

Advances in positron and electron scattering^{*}

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Abstract. The topical issue on “Advances in Positron and Electron Scattering” combines contributions from POSMOL 2015 together with others devoted to celebrate the unprecedented scientific careers of our loyal colleagues and trusted friends Steve Buckman (Australian National University, Australia) and Michael Allan (University of Fribourg, Switzerland) on the occasion of their retirements. POSMOL 2015, the XVIII International Workshop on Low-Energy Positron and Positronium Physics and the XIX International Symposium on Electron-Molecule Collisions and Swarms, was held at Universidade NOVA de Lisboa, Lisboa, Portugal, from 17–20 July 2015. The international workshop and symposium allowed 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.

1 Introduction

Following previous editions [1], the meeting held in Lisboa has attracted 150 participants (90 regular, 54 students, 6 accompanying), from twenty five different countries. POSMOL 2015 accommodated five plenary sessions covering experiments on electron energy loss spectra of gas phase molecules and ionic liquids, a tribute to the exceptional contributions of Jim Mitroy, the theory of low-energy positron scattering on atoms and molecules, swarms as an exact representation of weakly ionized gases and calculations of bound and continuum states of molecules using the R-matrix method. The international conference hosted eighteen thematic sessions, consisting of twenty eight topical lectures and four joint sessions on the most recent experimental and theoretical achievements on low-energy positron and positronium physics and electron-molecule collisions and swarms. The meeting also accom-

modated a poster session, allowing entry to more than one hundred presentations guaranteeing therefore an opportunity for more fruitful discussions. Throughout POSMOL 2015 both international advisory committee meetings for “EMS” and “POSITRON” were held.

2 New scientific insights

The topical issue on Advances in Positron and Electron Scattering has collected 43 contributions and is devoted to the state-of-the art developments on experimental and theoretical aspects in low-energy positron and positronium physics and electron-molecule collisions and swarms from leading research groups across the globe. These contributions include the most recent advances in the field and are also part of a special tribute to the outstanding scientific and technical career of Steve Buckman and Michael Allan, two loyal colleagues and trusted friends on the occasion of their retirement.

A study of sodium doping and reactivity in pure and mixed ice nanoparticles has been reported by Lengyel et al. [2]. Bray et al. [3] presented and discussed the internal consistency in the close-coupling approach to positron

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collisions with atoms. Investigating the role of vibrational excitation in simulating charged-particle tracks in liquid pyrimidine was presented by Brunger et al. [4] as part of a significant effort to understand radiation damage in biological matter. Smialek and Mason [5] have presented a photoelectron-photoabsorption database and photoelectron and threshold photoelectron valence spectra of pyridine [6]. Barboza and Bettega [7] have reported elastic cross sections for low energy electron collisions with the cyclic ether tetrahydropyran. Linert and Zubek [8] obtained a detailed study on electron energy-loss spectroscopy of excited states of the pyridine molecules in the energy range 3.5–9.0 eV. Donko and Dyatko [9] examined two particular effects that appear in electron transport: the negative differential conductivity and transient negative mobility, via conventional Boltzmann equation analysis and via a novel particle simulation method that is devoid of all approximations that are adopted in the Boltzmann equation solution. Screening effects of plasmas on the formation of antihydrogen ($\bar{\text{H}}$) in an arbitrary s-state from the ground state of the positronium atom (Ps) by antiproton ($\bar{\text{p}}$) impact have been studied within the framework of charge-conjugation and time-reversal invariance [10]. Mass spectra of electron ionized valine doped helium clusters for both cations and anions and up to 40 valine molecules have been reported by Weiberger et al. [11] whereas calculations of the ionization rate of the sodium atom in strong fields within the quasistatic regime were presented by Bunjac et al. [12]. The photodetachment of the negative ion of boron, $\text{B}^- \ ^3\text{P}$, was investigated by employing the B-spline R-matrix method for photon energies ranging from threshold to 12 eV [13] and new and original experimental data on the dissociative electron attachment (DEA) to 2-nitrophenol molecule, 2-nitrophenol clusters and heterogeneous clusters of 2-nitrophenol, argon and water was presented by Kocisek et al. [14]. Sauer et al. [15] reported on the calculation of dipole polarizability derivatives of adamantane and their use in electron scattering computations whilst Franz et al. [16] described density functional calculations (DFT) of elastic integral scattering cross-sections for positron collisions with argon, krypton, nitrogen and methane below the positronium formation threshold. Alves et al. [17], within the relevance of modelling oxygen-containing plasmas, reported on the presentation and validation of electron scattering cross sections, with atomic and molecular oxygen in the ground-state and excited states. Rotational excitation of H_2 by positron impact in adiabatic rotational approximation was presented by Zanin et al. [18] whereas the structure and dynamics of near-threshold electrons: scattering and bound states driven by dipolar interactions with polyatomic molecules has been reported by Carelli and Gianturco [19]. Rankovic et al. [20] reported the design and performance of an instrument for electron impact tandem mass spectrometry and action spectroscopy of mass/charge selected macromolecular ions stored in RF ion trap. Borrmann and Swiderek [21] presented experimental data on the formation of 2-propanol in condensed molecular films of acetaldehyde following electron impact

