27th International Symposium on Ion-Atom Collisions

ISIAC

satellite of

Book of Abstracts

Editor: **Katalin Nagy-Póra**

July 14-16, 2021 | Organized on-line

The International Symposium on Ion-Atom Collisions (ISIAC) is a biennial satellite of the International Conference on Photonic, Electronic and Atomic Collisions (ICPEAC). As usual, the symposium will cover all ion-atom collision phenomena including excitation, ionisation and charge transfer, from low to relativistic velocities as well as interactions of ions with surfaces, molecules and clusters.

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Wednesday, July 14, 2021

All times are in EET (UTC+3)

15.20	**Opening**	
	Chair: **Alain Dubois**	
15.30	**Alisher Kadyrov** Convergent close-coupling approach to ion-atom collisions: recent progress	INV-01
16.00	**Junwen Gao** Single and double electron capture in intermediate energy N^{5+}+H_2 collisions	INV-02
16.30	**Pablo de Vera** Electronic interactions of swift ions and their secondary electrons in biologically relevant materials	INV-03
17.00	**Nicolas Antonio** Modelling electron capture in Be ion collisions with hydrogen for charge-exchange spectroscopy	FL-01
17.05	**Tomasz Wasowicz** The role of charge transfer and complex formation in cation-induced fragmentation of pyridine	FL-02
17.10	**Maria Silvia Gravielle** Influence of surface defects in grazing-incidence fast atom diffraction	FL-03
17.15	**Break**	
	Chair: **Clara Illescas**	
17.45	**Nicolas Sisourat** Ion-atom collisions within helium clusters	INV-04
18.15	**Tom Kirchner** Interatomic Coulomb decay in low-energy ion-dimer collisions: a theoretical analysis based on independent-atom-model coupled-channel calculations	INV-05
18.45	**Madhav Dhital** Study of Higher-Order Contributions to The Few-Body Dynamics of Simple Atomic Systems at A Fully Differential Level	INV-06
19.15-19.45	**Poster Session**	

INV - Invited presentation
SH - Short presentation
FL - Flash presentation

Thursday, July 15, 2021

All times are in EET (UTC+3)

15.00-15.30	**Poster Session**	
	Chair: **Béla Sulik**	
15.30	**Xiaolong Zhu** Heavy N^+ ion transfer in doubly charged N_2Ar cluster	INV-07
16.00	**Max Kircher** A kinematically complete experiment on Compton scattering: Collision physics with photons	INV-08
16.30	**Svenja Lohmann** Ion-electron dynamics studied in a 3D-transmission approach	INV-09
17.00	**Abhijeet Bhogale** Ionization of water under the impact of 250 keV protons and C, O ions with energy of a few MeV/u	FL-04
17.05	**Péter Herczku** An experimental apparatus for systematic studies of molecular processes induced by ion and electron irradiation in astrophysical ice analogues	FL-05
17.10	**Pablo Ramón Batista Oliveira** Secondary ion emission from condensed N_2O irradiated by MeV heavy ions	FL-06
17.15	**Break**	
	Chair: **Maria Silva Gravielle**	
17.45	**Wania Wolff** Complete Break-up of Methane and Ammonia from Satellite States	INV-10
18.15	**Gisela A. Bocan** Anomalous KCl(001) Surface Corrugation from Fast He Diffraction at Very Grazing Incidence.	INV-11
18.45	**Kate Spicer** Singly dfferential direct scattering and electron capture cross sections of intermediate energy proton-helium collisions	SH-01
19.00	**Markus Schöffler** On the quest for projectile coherence in C^{6+}/He collisions	SH-02
19.15	**Zoltán Juhász** Binary ridges in the $O^+ + H_2 \rightarrow O + H^+ + H$ process as a signature of molecular rotation	SH-03

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Friday, July 16, 2021

All times are in EET (UTC+3)

15.00-15.30	**Poster Session**	
	Chair: **Xinwen Ma**	
15.30	**Lokesh Tribedi** Electron emission from large biomolecules and radiosensitizing effect	INV-12
16.00	**Jimmy Rangama** Coulomb-explosion imaging of carbon monoxide dimers	INV-13
16.30	**Andreas Jacob** Formation of $\bar{H}^+$ via radiative and nonradiative attachment of e^+ to $\bar{H}$	INV-14
17.00	**Victor Kartoshkin** Ionization of alkali atoms during the collisions with polarized metastable helium. Redistribution of the spin polarization	FL-07
17.05	**Abdelmalek Taoutioui** Transfer ionization cross sections in A^{+q} + He collisions	FL-08
17.10	**Mariel Elisa Galassi** Neonization method to calculate multiple ionization cross sections of water molecules by ion impact	FL-09
17.15	**Break**	
	Chair: **Michael Schulz**	
17.45	**Alain Dubois** Multi-electron effects in collisions of swift ions and atoms	INV-15
18.15	**Alejandra Mendez** Underlying scaling rules for the ionization of molecules	INV-16
18.45	**Yu Zhang** Hydrogen Migration in the Dissociation of Hydrocarbon Dications	SH-04
19.00	**Stefanos Nanos** Shell Effects on Electron Capture to the Continuum in MeV/u Collisions of Deuteron Ions with Multielectron Targets	SH-05
19.15	**David La Mantia** First Observation of RDEC for $F^{9,8+}$ Ions on Graphene	SH-06
19.30	**Closing**	
19.40	**International Advisory Board meeting**	

INV - Invited presentation
SH - Short presentation
FL - Flash presentation

List of Poster Contributions

Wednesday, July 14, 2021

P-01	**Cíntia A. P. da Costa and Enio F. da Silveira** Radiolysis of Valine by keV electrons
P-02	**Silvina Segui, Juana L. Gervasoni, Nestor R. Arista, Zoran L. Miskovic** Energy loss of relativistic charged particles in 2D materials, using the oscillator model
P-03	**R. Martinez, A. Domaracka, M.E. Palumbo, G. Strazzulla, P. Boduch, H. Rothard, E.F. da Silveira** Electronic Sputtering from SiO_2 Targets
P-04	**Claudia C. Montanari, Alejandra M. P. Mendez, Darío M. Mitnik, Jorge E. Miraglia** Stopping power in heavy atoms, the role of $4f$ electrons
P-05	**D. Schury, C. Bu, P.-M. Hillenbrand, X. Urbain, and D. W. Savin** Planned Laboratory Studies of N_2 reacting with H_3^+ Isotopologues
P-06	**Verónica B. Tessaro, Benoit Gervais, Floriane Poignant, Michael Beuve, Mariel E Galassi** MDM-Ion Monte Carlo code: swift ion tracks in water to study physical parameters of interest in hadrontherapy

Thursday, July 15, 2021

P-07	**Saed J. Al Atawneh and K Tőkési** Interaction of C^{5+} ions with hydrogen atoms
P-08	**Chandan Bagdia, Deepankar Misra, Abhijeet Bhogale, Lokesh C Tribedi** Double-to-single ionization ratio for a PAH molecule coronene ($C_{24}H_{12}$) in fast ion impact
P-09	**Ł Jabłoński, D Banaś, P Jagodziński, A Kubala-Kukuś, D Sobota, I Stabrawa, K Szary, M Pajek** Two electron processes in relaxation of Rydberg hollow atoms
P-10	**C T Plowman, K H Spicer, I B Abdurakhmanov, A S Kadyrov, and I Bray** Calculation of differential cross sections in proton-hydrogen collisions
P-11	**L. Wei, J. Han, B. Ren, B. Wang, W. Yu, Y. Zhang, Y. Zou, L. Chen, J. Xiao, and B. Wei** Absolute total single- and double-electron capture in $O^{6+} + (CO_2, CH_4, H_2 \text{ and } N_2)$ collisions
P-12	**R. Yanes-Rodríguez, R. Rodríguez-Segundo, P. Villareal and R. Prosmiti** Interactions and quantum effects on molecular ions' microsolvation process

Friday, July 16, 2021

P-13 **I. B. Abdurakhmanov, C. T. Plowman, A. S. Kadyrov and I. Bray**
Effective single-electron treatment of ion collisions with multielectron atomic targets

P-14 **M Al-Ajaleen, K Tőkési**
Interaction of electrons and positrons with protons aligned in one-dimension line

P-15 **Debasmita Chakroborty, S Phatak, C. Bagdia, A. Bhogale, L. Gulyas and L. C. Tribedi**
Differential cross section of emitted electrons from acenapthene under fast H-like Si ion impact

P-16 **Sergio Beneitez, Juana L. Gervasoni, Jorge G. Gallardo**
Adsorption energy of Hydrogen and Nitrogen in Tungsten

P-17 **V. A. Knyazeva, K. N. Lyashchenko, O. Yu. Andreev**
Photon polarizations in two-photon $2s \to 1s$ transitions in one-electron ions

P-18 **Tomasz J. Wasowicz**
Unusual overproduction of excited hydrogen atoms identified in the H_3^+ collisions with tetrahydrofuran

P-19 **I Ziaeian, K Tőkési**
State selective charge exchange cross sections in $Be^{4+} + H(1\,s)$ collisions

Convergent close-coupling approach to ion-atom collisions: recent progress

Alisher Kadyrov
Department of Physics and Astronomy, Curtin University, Perth, Australia
a.kadyrov@curtin.edu.au

Ion-atom collisions take place in various astrophysical and laboratory plasma environments. Therefore, an accurate knowledge of excitation, electron-capture and ionisation processes occurring in such collisions plays an important role for practical applications. A two-centre wave-packet convergent close-coupling (WP-CCC) approach developed in our group is capable of providing benchmark data on the integrated and differential cross sections for processes taking place in ion-atom collisions. The WP-CCC approach is based on expansion of the total scattering wave function using a two-centre pseudostate basis. This allows one to take into account all underlying processes, namely, direct scattering and ionisation, and electron capture into bound and continuum states of the projectile. The normalized wave packets constructed from the radial Coulomb wave functions are used to discretise the continuous spectrum of the target and projectile atoms. The generated orthonormal wave-packet bases are used in the two-centre expansion of the total scattering wave function. One of the favorable features of the WP-CCC method is its ability to generate target and projectile atom states with arbitrary energies and distribution. This, in addition to improving the accuracy of the calculations, also has a particular advantage in calculating differential ionisation cross sections where the energies of the pseudostates with different orbital quantum numbers are aligned. Discretisation of the continuum can be as dense as necessary. The utility of the method was demonstrated in our previous works on examples of proton and multiply-charged ion collisions with atomic hydrogen. The integrated, fully differential, as well as various doubly and singly differential cross sections for ionisation of hydrogen were calculated and a comprehensive set of highly accurate benchmark results obtained. Here we report on recent progress in applications of the method to collisions of fully stripped ions with atomic hydrogen and multielectron targets.

