POSITRON

XVIII International Workshop on Low-Energy Positron and Positronium Physics

Book of Abstracts

POSMOL 2015

17-20 July 2015, LISBOA, PORTUGAL

XVIII International Workshop on Low-Energy Positron and Positronium Physics &
XIX International Symposium on Electron-Molecule Collisions and Swarms
17 - 20 July 2015, Lisboa, Portugal

POSMOL 2015

XVIII International Workshop on Low-Energy Positron and Positronium Physics

	Friday	Saturday		Sunday		Monday	
	17/07/2015	18/07/2015		19/07/2015		20/07/2015	
08:30 - 09:00		OPENING REMARKS					
09:00 - 09:45		PL01 - ALLAN		PL03 - BRAY		PL05 - TENNYSON	
09:45 - 10:15		TL01 - VARELA		TL09 - SUGAWARA		TLE15 - ORLANDO	TLP15 - KURODA
10:15 - 10:45		TL02 - DANIELSON		TL10 - CHIARI		TLE16 - RACKWITZ	TLP16 - STORRY
10:45 - 11:15		COFFEE BREAK		COFFEE BREAK		COFFEE BREAK	
11:15 - 11:45		TLE03 - DENIFL	TLP03 - GRIBAKIN	TLE11 - URQUIJO	TLP11 - LISZKAY	TLE17 - SAJEEV	TLP17 - ERIKSON
11:45 - 12:15		TLE04 - PTASINSKA	TLP04 - BETTEGA	TLE12 - DONKO	TLP12 - ASAI	TLE18 - VÁSQUEZ	TLP18 - NATISIN
12:15 - 14:00		LUNCH		LUNCH |COMMITTEES MEETING		LUNCH	
14:00 - 14:45		PL02 - BROMLEY		PL04 - PETROVIC		DEPARTURE	
14:45 - 15:15		TLE05 - GAY	TLP05 - MICHISHIO	TLE13 - ALVES	TLP13 - TATTERSALL		
15:15 - 15:45		TLE06 - COSTA	TLP06 - BRAWLEY	TLE14 - BOYLE	TLP14 - HOGAN		
15:45 - 16:15		COFFEE BREAK		COFFEE BREAK			
16:15 - 16:45		TLE07 - SWIDEREK	TLP07 - JONES	EXCURSION			
16:45 - 17:15	WELCOME RECEPTION AND REGISTRATION	TLE08 - KUMAR	TLP08 - MACHACEK				
17:15 - 19:00		POSTER SESSION | WG1 CELINA MEETING					
19:00 - 00:00				CONFERENCE DINNER			

XVIII International Workshop on Low-Energy Positron and Positronium Physics
Lisboa, Portugal
17-21 July, 2015

Edited by:
Paulo Limão-Vieira
Filipe Ferreira da Silva
Guilherme Meneses
Emanuele Lange
Tiago Cunha

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XVIII International Workshop on Low-Energy Positron and Positronium Physics

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Editorial

Dear Colleagues,

Welcome to Lisboa and POSMOL 2015, the XVIII International Workshop on Low-Energy Positron and Positronium Physics & the XIX International Symposium on Electron-Molecule Collisions and Swarms. POSMOL 2015 permits to achieve a very privileged forum of sharing and developing our scientific expertise on current aspects of positron, positronium and antiproton interactions with electrons, atoms, molecules and solid surfaces, and related topics, as well as electron interactions with molecules in both gaseous and condensed phases. Particular topics include studies of electron interactions with biomolecules, electron induced surface chemistry and the study of plasma processes. Recent developments in the study of swarms are also fully addressed. We are very pleased to host in Lisboa for the first time POSMOL 2015 with 160 delegates from 25 countries.

POSMOL 2015 promises to be an exciting and stimulating conference with 5 plenaries, 4 joint topical lectures, 28 oral presentations and more than 100 posters providing a very privileged opportunity of scientific discussions on positron and positronium physics, electron-molecule collisions and swarms.

Just before the meeting, we have arranged to honour our loyal colleague and trusted friend Steve Buckman, Professor of Physics and School Director at the Australian National University, Canberra, Australia, on the occasion of his retirement in acknowledgement of his many achievements in Atomic and Molecular Physics.

POSMOL 2015 local logo has been envisaged from a Portuguese caravel, a sailing ship developed in the 15th century by the Portuguese to explore along the West African coast and into the Atlantic Ocean, together with two crows as symbol of Lisboa and guardians of the city. Both crows appear in red and blue colours which have been a while ago adapted as to represent the positrons and electrons & swarms communities.

We would like to express our gratitude to the local organizing committee, in particular to Susana Sério, Guilherme Meneses, Tiago Cunha, Emanuele Lange and Ana Luísa Cruz (local secretary) who worked so hard and made this meeting happen.

Last but not least, we wish you a successful meeting and a pleasant stay in Lisboa.

Paulo Limão-Vieira

Gustavo García

Filipe Ferreira da Silva

POSMOL 2015 Chairs

Lisboa, July 2015

General Information

ACCESS TO CAMPUS DE CAMPOLIDE

Lisbon airport is located in the city centre. It is easy to reach Campus de Campolide by metro from the airport, Red Line from Airport to S. Sebastião. Campus de Campolide can be reached within 10 minutes walking from S. Sebastião station.

REGISTRATION

The registration desk will be located at the atrium of the Rectorate building from 16:00 to 19:00 on Friday 17th July.

VENUE FOR SCIENTIFIC PRESENTATIONS

The POSMOL 2015 opening will be held on Saturday 18th July at 08:30 in room A. The plenary lectures, joint topical lectures and positron lectures will be held in room A, whereas EMS lectures will in room B. Poster session will be held on Saturday 18th July from 17:15 to 19:00 in the atrium of the building.

ORAL PRESENTATIONS

Room A and B are equipped with desktop computer. Speakers are recommended to bring their presentations in ppt, pptx or PDF format on a USB pen drive. Speakers should upload their presentations in advance. Speakers who want to use their Mac laptops should bring DVI-VGA or DisplayPort-VGA adapter.

POSTER PRESENTATIONS

Posters should fit A0 size suitable for the boards. Posters may be displayed from Friday 16th July and should remain until the end the conference.

BADGES

Please have your badge all the time.

WELCOME RECEPTION AND CONFERENCE DINNER

The welcome reception will be held on Friday 17th July at the atrium and front garden of the Rectorate building and the conference dinner on Sunday 20th July at “Estufa Real”, Ajuda botanic garden.

POSTER PRIZE

The International Advisory Committees will award a poster prize to the best posters in EMS and Positrons. The winners will be announced during the conference dinner and awarded a € 50 prize each.

INTERNET ACCESS

There is free Wi-Fi internet access in the rooms and in the atrium of the Rectorate building. Details will be provided at the conference.

EPJD SPECIAL ISSUE

An EPJ D Special issue on "Advances in Positron and Electron Scattering" has been commissioned on topics related to the Workshop and Symposium.

Guest Editors: Paulo Limão-Vieira (Universidade Nova de Lisboa, Portugal), Gustavo García (CSIC Madrid, Spain), E Krishnakumar (Tata Institute of Fundamental Research, India), James Sullivan

(Australian National University, Australia), Hajime Tanuma (Tokyo Metropolitan University, Japan), Zoran Petrovic (Institute of Physics, Serbia & Montenegro).

1. This special issue of EPJ D provides an opportunity to have only original material, refereed and published quickly.
2. Accordingly, authors making a contribution should, on their own initiative, submit their paper to https://articlestatus.edpsciences.org/is/epjd . The style files of EPJ D must be used - they can be found at www.epj.org (in the pull-down of the LaTeX manuscript button in the left margin).
3. Articles submitted must be strictly journal length and quality and each will be refereed like any regular paper of its kind submitted to EPJ D.
4. All manuscripts should be submitted no later than December 31 2015.

MEALS

Lunch and coffee break are provided on 18^{th}, 19^{th} and 20^{th} July.

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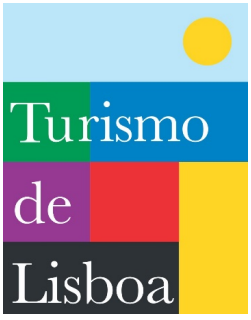
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QUINTA DA FOLGOROSA
PREMIUM WINES

SCIENTIFIC PROGRAMME OF THE XVIII INTERNATIONAL WORKSHOP ON LOW ENERGY POSITRON AND POSITRONIUM PHYSICS

Friday 17th July

16:45 – 19:00 REGISTRATION AND WELCOME RECEPTION (Campus Campolide)

Saturday 18th July

08:30 – 09:00 **Opening Remarks**

09:00 – 09:45 **Plenary Lecture** – Chair: E. Krishnakumar (Room A)
PL01: **M. Allan** (*University of Fribourg*)
"Nuclear dynamics in resonances, 2-dimensional EEL spectra, electrons and ionic liquids, electronic excitation and other stories."

09:45 – 10:15 **Session A** – Chair: M. Tachikawa (Room A)
TL01: **M. T. do N. Varella** (*University of São Paulo)*
"Electron-induced damage to biomolecules: from gas to condensed phase"

10:15 – 10:45 TL02: **J. R. Danielson** (*University of California*)
"Role of Vibrational Mode Coupling in Determining Positron Annihilation on Molecules."

10:45 – 11:15 COFFEE BREAK

11:15 – 11:45 **Session B** – Chair: R. Campeanu (Room A)
TLP03: **G. F. Gribakin** (*University of Nebraska)*
"Positronium scattering from noble-gas atoms at intermediate and low energies"

11:45 – 12:15 TLP04: **M. H. F. Bettega** (Federal *University of Paraná*)
"Cross sections for positron collisions with small molecules"

12:15 – 14:00 LUNCH

14:00 – 14:45 **Plenary Lecture** – Chair: S. Buckman (Room A)
PL02: **M. W. J. Bromley** (*University of Queensland*)
"The remorseless AMO physics of Jim Mitroy"

14:45 – 15:15 **Session C** – Chair: D. B. Cassidy (Room A)
TLP05: **K. Michishio** (*Tokyo University of Science)*
"Resonant Photodetachment of Positronium Negative Ions"

15:15 – 15:45 TLP06: **S. J. Brawley** (*University College London*)
"Positronium scattering below its break-up threshold"

15:45 – 16:15 COFFEE BREAK

16:15 – 16:45	**Session D** – Chair: V. Flambaum (Room A) TLP07: **A. Jones** (*University of California)* "Experiments with Rydberg Positronium"
16:45 – 17:15	TLP08: **J. R. Machacek** (Australian National University) "Positron scattering from molecules"
17:15 – 19:00	**Poster Session** **COST Action CM1301 CELINA WG1 Meeting**

Sunday 19th July

09:00 – 09:45	**Plenary Lecture** – Chair: Y. Nagashima (Room A) PL03: **I. Bray** "Theory of low-energy positron scattering on atoms and molecules"
09:45 – 10:15	**Session E** – Chair: G. Laricchia (Room A) TL09: **H. Sugawara** (*Hokkaido University)* "Electron behavior under characteristic magnetic fields applied to inductively coupled plasmas for control of charged particle transport"
10:15 – 10:45	TL10: **L. Chiari** (*Tokyo University of Science*) "Cross section measurements for positron and electron scattering from molecules of biological relevance"
10:45 – 11:15	**COFFEE BREAK**
11:15 – 11:45	**Session F** – Chair: J. Sullivan (Room A) TLP11: **L. Liszkay** (*CEA-DSM/IRFU)* "Progress with intense positron beams from compact electron accelerator based sources"
11:45 – 12:15	TLP12: **A. Ishida** (*University of Tokyo*) "New measurements of the Positronium Hyperfine Splitting"
12:15 – 14:00	**LUNCH**
14:00 – 14:45	**Plenary Lecture** – Chair: H. Cho (Room A) PL04: **Z. Lj. Petrovic** (*University of Belgrade*) "Swarms as an exact representation of weakly ionized gases"
14:45 – 15:15	**Session G** – Chair: J. Mohallem (Room A) TLP13: **W. Tattersall** (*Australian National University*) "Extending Monte Carlo transport simulations to dense structured fluids"
15:15 – 15:45	TLP14: **S. D. Hogan** (*University College London*) "Rydberg atom optics - from hydrogen to positronium"
15:45 – 16:15	**COFFEE BREAK**
16:15 – 19:00	**EXCURSION**
19:00	**CONFERENCE DINNER**

Monday 20th July

Plenary Lecture – Chair: I. Fabrikant (Room A)

09:00 – 09:45 PL05: **J. Tennyson** (*University College London*)
"Calculations of bound and continuum states of molecules using the R-matrix method"

Session H – Chair: D. Fursa (Room A)

09:45 – 10:15 TLP15: **N. Kuroda** (*University of Tokyo)*
"Production of an antihydrogen beam"

10:15 – 10:45 TLP16: **C. Storry** (*York University*)
"ATRAP Update"

10:45 – 11:15 COFFEE BREAK

Session I – Chair G. Gribakin (Room A)

11:15 – 11:45 TLP17: **S. Eriksson** (*Swansea University)*
"Towards laser spectroscopy of antihydrogen in the ALPHA experiment"

11:45 – 12:15 TLP18: **M. R. Natisin** (*University of California*)
"Ultra-high resolution, trap-based positron beams using a cryogenic buffer gas"

ABSTRACT INDEX

PL-01

Nuclear dynamics in resonances, 2-dimensional EEL spectra, electrons and ionic liquids, electronic excitation and other stories

Michael Allan and Khrystyna Regeta

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The talk will touch several subjects recently investigated in Fribourg:

2-D Electron Energy Loss spectra [1,2]. We show that 2D electron collision spectra contain rich information about the motion of a nuclear wave packet on a resonant potential surface - a key ingredient to understanding electron-induced chemistry. It is possible because the motion of the nuclear wave packet is characterized by a competition between propagation and detachment, the wave packet `rains down' along its path above the neutral potential surface and the final vibrational states carry (indirectly) information about where it rained down and thus allow us to `spy' on its trajectory. Changing the incident electron energy allows us to choose in which initial vibrational state (or boomerang state when the autodetachment is fast and the state is lifetime broadened) the resonance is prepared, i.e., into what direction (along what normal mode) is the nuclear wave packet initially sent. The spectra of the detached electrons carry information about the packet propagation, they tell us into what mode and into which quanta the wave packet dropped, and whether it changed modes by IVR.

Electrons and Ionic Liqids [3]. The instrument for low energy (0-30eV) electron impact spectroscopy, originally developed for gas phase molecules, is applied to room temperature ionic liquids (IL). Electron energy loss (EEL) spectra recorded near threshold, by collecting 0-2eV electrons, are largely continuous, assigned to excitation of a quasi-continuum of high overtones and combination vibrations of low-frequency modes. EEL spectra recorded by collecting 10eV electrons show predominantly discrete vibrational and electronic bands. The vibrational energy-loss spectra correspond well to IR spectra except for a broadening (~40 meV) caused by the liquid surroundings, and enhanced overtone activity indicating a contribution from resonant excitation mechanism. The spectra of four representative ILs were recorded in the energy range of electronic excitations and compared to density functional theory multireference configuration interaction (DFT/MRCI) calculations, with good agreement. The spectra up to about 8 eV are dominated by p-p^* transitions of the aromatic cations. The lowest bands were identified as triplet states. The spectral region 2-8 eV was empty in the case of a cation without p and p^* orbitals. The EEL spectrum of a saturated solution of methylene green dye in an IL band showed the methylene green EEL band at 2eV, indicating that ILs may be used as a host to study nonvolatile compounds by this technique in the future.

Electronic Excitation. Ethene, furan [4], benzene and pyrimidine will be compared and the common trends in the cross sections pointed out. The problem of connecting the electronic excitation cross section with neutral dissociation will be addresses by presenting an attempt to calculate the repulsive nature of the potential surfaces of the electronically excited states of $Pt(PF_3)_4$ [5].

References

[1] K. Regeta and M. Allan, *Phys. Rev. Lett.*, **110**, (2013), 203201.
[2] K. Regeta and M. Allan, *J. Chem. Phys.*, **142**, (2015), 184307.
[3] K. Regeta and M. Allan, *Phys. Chem. Chem. Phys.*, (2015), DOI: 10.1039/C5CP01417D
[4] K. Regeta and M. Allan, *Phys. Rev. A*, **91**, (2015), 012707.
[5] M. Zlatar, J. Fedor and M. Allan, (2015), in preparation.

PL-02

The remorseless AMO physics of Jim Mitroy

Michael W.J. Bromley

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In this lecture I will survey and attempt to summarise the scientific contributions that Prof. Jim Mitroy produced before his unexpected passing away in August 2014 [1]. Whilst he was never a dedicated follower of fashion, the research topics that he tackled during his lifetime were generally aligned with the scientific times. Over three decades he relied on a combination of computational approaches underpinned by an excellent theoretical understanding of Atomic, Molecular and Optical Physics. Armed with a keen nose for which problems were interesting enough and that he could remorselessly solve with the current generation of computers, he managed to regularly reinvent himself whilst still using many of the techniques that he developed early in his career. I will discuss, in loosely chronological order, his key discoveries, some of his nearly 200 papers, ideas, and modus operandi:

e^- Decade (1977-1989): The early years involved developing atomic structure methods and accurate (at the time) computer codes with an emphasis on electron-atom collisions:

- 1977-1983: PhD thesis in "Studies in atomic structure and (e, 2e) reactions" supervised by Ken Amos at The University of Melbourne.
- 1983-1986: Postdoctoral Researcher with Ian McCarthy at Flinders University in Adelaide.
- 1986-1988: Research Associate with David Norcross at JILA in Boulder, Colorado.
- 1988-1989: Research Fellow in Theoretical Physics at ANU in Canberra.

e^+ Decade (1990-2002): Began with his appointment in 1989 as a lecturer at the University College of Northern Territory (shortly thereafter renamed the Northern Territory University), and initially this period saw an adaptation of the electron-atom scattering methods to positron-atom collisions:

- 1993-1996: Sabbatical in 1993 with Andris Stelbovics at Murdoch University in Perth, sparked off a series of papers on positron-hydrogen scattering including re-arrangement [2].
- 1997-2000: Employed Gregory Ryzhikh (Ryjikh) to work on positron scattering off alkali metals, ended up discovering positronic lithium, and consequently a number of other positronic atoms along with myself (his only PhD student: 1998-2002) [3].
- 2000-2002: Employed Igor Ivanov, they solved the positronium-atom scattering problem.

Final Decade (2003-2014): His university changed its name to Charles Darwin University. He moved into photon-atom and atom-atom interactions, whilst maintaining positron related research. He enjoyed visiting San Diego, USA and Wuhan, China a number of times during this period:

- 2002-2003: Employed Sergey Novikov and described spin-orbit quenching of positronium.
- 2003-2014: Employed Jun-Yi Zhang, Li-Yan Tang, Jun Jiang and Yongjun Cheng. Computed atom-atom and photon-atom interactions, published a major review article in 2010 [4].
- 2006-2013: Core member of the Australian National Centre of Excellence for Antimatter-Matter Studies, and contributed broadly to its success. Led major method review article [5].