ionisation-induced proton transfer, and computed elastic cross section for positron scattering from beryllium and magnesium, using physically motivated, parameter free and local model potentials were reported by Poveda et al. [22]. Dora et al. [23] showed the first theoretical attempt to identify higher lying resonances that lead to dissociative attachment of CO, and Ridenti et al. [24] presented electron scattering data for biomass molecular fragments, indicating that low-energy resonances may have an important role in the de-lignification of biomass through a plasma pre-treatment. Ćurik et al. [25] determined shape resonances in acetylene negative ions through commercially available quantum chemistry software by use of the RAC method developed by the authors. Triple-differential cross sections for the ionization of NH_3 by positron impact in coplanar and perpendicular geometrical arrangements were presented by Toth et al. [26]. The first high resolution measurement of He^{*-} formation in helium droplets was reported by Al Maalouf et al. [27], the study of the radiative electron attachment and photodetachment processes for the $\text{C}_2\text{H}/\text{C}_2\text{H}^-$ and $\text{C}_4\text{H}/\text{C}_4\text{H}^-$ molecules by Khamesian et al., the theoretical study of a positron-attachment to vibrational excited states for non-polar carbon disulphide molecule by Takeda et al. [28] and low energy electron induced reactions in fluorinated acetamide yielding neutral stable molecules have been reported by Kopyra et al. [29].

The topical issue also accommodates other contributions related to the lowest autodetachment state of the water anion [30], high resolution ejected electron spectroscopy has been used to investigate a large number of Ar autoionizing states [31], the calculation of resonance states of positronic lithium atom [32], nuclear dynamics in resonances revealed by 2-dimensional EEL spectra, electron collisions with ionic liquids and electronic excitation of pyrimidine by Allan et al. [33], age-momentum correlation study of positron slowing down processes in dense Ar gases and free energy barrier for dissociation of the guanosine monophosphate anion in water [34]. Finally, we note a set of contributions on electron impact and electron transfer on:

- structure and energetics in dissociative electron attachment to $\text{HFeCo}_3(\text{CO})_{12}$ [35];
- effect of the third π^* resonance on the angular differential cross sections for electron-pyrimidine scattering [36];
- computational study of dissociative electron attachment to π -allyl ruthenium (II) tricarbonyl bromide [37];
- local orbital techniques to improve the scaling of electron-molecule scattering calculations, in order to facilitate accurate calculations on the large and complex targets, such as biomolecules, that are of increasing interest [38];
- extensive investigation on the negative ion resonances in carbon monoxide [39];
- change in resonance parameters of a linear molecule as it bends: evidence in electron-impact vibrational transitions of hot COS and CO_2 molecules [40];

- kinetic-energy release distributions of fragment anions from collisions of potassium atoms with D-ribose and tetrahydrofuran [41].

3 Summary

Although related to POSMOL 2015 the papers were submitted after the conference and have all passed the full editorial treatment and evaluation according to the high standards of the journal. The international advisory committees for the electron-molecule symposium and the positron workshop together with the local organizing committee hope that POSMOL 2015 was an excellent opportunity to share and develop scientific and technological expertise of current relevant aspects of positron, positronium and antiproton interactions with electrons, atoms, molecules and solid surfaces, and related topics, as well as single electron and electron swarm interactions with molecules in both gaseous and condensed phases. We are looking forward to POSMOL 2017, the XIX International Workshop on Low Energy Positron and Positronium Physics and the XX International Symposium on Electron-Molecule Collisions and Swarms, to be held at Amaro On Mandalay Resort, Magnetic Island, Queensland, Australia, from 23–25 July 2017.

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