

# Positron atomic physics – A look to the future

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## Abstract

This article is a brief overview of opportunities and challenges in the area of low-energy positron and positronium atomic physics. The ideas presented here come from discussion during the final, summary session of the XIII International Workshop on Low Energy Positron and Positronium Physics, Campinas Brazil, July 2005.

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As is the custom, the final session of the workshop was devoted to a group discussion regarding the challenges and opportunities in the area of low-energy positron and positronium physics. The session began with brief presentations by Michael Bromley (San Diego), Mike Charlton (Swansea), Gleb Gribakin (Belfast) and Nella Laricchia (London) on their views of the future and continued with a group discussion. The following is a brief overview of key points raised by the group. A more detailed report of the workshop, including this summary session, will be published elsewhere [1].

## 1. Positron sources, technology and facilities

Presently, most positron atomic physics experiments are done using  $^{22}\text{Na}$  sources. Typical  $^{22}\text{Na}$ -based beams using solid neon-moderators (i.e. the most efficient moderators available) have fluxes in the range from  $10^5$  to  $10^7$  positrons per second. For the past few years, almost all of these sources have come from one supplier. It was pointed out that the field would benefit by the availability of alternative means to obtain positron sources.

On the world scene, there are a few intense positron-beam facilities. Examples in Europe are the reactor-based beam at the University of Delft, and a new facility at the new reactor in Munich. Both operate with positron fluxes

in excess of  $10^8 \text{ s}^{-1}$ . Generally, the positron atomic physics community has not as yet exploited these resources that, at present, are used predominantly for condensed matter and materials science studies. There is a general sense that the opportunities presented by the availability of these intense beams should be more fully utilized for positron atomic physics.

In terms of new facilities, there are experiments in progress to make a more intense source using small accelerators and  $^{13}\text{N}$  (Washington State and U.C. Riverside). It was suggested that a long-term goal for intense positron facilities should be the establishment of beam lines made as “turn-key” as possible to facilitate a broad range of users and experiments. One important direction for an intense positron facility would be the development of a Ps beam line. The current method of choice for forming Ps beams involves the relatively inefficient process ( $\sim 10^{-3}$  Ps atoms per positron) of charge exchange in a gas cell, and thus Ps experiments would benefit greatly by the availability of a much more intense positron-beam.

The field has benefited by the recent development of cold, trap-based positron-beams. This technique produces a magnetized beam (i.e. in fields of strength  $\sim 0.01$ – $0.1 \text{ T}$ ; energy resolution  $\sim 20 \text{ meV}$ ). While this technique is superior to electrostatic beams, for example, for measurement of integral cross sections, it has disadvantages for other applications such as measurement of small cross sections and differential inelastic cross sections.

A question was raised as to whether high-brightness electrostatic beams with similar energy resolution could

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be developed. This does not appear to be out of the question using brightness-enhancing techniques currently under development. In this same vein, if such an electrostatic beam were available; it could, for example, be used with the COLTRIMS technique to measure multiple final-state projectiles resulting from a collision, and the “magnetic angle changer” technique to study scattering over a wide range of angles. Both of these latter techniques have made tremendous contributions in the conventional areas of electron and ion scattering.

The group was enthusiastic about the new positron atomic physics and materials science facility currently being established at the Australian National University in Canberra. As currently planned, the facility will have a magnetically guided, trap-based beam, using a  $^{22}\text{Na}$ /neon-moderator positron source.

The development of colder positron-beams (e.g. resolution  $\sim 1$  meV, FWHM), now in progress, would be a welcome development. Applications include more precise studies of threshold phenomena and searches for narrow resonances. In a similar vein, techniques to produce larger, denser and colder positron plasmas would facilitate increased production of low-energy antihydrogen and study of the  $\text{Ps}_2$  molecule, BEC Ps and electron–positron plasmas.

## 2. Positron and positronium interactions – experiment

There are many areas where further and/or more refined experiments are needed. Examples include positron-impact ionization (including positronium formation), which would benefit from study of the differential cross sections, for example, to provide more stringent tests of theory. Careful studies of annihilation and Ps formation up to and through the threshold would be of interest to test the precise theoretical predictions that are now available. There is a discrepancy between prediction and experiment for the peak in the positronium formation cross section in helium that should be further investigated. The formation of Ps on inner-shell orbitals has been the subject of considerable speculation and requires definitive experimental study.