References

[1] M.W.J.Bromley, S.J.Buckman, C.W.Clark , *Physics Today Obituary*, (2015). http://scitation.aip.org/content/aip/magazine/physicstoday/news/10.1063/pt.5.6137

[2] J.Mitroy, "Close Coupling theory of positron Hydrogen scattering", *Aust.J.Phys.,* **46** (1993), 751.

[3] J.Mitroy, M. W. J. Bromley and G. G. Ryzhikh "Positron and Positronium binding to atoms" *J.Phys.B,* **35** (2002), R81.

[4] J. Mitroy, M.S.Safronova, C.W.Clark, "Polarizabilities of atoms and ions" *J.Phys.B,* **43** (2010), 202001.

[5] J.Mitroy, S.Bubin, K.Varga, Y.Suzuki, W.Horiuchi, L.Adamowicz, W.Cencek, et al. "Theory and application of explicitly correlated gaussians" *Rev.Mod.Phys.,* **85 (**2013), 693.

PL-03

Theory of low-energy positron scattering on atoms and molecules

I. Bray, D. V. Fursa, A. S. Kadyrov, J. J. Bailey and M. C. Zammit

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In recent years there has been considerable progress in the theory of positron scattering on atoms and molecules. So much so that in the case of the atomic hydrogen target the collision system can be formulated without approximation and solved computationally. The major complexity, incorporation of the positronium (Ps) formation channels, can be done routinely with the usage of complete two-centre square-integrable expansions. The accuracy of such approaches can be tested internally, without reference to experiment.

In the case of targets more complicated than atomic hydrogen, such as helium or the hydrogen molecule, the complexities are immense. Yet from the perspective of theory the goal is to provide an accurate formalism that is valid at all energies, and is sufficiently general to apply to rearrangement collisions more broadly, such as in proton-atom/molecule scattering. In the talk we shall discuss the various unique aspects of the positron-atom/molecule collision systems and their computational complexity.

PL-04

Swarms as an exact representation of weakly ionized gases

Zoran Lj. Petrović, Saša Dujko, Dragana Marić, Danko Bošnjaković, Srđan Marjanović, Jasmina Mirić, Olivera Šašić, Snježana Dupljanin, Ilija Simonović, Ronald D. White*

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Often swarms are regarded as idealized ensembles of charged particles that may be realized in specialized experiments to provide accurate transport coefficients, which after some analysis, yield "complete" sets of cross sections and accurate representations of non-equilibrium electron energy distribution function (EEDF) for a given *E/N*. Generally it is believed nowadays that swarms are just a tool for modeling non-equilibrium (low temperature) plasmas, as some kind of an interface through which atomic physics enters plasmas. In this review we shall show some new results that extend that picture into several directions:

- New results for the cross sections in systems where information from beam experiments and binary collision theories are insufficient such as $C_2H_2F_4$ that is commonly used as a cooling gas in modern refrigerators and air conditioners, but also it is used in particle detectors and has a potential for plasma processing applications.
- Ionized gases where swarms are exact representation of the system. Those include weakly ionized gases such as atmosphere, gas breakdown, afterglow (after the breakup of the ambipolar field), steady state Townsend regime of discharges, conduction of electricity through gases, interaction of secondary electrons produced by high energy particles with the gas or liquid background and many more. A special example will be modeling of Resistive Plate Chambers, the most frequently used gas phase detectors of elementary particles in high energy experiments.
- Swarm studies provide best insight into non-hydrodynamic (or as plasma specialists call it non-local) development of the ionized gas. It is not only that simulations are simple but also some of the accurate experiments operate in such conditions and thus allow testing of such theories. One such example are the Franck Hertz oscillations. Temporal and spatial relaxation of properties of ensembles to the final distribution belong to this group as well and are of interest for a number of positron applications and trapping in general.
- Fluid models when applied to swarms provide a good way to test the fluid models as used in more general plasmas. This has yielded the need to generalize fluid equations and extend them to a one step further while using a higher order transport coefficients.
- Finally we shall address the open issues for transport theorists and atomic and molecular collision population in the attempt to represent transport of electrons, positrons and other particles in liquids, especially in water that has a strong dipole moment. Hydrated electrons and positrons are the actually particles of interest for modeling these particles in the human tissue.

As an interface between atomic and molecular collision physics on a lower phenomenological (but deeper) level and plasmas on a higher (but less fundamental) level swarm physics has the responsibility of providing plasma physics with its intellectual basis and fundamental importance. It is how we combine the building blocks of atomic and molecular physics, transport theory and other relevant elementary processes that will define generality of the conclusions about non-equilibrium plasmas that are all different and require a special approach.

The models that we provide here are simple, yet realistic and real systems that may be described by swarm models and that may be regarded as low ionization limits of some more complex non-equilibrium plasmas.

PL-05

Calculations of bound and continuum states of molecules using the R-matrix method

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The R-matrix method involves the division of space into an inner region, where the detailed physics of the process under consideration takes place, and an outer region where asymptotic methods can be applied. The method was originally developed by Wigner to look at resonances in nuclear reaction; it remains a particularly powerful procedure for characterising resonances. The R-matrix method is now widely used to study collision problems involving electrons and positrons, as well as photionisation [1]. In particular it is a popular method low-energy electron-molecule collision problems [2].

Besides the systematic push to study larger molecules, electron-molecule collision calculations are also becoming more reliable. Thus recent R-matrix studies of the bound [3] and continuum [4] states of N_2 have mapped out these states with an unprecedented level of detail and accuracy. Progress on the use of the R-matrix for electron-molecule collision calculations will be considered. This issue of how these studies might be adapted to incorporate uncertainties will be discussed.

Positron-molecule collision calculations are generally more challenging than their electron counterparts. The R-matrix with pseudostates method (RMPS) was originally developed to extend the energy range of low-energy electron collision studies. However the more rigorous treatment of polarisation effects obtained using RMPS procedures has been found to significantly improve the treatment of positron-molecule collisions.

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[3] D.A. Little and J. Tennyson, *J. Phys. B: At. Mol. Opt. Phys.*, **46**, (2013), 145102.
[4] D.A. Little and J. Tennyson, *J. Phys. B: At. Mol. Opt. Phys.*, **47**, (2014), 105204.
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TL-01

Electron-induced damage to biomolecules: from gas to condensed phase

Márcio T. do N. Varella, Lucas M. Cornetta, Fábris Kossoski, Sylvio Canuto, Kaline Coutinho

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The role played by secondary electrons in the radiation damage to biomolecules is well established both in the gas phase [1] and in aqueous solution [2]. In this process, electrons released along the track of high-energy photons attach to biomolecules and give rise to dissociative transient negative ions (TNIs) that induce DNA strand breaks.

In this talk, we will address the TNI spectra of 5-halouracils, a well-known class of radiosensitizing drugs (chemicals that can enhance the efficiency of the radiation treatment of cancer cells), as obtained from bound-state and elastic scattering calculations below the electronic excitation thresholds, i.e., accounting for stable anions and shape resonances. All 5-X-uracil molecules, with X=F, Cl, Br and I, present rich spectra comprising dipole bound states, valences bound states and shape resonances. While the energies of the π^* anion states are not strongly dependent on the halogen substituent, the σ^*_{CX} shape resonances are strongly stabilized from 5-F-uracil to 5-I-uracil, ultimately suppressing the electron-induced hydrogen elimination reactions in the heavier species.

We also address free-energy barriers for the dissociation of nucleotide anions in aqueous solution. While the gas-phase studies have proven essential to understand the basic mechanisms for dissociative electron attachment, at least some of these mechanisms would not be expected to be as important in aqueous environment, e.g., those triggered off by dipole bound states or those involving the elimination of hydrogen atoms (in gas phase) that take part in hydrogen bonding with solvent molecules. The nucleotides can be viewed as prototypes for the DNA strands, as they comprise the nucleobase, sugar and phosphate units. However, the study of these systems in solution would challenge the scattering methods, such that we restrict our calculations to stable anions, therefore employing bound-state electronic structure techniques. At the present stage, our main goal is developing a protocol to approach the dissociation in liquid phase, such that we explore a number of relevant technical aspects, namely the choice of basis sets, correlation-exchange functionals in density functional theory (DFT) computations, as well as the use of continuum (implicit) solvation models, wherein the solvent is treated as a polarizable dielectric, or explicit solvent (water) molecules.

We employ several well-established techniques in the present studies. The scattering calculations were carried out with the parallel implementation [3] of the Schwinger Multichannel Method implemented with pseudopotentials [4]. The implicit solvation studies employed the SMD approach [5], while explicit solvation was described with Monte Carlo techniques [6]. The bound state calculations were carried out with standard quantum chemistry techniques (DFT and coupled-cluster).

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TL-02

Role of Vibrational Mode Coupling in Determining Positron Annihilation on Molecules

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Positron collisions with molecules at incident positron energies in the range of the molecular vibrations can result in attached states formed *via* vibrational Feshbach resonances (VFRs) [1]. While the resulting positron-molecule complexes are not a true bound states, but resonances, the attached positron has an increased probability of annihilation. The resulting annihilation rate is determined by a competition between annihilation and vibrational auto-detachment. This talk summarizes our current state of knowledge regarding these effects - processes that dominate positron annihilation on most molecules at low energies - and current outstanding questions are highlighted.

A theory of resonant annihilation on isolated VFRs (so-called "entrance channels") is successful in predicting the annihilation rates for selected small molecules such as methyl halides [1]. However, the picture is typically more complicated. A key consideration (e.g., in alkanes and molecules with additional halogen substitutions) involves vibrational coupling to other modes (a process known in the chemistry community as intramolecular vibrational energy redistribution or IVR) [2]. The auto-detachment rate depends critically whether the molecular vibrational energy resides (or does not reside) in a mode that couples the attached positron to a continuum state. The former is dubbed an "escape" channel and the latter a "dark state."

These mode-coupling effects can be greatly enhanced by the close proximity of multimode vibrations to the entrance channel (i.e., near-resonant combination and overtone modes). For example, if one of the components of a multimode vibration is an escape-channel vibration, the VFR is strongly suppressed; and if the entrance channel couples strongly to dark-state multimodes (e.g., alkane molecules), the resonant annihilation can be greatly enhanced.

A simple model will be discussed that highlights the role that vibrational mode coupling plays in determining the strengths of the annihilation resonances, and the multimode vibrational structure of specific molecules will be related to observed annihilation-rate spectra [3]. With these pictures in mind, the relationship between the mode coupling effects studied in typical IVR experiments and those responsible for resonant positron annihilation will be discussed. The talk concludes with a focus on issues yet outstanding that need be addressed in order to make quantitative predictions of annihilation rate spectra when mode-coupling effects are operative.

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+ In collaboration with M. R. Natisin and C. M. Surko.

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TLP-03

Positronium scattering from noble-gas atoms at intermediate and low energies

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The starting point of our work was the observation of a striking similarity between the measured positronium (Ps) and electron total scattering cross sections for a number of atomic and molecular targets, including the noble gases, H_2, N_2, O_2, H_2O, CO_2 and SF_6 [1,2], when plotted against the projectile velocity for $v = 0.5{-}2$ a.u. This is particularly surprising given that one of the projectiles (Ps) is neutral, while the other (electron) is charged. Our calculations for Kr and Ar [3] show that this phenomenon can be explained quantitatively using the impulse approximation (IA). It is applicable to Ps collisions at intermediate energies since Ps is a diffuse system, and it allows one to express the scattering amplitude for the composite particle (Ps) in terms of the electron and positron scattering amplitudes. The latter are taken from the polarized-orbital calculations [4], and are mostly affected by the static and exchange (for the electron) potential of the target. For $v > 0.5$ a.u. we also include the contribution of the Ps ionization cross section [5]. In the velocity range of interest, the electron scattering cross section is considerably greater than the positron cross section, which ensures that the Ps-atom scattering cross section is close to the electron scattering cross section for the same velocity, as found in the experiment.

At lower energies ($v < 0.5$ a.u.) the electron and positron scattering are strongly affected by the long-range polarization potential. The IA is not valid for the low-velocity Ps, producing the scattering cross section much in excess of expected values. Here we develop an alternative approach and construct an effective Ps-atom potential using the electron-atom and positron-atom pseudopotentials [6]. The resulting "static-exchange" Ps-atom interaction is repulsive. Including the attractive van der Waals interaction (which plays a relatively small role) reduces the cross section at low velocities. When the Ps ionization cross section is added, the calculated cross section merges with the results of the IA calculation for $v > 0.5$ a.u. and is in good agreement with experiment [1]. We thus obtain a reliable picture of Ps scattering from atomic targets at both low and intermediate energies.

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TLP-04

Cross sections for positron collisions with small molecules

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In a recent joint theoretical and experimental effort involving research groups from Italy, Spain, Australia and Brazil, we investigated positron collisions with several molecular targets [1]-[8], by carrying out calculations of elastic and total cross sections and measurements of total cross sections. The total cross sections show differences when compared to previous measurements at low energies, which can be explained by differences in the angular discrimination of the experimental apparatus. The elastic cross sections were computed using the Schwinger multichannel (SMC) method [9], for energies up to 10 eV, in the static plus polarization approximation. In particular, these SMC calculations have not included the positronium formation channel. Total cross sections, including positronium formation, were computed using the IAM-SCAR method [10], which works well for higher energies. The elastic cross sections and the total cross sections differ at low energies. We will discuss possible reasons for these discrepancies. We will also discuss the presence of a virtual state and of a Ramsauer-Townsend minimum for non-polar molecules. Some recent results for elastic collisions of positrons with methylamine [11], propene and cyclopropane [12], and allene will also be presented.

Acknowledgments

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TLP-05

Resonant Photodetachment of Positronium Negative Ions

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The positronium negative ion, a bound state of two electrons and a positron, is one of the simplest three-body system interacting via Coulomb forces. This ion provides a good testing-ground for the quantum-mechanical three-body problem since its constituents have a unique mass ratio compared with H^- or H_2^+. Numerous theoretical studies on the ion have been addressed to elucidate the bound-state property not only for a ground state [1] but for the autoionization states [2-5], which were predicted in its photodetachment or positronium-electron scattering. However, because of the difficulty owing to low ion intensity and short annihilation lifetime (479 ps), experimental verifications were limited to few measurements of the annihilation rate [6]. More recently, we have found an efficient emission of positronium negative ions by implantation of slow positrons onto tungsten surfaces covered with sub-monolayer alkali-metals [7]. This opens up researches on observation of its photodetachment [8], subsequent generation of energy-tunable positronium beams [9] and further optical measurements.

In the present work, we demonstrate a laser spectroscopy of positronium negative ions, in which the ions were efficiently generated through this fashion. Bunches of the ions were generated by implantation of pulsed slow positrons from KEK Slow Positron Facility onto a tungsten surface covered with 0.3 monolayer Na. The photodetachment of the ions was induced by ultraviolet laser beams (225 - 230 nm) from a tunable dye laser, and the number of fragment positronium atoms was measured as a function of the wavelength. We have observed a $^1P^o$ shape resonance, in which the electron is temporarily trapped by a centrifugal barrier potential, slightly above Ps (n=2) formation threshold. The obtained resonance parameters (resonance energy and width) are in good agreement with three-body calculations [2, 3, 5]. The experimental details as well as the progress of the positronium negative ion spectroscopy will be discussed at the Workshop.

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TLP-06

Positronium scattering below its break-up threshold

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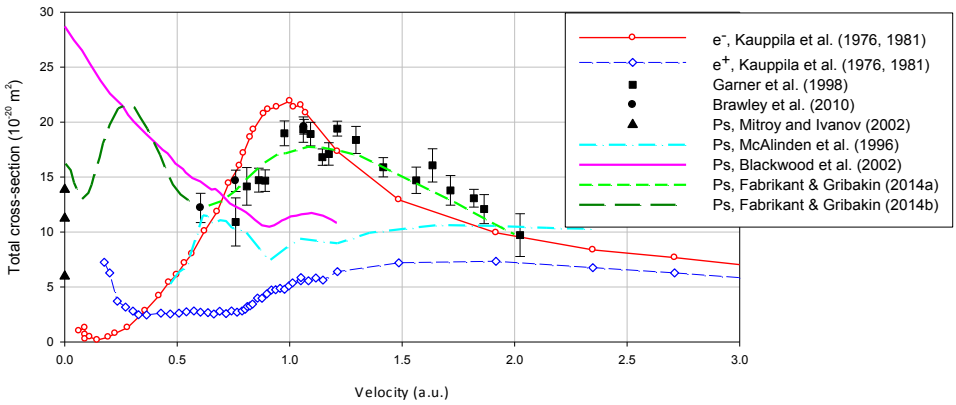
Scattering experiments with positronium (Ps), the unstable bound state of an electron and its antimatter partner, the positron, have thus far been performed at intermediate energies for a variety of atoms and simple molecules e.g. [1]. Within this range, ground state Ps atoms – formed from the interaction of a positron beam with a gaseous production target e.g. [2] – have been found to scatter with a similar total cross section to that for equivelocity electrons, even near velocities at which resonances have been observed [3]. Recently, an impulse approximation has been employed to provide a theoretical explanation of this similarity at intermediate energies [4] whilst, at low energies, a different approach [5] has predicted major differences between the projectiles (see Figure 1).

Figure 1. Total cross-section of Ps + Ar in comparison with theories and those for equivelocity electrons and positrons.



Until now, low Ps beam intensities had restricted measurements to energies greater than 7 eV (0.5 a.u.), with experiment thus unable to access the potentially rich structure suggested by low-energy electron scattering results. However, guided by new insights into the scattering of Ps [1], Ps beams have been successfully produced and are being employed down to 1.5 eV incident energy. New total cross section data will be presented for Ps collisions with Ar, Xe, CF_4, O_2 and N_2.

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TLP-07

Experiments with Rydberg Positronium

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I will report on recent experimental work done at UCR involving the preparation and control of Rydberg positronium (Ps) atoms [1-3]. We have constructed a TOF apparatus, in which Rydberg Ps are produced by 1S→2P laser excitation of Ps from a suitable target, followed by 2P→Stark-split states of principle quantum number *n* from 10 up to the term limit. The Rydberg Ps is detected at the end of a ~1.5 m flight path after flight times of up to ~50 μs. This apparatus provides us with precise measurements of the energies of individual atoms and therefore can be used to probe in detail the mechanisms of Ps production by various targets. The earliest realization of the device required a significant Doppler correction, which could be accurately applied from knowledge of the Ps TOF [4]. Later improvements to the design, using a crossed beam geometry, yielded measurements that were virtually first-order Doppler free [5]. Measurements of the energy spectra of Ps emitted from metal organic framework (MOF) targets have demonstrated conclusively the propagation of Ps through the crystals in Bloch waves, resulting in a series of narrow energy Ps peaks [6-8]. Measurements on a Cu(110) target at ~120K have yielded the Ps negative affinity 2.54±0.02 eV with a resolution comparable to that achieved via angle-resolved photoelectron spectroscopy (ARPES).

This work was supported in part by the US NSF under grant no. PHY 1206100, and by the DOE BES DE-FG02-13ER46972.

