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Editorial

Molecular collisions, photoionization and dynamics: honouring Professor Vincent McKoy

M. H. F. Bettega[1,a], S. J. Buckman[2], M. Khakoo[3], P. Limão-Vieira[4,b], and M. T. do N. Varella[5,c]

[1] Departamento de Física, Universidade Federal do Paraná, Caixa Postal 19044, Curitiba, Paraná 81531-980, Brazil
[2] Research School of Physics, Australian National University, Canberra, ACT 2601, Australia
[3] Department of Physics, California State University, Fullerton, CA 92834, USA
[4] Atomic and Molecular Collisions Laboratory, Department of Physics, CEFITEC, Universidade NOVA de Lisboa, 2829-516 Caparica, Portugal
[5] Instituto de Física, Universidade de São Paulo, Rua do Matão 1731, São Paulo, São Paulo 05508-090, Brazil

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Abstract. The topical issue "Advances on Molecular Collisions, Photoionization and Dynamics" encompasses a set of theoretical and experimental contributions honouring the unprecedented scientific career of our loyal colleague and trusted friend the late Professor Vincent McKoy. He has been a pioneer in implementing ab initio electron-molecule scattering and molecular photoionization theoretical methods, alongside with his collaborations across the globe, having contributed to different research fields that are now well-established and where he leaves a strong scientific legacy as noted by the testimony of his long-lasting collaborator, Carl Winstead. The contributions hereafter are related to the most recent achievements in electron interactions with molecules and molecular ions as a function of phase and stage of aggregation as well as key aspects of photoionization mechanisms therein. Particular topics include studies of photon and electron interactions (excitation, ionization and attachment) with biological, technological, astrophysical and aeronomic relevant molecules, electron transport phenomena and electron induced surface chemistry. Theoretical aspects of model potentials and molecular processes including nonadiabatic chemical reactions are also addressed in this special occasion.

1 Introduction

We have commissioned this topical issue that has attracted the contribution of more than a hundred authors and co-authors, from nineteen different countries and/or affiliated institutions, with a tribute to the exceptional contributions of the late Professor Vincent McKoy on electron-molecule scattering and molecular photoionization methods. The international scientific community promptly responded to pay tribute to Vincent McKoy's legacy and to celebrate his major theoretical achievements on key aspects involving electrons and photons with atoms and molecules.

2 New scientific insights

The topical issue on Molecular collisions, photoionization and dynamics has collected 29 contributions and is devoted to the state-of-the art developments on theoretical and experimental aspects of electron-molecule scattering and molecular photoionization theoretical methods from leading research groups across the globe. These contributions include the most recent advances in these fields and are also part of a special tribute to the outstanding scientific career of Professor Vincent McKoy, a loyal colleague and trusted friend, which is clearly testified in the contribution from Carl Winstead, the long-lasting and close collaborator of Vince [1].

A study on the absolute partial ionization cross sections for electron impact of R-carvone from threshold to 100 eV has been reported by Amorim et al. [2]. Luxford et al. [3, 4] presented and discussed the dissociative electron attachment mechanisms to methyl acetonitrile and isocyanide, respectively. New experimental data on the fragmentation of the tyrosine amino acid molecule and the formation of ionised products due to the low-energy electron impact were presented by Tamuliene et al. [5]. Takatsuka [6] has presented a methodology to unify electronic and nuclear quantum wavepacket dynamics in molecular processes including nonadiabatic chemical reactions whereas a R-matrix theory implemented using the pseudostate formalism has been used to calculate elastic and excitation processes in electron

[a] e-mail: bettega@fisica.ufpr.br
[b] e-mail: plimaovieira@fct.unl.pt (corresponding author)
[c] e-mail: mvarella@if.usp.br (corresponding author)

interactions with N_2H and HCO [7]. Suarez-Moreno et al. [8] have reported studies on electron interactions with formamide clusters as a model system to understand phenomena relevant to astrophysical, prebiotic and radiobiological processes. Silva and co-workers [9] reported on a joint theoretical–experimental investigation on the elastic and absorption electron collisions with acetaldehyde. Zavilopulo et al. [10] examined the ionization and fragmentation of valine molecules in the gas-phase by electron impact. A detailed study on electron impact elastic scattering from CH_4^+, NH_3^+, H_2O^+, NH_4^+ and H_3O^+ molecular ions is reported for the first time by using an optical model potential method [11]. Elastic and inelastic scattering of low-energy electrons from gas-phase C_{60}: elastic scattering angular distributions and coexisting solid-state features have been revisited by Tanaka et al. [12] while Cl^- kinetic-energy release distributions from chlorobenzene and related molecules in electron transfer experiments were presented by Kumar et al. [13]. A combined experimental and theoretical study of helium adsorption on cationic hexaphenylbenzene (HPB), a propeller-shaped molecule, was investigated [14], and molecular synthesis in ices triggered by dissociative electron attachment to carbon monoxide was presented by Schmidt et al. [15]. García-Abenza and co-workers [16] reported on a complete data set for the simulation of electron transport through gaseous tetrahydrofuran in the energy range 1–100 eV as a significant attempt to understand radiation damage in biological related molecules particle track simulations, whilst Randi et al. [17] described elastic, electronically inelastic, total ionization and total cross sections for the scattering of electrons by *trans*-formic acid. Falkowski et al. [18, 19], within the relevance of a model potential for computing total ionization cross sections of atoms and molecules by electron impact, reported on hydrogen, carbon, nitrogen and oxygen atoms and for hydrogen, nitrogen, water, methane and benzene molecules. For benzene, they calculated differential and integral cross sections for elastic and electronic excitation, as well as total cross sections, for electron scattering at impact energies in the 10–50 eV range. Computing resonance energies directly through a method comparison for a model potential was presented by Davis and Sommerfeld [20], Bandurin et al. [21] obtained the excitation of L-valine molecules by optical spectroscopy, and new routes in the formation of positively charged fragments upon electron attachment were investigated [22]. We also note a contribution on a set of cross sections and transport coefficients for electrons in C_2H_6O and its mixtures with Ar and Ne [23] while Sugawara and Nakata report an analytical study on elliptic vector loci of average electron velocity of an electron swarm in constant-collision-frequency model gas under ac electric and dc magnetic fields crossed at arbitrary angles [24]. A high-resolution, variable-energy electron beam from a Penning–Malmberg (Surko) buffer-gas trap has been reported by Buckman and co-workers [25]. The investigation of the elastic scattering of low-energy electrons and positrons by pyrazine (isomer of $C_4H_4N_2$) was carried focusing on the description of polarisation effects [26]. Freitas and co-workers obtained elastic cross sections for the scattering of low-energy electrons by cubane (C_8H_8) and discussed the shape resonance spectra and the presence of a Ramsauer-Townsend minimum and of a virtual state [27]. Finally, the last two contributions within the topical issue address low-energy electron elastic scattering by SF_6 [28] and competing ionization and dissociation in the H_2 gerade system [29].

3 Summary

The topical issue on Molecular collisions, photoionization and dynamics in honour of Professor Vincent McKoy has received 29 papers from researchers from all over the world. Within the scope of this topical issue, the scientific and technical contributions within each paper have all passed the full editorial treatment and evaluation according to the high standards of the journal. With this collection of manuscripts, we modestly pay our tribute to the contributions of the late Professor Vincent McKoy, hoping that his scientific achievements and legacy, within the scope of electron and photon interactions with atoms and molecules, will continue for the future generations to come.

Declarations

Data Availability Statement This manuscript has no associated data, or the data will not be deposited. [Authors' comment: This is an editorial and so not categorised as a contribution made of any set of data].

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