In the area of electronic excitation of molecules, sharp, near-threshold increases in the cross sections for excitation of the lowest-lying electronic states have been observed in  $\text{N}_2$  and CO. The origin of these features is not understood and currently the subject of considerable theoretical interest. There are also significant discrepancies between theory and experiment in the positron analogue of the “ $e \rightarrow 2e$ ” problem (i.e. correlation of final-state particles in direct ionization). These discrepancies and more refined electron–positron correlation experiments should be pursued. Comparative studies of positron- and electron-impact cross sections, such as those planned for the new Canberra positron facility, are likely to be very insightful.

While simple targets are of great interest, study of more complex systems would also be of value. Examples include the noble gas atoms, and related molecular sequences such as  $\text{CH}_4$ ,  $\text{CF}_4$ ,  $\text{CCl}_4$ ,  $\text{CBr}_4$ . This would, for example, aid in

the development and testing of theories, including their ability to describe strong electron–positron correlation effects in scattering, annihilation and positron binding. Such studies would also provide information about positron interaction with the vibrational degrees of freedom and their effect in enhancing annihilation rates.

The area of Ps scattering with atoms and molecules has been much less well explored. There are many open issues in this area, such as the details of inelastic collisions, Ps-breakup, target ionization and doubly inelastic processes.

## 3. New experiments

Thus far, most atomic and molecular targets have been studied at 300 K, particularly in experiments with trap-based beams. More work with heated and cooled targets would be very useful. One example discussed was study of atomic clusters such as  $\text{C}_{60}$ , where cage-like resonant states have been predicted. Another example is trap-based beam studies of alkali atoms.

It has been shown theoretically that positrons can bind to certain classes of atoms, and positron binding energies have been predicted for approximately ten atoms. This is a very important area for future experiments, although detection schemes to date appear to range from challenging to very challenging.

Should the new generation of planned cold positron-beams become a reality (i.e. with approximately meV energy resolution), it would open up a wide variety of possibilities, such as precise study of threshold phenomena and the investigation of narrow resonances. An example is the vibrational Feshbach resonances observed in positron annihilation on hydrocarbons, where the currently available resolution ( $\sim 20$  meV) is inadequate to resolve individual vibrational modes.

In the more challenging category, positron- and Ps-impact studies involving excited-state targets such as  $\text{He}(^3\text{S})$  and other metastable noble gas atoms would be of considerable interest and could possibly be done with the target species in an atom trap.

## 4. Positron and positronium interactions – theory

A number of recent developments and outstanding issues in positron atomic physics theory were discussed. The view was expressed that, for noble gas atoms, many-body theory now provides a good understanding of the role of correlation effects, both in low-energy elastic scattering and annihilation. Interestingly, it was found that this requires a nonperturbative description of virtual Ps formation (i.e. through calculation of the electron–positron, ladder-diagram series). The next challenge will be to extend the theory to higher positron energies, where the Ps formation channel is open. Another view is that a full, quantitative theory of positron annihilation has yet to be achieved. One issue mentioned is the role of p-waves in annihilation resonances, where open questions remain.

While various methods, such as coupled-channel approximations, the configuration interaction formalism, and many-body theory, have been used to make accurate (or relatively accurate) predictions about positron interactions with a variety of atoms, much less is known theoretically about positron interactions with molecules. It is likely, for example, that for many molecular systems, inclusion of the Ps channel (either open or closed) will be very important in describing such processes as electronic excitation and positron binding. A view was expressed that work by additional theoretical groups would be particularly welcome on polyatomic molecules, including the problem of vibrational excitation.

One key area for future work is positron binding to molecules. While there is strong experimental evidence that such an effect exists in large hydrocarbon molecules, at present, detailed theoretical models are absent. Small molecules could provide a theoretical test bed to understand the physical mechanisms that lead to positron binding using a variety of theoretical techniques. To date, the only molecules that have been shown to bind positrons are strongly polar species that bind due to the long-range dipole force, even in the static approximation (although this substantially underestimates the binding energy).

The Schwinger variational approach was also a topic of discussion. It has been used successfully to describe positron scattering from small molecules, however annihilation appears to be a more difficult problem. It was suggested that it might be useful to test the ability of this approach to describe correlation effects in atomic systems, where theory and experiment are in reasonably good accord. The group viewed as a positive development a new effort, just beginning, to calculate positron interactions with small molecules using the *R*-matrix formalism.