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TLP-08

Positron scattering from molecules

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We will discuss our recent experimental results for positron scattering with simple molecules. For this comparison we will focus on positron scattering from molecular hydrogen (H_2) [1] and water (H_2O) [2]. The aim of this work was to provide absolute positron scattering information for two small molecules. Since these results are absolute, they can be used as a benchmark for theory, which is particularly important about the positronium formation threshold. In both cases, comparisons will be made with the most recent theoretical results. Measurements to be presented include the grand total scattering cross section, positronium formation cross section, and the elastic scattering cross section and the total inelastic scattering cross section (other than Ps formation) as well as the elastic differential scattering cross section at a number of energies. An example of the comparisons to be made is shown in figure 1. The scope for further measurements in these systems will be discussed.

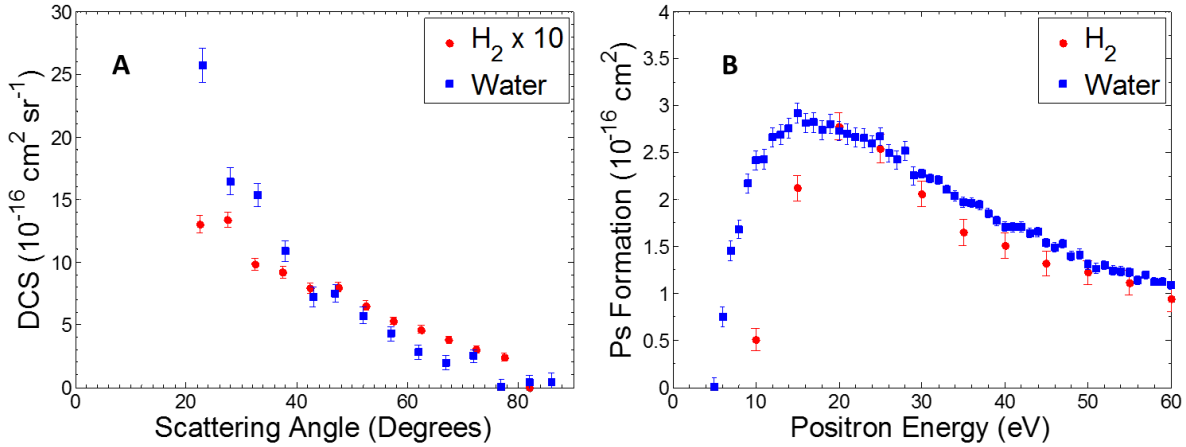

Figure 1: (**A**) Comparison of the elastic differential scattering cross section for water [2] and molecular hydrogen [1] for a scattering energy of 1 eV. (**B**) Comparison of the positronium formation cross section for water [3] and molecular hydrogen [1].

The experimental measurements were carried out using the low-energy positron beam line at the Australian National University. The magnetically confined positron beam can be tuned from below 1 eV up to 200 eV with a variable energy resolution, which was typically 60 meV. A calibrated capacitance manometer was used to determine the absolute number density of the target vapour. The scattered and unscattered positron beam was energy analysed. Details of the experimental operation will also be briefly covered in the presentation.

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TL-09

Electron behavior under characteristic magnetic fields applied to inductively coupled plasmas for control of charged particle transport

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Electron motions in inductively coupled plasmas under characteristic magnetic fields (***B*** fields), quadrupole magnetic field (QMF, fig. 1) and confronting divergent magnetic fields (CDMFs, fig. 2), are presented.

The QMF induced by three coaxial coils [1] consists of two pairs of antiparallel gradient magnetic fields (APGMFs) around a ring of $\boldsymbol{B} = 0$ called neutral loop (NL, corresponding to $x = z = 0$ in fig. 1). As well as gyration around magnetic field lines, electrons undergo directional drifts along the NL [2]. This directionality originates in the APGMFs [3] and is position-dependent; electrons under the weak ***B*** field near the NL meander to one direction, and those under the strong ***B*** field far from the NL gyrate and drift to the opposite direction [4,5] (the grad-*B* drift). This would result in a rectification of the loop plasma current along the NL in the coupling with the one-turn rf antenna. An experimental result [6] suggests an appearance of the rectification as an asymmetric rf emission. The rectification is an interesting effect to be confirmed by measurement.

The CDMFs formed by two coils [7] have a point of $\boldsymbol{B} = 0$ (X point). The plasma, driven by a planar spiral rf antenna, is divided into the upper and lower parts by the separatrix. The ***B*** field in the upper region guides the accelerated electrons sideways. This prevents the electrons from straight diffusion to the lower region. However, two ways of downward electron diffusion are considered. One is scattering near the separatrix. By the displacement of the gyrocenter, some of the scattered electrons transfer their guiding magnetic field lines from those of the upper region to those of the lower region. This is likely to occur for high-energy electrons with long gyroradii. The $\boldsymbol{E} \times \boldsymbol{B}$ drift synchronous to the rf ***E*** field also assists electrons to cross the separatrix. The other is passage through the weak ***B*** field around the X point. This process is easy even for low-energy electrons. The electron diffusion across the separatrix is controllable by the ***B*** field. Evaluation of the selectivity and efficiency would lead to active use of separatrix, e.g., as a magnetic shutter or filter.

This work was supported by JSPS grants-in-aid 22540500 and 25400528, and by ULVAC Inc.

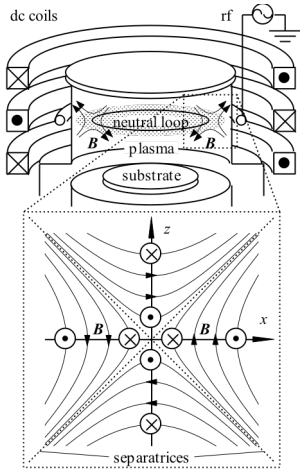

Figure 1. Quadrupole magnetic field. Directionality appears in the azimuthal electron drift.

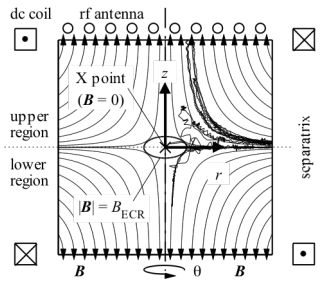

Figure 2. Confronting divergent magnetic fields. The separatrix suppresses downward electron diffusion. $B_{\mathrm{ECR}} = 2\pi(m/e)f_{\mathrm{rf}}$ is the rf-resonant magnetic field strength.

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TL-10

Cross section measurements for positron and electron scattering from molecules of biological relevance

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Ionising radiation is widely used in modern medical technologies, both for imaging and therapy. Positrons, in particular, lie at the heart of Positron Emission Tomography (PET), one of the most common tumour diagnostics. Positron thermalisation within the body, from the moment of release to positronium (Ps) formation or annihilation, involves an energy loss of six orders of magnitude and induces a cascade of ionisation events liberating several thousand low-energy electrons. Both the primary positrons and the secondary electrons may cause cell damage or mutations, e.g. by initiating DNA lesions. However, their energy deposition mechanisms remain mostly unknown. Hence investigations into low-energy charged-particle interactions with molecules of biological importance, such as the cellular components and their analogues, are needed to assess any potential charged-particle-induced damage.

We present cross sections measurements for positron and electron collisions with a variety of biologically relevant targets, including water [1], the sugars in the DNA backbone [2-4] and the nucleobases [5-7]. Total and integral cross sections, as well as angular distributions, are reported at incident energies from 1 eV to a few hundred eV. The positron experiments were carried out using two different spectrometers: the high-resolution buffer-gas trap and positron beam apparatus at the Australian National University and the very low-energy apparatus at the University of Trento. The electron-impact measurements were conducted using the cross-beam apparatus at Flinders University.

Accurate measured cross sections, in conjunction with energy loss and resonant dissociative electron attachment data, are fundamental in order to improve the current understanding of lepton interactions with living tissue. They also contribute to the development of more precise charged-particle track simulations and positron nano-dosimetry models, which will improve the current knowledge of the mechanisms of sub-cellular damage. This is essential for the future development of more efficient and safer positron-based medical technologies.

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TLP-11

Progress with intense positron beams from compact electron accelerator based sources

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Electron accelerator based slow positron sources are viable alternatives for sources based on radioactive isotopes. Electron linacs can generate slow positrons with significantly higher intensity than practically available beta sources. However, high energy electron accelerators used for positron production were large-scale devices, available often only intermittently or dedicated devices with high electron energy, consequently with a significant activation of the instrumentation when not in use.

Ideally, a slow positron source must be a compact device, with no remaining activity in the "off" state and no significant radiation dose outside the device other than low energy positrons and their annihilation gamma rays. The positron generator should provide both a continuous beam and pulses sufficiently short for positron lifetime spectroscopy, with high brightness in both modes. Finally, it should be compact enough to be implemented in any laboratory. We discuss to what extent compact electron linac –based positron generators can fulfil these requirements.

The group at CEA/IRFU, working on the positron source of the GBAR experiment (Gravitational Behaviour of Antihydrogen at Rest, CERN [1]), has built a slow positron generator in Saclay using a low energy (4.3 MeV) linear electron accelerator (linac). The positron generator serves not only the development of GBAR instrumentation but it is also a prototype of a possible new generation of compact, radioactive contamination-free positron sources. It can supply slow positrons with up to $3x10^6$ e^+/s intensity either in quasi-continuous mode to a beam line dedicated to positron spectroscopy or in pulsed mode to a positron accumulator. We discuss the performance of the source and possible improvements in beam intensity and quality on the basis of our experience.

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TLP-12

New measurements of the Positronium Hyperfine Splitting

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Positronium (Ps) is an ideal system for the research of the quantum electrodynamics (QED) in bound state. The ground state hyperfine splitting (HFS) of positronium gives a good test of the bound state calculations. Non-Relativistic QED calculations [1] have revealed a 16 ppm (4.5σ) discrepancy of Ps HFS value between the QED prediction and the previous experimental average [2,3]. The discrepancy might be because of possible common systematic uncertainties in all the previous experiments. One possibility is the unthermalized o-Ps contribution (Ps thermalization is a process that Ps loses its kinetic energy from initial energy E_0 to room temperature), which has already been shown to be significant in o-Ps lifetime puzzle [4,5]. Another possibility is non-uniformity of magnetic field.

We performed two new measurements of the Ps HFS. One was a precision measurement with conventional indirect method using the Zeeman effect which reduced the possible systematic uncertainties and provided an independent check of the discrepancy [6]. The other was the world's first direct measurement with a newly developed optical system using a frequency-tunable gyrotron and a Fabry-Pérot cavity [7]. The indirect method has an advantage of precision of HFS measurement over the direct method, while the direct method has an advantage that it is free from systematic uncertainties of static magnetic field because it does not use the Zeeman effect.Our indirect measurement was the first measurement which treated the Ps thermalization effect on HFS correctly. It resulted in a new independent value of HFS = 203.3942 ± 0.0016(stat., 8.0 ppm) ± 0.0013(syst., 6.4 ppm) GHz. This result is consistent with theory within 1.1σ, whereas it disfavors the previous experimental results by 2.6σ. It shows that the Ps thermalization effect is crucial for precision measurement of HFS.

The direct measurement obtained the Breit-Wigner resonance of the transition from o-Ps to p-Ps. The result was HFS = $203.39\ ^{+0.15}_{-0.14}$ (stat.) ± 0.11(syst.) GHz, which is consistent with theory within its uncertainty. This measurement also obtained the first direct measurement of p-Ps decay rate ($\Gamma_{p\text{-}Ps}$) at the same time, which resulted in $\Gamma_{p\text{-}Ps} = 11.2\ ^{+1.9}_{-2.3}$ (stat.) ± 1.3 ns^{-1}, which is also consistent with theory. Our system opens up new era of millimeter-wave spectroscopy, and enables us to directly determine both the HFS and $\Gamma_{p\text{-}Ps}$.

Both of the two measurements can be improved by forming Ps and performing spectroscopies in vacuum, using a high-intensity slow-positron beam. In this talk, details of the two measurements will be presented, followed by brief prospects for improved precision in future experiments.

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TLP-13

Extending Monte Carlo transport simulations to dense structured fluids

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Monte Carlo modeling is an effective method for predicting positron transport in soft-condensed matter for applications such as Positron Emission Tomography. However, there are a number of issues in existing models that we seek to overcome.

We have developed a new Monte Carlo model that implements a number of features not found in existing models. In particular, our model allows for fully-differential positron-impact ionization cross-sections, where the sharing of energy and momentum between the positron and the ejected electron is sampled from probability distributions. We will present new work [1] highlighting the importance of this effect, particularly on the spatial and temporal relaxation of positrons.

We have also developed two methods for including the effects of coherent scattering by a dense structured fluid. The first method employs a static structure factor, and requires similar approximations to those of Boltzmann equation solutions of the same system [2]. We will present our technique, showing its agreement with the equivalent Boltzmann equation solution for benchmark systems.

The second method directly samples the dynamic structure factor, which allows the rigorous modeling of positron transport in liquid-phase material, including both thermal effects and coherent scattering from temporally and spatially correlated scatterers. We highlight the importance of high-quality dynamic structure factors and scattering cross section sets.

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TLP-14

Rydberg atom optics - from hydrogen to positronium

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Atoms in highly excited Rydberg states can possess very large electric dipole moments. For states with principal quantum numbers $n > 16$ ($n > 11$ in positronium), these dipole moments exceed 1000 D. As a result inhomogeneous electric fields can be exploited to efficiently control the translational motion of samples in these states [1,2]. This has led, over the last decade, to the experimental realization of Rydberg atom optics elements including electrostatic mirrors [3], lenses [4], and traps [5,6]. In these devices atoms with initial kinetic energies of up to 40 meV can be decelerated to zero mean velocity, and trapped, in the laboratory-fixed frame of reference [7].

In high Rydberg states of positronium, the electron-positron annihilation rate is negligible and these states decay predominantly via radiative processes. For each value of n the resulting fluorescence lifetimes are twice as long as those in the hydrogen atom. These long lifetimes, and the possibility of generating dense thermal samples of positronium, with kinetic energies of ~25 meV, by implantation of positrons into room temperature silica targets [8], suggests that the Rydberg atoms optics elements listed above can also be implemented for the efficient manipulation of the translational motion of Rydberg positronium.

In this talk I will first describe experiments in which Rydberg atom optics elements have been used to decelerate and trap hydrogen Rydberg atoms. I will then discuss recent experiments in which positronium atoms have been excited to selected Rydberg-Stark states [9], with a view to implementing similar approaches for focussing, decelerating and trapping these samples. The resulting trapped or velocity-controlled beams of Rydberg positronium are expected to be well suited for (1) precision spectroscopic studies, (2) gravitational free-fall measurements, and (3) low-energy scattering.

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TLP-15

Production of an antihydrogen beam

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Antihydrogen atom, a positron bound to an antiproton, is one of the favorable target to test CPT symmetry via high resolution comparisons with hydrogen atom. The ASACUSA collaboration is aiming to perform a ground-state hyperfine spectroscopy of antihydrogen atom in-flight [1]. A cusp trap scheme to produce spin-polarized antihydrogen beams has been proposed [2]. The cusp trap consists of a magnetic field produced by an anti-Helmholtz coil and an electrostatic well by a multiple ring electrodes, which is utilized to synthesize antihydrogen atoms and produce anti-atomic beams [2,3]. Recently, important milestones had been reported; synthesis of antihydrogen atoms in the cusp trap[4] and detection of flow of antihydrogen atoms [5]. Since then, the collaboration has upgraded experimental apparatuses in order to perform the planned high precision spectroscopy. An asymmetric double-cusp magnetic field configuration was adopted to improve focusing power for and polarizability of antihydrogen beams. An antiproton trap and a positron accumulator were modified for the purpose as well. The latest status of the ASACUSA CUSP experiment for antihydrogen spectroscopy will be discussed.

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TLP-16

ATRAP Update

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Our ATRAP collaboration at CERN is focused on comparing the predicted symmetry between matter and antimatter in 2 ongoing experiments. In each case relativistic antiprotons are produced by collisions and then are slowed in a decelerating ring to energies of 5MeV. These antiprotons are ejected from CERNs accelerator/decelerator system to experiments and then are further slowed and captured in a Penning trap using a degrader foil, a gas tuning cell and a cloud of electrons to cool them to a temperature of 4 kelvin.

One of these antiprotons is held in a small Penning trap located within a strong magnetic gradient which shifts its motional frequencies depending on the particles quantum state. Measurements of the antiproton magnetic spin flip transition frequencies, a measure the particles magnetic moment, are identical to those in the proton at the present measurement precision. Increased precision in comparing the antiproton and proton magnetic moment are ongoing at CERN.

In our second experimental zone record numbers ($>10^7$) of antiprotons are loaded into the lower section and ($>4 \times 10^9$) positrons (e^+) are loaded into the upper section of a larger Penning trap cooled to ~1 Kelvin. The middle sections of this trap is surrounded by superconducting coils (Ioffe trap) which, when energized, produce a magnetic gradient of ~1T within the Penning trap electrode volume. In this apparatus the antiprotons and positrons are combined producing thermal antihydrogen atoms, some of which are trapped for up to 1000 seconds within the magnetic gradient, neutral particle trap. Our ATRAP collaboration is now assembling a continuous wave laser source at 121nm to cool these atoms further and a powerful laser system at 486nm for precise measurements of the 1S-to-2S, two-photon transitions in antihydrogen for comparison with matter hydrogen atoms.

In a separate experimental program also in atomic physics, a new exotic atom (e^+H^-) has been produced and detected for the first time in my labs at York University. Here a positron is captured in a hydrogenic, Rydberg, atomic state around a H^- ion by the process of radiative recombination. These experiments may be extended in our nuclear reactor based e^+ system (MIPBF) being developed. In this system a beam of 10^9 low energy e^+/s produced near the reactor will be directed to a number of ports. One of these brings e+ over a 10m distance to a e^+ accumulator optimized for these reactor e^+. Our record setting radioactive source based e^+ rates for slowing and trapping coupled with this reactor system has unprecedented potential for trapped e^+ research in atomic physics.

TLP-17

Towards laser spectroscopy of antihydrogen in the ALPHA experiment

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Antihydrogen offers a unique way to test matter/antimatter symmetry. Antihydrogen can reproducibly be synthesised and trapped in the laboratory for extended periods of time [1, 2] offering an opportunity to study the properties of antimatter at high precision. New techniques to study antihydrogen have emerged; the ALPHA collaboration at CERN can now interrogate the bound state energy structure with resonant microwaves [3], determine the gravitational mass to inertial mass ratio [4] and measure charge neutrality [5]. The results are not yet sensitive enough to draw conclusions on matter/antimatter symmetry but recent progress shows that experiments with trapped antihydrogen are possible and the collaboration is firmly en-route towards precision measurements. The trapping apparatus has been upgraded, improving access for both laser beams and microwave radiation. The apparatus includes a frequency stabilised laser system and a cryogenic enhancement cavity for two-photon excitation of the 1S – 2S transition in antihydrogen. Recent progress towards spectroscopy of trapped antihydrogen is presented.