Earlier the WP-CCC method was applied to calculate fully differential cross sections for single ionization of helium by energetic protons using a single-centre expansion [1]. The obtained results showed that the coupling between channels and multiple-scattering effects, combined with a more accurate treatment of the target structure, significantly improves the agreement between theory and experiment. We have now extended the method to intermediate energies where a two-centre expansion is required. We have calculated angular differential cross sections for direct scattering and electron capture, and singly differential cross section for ionisation [2]. The results agree well with available experimental data. We have also developed a computationally more efficient one-centre approach to two-centre rearrangement collisions involving multielectron targets [3] and applied to proton scattering on lithium. Recently, we have developed an effective single-electron treatment of ion collisions with multielectron targets that does not use the independent-event model [4] and applied it to calculate single-electron capture and single-ionization cross sections for proton collisions with alkalis. Obtained results are in very good agreement with experiment for electron capture, however, significant discrepancies between theory and experiment for single ionization of Na and K remains. We have used the WP-CCC approach to calculate the angular differential cross sections of elastic scattering, excitation, and electron capture, as well as the ionization cross sections differential in the ejected-electron angle, and in the ejected-electron energy [5]. We also report on calculations of the total and state-selective cross sections for bare beryllium ion collisions with hydrogen [6], where there have been discrepancies between different approaches for capture into excited states of the projectile.

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[6] N W Antonio, C T Plowman, I B Abdurakhmanov, A S Kadyrov, I Bray, submitted for publication

Single and double electron capture in intermediate energy N^{5+} + H_2 collisions

J. W. Gao[1], Y. W. Zhang[2], Y. Wu[3,2], J. G. Wang[3], N. Sisourat[4], and A. Dubois[4]
[1]*Institute of Nuclear Science and Technology, Sichuan University, 610064, Chengdu, China*
[2]*Center for Applied Physics and Technology, HEDPS, Peking University, 100871, Beijing, China*
[3]*Institute of Applied Physics and Computational Mathematics, 100088, Beijing, China*
[4]*Sorbonne Université, CNRS, Laboratoire de Chimie Physique-Matière et Rayonnement, 75005, Paris, France*
gaojunwen@scu.edu.cn

Over the past decades, electron capture processes induced by highly-charged ions colliding with H_2 molecules have been studied extensively because of the great importance in various domains, such as the understanding of x-ray emission from solar wind ions interacting with cometary neutral species [1] and the modeling of fusion plasmas for diagnostic purposes [2]. For the system N^{5+}-H_2, a substantial number of experimental investigations, e.g., [3-6], have been carried out for single electron capture (SEC) processes. In contrast, only very scarce data are available for the double electron capture (DEC) process [3]. From the theoretical point of view, investigating this collision system still remains challenging due to the strong coupling between various channels, the multicenter features of the H_2 molecular target as well as the role of the electronic correlation.

In the conference, we shall present our latest work [7] on single and double electron capture in intermediate energy N^{5+} + H_2 collisions. Total and partial cross sections are calculated using a three-center, two-active-electron, semiclassical nonperturbative approach. For SEC cross sections, the present results show an excellent agreement below 10 keV/u where theoretical and experimental data are available and discriminate between them when disagreement existed. In addition, it is shown that the cross sections for DEC into autoionizing states are particularly significant and thus contribute substantially to the total single electron capture cross sections through post-collisional autoionization. The cross sections for DEC into bound states of N^{3+} are also reported and show severe discrepancies with the rare available data. Furthermore, the molecular orientation effects for electronic processes have also been investigated, which leads to a discussion with respect to the mechanisms responsible for the corresponding electronic processes.

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Electronic interactions of swift ions and their secondary electrons in biologically relevant materials

Pablo de Vera[1], Andrea Pedrielli[1], Paolo E. Trevisanutto[1], Stefano Simonucci[2], Rafael Garcia-Molina[3], Isabel Abril[4], Simone Taioli[1], and Maurizio Dapor[1]
[1]*European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT*) and Trento Institute for Fundamental Physics and Applications (TIFPA), Trento, 38123, Italy*
[2]*School of Science and Technology, University of Camerino, 62032, Camerino, and INFN, Sezione di Perugia, 06123, Perugia, Italy*
[3]*Departamento de Física, Centro de Investigación en Óptica y Nanofísica, Universidad de Murcia, Murcia, 30100, Spain*
[4]*Departament de Física Aplicada, Universitat d'Alacant, Alacant, 03080, Spain*
pdeveragomis@ectstar.eu

Among the many applications of energetic ion beams, their exploitation in medicine is attracting much attention in recent years. Ions can be used for cancer treatment instead of the X-rays employed in conventional radiotherapy, which brings many advantages [1]: their characteristic depth-dose curve (known as the Bragg peak) allows the energy deposition within the tumour area sparing the surrounding healthy tissues; additionally, ions present an increased cell killing probability for the same amount of dose as compared to photons. The latter feature arises as a consequence of a chain of physico-chemical events happening on different space, time and energy scales [2], which connect the initial macroscopic propagation of the ions in the body to the final DNA damage in cells through the production, propagation and effects of secondary species, mainly low energy secondary electrons and reactive chemical species.

In this contribution, a series of methods which have been developed during recent years for the multiscale modelling of the physical processes underlying ion radiation biodamage will be reviewed. These include the calculation of high-quality electronic excitation spectra of condensed-phase materials by means of *ab initio* methods [3], the use of these spectra together with the dielectric formalism for reliably obtaining electronic cross sections for ions and electrons [4], as well as the use of the resulting cross sections in Monte Carlo simulations to estimate clustered DNA damage on the nanometre scale [3].

These methodologies are also very useful for getting physical insights into the processes behind newly explored cancer treatment modalities, such as the use of metal and metal oxide [5] nanoparticles as enhancers of ion beam cancer therapy.

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Modelling electron capture in Be ion collisions with hydrogen for charge-exchange spectroscopy

N. W. Antonio, C. T. Plowman, I. B. Abdurakhmanov, A. S. Kadyrov, I. Bray
Curtin Institute for Computation and Department of Physics and Astronomy, Curtin University, GPO Box U1987, Perth, WA 6845, Australia
nicholas.antonio@student.curtin.edu.au

The two-centre wave-packet convergent close-coupling (WP-CCC) approach is applied to bare beryllium ion collisions with atomic hydrogen to calculate electron-capture and ionisation cross sections relevant for charge-exchange spectroscopy. Specifically, total, n- and $n\ell$-resolved electron-capture cross sections (here, n and ℓ are the principal and angular momentum quantum numbers of the Be^{3+} ion, respectively) are calculated. The WP-CCC method expands the scattering wave function in terms of both target and projectile basis states. Through direct substitution of this constructed scattering wave function into the Schrödinger equation it is then possible to obtain a set of coupled differential equations for the expansion coefficients. These equations are solved for the expansion coefficients. The resulting coefficients then allow us to calculate the aforementioned cross sections.

Generally, the total, n- and $n\ell$-resolved cross sections obtained in this study display excellent agreement with different theoretical models. We have also addressed discrepancies between two different works in regards to the distribution of the n-resolved electron-capture cross sections at an incident energy of 100 keV/amu. Figure 1 displays the WP-CCC results for the n-resolved electron-capture cross section as a function of the final state n against previous theoretical works.

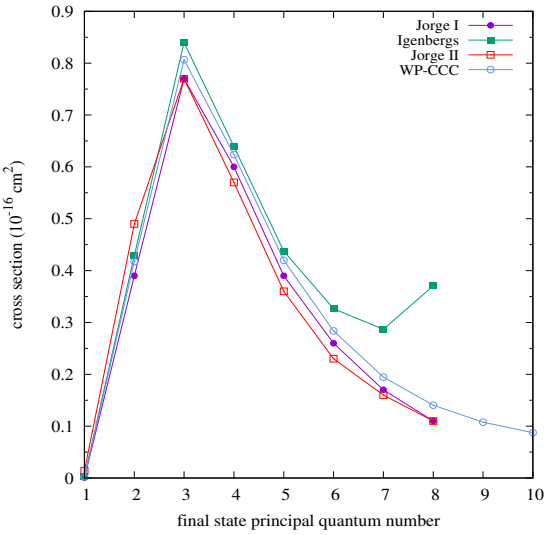

Figure 1: n-partial cross sections for electron-capture in Be^{4+}-H(1s) collisions at the incident energy of 100 keV/amu: The present WP-CCC results are compared to works by Igenbergs *et al.* [1] using an atomic orbital close-coupling method and Jorge *et al.* [2] with a time-dependent grid-numerical approach (I) and a classical trajectory Monte-Carlo approach (II).

