [1] began publishing a series of articles over a period of about 17 years on striations in collisional molecular gases in an anode centric divergent spherical geometry. The gases used were acetone and methanol in N_2 at pressures of $p > 0.1$ Torr. The most significant observation of theirs was the formation of spherically symmetric striations around the high voltage anode. They never reached a conclusive explanation of their existence and stability. Examples of such striations are shown in Figure 1. These are photographs of mine were taken of a gas discharge in H_2 containing a small mole fraction of N_2 (Childs, Clarage, and Anderson, *unpublished*). Performing Abel's transform on the scan shows that the emissivity of the bright regions is about three times that of the dark regions. These are double layers and more. The dark regions are potential minima where the electric field goes through zero and reverses. I proposed in 2015 [2] that the potential wells are due to negative ions. Indeed, even molecules used in the Russian experiments dissociate into more simple electronegative species such as CO and H_2. Measurements by others on very low pressure plasmas and my own modelling and simulation of this plasma show that dominant ions tend to be NH_3^+ and NH_4^+, the dominant neutral fragment is NH_3, and the negative ions are H^- and NH_2^-. The negative ions form at low E/N, *i.e.* in the dark regions.

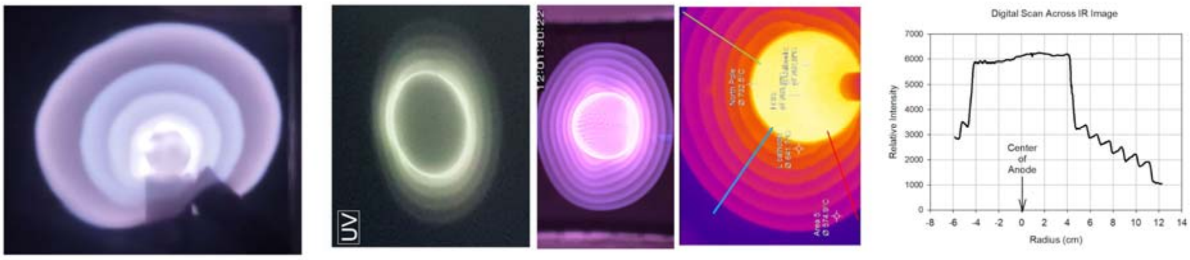

Figure 1: L to R: photo of H_2 plasma with 6mm anode; UV, Visible, IR images, the last showing an anode (diameter 8 cm) temperature of 763 C; a density scan across the IR image

My observations are that the plasma does not shift into the striated mode until there is a disturbance, such as a diffuse arc to ground or spikes in the applied DC voltage – I will show videos of this process. They tend to be preceded by anode spots. Once formed the striations are very stable and may persist for hours unless perturbed by voltage, current, or gas pressure and composition changes. The addition of a small amount of Ar, for example, destroys them.

Acknowledgement: The experiments were performed *sans* diagnostics by Childs, Clarage, and Anderson in Toronto. I took the photographs of computer monitors using a 24 MP Canon.

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Plasmas in Liquids

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Plasmas produced by creating electrical discharges in liquids have long been the subject of scientific investigations but the last ten years or so have seen an enormous increased interest in their study. This has been prompted by their expanding range of applications. Here, after an introduction, the focus will be on an investigation [1] of plasma ignition in saline solution using electrical and imaging diagnostics, along with simulations, to investigate the behaviour of the discharges created. The saline contains grounded and needle electrodes. As the voltage applied to the needle in the saline solution is increased, and prior to the observation of visible discharges, different regimes for the boiling of the saline solution are observed. As the electric field strengths are increased within the vapour region light emission from that region is observed. A shadowgraphy method is used to explore the initial vapour layer phase. Finite element method (FEM) based simulations are used to estimate the electric field strengths. Particle image velocimetry (PIV) measurements give us information of the velocities achieved in the liquid due to the plasma formation. Fast framing cameras, spectrometers and ICCD cameras are also usedAny figures will be reproduced in black and white so please take that into account when producing.

Aspects of the chemistry of these water vapour plasmas, where Zoran Petrovic has made very significant contributions to the data base, will also be discussed.

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The Petrovic Chronicles – Non-Equilibria Rules

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Professor Zoran Petrovic has been a unique, and major contributor to the field of Gaseous Electronics for almost 40 years. His research and applied work has been highlighted by the extensive international collaborations that it has involved, encompassing work on (at least) 4 continents. Zoran's unique contributions have been to straddle, and link, the gas discharge physics and AMO collision physics communities with both theoretical and experimental work, inject suggestions for new data needs and, where appropriate, suggest sets of collision cross sections that can be more broadly used in modelling and other studies.

The applications of his fundamental work in transport measurements, cross section derivations and optical emission from low temperature gas discharges (to name a few) are many and varied. His applied work cover fields as diverse as discharge and plasma diagnostics, microelectronics, wool treatment, seed germination, plasma medicine, surface treatment, gas breakdown and particle traps. This talk will attempt to summarise his main contributions to the field.

Positron Production and Cooling for Antihydrogen Production

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on behalf of the ASACUSA collaboration

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The ASACUSA Cusp collaboration at the Antiproton Decelerator of CERN aims at a precise measurement of the ground-state hyperfine splitting of antihydrogen, which promises to be one of the most sensitive tests of CPT symmetry. A dedicated antiproton-positron mixing trap serves as a source for a beam of antihydrogen atoms, which will undergo Rabi-type magnetic resonance spectroscopy [1]. Antiprotons are provided by the Antiproton Decelerator at CERN. Positrons come from a radioactive ^{22}Na source, which are slowed down using a neon rare-gas solid moderator and accumulated in a Surko-type buffer gas trap.

The collaboration has successfully observed antihydrogen 2.7 m away from the production region [2]. A measurement of the principal number distribution showed that most of the produced antihydrogen atoms are in high n states, which puts the next step on producing ground-state atoms. Calculations show that ground-state hydrogen production is best with a high density, low temperature positron plasma [3]. During the long shutdown 2 at CERN, in which antiprotons are not available, one focus will be on being able to provide cold positrons for the mixing process.

We will present our apparatus and methods used to produce, trap, accumulate, and condition positrons will be discussed. Planned new developments in positron temperature measurement and cooling will be shown, which will be important for improving the mixing efficiency for ground-state antihydrogen.

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