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TLP-18

Ultra-high resolution, trap-based positron beams using a cryogenic buffer gas

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Buffer-gas-trap (BGT) based positron beams are now used for a variety of scientific and technological applications [1]. These beams are produced by trapping and cooling positrons through interactions with a 300 K molecular gas and subsequently ejecting them in pulses. Using this technique, total energy spreads as low as ~40 meV FWHM have been obtained [2]. Presented here is work to create beams with significantly improved energy resolution. Because these beams are produced in a magnetic field, the total energy spread may be decomposed into spreads both parallel and perpendicular to the magnetic field. The parallel spread is largely set by the beam formation process, while the perpendicular spread depends only on the positron temperature [3]. Methods of reducing both of these components will be described.

Experimental measurements and simulation results of beam formation are described that highlight the key roles played by the positron ejection rate and axial bounce time in setting the parallel energy spread [3]. Measurements of positron cooling to 300 K through interactions with N_2, CF_4 and CO are also presented. When compared with a Born-approximation model of positron cooling on molecular vibrational and rotational modes, the measurements provide estimates of the relevant vibrational and rotational cross-sections [4]. This information was then used to predict the performance of these gases in cooling positrons to cryogenic temperatures.

A new apparatus is described that is designed to re-trap the 300 K BGT-based beam and further cool the positrons to 50 K using N_2 or CO cooled to 50 K. This cryogenic beam-tailoring trap (CBT) also has the capability to compress the positrons radially using rotating electric fields (the so-called rotating wall technique [1]). At the present stage of development, the resulting beam is consistent with a total energy spread of ~10 meV FWHM (a factor of 4 better than the previous state-of-the-art). It also has a ~1 μs FWHM temporal spread, and ~1 mm FWHM beam diameter. Simulations indicate that the current experiment should be capable of producing a beam with a total energy spread of 5 meV FWHM. Work is in progress to mitigate the currently limiting effect in order to achieve this goal.

Other key aspects of the new vibrational and rotation cross section measurements [4] and simulations of trap-based beam formation [3] will also be discussed as time permits.

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In collaboration with J. R. Danielson and C. M. Surko

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P-01

Rydberg-Stark states of Positronium for atom optics

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Positronium (the short-lived bound state of the electron and its antiparticle, the positron) has been produced in Rydberg states using a two-step optical excitation. This is feasible thanks to recent advances in positron trapping techniques [1] that allow intense pulses of positrons to be created, which are then directly implanted into an appropriate target to produce positronium (Ps). Since Ps is produced in nanosecond pulses, it is possible to address it with standard pulsed lasers. Ps was excited via similar methods to previous studies [2] using UV and IR lasers to excite the system to n = 2 and then to a high-n state, respectively. Fig. 1(a) shows the result of this process for values of $n \geq 9$. Exciting Ps atoms to a Rydberg state prevents self-annihilation and pro-vides the system with a large electric dipole moment that scales with n 2 . This property has been exploited to control the motion of Rydberg atoms and molecules in recent years [3, 4].

Now that Rydberg Ps has been produced as reported in this study, it is possible to design a system to manipulate these atoms in such a way that would allow them to be focused, decelerated and trapped.

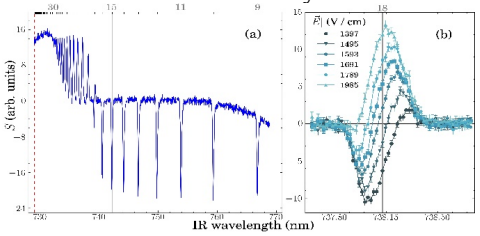

FIG. 1. (a) Rydberg spectrum at zero electric field. (b) Stark-state dependent change in sign of the signal in n = 18 due to electric field ionisation.

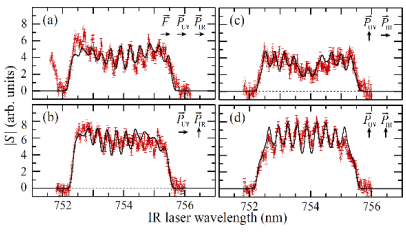

FIG. 2. Ps Stark spectra encompassing all states in n = 11 for different laser polarizations with respect to the applied electric field F .

However, this is only feasible if the dipole moment of the atom can be accurately selected, therefore Ps should be excited to a specific Stark state. This is shown in fig. 2. The outermost states in each manifold of Stark-states have the largest dipole moments and therefore allow for the most efficient control over the atomic motion. The difference in ionization electric field for states on the long- and short-wavelength sides of each Stark manifold has been used to filter states with different dipole moments. This appears as a change in sign in the signal in fig. 1(b).

These advancements will facilitate the design of Ps atom-optics which will be used for focusing, decelerating, and trapping. These techniques are ideally suited to the manipulation of Ps because although it moves at very high speeds, its kinetic energies are almost equal to those in beams of hydrogen and helium, for which deceleration and electrostatic trapping has previously been demonstrated. This will open the door to a wide range of new areas of research, ranging from spectroscopy to antimatter gravity measurements [5].

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P-02

Low Energy Positron Interactions with Uracil

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Positron emission tomography (PET) is a nuclear imaging technique widely used in medicine. To understand the atomic and molecular processes occurring in PET an understanding of positron interactions with biologically relevant molecules is required.

Low energy positron scattering for several biologically relevant molecules such as water, THF, and formic acid have been measured [1,2]. Studies of positron interactions with the DNA and RNA nucleobases are experimentally challenging as they are solid at room temperature and a vapour is required for scattering measurements. Experimental studies are only available for uracil at this time [3,4].

Positron interactions with Uracil were measured between 1 and 180 eV. Total scattering, total elastic scattering and positronium formation cross sections were measured. These measurements were completed using the Atomic and Molecular Positron Beamline of the Centre for Antimatter-Matter Studies' at the Australian National University. The apparatus produces a magnetically confined low energy, high resolution positron pulsed beam. The apparatus is described in detail in [5]. The positron beam had a typical energy resolution of 70 meV for these measurements. A heated scattering cell was used to obtain a sufficient vapour pressure from the solid uracil to measure scattering from single target molecules. Using this cell, uracil was heated to ~100° C and scattering measurements performed.

The present results are compared with previous experimental results and theoretical calculations. These results contribute to the body of knowledge of positron interactions with biomolecules, which can then be incorporated into models of positron transport in biological systems, as well as testing the latest theoretical calculations for complex molecular targets.

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P-03

Elastic positron scattering from H2, N2 e O2 using ab initio potentials.

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Positron scattering by molecules, even the simplest ones, is a difficult theoretical many- body problem, so that few applications aiming at the calculation of scattering cross sections can be found in the literature.

In this work we develop semi empirical local potentials for positron scattering from diatomic molecules. Since the positron is treated on the same footing of the nuclei here[1], the problem becomes to produce a PES for three-center systems. A set of ab initio points is obtained and the many-body-expansion (MBE) tecnique [2] for PES fitting is applied. We applied this methodology for positron scattering from H_2, N_2 e O_2.

The ad hoc inclusion of a long range polarization term is needed only for H_2, which gives our calculations an ab initio character. Scattering cross sections are obtained with a MCF [3] routine [4]. Our results is compared to different theoretical and experimental results with very good agreement.

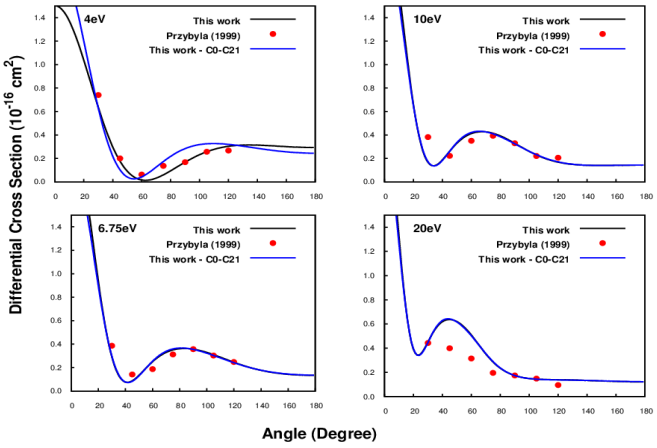

Figure 1: Differential Cross Section for positron scattering from O_2 using the ab inito local potential.

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P-04

Positronium excitation with a tunable, pulsed, solid state UV laser

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The Lyman-a transition (1S-2P) of positronium atoms (Ps) was excited by a tunable, pulsed, solid state UV laser [1]. Positrons from a two-stage buffer gas system [2], utilising recent advancements in rotating wall (RW) compression [3,4] and magnetron excitation techniques [5], were implanted into mesoporous silica in order to efficiently produce the Ps atoms [6], with an efficiency of up to 30% O-Ps determined by the technique of "single-shot positron annihilation lifetime spectroscopy" (SSPALS) [7]. The laser system, based on nonlinear processes of an unseeded optical parametric oscillator (OPO) and sum frequency generator (SFG) driven by the second and third harmonic of a commercial Nd:YAG respectively, has a frequency bandwidth of 225 ± 3 GHz and provides 1.5 mJ of energy in an 8 ns pulse at 243 nm. This power ensures saturation, while the large bandwidth provides significant overlap with the Doppler broadened transition of interest.

This result is the precursor to an efficient two-step process for the production of Rydberg Ps. To this end, a broadband (180-240 GHz), tunable (680-1064nm), pulsed, solid state IR laser capable of providing 40 mJ of power has been developed to excite Ps from 2P-Rydberg, and a further IR laser can be used to ionize the Rydberg Ps. In addition, in order to further increase the Ps yield, an independent positron trap (fed from the two-stage buffer gas system) has been installed and is currently capable of storing 2E7 positrons, with a confinement time >30 s.

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P-05

Vibrational kinetics in Cl_2 and O_2 low-pressure Inductively-coupled plasmas

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Low energy electrons can interact with molecules via resonances, leading either to the creation of negative ions (by dissociative attachment) or vibrational excitation (with detachment of the electron) Such vibrational excitation can lead to considerable electron power dissipation, and have a marked effect on the electron energy distribution function. Furthermore, the presence of vibrationally excited states may have a significant effect on the chemical kinetics. The actual steady-state vibrational distribution is a function of both the electron-impact excitation rates and the rates of V-V and V-T energy transfer processes. However, with the exception of N_2 and H_2 plasmas, very little attention has been paid to either measurement or modeling of vibrational distributions in plasmas of even simple diatomic gases. We have recently implemented a novel high-sensitivity ultra-broadband UV absorption bench for plasma diagnostics[1], which allows spectra to be recorded with baseline stability and noise as low as $2x10^{-5}$ over wavelength ranges up to 250nm. This allows complete vibronic bands to be recorded, and determination of vibrational states distributions. We applied this diagnostic to radiofrequency inductively-coupled plasmas in low pressure (5-50 mTorr) pure O_2 and pure Cl_2. The plasma reactor is described in the literature[2]. In O_2 plasmas we were surprised to observe multiple structured absorption bands across the spectral region 200-350nm[1]. These bands can be attributed to B-X Schumann-Runge transitions originating from highly vibrationally excited O_2 with energy half-way to dissociation of the molecule (v" up to 18) and with a vibrational temperature (for v"=12 to 16) of about 10,000K. Furthermore, high-resolution spectra of individual bands allowed the gas rotational temperature to be determined, reaching 900K at 50 mTorr 500W power. Ground state Cl_2 molecules show a broad UV absorption spectrum in the region 250-400nm. Vibrationally excited Cl_2 molecules have distinctly different absorption spectra[3], and should therefore be easy to detect. Furthermore, a recent compilation of e – Cl_2 collision cross-sections suggested that vibrational excitation could be very significant[4]. However, our measurements indicated that only a small fraction of the Cl_2 molecules are in vibrationally excited states (v=1 to 3). This can partly be attributed to strong gas temperature (and density) gradients, such that the spectra are dominated by cold, dense gas at the reactor radial edges. However, it appears that the Cl_2 vibrational temperature is close to equilibrium with the local gas translational temperature (which can reach 1000K at the reactor centre), in contrast to O_2. We are currently working on a global model of O_2 discharges including vibrational state kinetics. The differences between the two gases will be discussed in terms of the rates of the respective energy transfer processes. This work was performed within the LABEX PLas@par project and received financial state aid, managed by the Agence National de la Recherche (ANR), as part of the programme "Investissements d'avenir" (ANR-11-IDEX-0004-02). It was also partly funded by the Portuguese FCT - Fundação para a Ciência e a Tecnologia, under Project UID/FIS/50010/2013.

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P-06

Low-energy photon-positronium scattering cross-sections

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There is continual interest in the laser manipulation and spectroscopy of Ps, most notably from the Mills group at UCR, and the Cassidy group at UCL with an emphasis towards the production of Rydberg states[1]. We report the fundamental photon-positronium scattering cross-sections both below and above ionization threshold. From a single atomic structure calculation we simultaneously compute the scattering processes of Rayleigh, Raman, Compton and photoionisation. We rely on our recently developed computational method, using a large expansion over pseudostates to describe the continuum, which has been successfully applied to describe low-energy photon-hydrogen scattering[2].

The atom-photon electromagnetic coupling Hamiltonian has two terms in it that are easily written down as the Kramers-Heisenberg-Waller matrix elements. Solving them however, has proved challenging. The Waller term was only recently computed for Compton scattering of positronium by Zaliman, Pisk, and Pratt[3], followed by their computation of both photoionization and also the Compton differential scattering cross-sections using both the Kramers-Heisenberg and Waller terms[4], based on the analytic results of Gavrila[5]. However, the ab-initio analytic calculation of the Kramers-Heisenberg terms results in an infra-red divergence, which makes the numerical integration of the differential cross sections problematic, which is perhaps why total cross sections were not evaluated[4].

We use the reduced mass transformation to transform positronium into the effective one-body problem, and then compute the Kramers-Heisenberg terms (at photon energies where the Waller term can be neglected). Our numerical treatment diagonalises a large Laguerre-based basis set, resulting in a set of bound states and a set of pseudostates that discretise the continuum. Using the transition matrix elements between both bound-bound, bound-pseudo, and pseudo-pseudo we compute the complex transition polarisabilities by adapting the Raman-based formulae of Delserieys *et al*.[6] to the case of Compton scattering. Our atom-in-a-box calculations of the Compton scattering cross-sections do not appear to suffer from the infra-red divergence.

This work follows on from our benchmark calculations of photon-hydrogen scattering which provides a near complete picture of the various processes. As Zaliman and Pisk found for the Compton differential cross-sections[4], we find that the total cross sections for photon-positronium scattering are larger than those of hydrogen, and significantly more than the Thomson scattering cross-section of a single free-electron. As an example, the static dipole polarisability of H is 4.5 atomic units, while Ps experiences an increase of a factor of 8 (to 36 atomic units). Since the cross sections depend on the square of the polarisability, we expect factors of 64. Our total cross-sections show such enhancements.

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P-07

Quenching of positronium by laser induced paramagnetic centers in mesoporous silica at cryogenic temperatures.

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The use of mesoporous silica films for the production of positronium has become widespread in recent years [1]. In some applications it may be desirable to use such materials in a cryogenic environment, for example in the cold bore of a superconducting magnet for antihydrogen experiments [2] or in experiments conducted with Rydberg Ps where black body radiation may be undesirable [3]. In UHV conditions mesoporous silica is expected to be unaffected by cooling to cryogenic temperatures [4] since the Ps formation process is not thermal. However, this may not be the case if the sample is also exposed to radiation, as demonstrated for similar materials by Saito *et al.* [5] We have observed a drastic reduction in the positronium formation efficiency of a porous SiO_2 sample [1] following UV laser irradiation at 12 K. Positrons from a, two-stage Surko trap [6], were implanted into a porous target in 6 ns wide pulses at a repetition rate of 1 Hz. The subsequent formation of Ps was measured using single shot positron annihilation spectroscopy (SSPALS) [7]. With the sample kept at room temperature the observed Ps fraction was stable. At 12 K the positronium formation efficiency was slightly reduced due to the adsorption of residual gas by approximately 2% per day. However, following irradiation with UV laser light (l = 243 nm) at 12 K the Ps fraction dropped significantly, as shown in FIG 1. No effects from laser irradiation were observed at room temperature, and the low temperature laser induced damage was fully annealed out after warming the target to room temperature. These observations are consistent with the formation of paramagnetic centers, as observed by Saito et al [5], who observed quenching of ground state Ps atoms by surface paramagnetic centers in silica aerogels.

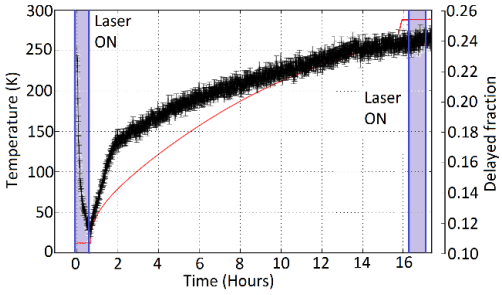

Figure 1: The delayed fraction, which is proportional to the positronium formation efficiency decays following laser irradiation of the target at 12 K. A full recovery is observed as the sample is warmed to room temperature where the laser has no

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P-08

Laser-enhanced time-of-flight measurements of positronium emitted from nanoporous silica

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Using a two-stage Surko trap [1] we have produced positronium (Ps) atoms in a short (5 ns) burst that is well-suited to interrogation by pulsed lasers. This allows us to perform resonance-enhanced multi-photon ionisation (REMPI) of Ps, in which 1S-2P transitions are driven by a UV laser (λ = 243 nm) then the excited atoms ionized by coincident green light (λ = 532 nm). This process is observed via changes in the Ps decay rate, measured using a fast gamma-ray detector and the technique of single-shot positron annihilation lifetime spectroscopy [2]. In this way we have determined the Doppler-width of the Lyman-α transition [3], from which we infer the velocity-spread of the Ps distribution along the direction of the laser path. Furthermore, by restricting the Ps/ laser interaction to a well-defined region and varying the laser delay (see Fig. 1) the velocity distribution perpendicular to laser path has also been measured by time-of-flight (TOF) [4]. Extrapolating the Ps flight path from several positions to the surface of the nanoporous silica wherein they form gives an estimate of the rate of emission of the atoms from the pores. Together with Doppler spectroscopy, laser-enhanced TOF provides a rich analysis of the Ps converter, however, the TOF spectra are complicated by the variation in probability of Ps ionisation depending upon the time spent by each atom within the laser field, and therefore a correction function is needed to estimate the velocity distribution accurately. For cold distributions and intense laser fields this effect becomes negligible; accordingly, laser-enhanced TOF may prove crucial for precise measurements of ultra-cold Ps sources, becoming limited by the spatial extent of the lasers, which could in principal be focused to less than 50µm across.

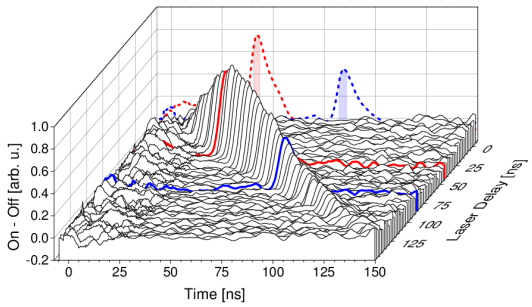

Fig. 1 Background subtracted and o-Ps decay corrected SSPALS spectra for various laser delay times. The diagonal ridge indicates an excess in annihilations due to photoionisation of the Ps atoms passing through the beam. (Fig. 6 in Ref. [4])

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P-09

Pseudopotential calculation of positronium collisions with the H_2 molecule

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Scattering cross sections for Ps collisions with atoms and molecules are very sensitive to the exchange interaction between the Ps electron and the target electrons. On the other hand, inclusion of this interaction by a completely *ab initio* method is a very challenging task, even for simple targets. In Ref. [1] we developed a pseudopotential approach which uses the electron scattering phase shifts to construct an *l*-dependent potential for electron scattering which can be used then for Ps scattering by the same target.