References

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The role of charge transfer and complex formation in cation-induced fragmentation of pyridine

Tomasz J. Wasowicz[1]
[1]*Department of Physics of Electronic Phenomena, Gdańsk University of Technology, ul. G. Narutowicza 11/12, 80-233 Gdańsk, Poland*
tomasz.wasowicz1@pg.edu.pl

The interaction of energetic photons or particles usually leads to the fragmentation of molecules. The collisions with photons or electrons typically cause the dissociative excitation or ionization of the target. In the heavy charged particles' impact, electrostatic interactions between reacting species preceding decomposition may additionally occur. Indeed, the charge transfer and the transient complexes formation are the processes in which the corresponding ion−molecule components remain bound by ion−dipole attraction. These reactions are of particular interest because they are involved in various chemical and biological phenomena, such as oxygenic photosynthesis or cellular respiration. Moreover, the cation beams are effectively used in hadrontherapy [1], and extensive studies have been recently performed to understand the mechanisms underlying the ion-induced fragmentation of biomolecules (see, e.g. [2], [3]).

Therefore this work is concentrated on unraveling these collisional processes leading to the fragmentation of pyridine molecules under the $H^+/H_2^+/He^+$ cations impact in the velocity range ~20–440 km/s. Pyridine is a heteroaromatic building block of vitamins, pharmaceuticals, and agrochemicals. The experiments were performed at the University of Gdansk. We have utilized collision-induced emission spectroscopy [4] to explore the collisional excitation products and the spectral signatures of collisional mechanisms (see examples in Figures 1a and 1b). In particular, the conditions of the electron capture mechanism and the transient complexes formation will be discussed.

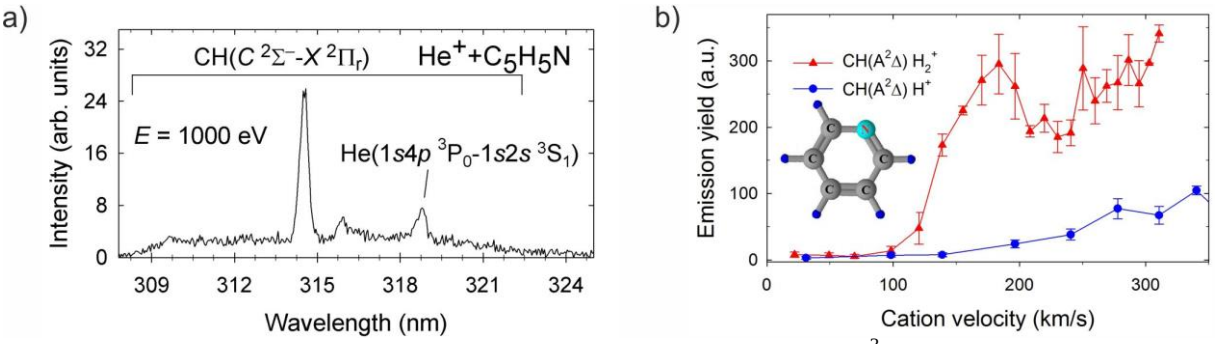

Figure 1: a) The luminescence of helium atoms excited to the 1s4p $^3P_0$ state. Since the helium atom is not a structural unit of pyridine, the corresponding emission points to the electron transfer reaction. b) The relative cross-sections of CH($A^2\Delta$). The prominent resonance-like maximum suggests the formation of the $[H_2{-}C_5H_5N]^+$ transient complex before decomposition.

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Influence of surface defects in grazing-incidence fast atom diffraction

L. Frisco[1], M.S. Gravielle[1]
[1]*Instituto de Astronomía y Física del Espacio (UBA-CONICET), Buenos Aires, Argentina*
msilvia@iafe.uba.ar

Grazing-incidence fast atom diffraction (GIFAD) is an exceptionally sensitive technique of surface analysis, which provides detailed information of the topmost atomic layer [1]. GIFAD patterns are produced by well-ordered crystal targets. But such a periodic ordering requirement is particularly crucial along the axial direction, since grazing projectiles probe long distances of the surface along the incidence channel. Therefore, surface preparation is an important issue in GIFAD experiments. However, even under extremely good cleanness conditions, real crystals present defects that might affect the interference structures [2].

In this work we study the influence of defects on diffraction patterns for He atoms grazingly impinging on a LiF(001) surface, collision system that can be considered as a prototype for GIFAD. In particular, we analyze the presence of terraces on the LiF sample, which are assumed as placed parallel or perpendicular to the axial channel. For an ideal crystal, the GIFAD pattern is formed by sharp peaks laying on a circular annulus - the Laue circle - due to the energy conservation associated with the elastic scattering (Fig. 1 (a)). But the presence of an outward (inward) step, oriented perpendicular to the axial channel, introduces a broad background above (below) the Laue circle (Fig. 1 (b)). This effect might be present in experimental GIFAD patterns, in addition to inelastic [3] and thermal [4] contributions, allowing us to study surface defects.

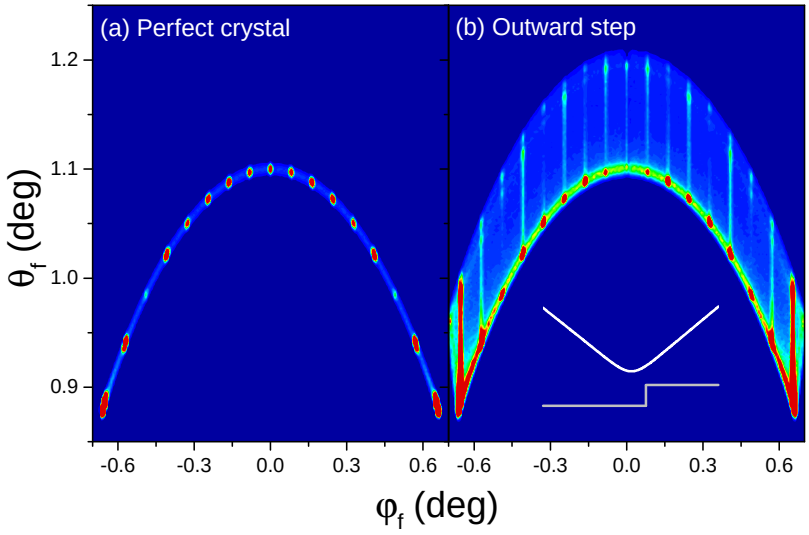

Figure 1: SIVR distributions for 1.25 keV ^{4}He → <110> LiF(001) at the grazing angle θ_i = 1.1 deg, considering: (a) perfect crystal and (b) surface with a perpendicular step (height 0.1 a.u.).

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Ion-atom collisions within helium clusters

Nicolas Sisourat[1]
[1]*Sorbonne Université, CNRS, Laboratoire de Chimie Physique - Matière et Rayonnement , F-75005 Paris, France nicolas.sisourat@sorbonne-universite.fr*

Interatomic/Intermolecular Coulombic Decay (ICD) is an ultrafast non-radiative electronic decay process wherein an excited atom or molecule transfers its excess energy to a neighboring species leading to the ejection of an electron from the latter [1]. In a helium cluster, ICD can take place after simultaneous ionization and excitation of one helium atom within the cluster [2]. After ICD, two helium ions are created and the system undergoes Coulomb explosion. Following this ultrafast dissociation several ion-atom collisions within the cluster may take place.

In this talk, we will report on the theoretical approach we have developed to describe the electronic and nuclear processes taking place in this original type of ion-atom collisions [3]: our approach combines a semiclassical method with a Diatomics-In-Molecule approach allowing us to consider helium clusters containing thousands of atoms. Several examples will be presented and discussed [4], providing new insights into ion-atom collisions in the condense phase.

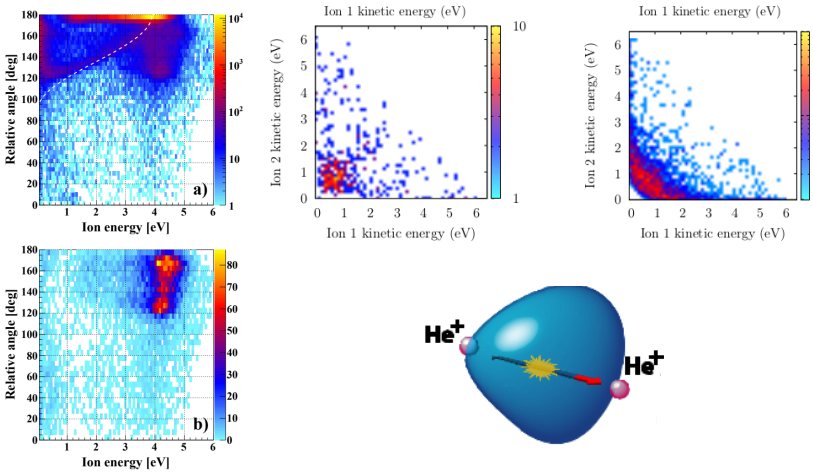

Figure 1: ICD can take place after simultaneous ionization and excitation of one helium atom within a helium cluster. The excited ion transfers its excess energy to another helium atom which is ionized as a result. After the energy transfer, the two ions repel each other due to Coulomb repulsion. The ions thus created may undergo ion-atom collisions within the cluster.