The problem of positron binding to large molecules appears to be considerably more challenging. A method sensitive to electron–positron correlations appears to be required to describe positron resonances and binding, and the detailed vibrational dynamics of the molecule must be included as well. At present, this problem may be more amenable to study using model approaches, such as use of zero-range potentials. In general, comparison of electron–molecule and positron–molecule attachment will likely be of considerable interest. In this regard, the standard picture of electron capture by molecules is based on the intersection of potential surfaces corresponding to the electronic terms describing the neutral molecule and negative ion. In the case of positron capture (which underpins huge enhancements in annihilation rates observed for large molecules), it is presently unclear whether a similar picture will be useful or whether a different model of capture will be required.

## 5. Intersection of theory and experiment

Traditionally, hydrogen and helium are systems where the predictions of accurate theories could be compared in detail with experimental results. There is a great need for

additional benchmarks so that theory and experiment can be compared with precision. This includes elastic scattering; rotational, vibrational and electronic excitation; single and double direct ionization; Ps formation; and direct annihilation. While considerable data exists for some of these processes, such as elastic scattering and direct ionization, very little is available for others such as rotational excitation and double ionization. The field suffers in this regard from the small number of cases where there is more than one experimental data set for a particular quantity to test theory. Similarly, there is frequently only one calculation to compare with a set of measurements. To have multiple theoretical and experimental groups focus on specific benchmark problems would be very beneficial. Examples include precision studies of simple systems such as He and H<sub>2</sub>. Other important targets include H<sub>2</sub><sup>+</sup> (including the dissociation channel) and H<sub>2</sub>O.

A number of interesting and important issues were mentioned regarding the many-positron, many-electron system (i.e. electron–positron many-body systems). They include the formation and study of the Ps<sub>2</sub> molecule (experiment in progress) and the related effort to create BEC positronium in cavities below a material surface. These experiments involve cold collisions, where for example, the scattering length is a critical parameter. The physics here has important synergies with current research on ultra-cold gases.

Another very important problem is the formation of low-energy antihydrogen. The most successful formation process developed to date involves the merging of cold positron and antiproton plasmas in a strong magnetic field. This produces a broad range of excited states, including strongly magnetized, high-Rydberg atoms (i.e. so-called guiding-center atoms). These guiding-center atoms have interesting and unusual properties that are likely to be the focus of much theoretical and experimental interest for the foreseeable future. One important issue is the development of detailed and realistic simulations of situations relevant to experiment to predict the range of excited states produced and how these atoms are further transformed in subsequent collisions. A related problem is the formation of cold Ps atoms via merged positron and electron plasmas.

Another related problem discussed at the workshop is the physics of antihydrogen–matter interactions (e.g. such as collisions of antihydrogen with hydrogen or helium atoms or H<sub>2</sub>). At low temperatures, description of these collisions is believed to require going beyond the Born–Oppenheimer approximation to use of a non-adiabatic formalism. Somewhat surprisingly, strong antiproton–nucleus interactions proved to be very important in particular cases. This area of antihydrogen collisions with matter also has important synergies with current work on ultra-cold gases.

## 6. Concluding remarks

This summary highlights the wealth of interesting scientific questions, which can and should be investigated, ones

that will quite likely lead to interesting scientific results. In the broader view, there is a continuing belief that the field would benefit greatly by actively seeking more connections to other areas of science. With this in mind, selectivity was recommended in studying positron processes and phenomena with an eye toward the broader impacts of the research. Given the range of applications of positron physics (e.g. from astrophysics to PET scans), it would be both appropriate and beneficial for positron atomic physics to lose the “exotic particle” tag. One example in this regard is exploiting the synergy between electron-driven and positron-driven processes. More work relevant to materials and bioscience would also aid in achieving this objective.

The availability of additional intense-beam and otherwise dedicated positron facilities presents additional opportunities. Not only can one achieve much higher data rates and develop a range of instrumentation hard to justify in

a single laboratory, but these user facilities can be expected to enable a broader range of scientists to exploit positron processes to address a wide range of scientific issues.

Finally, it should be remarked that the international nature of the theoretical and experimental positron community has led to much progress and can be expected to do so in the future. The workshop highlighted the extensive collaborative efforts that exist across the world on both experimental and theoretical problems of interest. This valued tradition can be expected to serve the field well.

### Reference

- [1] G. Laricchia, M.W.J. Bromley, M.A.P. Lima, *Physica Scripta: Comments on Atomic, Molecular and Optical Physics* (to be submitted for publication).