In the present work we use the same ideas to calculate elastic scattering cross sections for Ps-H_2 collisions. The hydrogen molecule, in a very good approximation, can be described as a spherically symmetric target. We use a modification [2] of the Hara local exchange potential for the *e*-H_2 interaction to construct a nonlocal pseudopotential describing the Ps-H_2 interaction. We also add the van der Waals interaction with an effective cut-off at small Ps-H_2 distances similar to that used in [1]. For comparison with the experimental results [3] for the total scattering cross section, we also calculate the Ps ionization cross section using the binary-encounter approximation. The results agree very well with the experiment [3], and also with the experiment [4] on low-energy Ps degradation in H_2 gas.

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P-10

Investigation of possible structures in positronium total cross sections

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For the first time, positronium total cross sections have been measured at energies as low as 1.5eV (0.23 a.u.) using the quasi-monoenergetic ground-state ortho-positronium beam at University College London. The beam is produced by neutralizing a magnetically-guided beam of positrons through a suitable gas [e.g.1]. Collision between positronium, Ps, and the atoms/molecules of interest occur in a second scattering cell, as described in [e.g. 2]. Our investigative capability has been expanded to low energies by using Ar as the neutralizing gas [1]; the method will be described in some detail.

Similarities between the electron and Ps total cross sections at the same velocity have previously been reported [3]. Recently, an impulse approximation has been employed to provide a theoretical explanation of this similarity at intermediate energies [4] whilst, at low energies, a different approach [5] has predicted major differences between the projectiles.

Experimental investigations are currently being made at low energies to explore potential structures [6], including Ramsauer-Townsend minima (e.g. 0.23 a.u. in the Xe electron total cross section) and shape resonances (e.g. 0.41 a.u. $^2\Pi_g$ shape resonance in N_2), illustrated in figure 1. Results will be presented at the conference.

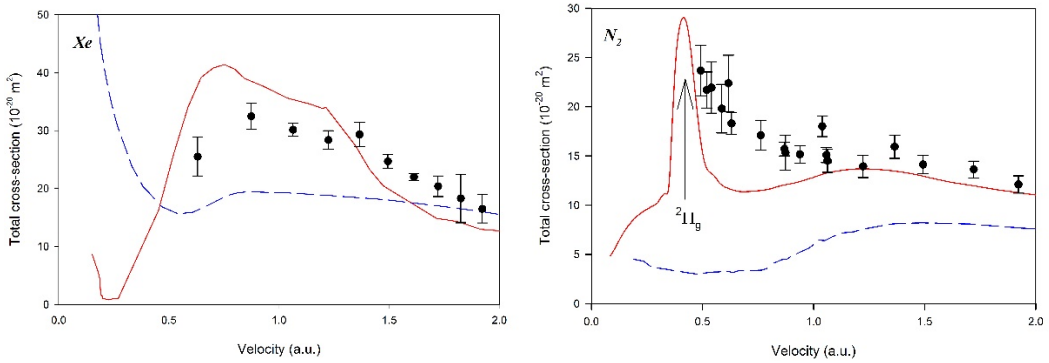

Figure 1: Previous determinations of total cross sections for positron (dashed line) [7, 8], electron (solid line) [9, 10] and Ps (points) [3] compared by particle velocity

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P-11

Periodic table of positronic atoms

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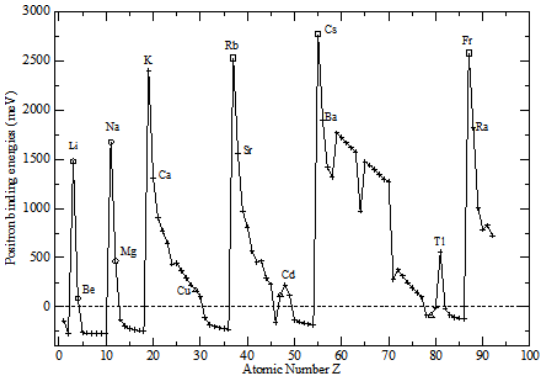
The calculation shows that more than half of the atoms in the Periodic Table bind the positron in their ground state. A number of atoms also bind positrons in excited states forming discrete spectrum and low-lying resonances.

Binding of positron to an atom with several valence electrons is a challenging problem. This is mainly due to the strong electron-positron correlation effects and virtual positronium (Ps) formation [1]. In Ref. [2] we presented calculations of the positron binding energies to all atoms in the Periodic Table. The most accurate previous calculations involving Li, Na, Ag, Cu, Au, Be, Mg, Ca, Zn, Sr and Cd atoms [3, 4] have been included and used to correct our values for the binding energies of positron to other atoms. We hope that the recommended positron binding energies to all atoms in the Periodic Table stimulate the experimentalist to detect the positron-atom bound states. The ordinary Periodic Table is constructed due to the similar chemical properties of atoms with the same number of valence electrons in external subshells. We have obtained similar periodicity in the positron-atom bound states, see the figure.



For atoms with ionization potential I such that $I > 6.80$ eV, the Ps-formation channel is closed. The closest decay channel will be $e^+ + A$. On the other hand, for $I < 6.80$ eV the lowest decay channel is Ps+A^+. On the figure, the positron binding energies ε_b have been presented relative to the decay channel $e^+ + A$. The binding energies relative to different channels are related by an equation $\varepsilon_b = \varepsilon_{Ps} - I + 6.80$ eV, where ε_{Ps} is the positron binding energy relative to the channel Ps+A^+, and 6.80 eV is the binding energy of positronium (Ps). A number of atoms also bind positrons in excited states forming discrete spectrum and low-lying resonances. These resonances may be used for experimental detection of positron-atom bound states via resonant annihilation or scattering [5]. Figure 1. Recommended positron binding energies relative to the dissociation threshold $e^+ + A$. The results based on current study are shown with + sign. The circle shows the results of the previous best calculations based on configuration interaction (CI) or stochastic variational methods (SVM). ‣ shows the previous result of the relativistic method for Cu, Ag, and Au in our group.

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P-12

Detecting Positron-Atom Bound States through Resonant Annihilation and Scattering

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A method is proposed for detecting positron-atom bound states by observing enhanced positron annihilation due to electronic Feshbach resonances. Relativistic coupled-cluster single-double approximation with third-order corrections is used to calculate positron binding energies and resonances for all atoms in Periodic Table.

In spite of wealth of predictions [1, 2, 3, 4], experimental verification of positron binding to neutral atoms is still lacking. We proposed a realistic experimental scheme to detect positron-atom bound states of open-shell atoms by measuring *resonant positron-atom annihilation* [5]. Therefore it is important to calculate positron binding energies to the ground state and excited configurations.

In resonant positron-atom annihilation process $A + e^+ \to A^* e^+ \to A^+ + 2\gamma$, the positron first loses energy by exciting the atom and becoming trapped in the bound state with the excited atom. It then annihilates with one of the electrons, and the resulting gamma quanta can be detected.

The observable effect may be obtained by averaging the normalized dimensionless annihilation rate $Z_{eff} = \sigma_a k/(\pi r_0^2 c)$ over the energy distribution in the positron beam. Here σ_a is the resonant positron-atom annihilation cross section, k is the positron momentum, r_0 is the classical electron radius. The state of the positron bound to the excited atom, which lies above the atomic ground state, is a Feshbach resonance. Its total width Γ is the sum of the annihilation width Γ^a and the elastic width Γ^e. The latter gives the decay rate of this quasibound state into $A + e^+$ the continuum, and also characterizes the probability of its formation in positron-atom collisions. Strong annihilation resonances require $\Gamma^e \gg \Gamma^a$.

The current study presents a first adaptation of the linear coupled-cluster single-double (SD) method with the third-order perturbation theory for the problem of positron-atom bound states. The calculations [6] for the positron binding energies to the closed-shell atoms (Be, Mg, Ca, Zn, Cd, and Hg) provide an estimate of an accuracy of our method (~100 meV) since various calculations for them are available in the literature [3]. In this approach, if the positron is found to be bound to an atom in a given configuration, it is assumed to be bound to all states (ground or excited) with the same configuration. In this way, we show that many atoms do bind a positron not only in the ground state, but also in excited states. The resonant and binding energies related to each other by $\varepsilon_r = E_{ex} - \varepsilon_b$, where E_{ex} is the atomic excitation energy measured with respect to the ground. To observe a narrow resonance, one requires $\varepsilon_r > 0$ and that ε_r is smaller than positronium (PS) formation threshold. According to these criteria, we have obtained many low-lying resonances for many atoms [6].

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P-13

Exchange-assisted tunneling and enhancement of positron annihilation with inner-shell electrons

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Exchange interaction and correlations radically change behavior of a quantum particle in a classically forbidden region. Exchange produces power-law decay instead of the usual exponential decrease of the wave function. Exchange-assisted tunneling enhances annihilation of positron with inner-shell electrons and produces other observable effects.

Exchange interaction strongly influences the long-range behavior of localized electron orbitals and quantum tunneling amplitudes. It produces power-law decay instead of the usual exponential decrease at large distances. For inner orbitals inside molecules decay is $1/r^2$, for macroscopic systems $\cos(k_F r)/r^\nu$, where k_F is the Fermi momentum and $\nu = 3$ for one-dimensional, $\nu = 3.5$ for two-dimensional, and $\nu = 4$ for three-dimensional crystals [1]. Correlation corrections do not change these conclusions [1, 2, 3]. Slow decay increases the exchange interaction between localized spins and the under barrier tunneling amplitude. The under barrier transmission coefficients in solids (e.g., for point contacts) become temperature dependent.

Exchange-assisted tunneling enhances annihilation of positron with inner-shell electrons [4].

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P-14

New precise measurement of the hyperfine splitting of positronium

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Positronium (Ps) is an ideal system for the research of the quantum electrodynamics (QED) in bound state. The ground state hyperfine splitting (HFS) of positronium gives a good test of the bound state calculations. Non-Relativistic QED calculations [1] have revealed a 16 ppm (4.5σ) discrepancy of positronium HFS value between the QED prediction and the previous experimental average [2,3]. The discrepancy might be because of possible common systematic uncertainties in all the previous experiments. One possibility is the unthermalized o-Ps contribution (Ps thermalization is a process that Ps loses its kinetic energy from initial energy E_0 to room temperature), which has already been shown to be significant in o-Ps lifetime puzzle [4,5]. Another possibility is non-uniformity of magnetic field.

We performed a new experiment which reduced the possible systematic uncertainties and provided an independent check of the discrepancy using the following three new methods: a β-tagging system to get timing information, a large bore superconducting magnet to produce the static magnetic field B~0.866 T with an inhomogeneity of 1.5 ppm RMS using compensation coils, and high performance γ-ray detectors using $LaBr_3$(Ce) scintillators.

We also measured Ps thermalization function in i-C_4H_{10} gas, which was used in our HFS measurement to form Ps, with a Ge detector. We used `pick-off technique' [4,6]. The result of σ_m (momentum-transfer cross section) = 47.2 ± 6.7 Å^2 for o-Ps below 0.17 eV was obtained.

Using the result of the thermalization measurement, our new HFS measurement revealed that the Ps thermalization effect was as large as 10 ± 2 ppm. Treating the thermalization effect correctly, a new result of HFS = 203.3942 ± 0.0016(stat., 8.0 ppm) ± 0.0013(syst., 6.4 ppm) GHz was obtained [7]. This result is consistent with theory within 1.1σ, whereas it disfavors the previous experimental result by 2.6σ. It shows that the Ps thermalization effect is crucial for precision measurement of HFS. A brief prospects for improved precision in future experiment will also be presented.

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P-15

Optical model for the positronium formation cross section in positron helium and neon scattering

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Positron-atom interaction is of importance not only in atomic physics but in many fields utilizing positron annihilation in matter. A positron can be alternative probe to an electron for investigation of atom/molecule because of its opposite sign of charge. The most difference between the positron and electron is a positronium (Ps) formation which is an rearrangement reaction where coordinates of the system should be changed to satisfy asymptotic boundary conditions. Since the wavefunction of the positron and atom system is not orthogonal to that of the Ps and residual cation system, there are several problems, such as overcompleteness problem, in theoretical calculations. An optical model is useful method to investigate the coupling between the elastic channel and Ps formation rearrangement channel, and has been applied for variety of scattering problems. The Ps formation channel is treated as absorption of the flux of the incident positron by introducing an imaginary part of the potential.

In the present paper, we determine the optical potential for positron-helium and positron-neon scattering, and obtained Ps formation cross sections. Recently, several precise low energy positron and rare gas atom scattering experiments have been performed. These systems are simple and basic systems containing many interesting phenomena, such as Ramsauer-Townsend effect, relativistic effect, Ps formation, and positron slowing-down. The optical model approach has also been applied, but we adopt more precise effective potential obtained recently in positronic alkali atom caion having the same electron structure as rare gas atom. The interaction between positron and the atom is assumed to be a sum of static, polarization potential and imaginary potential. Real part of the potential is determined to reproduce the elastic cross sections below the Ps formation threshold energy. The shape of the imaginary part is assumed to be proportional to the form-factor of the outermost s-wave electrons in the target atom because the low energy positron cannot pick up inside electrons having large binding energy and low energy Ps formed from s-wave positron and p-wave electron cannot get over the centrifugal potential.

Figure 1 shows observed total cross sections and calculated total, elastic, and Ps formation cross sections in positron-neon atom scattering. The cross sections consist of up to d-wave. At the energy of 0.8 eV, s-wave cross section is zero resulting from a Ramsauer-Townsend minimum. In the case of electron-rare gas atom scattering, the s-wave phase shift is known to be π at the minimum, because the phase shift increases as an increase of the kinetic energy owing to attractive static and polarization potentials. In the case of positron scattering, on the other hand, the calculated s-wave phase shift is zero. The phase shift increases and then decreases as an increase of the kinetic energy. At the low energy region, long-range attractive polarization potential is dominated. As the kinetic energy increases, contribution of the repulsive static potential increases. At the Ps formation threshold energy, slope of the elastic cross section changes sharply, and decreases above the threshold, on the contrary. Because of the Ps formation, the flux of the elastic channel attenuates, and elastic cross section decreases.

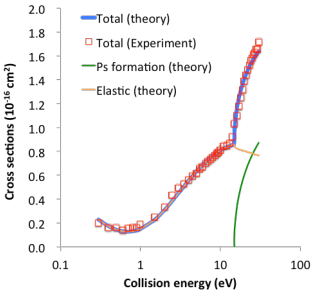

Figure 1. Cross sections in positron-neon atom scattering. Experimental value is taken from A.C.L.Jones *et al.*, *Phys.Rev.A***83**,032701 (2011).

P-16

Theoretical study of the effect of molecular vibrations on the positron binding to polyatomic molecules with multi-component molecular orbital and quantum Monte Carlo methods

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The positron, which is the anti-particle of the electron, is now widely used in both scientific and technological areas such as physics, chemistry, material science, medicine, and their interdisciplinary areas. The detail mechanism of such processes, however, are still unclear in the molecular level. A positron affinity (PA), which is a binding energy of a positron to an atom or molecule, is one of the most important properties for studying positron attachment process. The PA values have now been experimentally measured by Surko and co-workers for many molecular species such as some hydrocarbons (alkanes, alkenes, and aromatics), alcohols, and halogenated hydrocarbons [1]. Their PA measurement is based on the vibrational Feshbach resonance (VFR) by incident low-energy positrons, in which the formation of a positron-molecular complex at the molecular vibrational excited states is suggested. Thus, in order to elucidate the mechanism of the positron binding to molecules in vibrational excited states in detail, the theoretical analysis including the effect of the molecular vibrations is indispensable.

In this study, we developed a new theoretical method for analyzing the effect of molecular vibrations on positron affinities in order to elucidate the mechanism of the positron binding to molecules in vibrational excited states. Our method is based on both the anharmonic vibrational state theory with quantum Monte Carlo (QMC) technique [2] and *ab inito* multi-component molecular orbital (MC_MO) theory [3,4] that enable us to solve the electronic and positronic wave functions simultaneously. To demonstrate the effect of molecular vibrations to the positron bindings with our method, we show the characteristic features of the positron binding to some small molecules such as hydrogen cyanide (HCN)[2], formaldehyde (CH_2O)[5] molecules, *etc*. By analyzing the PA values at vibrational excited states, we found that (i) for HCN molecule, the vibrational excitations of the CN and CH stretching modes enhance the PA value compared to that of the vibrational ground state, whereas the excitation of bending mode deenhances it, and (ii) for CH_2O molecule, the vibrational excitations of the C=O stretching mode enhances the PA value, whereas the excitation of CH_2 rocking mode deenhances it. We also confirmed that such PA enhancement/deenhancement arises from the change in both the permanent dipole moments and dipole-polarizability at each vibrational excited state for both molecules.

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P-17

Do positrons measure atomic and molecular Diameters?

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The question of atomic "dimensions" became recurrent with the advent of quantum wave mechanics that eliminated idea of electron orbits. Diameters of some equivalent "hard spheres" are needed, for example, in evaluation gas pressure from viscosity or electron diffraction. Different approaches, say from van der Waals gas-phase radii, from liquids' viscosity, from crystallography and from quantum-mechanics outermost orbitals give for some targets, like He and Ar contradictory evaluations.

Measurements of total cross sections for positron scattering on H_2, N_2, Ar, benzene, cyclohexane at Trento University [1] performed with a high beam stability and good angular resolution showed almost constant values in the region between a few eV and the positronium formation threshold. Further, these constant values are of a few $Å^2$, in agreement with some other "hard-sphere" evaluations. The idea that positrons measure molecular diameters was launched at Einstein's Anniversary Congress [2]. However, such a result is in a very contrast with ideas of quantum mechanics, see [3] and cannot be reproduced with the classical mechanics, either [4].

From 2007 a new apparatus at Australian National University in Canberra, conceptually different from that in Trento, measured several targets including Ar and H_2 [5, 6]. Even if some differences in absolute values exist with Trento data [1], constant cross sections are visible within the experimental error bars. From the theoretical point of view, an extensive work by Gribakin and co-workers for noble gases [7] show that in order to reproduce constant cross sections, the virtual-positronium formation process has to be included into calculations. In case of H_2, the convergent close-coupling method shows that virtual electronic excitation states should be taken into account [8, 9]. Our trials using density functional Hamiltonian [10, 11] without such states (and therefore producing lower results than the experiment) confirm these conclusions.

A question arises: in what way does the elastic channel sum up with the virtual positronium contribution to give a constant, hard-sphere (or rather a sticky ball) cross-section? In other words: why does Quantum Mechanics yield exactly the classical result?