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Interatomic Coulomb decay in low-energy ion-dimer collisions: a theoretical analysis based on independent-atom-model coupled-channel calculations

Tom Kirchner, Dyuman Bhattacharya
Department of Physics and Astronomy, York University, Toronto, Ontario M3J 1P3, Canada
tomk@yorku.ca

We consider few keV/amu ion collisions with Ne_2 and present an analysis of the electron removal processes which are associated with various dimer fragmentation channels, interatomic Coulomb decay (ICD) being one of them. The ion-dimer system is described within the independent atom model and the coupled-channel basis generator method is used to solve the underlying ion-atom problems. Relative yields for the fragmentation channels of the dimer are obtained from an impact parameter by impact parameter analysis of the electronic processes of interest for three mutually perpendicular orientations, and are compared with recent experimental data and classical over-the-barrier model calculations for triply-charged ion impact at $E = 2.81$ keV/amu [1]. We find fair agreement with the measurements for O^{3+} impact; in particular, we can confirm that ICD is a significant reaction channel in this system. The situation changes when the screened O^{3+} projectiles are replaced by bare Li^{3+} ions, i.e., the occurrence of ICD depends on the electronic structure of the projectile and cannot be explained simply by its asymptotic charge [2]. We will also show that using He^{2+} ions as projectiles would make ICD *the* dominant dimer fragmentation channel in the few keV/amu impact energy regime.

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Study of Higher-Order Contributions to The Few-Body Dynamics of Simple Atomic Systems at A Fully Differential Level

M. Dhital[1], S. Bastola[1], A. Silvus[1], J. Davis[1], B.R. Lamichhane[1], E. Ali[2], M.F. Ciappina[3,4], R.A. Lomsadze[5], A. Hasan[6], D.H. Madison[1], and M. Schulz[1]
[1]*Missouri University of Science and Technology*
[2]*Northwest Missouri State University*
[3]*ICFO-Institut de Ciencies Fotoniques*
[4]*ELI Beamlines*
[5]*Tbilisi State University*
[6]*UAE University*
madhavd@ucr.edu

Atomic scattering research has played a crucial role in advancing our understanding of the few-body problem in simple atomic systems. In perturbation theory, understanding the relative contribution of first vs higher-order mechanisms is essential in accurately describing the few-body dynamics. We have performed kinematically complete experiments on ionization of He and H_2 by 75keV proton impact in the kinematic regime where a higher-order process known as post-collision interaction (PCI) is significant. In PCI, the projectile and the electron ejected in the primary interaction attract each other in a second interaction in the outgoing part of the collision. We measured all the momentum components of the scattered projectile and the recoiling ion produced in the interaction, in coincidence. Then the ejected electron momentum was deduced from momentum conservation. Fully differential cross sections (FDCS) were extracted for several electron energies ranging from well below to well above the projectile-electron velocity matching regime [PCI maximizes at the projectile-electron velocity matching regime]. Moreover, for each electron energy, FDCS were obtained for several fixed projectile scattering angles. Pronounced post-collisional effects between the projectile and the ejected electron were observed in the projectile scattering angle dependence, the electron emission angle dependence, and the electron energy dependence of the FDCS. The data were compared to two different, but conceptually similar distorted wave calculations. Our results indicate the limitations of perturbative models in the kinematic regime where PCI is strong and thus the need for non-perturbative approaches to advance our understanding of the few-body dynamics in simple atomic systems.

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Heavy N^+ ion transfer in doubly charged N_2Ar cluster

Xiaolong Zhu[1,2*], XiaoQing Hu[3], ShunCheng Yan[1,2], YiGeng Peng[3], WenTian Feng[1], DaLong Guo[1,2], Yong Gao[1], ShaoFeng Zhang[1,2], Amine Cassimi[4], JiaWei Xu[1,2], DongMei Zhao[1], DaPu Dong[1,2], Bang Hai[1,2], Yong Wu[3], JianGuo Wang[3] and X. Ma[1,2*]

[1]*Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China.*

[2]*University of Chinese Academy of Sciences, Beijing 100049, China.*

[3]*Institute of Applied Physics and Computational Mathematics, Beijing 100088, China.*

[4] *CIMAP, CEA/CNRS/ENSICAEN/UNICAEN, BP5133, F 14070 Caen, France*

zhuxiaolong@impcas.ac.cn x.ma@impcas.ac.cn

Van der Waals (vdW) clusters are weakly bound atomic/molecular systems and are ubiquitous in nature. They are an important medium for understanding micro-environmental chemical phenomena in bio-systems. In hydrogen-bond clusters, the proton transfer process plays an important role as well, it involves mass and charge migration over large distances within the cluster and results in fragmentation of the latter. Nevertheless, this transfer process is limited to hydrogen-bond clusters. Since these processes are known to be of relevance in biophysics and radiation therapy, **a question arises, whether a massive ion could be transferred in biochemical processes and lead to fragmentation? In a complex bio-environment, does heavy ion transfer play a role?** Van der Waals clusters may be an ideal candidate for these kinds of studies. In the present work, we use neutral vdW cluster N_2Ar as a target in collisions with 1 MeV Ne^{8+} ions to produce doubly charged cluster $(N_2Ar)^{2+}$. Surprisingly, an exotic heavy N^+ ion transfer channel $(N_2Ar)^{2+} \rightarrow N^+ + NAr^+$(Fig. 1 indicates (4)) has been observed. This bound-bound state transition involving heavy ion transfer process and the consequent formation of NAr^+ have never been reported so far. Our work demonstrates that this channel originates from the dissociation of parent doubly-charged cluster $N_2^{2+}Ar$ generated by the "N_2-site" two-electron loss process. Theoretical calculations show that the polarization interactions between Ar and N_2^{2+} lead firstly to an isomerization process of $N_2^{2+}Ar$ from its initial T-shape to linear-shape (N-N-Ar). Besides, the neighboring neutral Ar atom decreases the N_2^{2+} barrier height and width, resulting in significant shorter lifetimes of metastable molecular ion state $N_2^{2+}(X\ ^1\Sigma_g^+)$. Consequently, the breakup of the covalent N^+-N^+ bond, the tunneling out of the N^+ ion from N_2^{2+} potential well, as well as the formation of N-Ar^+ bound system take place almost simultaneously. Then the Coulomb explosion starts between N^+ and NAr^+ ion pairs. This mechanism might be general for molecular dimer ions in the presence of neighboring atom, and be of potential importance in understanding micro-dynamics of biological systems [1]. Recently, we also observed this mechanism in Ar^{2+}-N_2Ar collisions at low energy of 40 keV.

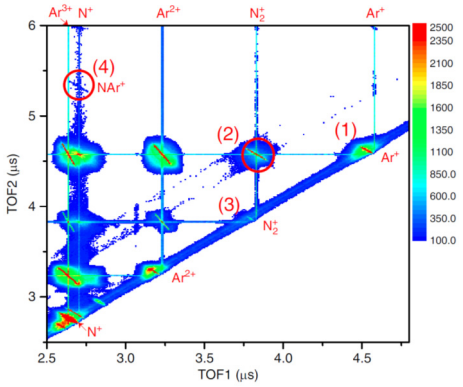

Figure 1: The two-dimensional TOF correlation map shows the time-of-flights between the first and the second fragment ions arriving at the recoil detector.

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A kinematically complete experiment on Compton scattering: Collision physics with photons

M. Kircher,[1] F. Trinter,[1,2] S. Grundmann,[1] I. Vela-Perez,[1] S. Brennecke,[3] N. Eicke,[3] J. Rist,[1] S. Eckart,[1] S. Houamer,[4] O. Chuluunbaatar,[5,6,7] Y. V. Popov,[8,5] I. P. Volobuev,[8] K. Bagschik,[9] M. N. Piancastelli,[10,11] M. Lein,[3] T. Jahnke,[12] M. S. Schöffler,[1] and R. Dörner[1]

[1] *J. W. Goethe Universität, Max-von-Laue-Str. 1, D-60438 Frankfurt, Germany*

[2] *Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin, Germany*

[3] *Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany*

[4] *University Sétif-1, 19000, Setif, Algeria*

[5] *Joint Institute for Nuclear Research, Dubna, Moscow region 141980, Russia*

[6] *Mongolian Academy of Sciences, 13330, Ulaanbaatar, Mongolia*

[7] *Peoples' Friendship University of Russia (RUDN University), 117198, Moscow, Russia*

[8] *Lomonosov Moscow State University, Moscow 119991, Russia*

[9] *FS-PETRA-S, DESY, Notkestr. 85, D-22607 Hamburg, Germany*

[10] *Sorbonne Universités, CNRS, UMR 7614, F-75005 Paris, France*

[11] *Uppsala University, P.O. Box 516, SE-751 20 Uppsala, Sweden*

[12] *European XFEL, Holzkoppel 4, Schenefeld, D-22969, Germany*

kircher@atom.uni-frankfurt.de, doerner@atom.uni-frankfurt.de

In collision experiments like (e,2e) or (p,e), the Coulomb field of the charged projectiles always disturb the initial and final states of the target. Using photons as projectiles removes this perturbation. However, the only "collision"-like photon-atom interaction is Compton scattering, which has an extremely small cross section ($\sim 10^{-24}$ cm^2), much smaller than those of classical collision experiments, making kinematically complete coincidence measurements very challenging. Due to the rise of high-intensity synchrotron light sources and the highly efficient COLTRIMS technique [1], we were able to perform a kinematically complete measurement of Compton scattering on helium with a photon energy of $h\nu = 2.1$ keV [2]. We measured the momenta of the electron and helium ion in coincidence, and, exploiting momentum conservation, derived from these the photon momentum. The resulting electron momentum distributions (Fig. 1) resemble the bimodal distributions known from (e,2e) or (p,e) contexts without any post-collision effects of an outgoing projectile.