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P-18

Radiative electron attachment to molecules of astrophysical interest: Direct and indirect mechanisms

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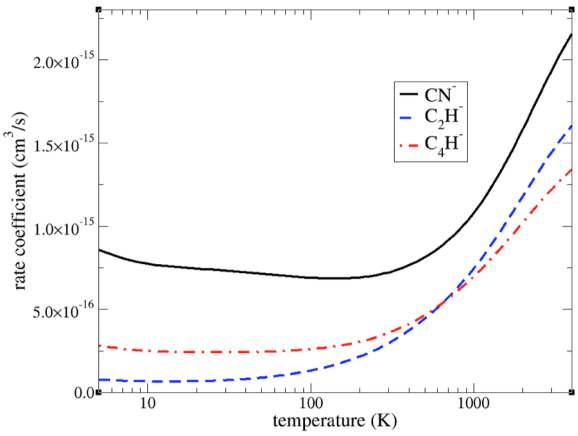
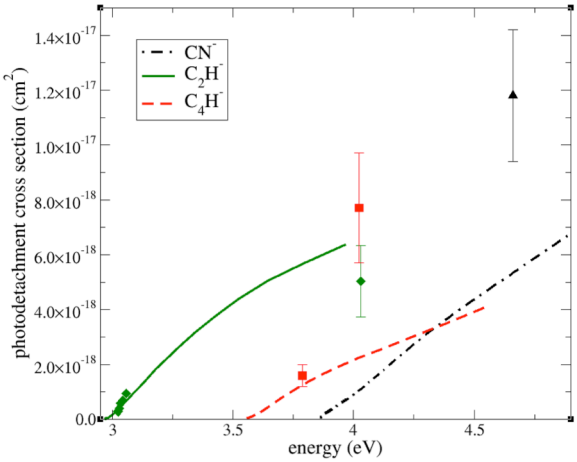
A first-principle theoretical approach to study the process of radiative electron attachment is developed and applied to the negative molecular ions CN^-, C_4H^-, and C_2H^-. Among these anions, the first two have already been observed in the interstellar space. Cross sections and rate coefficients for formation of these ions by radiative electron attachment to the corresponding neutral radicals are calculated. For completeness of the theoretical approach, two pathways for the process have been considered: (i) A direct pathway, in which the electron in collision with the molecule spontaneously emits a photon and forms a negative ion in one of the lowest vibrational levels, and (ii) an indirect, or two-step pathway, in which the electron is initially captured through non-Born-Oppenheimer coupling into a vibrationally resonant excited state of the anion, which then stabilizes by radiative decay. We have developed a general theoretical model to describe the two pathways. The contribution of the indirect pathway to the formation of cosmic anions was found to be negligible in comparison to the direct mechanism. The obtained total rate coefficients of radiative electronic attachment at 30K are $7x10^{-16}$ cm^3/s for CN^-, $7x10^{-17}$ cm^3/s for C_2H^-, and $2x10^{-16}$ cm^3/s for C_4H^-. These rates weakly depend on temperature between 10K and 100 K. The validity of our calculations is verified by comparing the present theoretical results with data from recent photodetachment experiments performed for the CN^-, C_4H^-, and C_2H^- ions.



Calculated rate coefficients for radiative electron attachment to the CN, C_2H, and C_4H molecules.



Comparison of the present theoretical cross sections with available experimental data for the process of photodetachment of the CN^-, C_2H^-, and C_4H^- ions.

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P-19

Positron scattering from He and Kr in a field-free interaction region

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A new electrostatic positron beam at UCL [1], illustrated in figure 1 (lhs), is being employed to measure the total cross sections of positron scattering from krypton and helium in the energy range of (10-200)eV. This work has been stimulated by recent results for helium [2] and neon [3], also determined using an electrostatic beam. These works showed significant discrepancies at low energies, as pictured for helium in figure 1 (rhs), with respect to previous measurements performed on systems using magnetic-field beam transport.

In transmission experiments, the largest source of systematic errors arises from the accidental inclusion of forward scattered particles in the measurement of the unscattered beam. This effect, which leads to an artificially lower total cross section, may be more easily reduced in the absence of external fields, which enable higher, energy-independent angular-discrimination ($\cong 2^o$ in the present apparatus). New results will be presented at the conference.

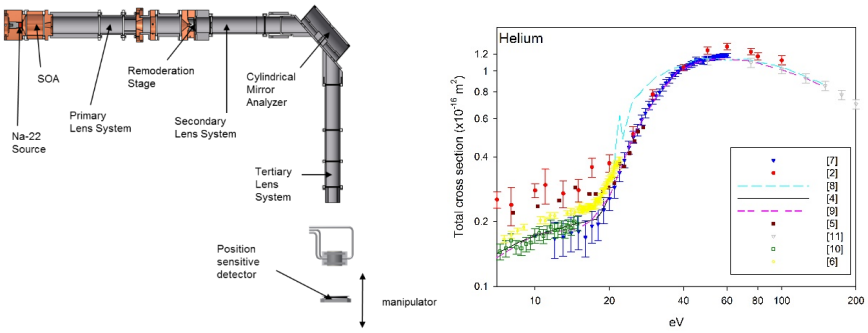

Figure 1: (lhs) positron beam; (rhs) positron-helium total cross section results.

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P-20

A resonance trend in the ICS for positron scattering from alkaline earth targets: Be, Mg and Ca.

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Low energy positron scattering by atoms has been subject to intensive research efforts. Common scattering patterns for chemically similar targets give insights to the deeper understanding of the interaction. For noble gases it is already possible to perceive a convergence between experimental and theoretical results [1]. It becomes important to move to atomic targets of the first and second rows of the Periodic Table.

Here, calculations for slow positron scattering from Beryllium, Magnesium and Calcium at energies from 10^{-5} to 10eV are reported. The computations are allowed by a model potential approach previously proposed for noble gases [2,3]. Integral and differential elastic cross sections, phase shifts and scattering lengths are focused on. The predictions for Be and Mg are in good agreement with previous reports, while original results are reported for Ca. This application to three alkaline-earth elements allows the prediction of shape resonance and shoulder trend in the ICS for these targets, as shown in the figure, as well as their connections to the partial wave contributions.

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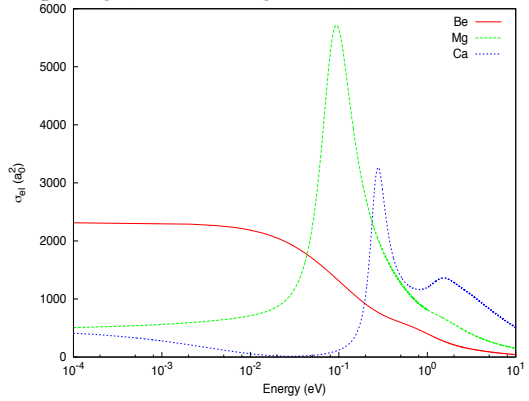

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P-21

Positronium emission from Na coated tungsten surfaces

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When slow positrons impinge on metals, they penetrate into the bulk and lose their energy until they thermalize. Afterwards, some of them diffuse back to the surface. If the positron work function ϕ_+ is negative, a fraction of the positrons are emitted with a kinetic energy $|\phi_+|$. Emission as positronium (Ps) is also a possible channel, since Ps affinity

$$\phi_{Ps} = \phi_+ + \phi_- - 6.8\text{eV},$$

where ϕ_- is the electron work function, is negative for most metals. Some of the positrons are also trapped in the surface potential well. When the metal is heated up, Ps yields increase due to the thermal desorption of Ps atoms formed from positrons at surface states. An increase in the yield of Ps emitted from Si surface has been observed when the surface was coated with Cs [1]. This was interpreted as the desorption of Ps formed from positrons trapped in the surface potential well with electrons whose work function had been lowered by the coating. Moreover, thermal desorption of Ps from Cs coated Ni surfaces was reported even at room temperature [2].

In the present work, we have investigated Ps emission from Na coated polycrystalline tungsten surfaces by measuring Ps time-of-flight spectra [3]. The data show that the maximum emission energy of Ps formed from thermalized positrons and conduction electrons, is not affected by the Na coating. The experiment also shows a significant increase of the Ps channel as a function of coating. Previous Ps emission models used for Si and Ni surfaces do not explain the present experiment. Therefore, an attempt is made to explain the increase of the Ps channel by showing that the low electron density surface layer produced by the coating facilitates the Ps production.

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P-22

Triple differential cross sections for the ionization of NH_3 by positron impact

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Ionization of molecules by electron and positron projectiles has attracted much interest in the last years. Most of the studies were performed for electron projectiles. Positron impact ionization studies are less abundant, due mainly to the limitations of producing high intensity positron beams. The measured physical quantity of interest, providing the most details of the process, is the triple or fully differential cross section (TDCS).

Previously, we have calculated TDCSs for several molecular targets, mostly for electron impact ionization and for coplanar geometrical arrangements. Recently, these studies were extended for non-coplanar geometries and for low emission energies. In particular, we have calculated TDCSs for the electron impact ionization of NH_3 both in the scattering and perpendicular planes and for equal energies and ejection angles of the outgoing electrons [1]. These cross sections have reproduced the main features of the experiments presented in [2]. The study also showed the importance of taking into account the post collision interaction (PCI) between the outgoing electrons at low energies in order to obtain correct TDCSs.

In our present study we calculate TDCSs for the kinematical parameters given in [2], but for positron impact ionization of NH_3 and compare the results with the previously obtained results for electron projectiles. This comparison is important in order to assess the effect of the projectile's charge and consequently the PCI effects on the cross section. The calculations are performed both in the scattering and perpendicular planes, for symmetric ejection of the equally energetic outgoing particles.

In order to describe the states of the free particles we have employed distorted waves calculated in the spherically averaged potential of the molecule or the molecular ion. The initial state of the target is approximated by Gaussian multi-center wavefunctions, which are linear combination of Gaussian atomic orbitals. The Gaussian atomic orbitals were obtained as contractions of Gaussian primitive functions using the Gaussian software package [3]. The PCI effects between the outgoing particles are taken into account by the inclusion of the Coulomb distortion factor or the Gamow factor in our models. These factors are described in [4] and [5] for electrons. In the present study we modified them to account for the interaction between a positron and an electron.

Our results are compared with the calculated TDCSs obtained for electron impact ionization due to the lack of experimental data for the employed kinematical conditions in case of positron projectiles.

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P-23

Free volume change of the electron-beam irradiated polyethylene during long-term storage

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Polyethylene is widely used for an insulator, a covering material, etc., of nuclear plant and/or accelerator. The irradiation effect and the degradation of polyethylene have been studied because they are very important for the safety of the equipment and the facilities.

Additive free high density polyethylene (HDPE) and low density polyethylene (LDPE) were used. An electron beam was irradiated up to 1000 kGy under vacuum at room temperature. After the irradiation, samples were stored in air at room temperature. Change of chemical structure, mechanical property and nanostructure of HDPE and LDPE were examined by micro-FT-IR spectroscopy, tensile test, and positron annihilation lifetime spectroscopy, respectively. Application of positron annihilation lifetime spectroscopy relies on the fact that some of the positrons injected into a polymer combine with an electron to form the hydrogen-like bound state, positronium. In a polymer, spin-parallel *ortho*-positronium (*o*-Ps) annihilates by pick-off annihilation in a free volume with one of the surrounding electrons and the lifetime of *o*-Ps increases with increasing hole size [1,2], so we can estimate the free volume size from the lifetime of *o*-Ps. In this work, positron lifetime spectra were recorded with a conventional fast-fast coincidence system by determining the time interval between the detection of a 1.27 MeV gamma-ray from the β^+ decay of a ^{22}Na source and the detection of one of 0.511 MeV annihilation photons [3,4]. Two identical samples sandwiched the ^{22}Na source sealed between two Kapton foils with a thickness of 7.5 μm [5].

The yield of carbonyl groups for HDPE increases with increasing the absorbed dose, and the tensile strength increases with the absorbed dose whereas the elongation at break decreases. These results indicate that oxidation of HDPE via allyl radical which produced with the irradiation leads the degradation of HDPE, on the other hand, HDPE becomes stiff due to the cross-linking.

Free volume size of the HDPE immediately after the irradiation is comparable to that of the unirradiated sample, but after 3 months, it seems to decrease for the samples whose absorbed dose are higher than 200 kGy. On the other hand, the yield of carbonyl groups for HDPE increases with the elapsed time (~ 3 months) after the irradiation which is due to the long-term oxidation via hydroperoxide, whereas no obvious change of the mechanical properties is observed. The post-irradiation effects, especially the change of the free volume size, will be discussed.

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P-24

Scattering of positron by Lithium atom with electron exchange

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We present the formalism of Time-dependent Exchange Perturbation Theory (TDEPT) built to all orders of perturbation, for the arbitrary time dependency of perturbation. The theory takes into account the rearrangement of electrons among centres. The elements of the scattering S-matrix and transitions T-matrix and the formula for the electron scattering differential cross section are derived. The application of the theory to scattering and collision problems is discussed on an example of positron scattering on a Lithium atom, calculating the differential and total cross-sections.

The strength of the interaction between particles during collisions is described by a scattering cross-section, or a differential cross-section. We consider the collision associated with the redistribution of electrons, as the collisions of positrons with neutral atoms accompanied by charge transfer. Here we would like to emphasize the advantages of applying the EPT method. The obtained matrix element contains the exchange and super-exchange integrals. These integrals take into account the permutations of the electrons between the centers. The signs of these integrals are defined by the Young diagrams and depend on the total spin value.

A simulated differential cross section as a function of the scattering angle at different energies of the incident positron. One can observe regions of a “twisted ridge” for certain values of wave vector k and a scattering angle θ. It has been previously reported that under similar conditions, but when an alpha-particle is colliding with a Lithium atom [1], the differential cross-section has a smooth appearance without ridges. The same “twisted ridge” were theoretically predicted for the scattering of proton by Lithium atom, for other values of vector k and angle θ [2].

The formalism of the time-dependent exchange perturbation theory allows the scattering processes of complex particles (atoms, molecules) to be described, taking into account the indistinguishability of electrons participating in multi-center collisions, even in cases where the permutations of electrons occur between different centers and are associated with non-orthogonal states. This formalism is applicable to cases of restructuring colliding particles, such as ion charge exchange processes.

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P-25

Multi-component *ab initio* study on positron attachment to weakly polar FH molecule: The role of molecular vibration and the electron-positron correlation

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According to Crawford's model, a positron should be able to form an infinite number of bound states with molecules if the molecule has a dipole moment with a value greater than 1.625 debye [1]. The hydrogen fluoride (FH) molecule have permanent dipole moment (1.83 debye), which is slightly larger than the critical value of Crawford. Although FH is good target molecule to investigate the possibility of positron binding, only a few calculations have been performed for [FH; e^+] [2-4] and the value of positron affinity (PA) in those previous studies are very small. It has been suggested that the effect of molecular vibration is important for positron attachment to FH, since the dipole moment and polarizability increase as the F-H internuclear distance *R* becomes longer [4]. However, Hartree-Fock method generally underestimate the magnitude of PA value due to the lack of the electron-positron correlation[5]. In this study, we have thus investigated the role of molecular vibration and the electron-positron correlation in positron attachment to FH.

Figure 1 shows the vibrational averaged positronic density[6] at $\nu = 0$ for [FH;e^+], where ν is a vibrational quantum number. The positronic density is situated at outer region of the F nucleus, which is in qualitative agreement with the previous study of Wołcyrz *et al*.[4]. However, the magnitude of the positronic density in the present study is more than 1000 times larger than that in the previous study. This means that our positronic density has more compact distribution and the positron is more tightly bound to FH.

Figure 2 shows the ν dependence on the vibrational averaged PA (vib. PA) [6,7] for FH. Though the vib. PA are less than 1 meV for $\nu \leq 6$, it becomes large as ν increases. This may be due to the synergetic effect of the following two reasons: (i) the vibrational wavefunction spread to large *R* region as ν increase. (ii) the dipole moment and polarizability are enhanced at large *R* region. As in the figure 2, weak but significant positron attachment to FH has been confirmed for $\nu \geq 7$.

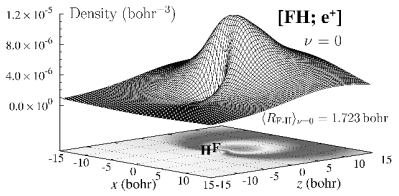

Fig. 1: The vibrational averaged positronic density for [FH; e^+].

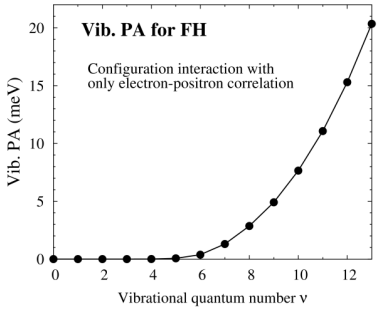

Fig. 2: The vibrational averaged PA for FH as a function of ν.

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P-26

Producing the positive antihydrogen ion $\bar{H}^+$ via radiative attachment

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In a prior paper [1] we provided an estimate of the cross section for the radiative attachment of a second positron into the $\left(1s^2\,{}^1S^e\right)$ state of the $\bar{H}^+$ ion using Ohmura and Ohmura's [2] effective range theory and the principle of detailed balance. Here we improve accuracy by utilizing a 200-term wave function [3] composed of explicitly correlated exponentials of the kind introduced by Thakkar and Smith [4]. Building on Keating's method [5] for analytically integrating the resulting three body integrals, we were able to also solve the temperature integrals to give an analytical form for the rate coefficient a_{PA} for attaching a second positron to antihydrogen to form $\bar{H}^+$. We compare our results to Bhatia's [6], who uses a 364-term Hylleraas wave function with both short-range and long-range correlations, and provide results for temperatures below 1000K.

Our motivation to produce $\bar{H}^+$ is for its potential use as an intermediary to cool antihydrogen to ultra-cold (sub-mK) temperatures for spectroscopic studies and probing the gravitational interaction of the anti-atom.

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P-27

Vibrational excitation of the ν_3 mode of Fluoromethane by positron impact. A time-dependent wave packet dynamics

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The scattering of a low energy positron (less than 1 eV) from Fluoromethane, involving the vibrational excitation of the ν_3 mode of the target, was studied using time-dependent wave-packet dynamics. The interaction between the positron and the C-F vibrational mode have been modeled through a two-dimensional *ab initio*-based potential energy surface (PES), which describe the collinear approaching: $e^+\cdots$F-CH_3. The PES, computed using the finite mass correction methodology [1], couple the translational (r) and vibrational (R) coordinates, and include a R-dependent dipole term of the form $\mu(R)/r^2$, which account for the long-range interactions. The method used to compute the scattering cross sections was adapted from a previous proposal, developed to obtain reactive cross sections in molecular collisions [2]. Thus, the integral cross sections for the first and second vibrational channels were computed by Fourier transform of the coefficients, which resulted from projecting the total scattered time dependent wave function on the target vibrational states. So far, our obtained cross sections present the expected sharp onset at threshold, exhibiting vibrational resonances at the excited channels [3]. In this moment we are engaged in the diminishing of possible errors related to the Gibbs phenomenon [4] and other associated to the wave-packet propagation parameters [5]. We argue that the present approach may unveil important details concerning the excitation of a molecular target by positron impact.