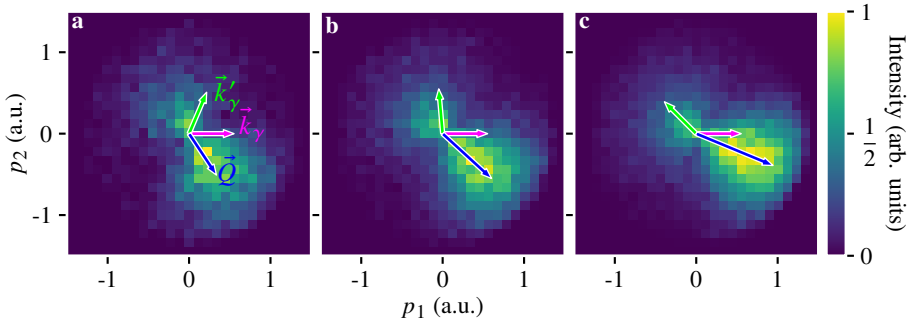

Figure 1: Electron momentum distributions in the scattering plane for different magnitudes of the momentum transfers $\vec{Q} = \vec{k}_\gamma - \vec{k}'_\gamma$.

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Ion-electron dynamics studied in a 3D-transmission approach

Svenja Lohmann[1,2], Radek Holeňák[1], Pedro L. Grande[3], Daniel Primetzhofer[1]
[1]*Department of Physics and Astronomy, Uppsala University, Box 516, 751 20 Uppsala, Sweden*
[2]*Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR), 01328 Dresden, Germany*
[3]*Physics Department, Institute of Physics, Federal University of Rio Grande do Sul (UFRGS), CEP 91501-970, Porto Alegre, RS, Brazil*
svenja.lohmann@physics.uu.se

We present experiments demonstrating trajectory-dependent electronic excitations at low ion velocities attributed to charge-exchange events. Experiments were performed with the time-of-flight medium energy ion scattering set-up at Uppsala University [1]. We employed pulsed beams of singly charged ions with masses from 1 (H^+) to 40 u (Ar^+) and energies between 20 and 300 keV. Ions are transmitted through self-supporting Si(100) nanomembranes and detected behind the sample. Fig. 1 demonstrates our experimental approach, in which ion energy loss is measured together with angular distributions for different beam-crystal alignments. We have analysed both trajectory-dependent electronic stopping and electronic energy-loss straggling. Our results show higher electronic stopping for random than for channelled trajectories for all studied ions [2]. For ions heavier than protons, direct core-electron excitations at employed ion velocities are inefficient. We, therefore, explain our observation by reionisation events occurring in close collisions of ions with target atoms mainly accessible in random geometry [3]. These events result in trajectory-dependent mean charge states, which heavily affects the energy loss. The electronic energy-loss straggling likewise exhibits a strong dependence on ion type, velocity and trajectory. For all ions, straggling in random geometry is higher than in channelling orientation. While for He straggling increases with ion velocity, for B travelling along random trajectories a minimum is observed in the studied velocity range. We compare experimental results for these two ions with predictions by the Chu model and transport cross section calculations (Penn-TCS model). We provide strong evidence that electron-hole pair creation alone cannot explain electronic excitations by slow ions other than protons. Especially for heavy ions, additional energy-loss processes such as charge exchange and autoionisation including possible alterations of the scattering potential [4] have to be taken into account.

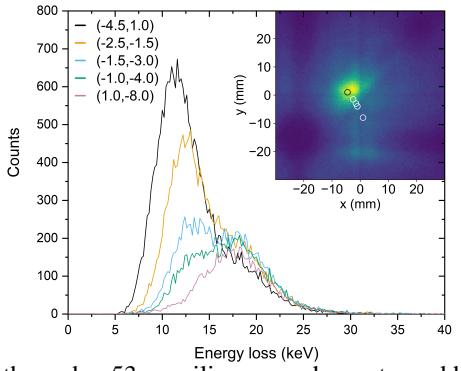

Figure 1: 150 keV Ne^+ transmitted through a 53 nm silicon membrane turned by (2°,4°) out of channelling geometry. The main plot shows energy-loss curves for different regions of interest on the detector. The inset shows the spatial distribution of ions with ROIs from the main plot indicated by circles.

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Ionization of water under the impact of 250 keV protons and C, O ions with energy of a few MeV/u

A. Bhogale[1], M. Roy Choudhury[1], C. Bagdia[1] J. M. Monti[2], A. Jorge[4], M. Horbatsch[3], T. Kirchner[3], R. D. Rivarola[2], L. C. Tribedi[1]

[1]*Tata Institute of Fundamental Research, Homi Bhabha Road, Colaba, Mumbai 400005, India*

[2]*Inst. de Fisica Rosario (CONICET-UNR), Universidad Nacional de Rosario, 2000 Rosario, Argentina*

[3]*Department of Physics and Astronomy, York University, Toronto, Ontario, M3J 1P3 Canada*

[4]*Departamento de Qumica, Universidad Autnoma de Madrid, Madrid, 28049, Spain*

abhibhogale@gmail.com; lokesh@tifr.res.in

The study of the DDCS for emitted electrons from water vapour by energetic proton impact gains importance in radiobiology. To explore the science behind the radiobiology related to the hadron therapy of cancer, and, in general for radiation damage by high energy particles, it is importannt to understand the characteristics of the ionization process and the energy loss in water molecules [1]. The ions interact with the water molecules to give rise to processes like ionization, electron capture or dissociation etc. The prominent process is the emission of electrons with different energies in all directions which may cause further damage [2, 3]. Emitted electrons are detected using hemispherical electrostatic analyzer for emission angles within 30 to 160 degree. The highly collimated proton beam of energy 250 keV was available from the 14.5 GHz ECR based ion-accelerator in the TIFR, Mumbai.

The absolute DDCS, $d^2\sigma/d\varepsilon_e d\Omega_e$, as a function of the emission energy (ε_e) and emission angle (Ω_e), have been obtained and compared with the CDW-EIS and CTMC [4] calculations. The CTMC calculations show excellent agreement with the experimental DDCS data particularly in the backward angles. In case of forward angles both the CDW-EIS and the CTMC provide reasonable agreement (Figure 1). The TCS values as obtained from the experiment, however falls about 30% below the CTMC predictions. We will also display the similar experimental data on water in higher energy ($\sim$ MeV/u) collisions involving C and O ions which are very well reproduced by the CTMC model. Energy scaling of cross section data will also be presented.

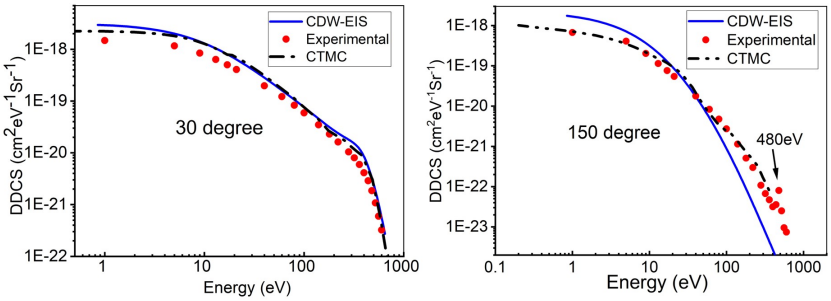

Figure 1: e-DDCS of water induced by 250keV protons for mission angles (a) 30° and (b) 150° with CDW-EIS (solid-blue line) and CTMC (dashed black line) predictions.

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An experimental apparatus for systematic studies of molecular processes induced by ion and electron irradiation in astrophysical ice analogues

P Herczku[1], D V Mifsud[1,2], Z Juhász[1], S T S Kovács[1], B Sulik[1], P A Hailey[2], Z Kaňuchová[3,4], A Traspas Muiña[5], S Ioppolo[5], R W McCullough[6], B Paripás[7] and N J Mason[2]
[1]*Institute for Nuclear Research (Atomki), Debrecen, H-4026, HU*
[2]*Centre for Astrophysics & Planetary Science, University of Kent, Canterbury, CT2 7NH, UK*
[3]*Astronomical Institute, Slovak Academy of Sciences, Tatranska Lomnicá, SK-059 60, SK*
[4]*INAF Osservatorio Astornomico di Roma, Monte Porzio Catone, RM-00078, IT*
[5]*School of Electronic Engineering & Computer Science, Queen Mary University of London, London, E1 4NS, UK*
[6]*School of Mathematics & Physics, Queen's University Belfast, Belfast BT7 1NN, UK*
[7]*Department of Physics, University of Miskolc, Miskolc, H-3515, HU*
herczku.peter@atomki.hu

From the first observation of molecular species in space (see [1] and refs. therein), much interest has been devoted to the formation and fates of interstellar molecules. To study the formation processes and reactivity of these molecules, we have to simulate the interstellar environment. Astrophysical ice analogues have been processed with Lyman-α, vacuum- or extreme- UV photons, electrons and ions [2] for a long time. Experiments have revealed much information on the chemical reactivity. However, systematicity, repeatability, and reproducibility have sometimes been difficult to achieve [3,4].