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P-28

Formation of antihydrogen in antiproton-positronium collisions embedded in plasmas

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Atomic collisions phenomena in plasma environments have received considerable interest in the recent years [1]. This is basically due to the important role played by plasma-embedded atomic collision processes in the interpretation of various phenomena associated with astrophysics, hot plasma physics, and experiments performed with charged ions. In the present work we focus our attention to investigate the effects of plasma screening on the formation of antihydrogen in $\bar{p} + Ps \rightarrow \bar{H} + e$ by using charge-conjugation invariance and time-reversal invariance processes [2]. Calculations for positronium formation cross section for the ground state have been performed by applying a formulation of the three-body collision problem in the form of coupled multi-channel two-body Lippmann-Schwinger equations [1], and the cross sections for the excited states have been obtained within the framework of a distorted wave theory in the momentum space [3]. Two types of plasma environments have been considered, namely weakly coupled plasma and dense quantum plasma. In weakly coupled plasma the interactions among the charged particles have been represented by static screened Coulomb potential (SSCP) with screening parameter μ: $V(r_{ij}) = (-1/r_{ij})e^{-\mu r_{ij}}$, (in a.u.), where r_{ij} denotes the distance between particles i and j. Whereas in dense quantum plasma those have been taken care of by exponential cosine-screened Coulomb potential (ECSCP) with screening parameter μ: $V(r_{ij}) = (-1/r_{ij})e^{-\mu r_{ij}} \cos(\mu r_{ij})$, (in a.u.). Effect of plasma screening on the formation of antihydrogen in the ground state as well as in excited states has been investigated. Total antiproton formation cross section has been obtained for a wide range of antiproton energy (20-10000kev). It is seen that effect of plasma screening on the total cross section in both cases is significant. Moreover, when quantum behavior of the background plasma medium is considered effect of screening on the cross section is rather stronger.

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P-29

Elastic Collision between Ps and H-like atoms when both are in ground states

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The elastic collision between positronium (Ps) and hydrogen-like atoms e.g. Ps and Ps, Ps and muonium (Mu), Ps and hydrogen (H), Ps and Deuterium (D) and Ps and Tritium (T) are studied to find the s-wave elastic phase shifts and the scattering lengths for both the singlet and triplet channels. The ab-initio static-exchange model (SEM) with a coupled-channel methodology is used [1] when both the atoms are in their ground states. The system is treated exactly with exchange considering it as a four-body Coulomb problem in the center of mass frame [2,3]. A systematic variation of scattering length with the reduced mass of the system is observed and are presented in Table 1.

Table 1. The variation of scattering length with reduced mass of the system.

Systems		Ps-Ps	Ps - Mu	Ps - H	Ps - D	Ps - T
Reduced Masses (a. u.)		1.0	1.9809	1.9978	1.9989	1.9993
Scattering lengths (a.u.)	Singlet (+)	9.35	7.40	7.24	7.18	7.14
	Triplet (-)	3.25	2.50	2.48	2.46	2.45

The observed dependence of scattering length on reduced mass of the system could explain the electron-like scattering of Ps [4] since the reduced mass of the system in Ps – atom and electron – atom collisions are almost the same and the difference decreases as the atom becomes heavier.

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The dependence of scattering length on reduced mass of the system

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The elastic collision between two hydrogen-like atoms with different reduced masses are studied using static-exchange model (SEM) to find the s-wave elastic triplet phase shifts and corresponding scattering lengths at low/cold energies. The new SEM code develop by Ray [1] to study a four-body Coulomb problem in center of mass frame following a coupled channel methodology in momentum space is used. All the Coulomb interaction terms in the direct and exchange channels to define the Born-Oppenheimer amplitude [2] that act as input to deduce the SEM amplitude are calculated exactly. The H-like two atomic systems of present interests are (i) Muonium (Mu) and Mu, (ii) Mu and H, (iii) Mu and Deuterium (D), (iv) Mu and Tritium (T), (v) H and H, (vi) H and D, (vii) H and T, (viii) D and D, (ix) D and T and (x) T and T. The reduced masses (μ) of these systems in atomic units are respectively (i) $\mu = 103.9$, (ii) $\mu = 186.7$, (iii) $\mu = 196.7$, (iv) $\mu = 200.2$, (v) $\mu = 918.5$, (vi) $\mu = 1224.5$, (vii) $\mu = 1377.6$, (viii) $\mu = 1836.5$, (ix) $\mu = 2203.7$, (x) $\mu = 2754.5$. The s-wave elastic triplet phase shift and the corresponding scattering length are calculated following the standard procedure described in references [1-5]. A systematic and interesting resemblance is observed between the scattering length and reduced mass of the system are observed for first time and are presented in **Table 1** below. In Ps-Ps system $\mu = 1$ and the triplet scattering length is 3.25 a.u. [5] using the present code.

Table 1. The variation of triplet scattering length with reduced mass of different H-like systems.

System →	Mu-Mu	Mu-H	Mu-D	Mu-T	H-H	H-D	H-T	D-D	D-T	T-T
Reduced mass → in a.u.	103.9	186.7	196.7	200.2	918.5	1224.5	1377.6	1836.5	2203.7	2754.5
Scattering length → in a.u.	4.54	4.76	4.88	4.95	5.88	6.25	6.37	6.58	6.68	6.90

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P-31

The dependence of scattering length on van der Waals interaction

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The modified static-exchange model (MSEM) recently introduced by Ray [1] is adapted to study the H(1s)-H(1s) elastic scattering considering the system as a four-body Coulomb problem in the center of mass frame where all the Coulomb interaction terms in direct and exchange channels are treated exactly. The model includes the nonadiabatic short-range effect due to electron-exchange and the long-range effect due to induced dynamic dipole polarizabilities between the atoms. The minimum value of the interatomic distance appears to be the most important parameter to determine the strength of the effective interatomic potential. The s-wave elastic phase shift and corresponding scattering length for different minimum value of interatomic distance (R_0) as R_0= $2a_0$, $3a_0$, $4a_0$, $5a_0$, $6a_0$, $7a_0$, $8a_0$, $9a_0$, $10a_0$, $11a_0$, $12a_0$, $15a_0$, $20a_0$ are deduced using the present MSEM code and compared with the data obtained using the static-exchange model (SEM). In **Table 1**, the calculated scattering lengths are presented and compared with SEM and other available data [2-6]. The variation of scattering length with R_0 in H(1s)-H(1s) elastic scattering is being reported

Table 1. The scattering length in atomic units using SEM and MSEM for different values of R_0.

Scattering length in atomic unit (a.u.)														
Using SEM	Using MSEM with R_0 =													Data of others
	$20a_0$	$15a_0$	$12a_0$	$11a_0$	$10a_0$	$9a_0$	$8a_0$	$7a_0$	$6a_0$	$5a_0$	$4a_0$	$3a_0$	$2a_0$	
5.88, 5.90[a]	5.80	5.68	5.26	5.11	4.89	4.63	4.38	4.03	3.77	3.68	3.63	3.60	3.58	2.04[a], 1.91[b], 1.22[c], 1.34[d], 1.3[e]

[a]Sen, Chakraborty and Ghosh [2];
[b]Jamieson, Dalgarno and Yukich [3];
[c]Jamieson and Dalgarno [4];
[d]Williams and Julienne [5];
[e]Koyama and Baird [6].

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P-32

Experimental determination of absolute differential positronium-formation cross-sections

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Experimental values of the absolute differential cross-sections for the formation of ground state positronium will be presented for a variety of atomic and molecular targets, including He, Ar, H_2 and CO_2 [1]. They have been determined by measuring the efficiency for collimated Ps production within a small angle (~1^o) around 0^o [e.g. 2-4].

In order to discern the degree of forward collimation of the Ps formed from each target, the energy dependence of the ratio of the differential and integrated cross-sections for each target has also been computed and compared with theories. The ratio highlights the greater probability for forward-emission of positronium formed from low Z targets [1].

The great sensitivity of theoretical angular-resolved cross-sections to the details of the various approximations (illustrated in Figure 1) may also impact on the resolution of discrepancies among *integral* Ps formation cross-section results.

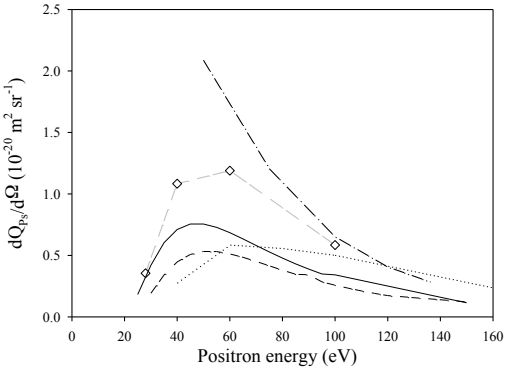

Figure 1. Theoretical prediction of the differential Ps formation cross-section for He. (diamond) FBA [5]; (□) DWA [5]; (·····) close-coupling [6]; (— · —) eikonal approximation [7]; (- - - - - -) DWA [9]; (——) second order DWA [10].

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Low-energy positron collisions with allene molecule

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In this work we will present calculated cross sections for low-energy positron collisions with allene (C_3H_4) molecules. We employed the Schwinger multichannel method for positron scattering [2] in the static plus polarization approximation, for energies up to 10 eV. Positron scattering calculation is a difficult task due the importance of a correct description of the polarization effects of the target electronic cloud. In order to investigate the role of polarization description in the calculated cross sections we performed calculations with different scattering basis set. We found a virtual state and a Ramsauer-Townsend minimum in the integral cross section and we analyze the different calculations with respect to these phenomena. We also compare the calculated integral cross sections with experimental total cross section available in the literature [3]. But it is worth mentioning that since the positronium formation channel is not included in the SMC method we do not expect agreement between calculated integral cross section and experimental total cross sections for energies above the positronium formation energy threshold.

Acknowledgments
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Calculation of Ps-atom phase shifts using a spherical cavity

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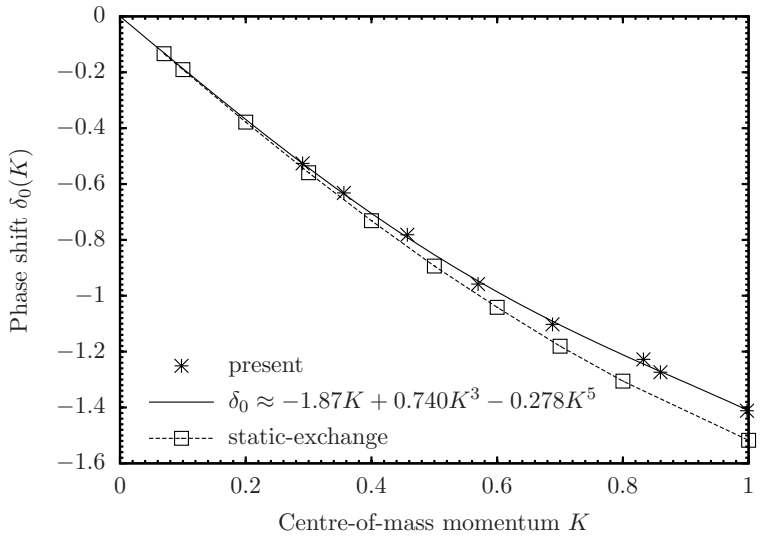
The interaction of positronium (Ps) with matter and antimatter is an important topic with applications to many areas of physics [1]. In this work we focus on low-energy Ps scattering from noble-gas atoms. To date there have been many studies of Ps scattering from He (e.g., [2, 3]) and several studies of Ps scattering from the other noble-gas atoms (e.g., [3, 4]). Here we use a *B*-spline basis to construct states of Ps in the field of an atom within a spherical cavity of radius *R*. The atom is described in the Hartree-Fock approximation.

By first calculating states of Ps from constituent electron and positron basis states in an otherwise empty cavity, the dependence of the radius ρ of Ps on its centre-of-mass momentum K can be determined [5]. Then when the atom is placed at the centre of the cavity, the phase shifts δ_L can be calculated through $\tan\delta_L(K) = J_{L+1/2}(K[R-\rho])/Y_{L+1/2}(K[R-\rho])$, where J_ν and Y_ν are the Bessel and Neumann functions, respectively. Thus we can obtain information about scattering from the bound-state problem. *S*-, *P*- and *D*-wave phase shifts have been calculated for Ps interactions with He, Ne, Ar, Kr and Xe. The figure below shows the *S*-wave phase shifts obtained for Ps(1*s*) scattering on He in comparison with existing static-exchange calculations [2]. There is excellent agreement, especially for low *K*.

The next stage of this research will be to include the long-range van der Waals interaction between Ps and the noble-gas atom, and then we will proceed to investigate Ps-atom scattering using many body theory to account for the electron-atom and positron-atom correlation interactions and screening of the electron-positron Coulomb interaction by the atom.



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P-35

Theoretical analysis of positron-molecular complexes: from small molecules to large biomolecules

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The positron 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 [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 our group, we have recently developed a new theoretical method for analyzing the effect of molecular vibrations on positron affinities. Our strategy is based on ab initio multi-component quantum Monte Carlo (QMC) [2] and molecular orbital (MCMO) [3, 4] methods for the electronic and positronic wave functions simultaneously, and the anharmonic vibrational state theory using quantum Monte Carlo (QMC) method [5, 6].

In the presentation, we will show the recent rigorous results of positron-attachment to small molecules such as HCN [2], H_2CO [3, 4, 6], and CS_2 [5] molecules. We would like to show some application of that to large BIOmolecules such as amino acids [7] and DNA species [8].

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P-36

Implementation of model potential in *ab initio* calculation of positronic compounds

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A positron affinity (PA), which is a binding energy of a positron, has now been experimentally reported by Surko and co-workers for many molecules such as hydrocarbon (alkanes, alkenes and aromatics), alcohols and halogenated hydrocarbons [1,2]. In theoretical approaches with first-principle techniques, there are two successful quantitative methods, variational calculations with explicitly correlated Gaussian basis set [3] and quantum Monte Carlo (QMC) method [4]. The theoretical PA values obtained with both methods are highly accurate, but the system size with both methods is still limited to small atomic/molecular systems due to its quite high computational costs.

In this study, we propose the use of Model Core Potential (MCP) [5] in Multi-Component Molecular Orbital (MC_MO) method [6] in order to reduce the computational costs in *ab initio* calculations of positronic compounds. The MC_MO method allows us to treat both electrons and positron as quantum-mechanically. The MCP is one of pseudo potentials used to reduce the number of electrons in *ab initio* calculations, and is able to describe accurate nodal structure in a wave function for valence electrons. Our final goal is to achieve an accurate PA estimation for large molecular systems using QMC method with MCP, but in this presentation, we would like to report a theoretical accuracy for PA values of some atomic and molecular systems obtained from MCP calculations at the Hartree-Fock (HF) level of MC_MO theory.

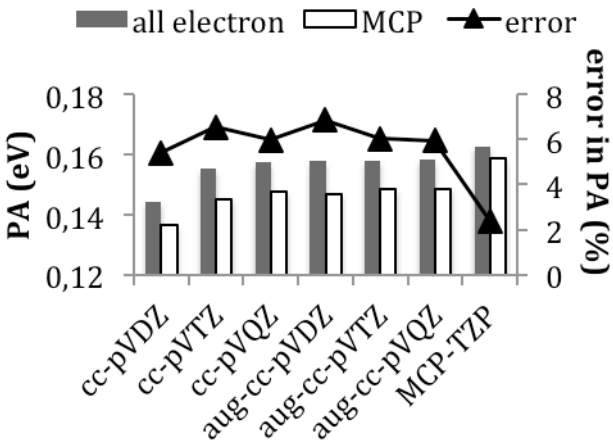

Fig.1 The PA values of LiH molecule at HF level. The values with all electron and MCP calculations are shown in gray and white bars, respectively. The line with triangle symbol shows error in PA from all electron calculations.

Figure 1 shows the PA values of LiH molecule at the HF level of calculations with various electronic basis sets. The MCP calculations reproduce the values with all electron and MCP calculations are obtained with the MCP calculations with MCP-TZP electronic basis set. We note that the fitted parameters in MCP have been parameterized with MCP-TZP electronic basis set. Further details and radial distribution function for both electrons and positron will be presented.

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P-37

Low energy positron collisions with NH_3

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Synopsis: We employed the method of continued fractions combined with the positron correlation potential (PCOP), in order to obtain the elastic cross sections for low energy positrons colliding with NH_3 molecules.

Positron molecule collisions is an interesting object of study, and differs from electron collision studies because the scattering positron is distinguishable from the molecular electrons. This difference is very important, since there is no need to consider exchange interactions. Another difference is the form of the polarization potential, and some models to account this interaction are available in the literature.

The PCOP model [1] is proven to give reliable differential and integral cross sections for positrons colliding with polar molecules [2], so it is adequate to represent the polarization of NH_3 molecules in the presence of low energy positrons.

Once the interaction potential in the static plus polarization was defined, we applied the method of continued fractions [3] in order to obtain elastic cross sections in the 0.1 to 10.0 eV energy range.

As NH_3 is a polar molecule with strong permanent dipole moment (1.47 D), a Born-closure scheme has been used to account the forward scattering. Thus, the differential cross sections have been found in order to obtain the integral cross sections which are compared with the measurements of Sueoka *et al* [4] and the calculations of Gianturco *et al* [5]. The agreement between the present results and the experimental data is found to be very good, including the forward scattering conditions. The comparison of the present results with the theoretical calculations of Gianturco et al [5] is reasonable in the whole energy range, but can be considered good only for energies lower than 4 eV.

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Low energy positron collisions with CH_4

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Synopsis: We employed the method of continued fractions combined with the polarization potential proposed by Burke and Chandra [1] (BC potential), in order to obtain the elastic cross sections for low energy positrons colliding with CH_4 molecules.

The collisions of positrons and molecules is a non-trivial problem. Even with no need to consider exchange effects between the projectile and target particles, a detailed polarization potential for short range effects should be considered and applying different polarization models to the same molecular target may give us some insight about the collisional process.

Following the work of Jain and Thompson [2], we applied the BC potential to the positron CH_4 collision problem, for some cutoff radius parameters. The resulting cross sections can be compared directly with other studies, that considered the short range effects in a different way. The most recent of such studies is the work of Zecca *et al* [3], which employed an *ab initio* methodology in order to discuss the polarization effects. It is interesting to notice that even for very different scattering methodologies, the resulting cross sections can be very similar. This is true for the comparison of the present results with those of reference [3] and for an application of the positron correlation potential (PCOP) model, as presented in the work of Jain and Gianturco [4].

The observed similarities between the theoretical approaches are present in the integral and differential cross sections. However, the theoretical correspondence with the TCS measurements of Zecca *et al* [3] is still a matter of discussion and some further theoretical work is needed.

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P-39

Resonances with natural and unnatural parities in positron-sodium scattering

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We present an investigation of resonances with natural and unnatural parities in positron-sodium. The e^+Na system is formulated as a three-body system: a frozen core, a positron and an electron. In this way, the system resembles the hydrogen-positron system, but there are some qualitative differences. First, the interaction between the Na^+ core and the active electron is Coulombic only at very long range. At shorter distances the nuclear charge is only partially screened, which makes it necessary to employ some sort of model potential for the e^-Na^+ interaction. More generally this interaction should also include electron exchange, but this has not been explicitly included in our study. The e^+Na interaction is, like the e^+H interaction, at long distances dominated by the polarizability of the atom, giving a potential $\propto r^4$. The polarizability of Na (162 atomic units) is however larger than that of H (4.5 atomic units), which allows the formation of a truly bound state of the e^+Na system [1]. Furthermore, the hydrogen atom has energy levels degenerate with respect to orbital angular momentum (neglecting fine structure) whereas the alkali atoms do not. Another characteristic of a positron-Na system is that the ionization energy of Na (0.19 a.u.) is smaller than the binding energy of Ps (0.25 a.u.), allowing for positronium formation even at zero impact energy.