Here we report a new facility for ion and electron irradiation studies relevant to experimental astrochemistry located at the Institute for Nuclear Research (Atomki) in Debrecen, Hungary.

The Chamber for Astrophysics-Astrochemistry (ICA) is designed to carry out systematic studies wherein a selected number of parameters (e.g. ice thickness, morphology, temperature, projectile ion nature and energy, etc.) may be controlled and varied. The main advantage of the ICA set-up lies in its provision for four deposition substrates, allowing the creation of ice replicates under identical conditions. Thermal, ion and electron, processing are available, allowing for various combinations of them. Heavy ion beams in the mid-energy (0.2-18 MeV) range may be delivered to ices deposited on cold (20-300 K) ZnSe substrates. These substrates are vertically mounted on an OFHC copper holder connected to a closed cycle cryostat, a 360° rotation stage and a z-linear manipulator. The ions may cross the ice layer with relatively small energy losses, or may implant into the ice. Irradiation induced physico-chemical changes are monitored by FTIR spectroscopy. A temperature controller allows us to perform thermal annealing studies on both non-irradiated and irradiated ices. Sublimating volatiles, particles sputtered during irradiation and molecules desorbed during annealing are monitored by a quadrupole mass spectrometer (QMS). Ice layers are created through background deposition. The gas-mixtures are prepared in a dosing-line and introduced into the main chamber by means of an all leak metal valve. The set-up is equipped with an electron gun which provides electron beams of a few μA in the 5 eV – 2 keV energy range. At the conference, we will present preliminary results of e-, H^+ and S^{2+} impact on ice mixtures deposited at 20 K.

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Secondary ion emission from condensed N_2O irradiated by MeV heavy ions

P. R. B. Oliveira[1], R. Martinez[2], D. Fulvio[3], E. F. da Silveira[1]
[1]*Departamento de Física, Pontifícia Universidade Católica do Rio de Janeiro, Rua Marquês de São Vicente, 255, Rio de Janeiro 22452-970, Brazil*
[2]*Universidade Federal do Amapá – UNIFAP, Departamento de Física, Rod. Juscelino Kubitschek, km 02, 68903-419, Jardim Marco Zero – Macapá – AP, Brazil*
[3]*Istituto Nazionale di Astrofisica, Osservatorio Astronomico di Capodimonte, Salita Moiariello 16, I-80131 Naples, Italy*
pablo@aluno.puc-rio.br

Astrophysical ices are the main surface material of many Solar system bodies, such as comets and trans-Neptunian objects. On these surfaces, solar wind ions and cosmic rays induce chemical reactions stimulating secondary ion emission to the gas phase. The effects of energetic processing of ices at low temperature have been analyzed through laboratory investigation, revealing in particular the production of molecules and free radicals of astrophysical importance. Since nitrous oxide (N_2O) was already observed in star-forming sites, this molecular species is expected to be present in ices covering some minor bodies in the outer Solar system. In the current work, N_2O ice is irradiated at 10 K by energetic (MeV/u) multicharged heavy ions (e.g. ^{105}Rh and ^{140}Ba); the sputtered positive and negative secondary ions were detected and analyzed by the TOF-PDMS technique (time-of-flight plasma desorption mass spectrometry). Several ionic species were identified, indicating strong molecular fragmentation: N^+, N_2^+, NO^+, O^+, and O^-. The bombardment also induces the formation of ion cluster series: $(N_2)_nR_m^+$, $(NO)_nR_m^+$, $(N_2O)_nR_m^+$, where R = N^+, N_2^+, NO^+, N_2O^+, O_m^+ (n up to ~ 10, m = 1−3). As illustrated in Figure 1, their sputtering yield distributions follow the sum of two decreasing exponentials one fast -F (k_F) and another slow -S (k_S), suggesting a two-regime formation. Almost all of the yield distributions have the same exponential decay constants, with $k_F \sim 1.4$ and $k_S \sim 0.15$ u^{-1}. Based on these results, an emission description for aggregates is proposed; which may improve the understanding of the processes by which, in space, neutral and ionized molecular species are delivery to the gas phase.

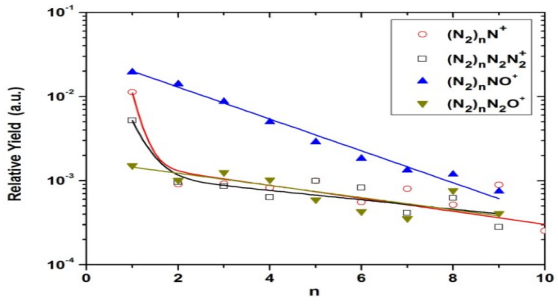

Figure 1: Relative sputtering yield distribution of ion clusters emitted by N_2O ice bombarded by MeV projectiles. Data obtained by Time-of-Flight Mass Spectrometry [1].

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Complete Break-up of Methane and Ammonia from Satellite States

Wania Wolff, H. Luna and E. C. Montenegro
Instituto de Física, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brasil
wania@if.ufrj.br

The ionization and subsequent dissociation of ammonia and methane molecules in a gas phase was investigated experimentally by impact of protons in a wide range of energies from 125 to 2700 keV [1,2]. Coincidence measurements, including electron-ion and electron ion-pairs, were performed and allowed us to extract clean discriminated single from multiple ionization cross sections and uncover the processes present in the dissociative single and multiple ionization. For the pure single ionization analysis, a semiempirical fragmentation matrix model based on the Born Approximation was used to obtain the contribution from the single hole vacancy (vertical transitions) and from the double-hole one particle (2h-1p) satellite states. The role of the charge sign of the projectile was analysed through a comprehensive comparison of the proton and the electron impact data, which despite extensively investigated, shows specially for ammonia a large dispersion among the absolute cross sections. Marked contrasts and similarities between both projectiles in the fragment ion production were observed for both molecules. This systematic investigation of the single and multiple ionization of ammonia and methane by protons is of interest to several physical chemical environments, across the interstellar medium, on the atmosphere and surface of planetary bodies and in the evolution of terrestrial life.

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Anomalous KCl(001) Surface Corrugation from Fast He Diffraction at Very Grazing Incidence.

G. A. Bocan[1], H. Breiss[2], S. Szilasi[2], A. Momeni[2,3], E. M. Staicu Casagrande[2], M. S. Gravielle[4], E. A. Sánchez[1], H. Khemliche[2]
[1]*Instituto de Nanociencia y Nanotecnología (CONICET-CNEA) and Instituto Balseiro (U. N. Cuyo), Bariloche, Argentina*
[2]*Université Paris-Saclay, CNRS, Institut des Sciences Moléculaires d'Orsay, Orsay, France*
[3]*CY Cergy Paris Université, Cergy, France*
[4]*Instituto de Astronomía y Física del Espacio (CONICET-UBA), Buenos Aires, Argentina*
gisela.bocan@cab.cnea.gov.ar

The substrate surface corrugation is a key feature in quasiepitaxy, driving the overlayer orientation even for weakly interacting interfaces. In this invited talk we will address the corrugation of the KCl(001) surface by means of grazing incidence fast atom diffraction (GIFAD) [1]. The unexpected $\sim 85\%$ corrugation increase below 100 meV we obtain for ^{4}He$\rightarrow\langle 110\rangle$KCl(001) suggests that KCl could outperform the usual NaCl or LiF layers often used in organic electronic devices to improve charge injection.

Experimental GIFAD patterns were recorded for ^{4}He$\rightarrow$KCl(001) along $\langle 110\rangle$ and $\langle 100\rangle$ channels. In Fig. 1 we show the corrugation $\Delta Z(E_\perp)$ obtained from the processing of these patterns, together with two sets of theoretical corrugations: ΔZ^{PES}, calculated on three high-precision DFT-based He-KCl(001) potential energy surfaces (PESs), two of which included van der Waals (vdW) interactions, and ΔZ^{SIVR} obtained from the processing of simulated GIFAD patterns, built by means of the surface initial value representation (SIVR), a semiquantum approach to the scattering dynamics under a given PES.

From the analysis of the potential and the SIVR phase we conclude that: i) For $\langle 110\rangle$, the increase in ΔZ for decreasing $E_\perp$ is not vdW in origin; ii) The increase of ΔZ^{PES} for $\langle 110\rangle$ is due to the late fading of the He-K$^+$ interaction; iii) For both channels, the difference $\Delta Z^{SIVR} - \Delta Z^{PES}$ is due to dynamical effects, traceable to a shallow attractive region, neither vdW nor polarization in origin; iv) Dynamical effects take hold when $E_\perp < 30$ meV, yielding the slope sign change for $\langle 100\rangle$ and the sharp increase for $\langle 110\rangle$. v) GIFAD provides satisfactory structural information for both channels in the $E_\perp > 30$ meV range.

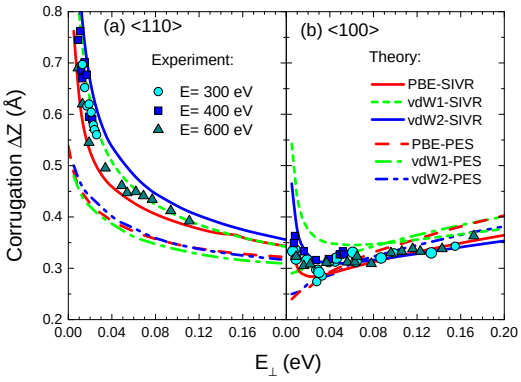

Figure 1: Corrugation for He-KCl(001) as a function of the normal energy $E_\perp$

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Singly differential direct scattering and electron capture cross sections of intermediate energy proton-helium collisions

K. H. Spicer[1]*, C. T. Plowman[1], Sh. U. Alladustov[2], I. B. Abdurakhmanov[1], A. S. Kadyrov[1], and I. Bray[1]

[1]Curtin Institute for Computation and Department of Physics and Astronomy,Curtin University, GPO Box U1987, Perth, WA 6845, Australia

[2]Uzbek-Israel Joint Faculty, National University of Uzbekistan, Tashkent, 100174, Uzbekistan

Synopsis We investigate the four-body proton-helium differential scattering problem using the two-center wave-packet convergent close-coupling approach in the intermediate energy region. For comparison, a recently developed method that reduces the target to an effective single-electron system is also used. The results of the two methods exhibit a very good level of agreement with experiment. It is concluded that both versions provide a realistic picture of they processes taking place in proton-helium collisions.

We present an investigation of the four-body proton-helium differential scattering problem using the two-center wave-packet convergent close-coupling (WP-CCC) approach. The approach uses fully-correlated two-electron wave functions for the helium target. Here, we focus on the angular differential cross sections for direct-scattering and electron-capture processes in the intermediate energy (75–300 keV) region where coupling between various channels is important.

A brief overview of the theoretical approaches to the differential proton-helium scattering problem indicates that different approaches have only been applied to isolated reaction channels. Some found agreement in their chosen process, however, could not provide information on other concurrent channels. There has been no attempt to calculate all the interconnected processes on equal footing at the same time and in a systematic fashion. The aim is to test if the WP-CCC approach is capable of providing a complete differential picture of all the simultaneous interrelated processes occurring during the collision and, thereby, filling this gap.

For comparison, we also use a recently developed approach [**?**] that allows one to reduce the two-electron helium atom to an effectively single-electron system convenient for scattering calculations.

We report results for angular differential cross sections for elastic scattering, excitation into the $n = 2$ states (where n is the principal quantum number of the atom in the final state), and state-selective electron capture obtained using both methods. Results for the angular differential cross sections of excitation and electron capture agree well with experiment. For elastic scattering, significant disagreement between the experiment at 100 keV and theory still remains, though agreement in shape between the experiment and the two-electron WP-CCC results is excellent. We suggest that there could be a normalisation error in the experiment. New experiments and independent calculations would shed more light on the situation. We also present results using a recently developed effective single-electron description of the target. Results from this alternative, computationally more efficient, treatment of the target structure exhibit generally good agreement with the correlated two-electron WP-CCC calculations.

It is concluded that both the fully-correlated two-electron and less expensive effective single-electron WP-CCC approaches are capable of providing a complete and reasonably accurate differential picture of the binary processes taking place in proton-helium collisions. We will next turn our attention to proton-helium differential ionisation where there is an abundance of experimental data to compare with.

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*E-mail: kate.bain@student.curtin.edu.au

On the quest for projectile coherence in C^{6+}/He collisions

L. Ph. H. Schmidt[1], J. Rist[1], M. Kircher[1], A. Mery[2], J. Rangama[2], S. Grundmann[1], I. Vela-Perez[1], D. Tsitsonis[1], D. Trabert[1], S. Eckart[1], G. Kastirke[1], K. Fehre[1], T. Jahnke[1], R. Dörner[1], R. Moshammer[3], J. Ullrich[4], D. Fischer[4], M. Schulz[5], A. Cassimi[2], M. S. Schöffler[1]

[1] Institut für Kernphysik, Goethe-Universität, Frankfurt Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany
[2] CIMAP Caen, GANIL, Bd Henri Becquerel, BP 55027 14076 Caen Cedex 05, France
[3] Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany
[4] Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany
[5] Physics Department and LAMOR, Missouri University of Science and Technology, Rolla, Missouri, USA

schoeffler@atom.uni-frankfurt.de

20 years ago, single ionization of Helium induced by 100 MeV/u C6+ projectiles was investigated in a kinematically complete experiment [1]. The experimentally obtained results, which were in strong contrast to state of the art theories at this time and even most recent calculations. While the electron momentum distribution should exhibit two well separates lobes, the so-called binary- and recoil-lobe, the node between them was mostly filled. This launched an avalanche of controversial discussions, which are still ongoing today. The most heavily debates explanations are a) experimental issues/limited resolution and b) transversal coherence of the projectile, a concept introduced in 2011 by Schulz and coworkers [2].

In order to solve the "C^{6+}-mystery", we used a state-of-the-art COLTRIMS (COLd Target Recoil Ion Momentum Spectroscopy) Reaction-Microscope and redid the initial experiment in Cave D4 of GANIL. As insufficient momentum resolution might have been an issue in the original experiment, ion arm of the spectrometer was built in a time- and space-focusing geometry in order to reduce the diminishing influence of the extended target size. The electron arm was built in a time-focusing Wiley-McLaren-Geometry. On both ends of the spectrometer, hexagonal delay-line-detectors were used, which have an overall non-linearity <100 µm. Also the gas jet was precooled to 80 K and for both, electrons and ions, separate calibrations, using an additional 25 keV ion source were used. With this, the ion momenta were calibrated, focusing on discrete structures in momentum space as a result of single electron capture ($He^{2+} + He \rightarrow He^{+} + He^{+}$ and $He^{+} + He \rightarrow He^{0} + He^{+}$). A momentum resolution of $\Delta p<0.1$ au for He^{+} recoiling ions was achieved. The electron arm of the spectrometer was calibrated via autoionizing states of a Neon target ($He^{2+} + Ne \rightarrow He^{+} + Ne^{2+} + e^{-}$), which create a dozen (below 15 eV) of energetically sharp isotropically emitted electrons.

The experiment was performed in March 2021. Therefore the data are currently being analyzed and the results will be presented.

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Binary ridges in the $O^+ + H_2 \rightarrow O + H^+ + H$ process as a signature of molecular rotation

Z Juhász[1*], V Vizcaïno[2], J-Y Chesnel[2], S T S Kovács[1], P Herczku[1], S Demes[1], R Rácz[1], S Biri[1], N Sens[2], D V Mifsud[3,1], L Ábrók[1] and B Sulik[1]
[1] *Institute for Nuclear Research (Atomki), Debrecen, H-4026, Hungary*
[2] *Normandie Univ, ENSICAEN, UNICAEN, CEA, CNRS, CIMAP, Caen, 14000, France*
[3] *Centre for Astrophysics and Planetary Science, School of Physical Sciences, University of Kent, Canterbury CT2 7NH, United Kingdom*
zjuhasz@atomki.hu

Emission of low-energy fragment ions is a significant output channel following excitation and moderate ionization of the target molecules by singly charged ions. Its experimental investigation is difficult since slow ions are sensitive to disturbing electric fields. A time-of-flight setup was thus developed at Atomki for reliable measurement of absolute cross sections for emission of fragment ions with kinetic energies down to 0.1 eV. The emitted ions fly through a well-shielded field-free region before their detection on a 2D position sensitive detector which is rotatable around the center.

We measured the velocity distribution of the H^+ (or D^+) fragments ejected from H_2 (or D_2) molecules bombarded with 10-keV O^+ ions (see Fig. 1). The maximum at velocities close to 0.001 a.u., is most likely due to dissociation of H_2^+ (or D_2^+) ions created by single electron capture. The velocity distributions also show a ridge structure due to enhanced fragment emission in the transverse direction after binary knock out by the projectile. Compared to its expected position for a target at rest, this binary ridge is split and shifted towards two opposite directions. These shifts are due to the speed of the atoms in the rotating target molecule. As expected from their mass ratio, the shift is found to be twice as large for H_2 as for D_2. The shift towards a negative longitudinal velocity component is found to be more likely than that towards a positive component, showing that the active target atom is attracted by the incoming projectile. This result provides evidence for rotational excitation of the target molecule before dissociation. The velocity distributions were measured at different temperatures and positions of the target gas nozzle. We observed changes in the binary structures, which may be attributed to target coherence effects.

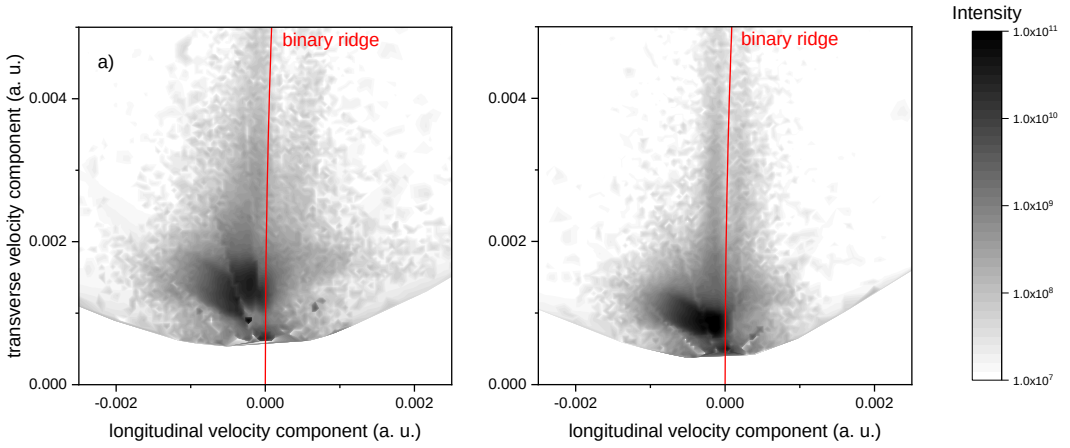

Figure 1: Velocity distribution of H^+ (panel a) and D^+ (panel b) fragments stemming from 10-keV $O^+ + H_2$ or D_2 collisions, respectively. The longitudinal velocity component is the component along the beam axis.