S-, P-, and D-wave resonances are calculated for energies extending up to the positronium (Ps) *n=2* formation thresholds for natural parity. Resonance states for P^e and D^o below the Na(4d, 4f, 5p) excitation and Ps *n=2,3* formation thresholds are calculated for unnatural parity which has not been previously reported. Below both positronium thresholds we have found a dipole series of resonances, with binding energies scaling in good agreement with expectations from an analytical calculation [2]. The present results are compared with those in the literature [3-6].

Explicitly correlated Gaussian trial functions expressed in Jacobi coordinates spanning all three rearrangement channels have been employed to include the correlation effects between the outer electron, the positron and the core. The complex scaling method has been used. Two different types of analytical model potentials are used to represent the interaction between the core and outer electron. Of the earlier works, our method is most similar to the stabilization method [4,5], but allows more accurate description of resonances by going into the complex plane. It is also different in the coordinate system and functional forms it uses for representing the wave-function, allowing relatively large basis sets to be used.

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Theoretical analysis of H/D isotope effect on positron affinity of hydrogen cyanide molecule

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The positron is the anti-particle of the electron and therefore has the same mass and spin, but the opposite charge. The positron undergoes a pair-annihilation with an electron together with a gamma-ray emission, and the positron spectroscopy using the gamma-ray are now widely used in various scientific and technological areas such as physics, chemistry, material science, medicine, and their interdisciplinary areas [1]. Positrons injected into a liquid or solid induce processes such as ionization, electronic excitation, the formation of positronium (a temporary bound state of a positron and an electron), and the formation of positron-molecular complexes before the pair-annihilation.

Recently, Surko and coworkers have experimentally measured a positron affinity (PA), which is the binding energy of a positron, for various kinds of molecular species with vibrational Feshbach resonance technique, in which a positron-molecular complex can be formed at vibrational excited states [2]. They also found the H/D isotope effect on the PA values for acetone, acetonitrile, and acetaldehyde molecules [3]. The origin of the H/D isotope effect, however, is still unclear both experimentally and theoretically.

In this study, thus, we theoretically analyzed the PA values of hydrogen cyanide (HCN) molecule, which is the smallest nitrile species, and its isotopologues (DCN), in order to elucidate the origin of H/D isotope effect on the binding of a positron to this molecule. In our analysis, the PA values at molecular geometries deformed along all vibrational coordinates are calculated with the configuration interaction (CI) level of multi-component molecular orbital method, and are averaged with a vibrational probability density obtained with quantum Monte Carlo method [4,5]. Figure 1 shows the H/D isotope shifts in PA values at each vibrational state of HCN molecule. We found that PA values at the vibrational excited states of the CD stretching mode become smaller than those of the CH stretching mode.

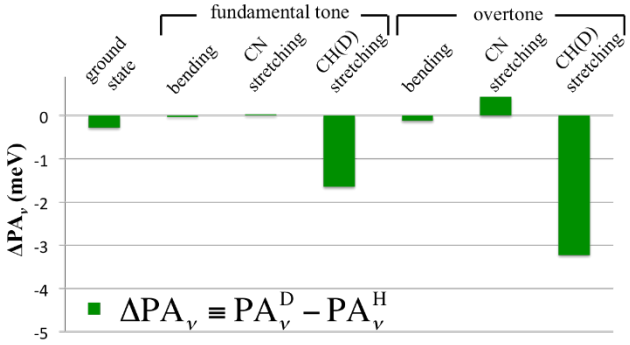

Figure 1: H/D isotope shifts in PA values at each vibrational state of HCN molecule

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A comparison of positron, electron and positronium low-energy scattering from hydrogen

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Experimental findings of Brawley *et al.* [1,2] have shown that for many targets, equal velocity e^- and Ps scattering cross sections are similar between 0.5 and 2.0 a.u. A similar conclusion was made by Fabrikant and Gribakin [3] from their theoretical analysis of e^- and Ps scattering from Kr and Ar. The tentative conclusion is that the positron plays a much smaller role in the scattering process than the electron in Ps-atom and in Ps-molecule scattering, this is despite the fact that Ps is a very polarisable neutral bound system.

We plan to present a comparative study of the low energy elastic scattering of e^+, e^- and Ps from H, using the Kohn variational method in all cases, in order to make a detailed analysis of the similarities and difference between them [4,5,6]. Our preliminary results indicate also a similarity of the integrated cross sections for e^- and Ps scattering; however, we find more significant differences in the differential cross sections.

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Binary encounter approach to positronium collisions with atoms and molecules

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The impulse approximation turned out to be efficient for description of Ps collisions with atoms [1,2] helping to explain the observed [3] similarities between Ps-atom and electron-atom scattering. However, its applications require on-shell reduction of electron-atom and positron-atom scattering amplitudes that leads to ambiguities, especially at low collision energies comparable to the Ps ionization threshold (6.8 eV).

In the present work we develop a semiclassical version of the impulse approximation for Ps-atom collisions based on the binary encounter approach to Rydberg atom collisions developed by Smirnov [4] and Flannery [5]. We apply this method to Ps ionization in collisions with atoms and molecules, i.e. to the process

$$B + \mathrm{Ps} \rightarrow B + e^+ + e^-$$

where B is a neutral target. The basic equation for the ionization cross section is

$$\sigma_{ion} = \frac{1}{v_B}\langle |\boldsymbol{v} - \boldsymbol{v}_B| \int d\sigma \rangle \qquad (1)$$

where $\boldsymbol{v}_B$ is the velocity of B relative to Ps, $\boldsymbol{v}$ is the electron velocity relative to the Ps center of mass, and $d\sigma$ is the differential cross section for e-B collisions. Integration occurs over the range of scattering angles resulting in the energy transfer $\Delta E > I$ where $I = 6.8$ eV is the Ps ionization potential. The average is over the electron velocity distribution in Ps. Eq. (1) describes the contribution of $e^- + B$ collisions to ionization. A similar contribution results from $e^+ + B$ collisions. The method requires the knowledge of scattering cross sections rather than amplitudes, and therefore is free of ambiguities associated with the on-shell reduction.

Calculation for ionization of Ps in collisions with rare-gas atoms show a good agreement with more sophisticated methods based on the quantum version of the impulse approximation [1].

This work has been supported by the US National Science Foundation.

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Positron moderation and diffusion: W meshes and foils

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Moderators are a crucial component for the production of quasi-monoenergetic positron beams, reducing the phase space distribution of β^+ particles emitted from radioactive decay (or pair production), whilst reducing their energy down to a few electron volts [e.g. 1, 2, 3].

We have investigated the efficiency of tungsten meshes and thin foils for moderation of fast positrons from Na-22 in transmission geometry and a fair agreement has been found with previous results [4]. For foils, we obtained a dependence on material thickness similar to the theoretical prediction of [5], however the magnitude is 5-10 times lower, as was found across a variety of earlier experiments. In order to investigate this discrepancy, we have developed a three dimensional diffusion model [4] in which we allow the thermalized positrons to diffuse isotropically. The results of this new model are in significantly better agreement with experiments. We have also found that for a given thickness, meshes are generally better than foils by around a factor of 10 with a maximum efficiency ($\sim 10^{-3}$), comparable to that achieved with thin single crystal foils and in accordance with previous measurements and the results of the present 3D model.

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Elaborate calculations of low-energy Ps-H collisions

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Ps-H scattering is a fundamental four-body process. Using the Kohn variational method and variants of the method (inverse Kohn, generalized Kohn, S-matrix complex Kohn and T-matrix complex Kohn), we compute phase shifts for this process for the first six partial waves.
We consider energies up to the Ps(n=2) threshold [1]. The work is an extension of prior calculations of the ^{1,3}S and ^{1,3}P phase shifts using the Kohn and inverse Kohn Variational methods [2]. We obtain singlet resonances below the Ps(n=2) threshold for the partial waves up to the ^{1}F-wave [1]. Using the S-matrix complex Kohn phase shifts, we determine for the ^{1,3}S-waves the scattering length and effective ranges, and we determine for the ^{1,3}P-waves the effective range [1]. We compare the results we obtain of the ^{1,3}S, ^{1,3}P and ^{1,3}D phase shifts, resonance parameters, scattering lengths, and effective ranges with results from other calculations.

We determine the elastic differential, elastic integrated and momentum transfer cross sections [1]. As the energy of the incoming Ps increases from zero energy, the scattering changes from isotropic to backward peaked to strongly forward peaked, indicating interesting behavior of the differential cross section. The maximum value of the differential cross section in the forward direction occurs at about 1eV.

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Computational resources were provided by UNT's High Performance Computing Services.

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P-45

Calculation of resonance states of positronic alkali atoms

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Positron-atom interactions have been one of the fundamental problems for positron science. Recently, there have been high-precision experiments associated with internal properties of atoms and molecules——for example, a precise measurement of hyperfine splitting of Ps in low density organic gas (i-C_4H_{10}) [1]. Theoretical investigations to the complex state of a positron and atoms/molecules are essential for the experimental studies. Compared with the experiments for bound and resonance states of positronic molecules, those for bound and resonance states of positronic atoms have been hardly studied. Some experiments to detect bound and resonance states of the positronic atom have been proposed [2, 3] recently. Precise calculation is crucial because the widths of the resonances are quite narrow.

Positronic alkali atoms ($LiPs^+$, $NaPs^+$) are good testing grounds to examine positron-atom and Ps-ion interactions. These systems can be calculated precisely within a three-body approximation composed of a positron, the valence electron and residual ion core of the atom. Resonance states of positronic alkali atoms are appropriate to investigate long-range interactions of positron-excited atom and excited Ps-ion. In previous studies, although some resonance states have been found, the existence and mechanism of resonance states, namely, a shape resonance [4] or Feshbach resonance [5], have not been confirmed.

In this work, we calculate resonance states of $LiPs^+$ and $NaPs^+$ with a high-precision effective potential constructed in our previous bound state calculation [6]. Resonance energies and widths are determined with a stabilization method. **Figure 1** shows correlation functions of the valence electron in Feshbach resonances below Na (4s) and Ps (n=2) threshold, and a shape resonance above Na (4s) threshold, together with the probabilities of finding in the excited states of Na and Ps atom. We examine the shapes of wavefunctions and analyze the structures of the resonance states. The resonances are found to be supported by attractive potential caused by polarization of the excited states of Na or Ps. From the deformation of the wavefunctions of the excited states, energy levels can be attributed to the resonances associated with threshold energy levels, even though the different series of resonances are intermixed.

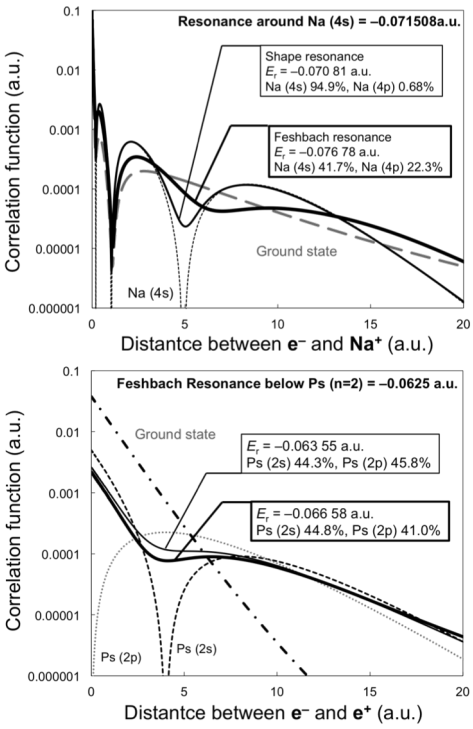

Figure 1. Correlation functions of resonance states of $NaPs^+$.

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Age-momentum correlation study of positron slowing down processes in dense Ar gases.

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A high energy positron injected into Ar gas loses its kinetic energy by a fast inelastic scattering slows down to 11.7 eV which is the first excitation energy of Ar atom. Below the kinetic energy of 11.7 eV, the positron can lose its energy by a slow elastic scattering whose momentum transfer is extremely low. Since the annihilation probability decreases with an increase of the kinetic energy of positron, a positron annihilation rate in epithermal energy region (11.7–0.04 eV) is smaller than that in thermal energy. Therefore, Positron annihilation lifetime spectrum (PALS) of Ar gas has a characteristic shoulder structure which can not be reproduced by a summation of exponential functions [1]. The positron termalizaition time was, therefor, defined from the shoulder structure of the PALS [2,3]. In order to investigate positron slowing down process directory, we performed a positron annihilation age-momentum correlation (AMOC) measurement [4] in dense Ar gas (7.5 MPa) at room temperature [5,6].

The positron source (^{22}Na, 0.5 MBq) was sandwiched between two sheets of 5 μm of the Ni foil (purity > 99%) [7], and was placed in the center of a cylindrical high-pressure vessel with a diameter of 2.8 cm and a height of 5.0 cm. We reconstructed the AMOC system by replacing plastic scintillator with BaF2 scintillator and adopting a digital oscilloscope. Time resolution of the PALS was 300 ps at the full width at half maximum (FWHM). Our results of the thermalization time and density dependence of lifetimes of thermalized positron and *o*-Ps were in good agreement with previous results [8]. Energy resolution of the two-photon annihilation (511 keV) was 1.23 keV at FWHM. In the present study, we resolved the Doppler broadening into two components (*p*-Ps and other free positron component). The intensity of *p*-Ps was determined from the PALS. We discuss the positron sowing down process not only S-parameter of the free positron component [5] but also W-parameter. We successfully obtained the positron age dependence of the two parameters from 0 to 1 ns.

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P-47

Positronium laser excitation and cooling, for the AEgIS collaboration

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The A.E.G.I.S: Antimatter Experiment: Gravity, Interferometry, Spectroscopy[1], is one of the experiments carried out at CERN which uses the CERN Antiproton Decelerator to produce antihydrogen ($\overline{\mathbf{H}}$). The goal is to answer fundamental questions concerning antimatter such as: Does anti-matter behave identically to matter under gravity? Is anti-matter similar to matter from the spectroscopic point of view? Comparison between matter (H) and antimatter ($\overline{\mathbf{H}}$) intends to test the famous CPT theorem linked with Lorentz invariance.

Another goal of the AEgIS experiment is to study Positronium physics. Indeed, AEgIS proposes to create colder antihydrogen, based on a charge exchange reaction between excited (Rydberg) positronium and cold trapped antiprotons:

$$Ps^* + \bar{p} \rightarrow \overline{H^*} + e^-$$

Thus, studying Ps physics is crucial for our experiment, and requires adapted lasers systems. In order to excite Ps up to its Rydberg states ($\simeq 20$) in presence of a high magnetic field (1T), two broadband pulsed lasers have been developed. The first one at 205.04 nm performs the $n = 1 \rightarrow n = 3$ transition, whereas an IR laser around 1670 nm excites Ps from $n = 3$ to Rydberg states[2].

In parallel to this system, two dyes narrowband lasers have been set up in order to perform Rydberg spectroscopy. Cooling of Ps is also considered for a future experience, cycling the $n = 1 \leftrightarrow n = 2$ transition.

We here intend to present recent laser excitations results on AEgIS and some encouraging Doppler laser cooling simulations.

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P-48

Rotational Excitation of H_2 by Positron Impact

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Synopsis: We present rotational excitation cross sections for low energy scattering of positrons by H_2 below positronium formation threshold (8.2 eV). The cross sections were computed from fixed-nuclei scattering amplitudes generated with the Schwinger multichannel method using the adiabatic rotational approximation. Comparison with other similar theoretical results is performed and discussed.

Below the ionization, positronium formation and electronic excitation thresholds, atoms steal the positron energy basically by momentum transfer. This situation is radically different for molecules, where the vibrational and rotational degrees of freedom can work more efficiently as cooling agents [1]. Recently, Natisin et al [2] measured the cooling rate of positrons in N_2. H_2 and N_2 are non-polar molecules with dipole inactive degree of freedom. It means that positron cooling works basically by rotational excitation in both systems. Under these conditions, it becomes interesting to compute the rotational cross sections for positron scattering by H_2 in the low energy domain. Our focus is for energies below 8.2 eV, where the positronium formation channel becomes energetically accessible for this system.

Following Cheng and Temkin [3], the rotational excitation cross sections are computed as

$$Q^{J_i \to J_f} = \frac{1}{2J_i+1}\frac{k_f}{k_i}\sum_{M_i,M_f}\int d\hat{k}_f \, |f(\vec{k}_f)^{J_i,M_i \to J_f,M_f}|^2$$

with

$$f(\vec{k}_f)^{J_i,M_i \to J_f,M_f} = \int d\Omega \, (Y_{J_f,M_f}(\theta,\phi))^* f^{LF}(\vec{k}_f) Y_{J_i,M_i}(\theta,\phi)$$

where $f^{LF}(\vec{k}_f)$ is the fixed nuclei scattering amplitude transformed to the Lab-Frame, Y_{J_i,M_i} and Y_{J_f,M_f} are the initial and final rotational states, here considered in the rigid-rotator approximation. The fixed-nuclei amplitude was computed with the Schwinger multichannel method [4]. It means that while the scattering dynamics is treated in an adiabatic formalism, the scattering potential is treated ab initio. We compare our results with previous ones generated by dell Vale and Gianturco [5].

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A coincidence study of electron and positron impact ionization of argon

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Very recently there have been complementary fully coincidence experiments performed using relatively high energy beams of electrons and positrons on an argon target [1]. We have performed calculations for the same kinematics using the distorted wave Born approximation (DWBA)[2-4]. For the electron calculation the distorted waves for the incoming and outgoing electrons are calculated in the static-exchange potential of the atom and for the slow electron in the singlet static-exchange potential of the ion. We consider the use of both the Gamov factor [5] and the Ward and Macek factor [6] to correct for post-collisional interaction (PCI). For positron impact ionization in the DWBA there is only a direct scattering amplitude, the distorted waves for the incoming and outgoing positrons are calculated in the static potential of the atom and the distorted wave for the ejected electron in the spin-singlet static-exchange potential of the ion. Agreement with [1] is not good. The experimental data is shifted well away from the direction of momentum transfer, while the theoretical binary maximum lies close to this direction. The one thing theory and experiment agree on is that the positron cross section is larger than the equivalent electron one but there is little in the way of quantitative agreement. PCI has a very small effect in both cases. Experimental studies of *(e,2e)* are well developed and it is therefore of interest to look for similar kinematics. There have been *(e,2e)* experiments reported by Avaldi and collaborators [7] in an experimental arrangement which is very close to that of [1]. We have performed DWBA calculations to compare with [7]. Here both theory and experiment are nearly symmetric about the direction of momentum transfer and agreement is encouraging. We thus conclude that there must be some unresolved issues with the experiment of [1].

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