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Electron emission from large biomolecules and radio-sensitizing effect

Lokesh C Tribedi

Tata Institute of Fundamental Research, Colaba, Mumbai 400005, India

Email: lokesh@tifr.res.in

. Heavy ion beams, such as, protons and carbon ions, with high (~GeV) energy obtained from large accelerator centers worldwide are typically used for the removal of cancerous tumor in human body. The hadron therapy combined with nanotechnology has been proposed to be an elegant alternative for cancer treatment. Internal amplification of low energy e-emission due to the inserted metal atoms causes the radio-biological effectiveness in nano-inserted biomolecules which is of prime importance for such treatment to reduce the incident dosage. The enhancement in the low energy electron emission due to the insertion of such atom has been measured here for a class of molecules namely halouracil. In particular the iodouracil (IUr) and bromouracil (BUr), obtained by replacing a H-atom in a RNA base molecule uracil, have been used for these measurements. We will discuss our recent results on the enhancement in the e-emission cross sections for IUr and BUr under the influence of fast proton and carbon-ions. The e-emission from is found to be substantially enhanced over uracil and water. The enhancement is much larger then the CDW-EIS model prediction. The sensitizing factor at least for the IUr is explained in terms of atomic giant dipole resonance (GDR) of strongly correlated 4d-electrons for the iodine atom. Some of the recent references are added [1-11] including two recent reviews [1,2].

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Coulomb-explosion imaging of carbon monoxide dimers

A. Méry[1], V. Kumar[1], X. Fléchard[2], B. Gervais[1], S. Guillous[1], M. Lalande[1], J. Rangama[1], W. Wolff[3], and A. Cassimi[1]

[1]*CIMAP, CEA, CNRS, ENSICAEN, UNICAEN, Normandie Université BP5133, 14050 Caen Cedex 04, France*

[2]*LPC Caen, Normandie Université, ENSICAEN, UNICAEN, IN2P3, CNRS, 14000 Caen, France*

[3]*Instituto de Física, Universidade Federal do Rio de Janeiro, Cidade Universitária Rio de Janeiro, Rio de Janeiro 21941-590, Brazil*

mery@ganil.fr

Carbon monoxide dimers $(CO)_2$ have been studied since the 1990s using infrared and millimeter-wave spectroscopy. However, the interpretation of the measured rovibrational spectra has been puzzling for many years because of the possible contribution of two distinct isomers of the dimer with very little binding energy difference. The lowest in energy has been assigned to a planar C-bonded geometry in which the carbon atoms of each CO molecule are located in the inner region of the dimer. In contrast, the other isomer would correspond to a planar O-bonded configuration with two inner oxygen atoms. Moreover, these two isomers have been found to have different equilibrium intermolecular distance R_e. The corresponding three-dimensional structures of the dimer can be described using four independent parameters: the intermolecular bond length R_e, the relative orientations θ_1 and θ_2 of each molecule with respect to the dimer axis, and the torsional angle ϕ (see Fig. 1).

We report on experimental results obtained from collisions of slow highly charged Ar^{9+} ions with a carbon monoxide dimer $(CO)_2$ target [1]. A cold target recoil ion momentum spectroscopy setup and a Coulomb explosion imaging approach are used to reconstruct the structure of the CO dimers. The three-dimensional structure is deduced from the two-body and three-body dissociation channels from which both the intermolecular bond length and the relative orientation of the two molecules are determined. For the three-body channels, the experimental data are interpreted with the help of a classical model in which the trajectories of the three emitted fragments are numerically integrated.

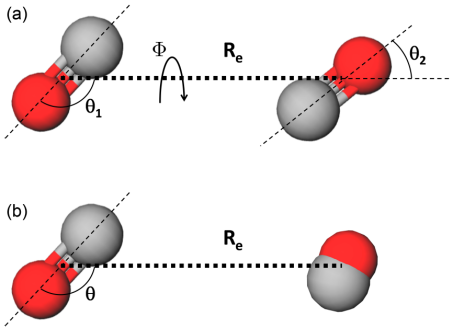

Figure 1: (a) Complete three-dimensional geometry (θ_1, θ_2, ϕ, R_e). (b) Partial geometry accessible through the two-body and three-body dissociation of the dimer (θ, R_e).

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Formation of $\bar{H}^+$ via radiative and nonradiative attachment of e^+ to $\bar{H}$

A. Jacob[1], C. Müller[1] and A. B. Voitkiv[1]
[1] *Institut für Theoretische Physik I, Heinrich Heine Universität Düsseldorf, Universitätsstr. 1, 40225 Düsseldorf, Germany*
andreas.jacob@hhu.de

The formation of positive ions of antihydrogen $\bar{H}^+$ via radiative and nonradiative attachment of free positrons (e^+) to antihydrogen ($\bar{H}$) is studied for positron energies ranging from sub-meV to eV. The $\bar{H}^+$ ion is of great interest as an intermediate particle in free fall experiments on the behavior of $\bar{H}$ in the gravitational field of the Earth (GBAR experiment, see e.g., [1]).

We consider the following radiative attachment mechanisms [2]: (I) Spontaneous radiative attachment (SRA), in which an incident e^+ is captured into the ground state of $\bar{H}^+$ via emission of a photon. (II) Laser-induced radiative attachment (LIRA), in which $\bar{H}^+$ is formed due to photo emission induced by a laser field. (III) Two-center dileptonic attachment (2CDA), where an incident e^+ is captured by $\bar{H}$ moving in a gas of matter atoms B and capture proceeds via resonant transfer of energy excess to B which becomes excited and then stabilizes via spontaneous radiative decay [3]. As an example of 2CDA, we consider that positrons and a beam of slow $\bar{H}$ move in a (dilute) gas of Cs atoms and positron capture by $\bar{H}$ involves the $6^2S_{1/2} \to 6^2P_{3/2}$ dipole transition in Cs. We compare mechanisms (I)-(III) with each other and show that LIRA and 2CDA can strongly dominate over SRA.

Besides, we discuss (nonradiative) three-body attachment with an assisting electron (3BAe), where free positrons are incident on $\bar{H}$ embedded in a gas of low-energy ($\sim$ meV) electrons and a positron is attached to $\bar{H}$ whereas an electron carries away the energy excess [4]. It is by far the dominant attachment mechanism at very low positron energies $\lesssim 10^{-2}$ eV, which is considerably smaller than the range of positron energies ($\simeq 1$ eV) where the radiative attachment mechanisms are most efficient (see Figure 1).

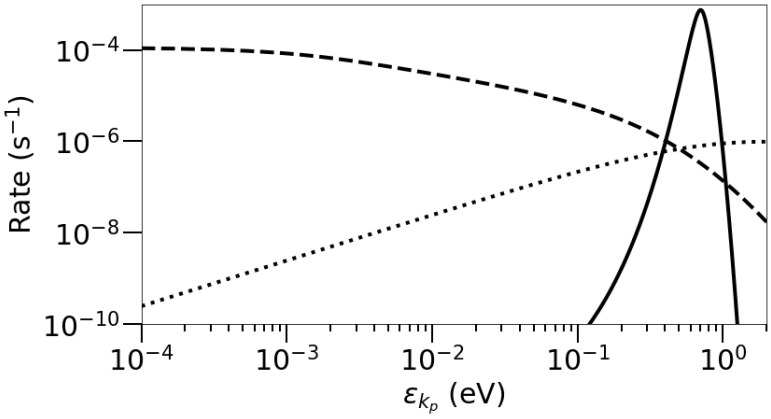

Figure 1: $\bar{H}^+$ formation rate (per $\bar{H}$) for SRA (dotted), 2CDA involving Cs (solid) and 3BAe (dashed).

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Ionization of alkali atoms during the collisions with polarized metastable helium. Redistribution of the spin polarization

V.Kartoshkin, S.Dmitriev, N.Dovator
Ioffe Institute. 26 Politekhnicheskaya, St Petersburg 194021, RUSSIA
victor.kart@mail.ioffe.ru

The observation of the magnetic resonance signals of rubidium atoms (^{85}Rb and ^{87}Rb isotopes) when using the indirect optical orientation in conditions of helium–rubidium gas discharge plasma is discussed. It has been demonstrated that optical pumping of alkali atoms in gas discharge results to a highly efficient indirect optical orientation of metastable He (2^3S_1) atoms [1]. However, in an attempt to perform the inverse experiment the result was quite unexpected: the magnetic resonance signal of Rb atoms was very weak. The experimental results have been considered, and an explanation of the observed anomaly in the signals is done.

At the optical orientation of metastable helium atoms in the Rb–He mixture and under conditions of a gas discharge, the polarization of rubidium atoms is possible as a result of two collisional processes. The first process is the inelastic process (it is the ionization of Rb atoms by metastable He atoms). The second process is the elastic process (so-called spin exchange process).

The idea of the experiment was as follows. Direct optical orientation of metastable (in the 2^3S_1 state) ^{4}He atoms was implemented by circularly polarized light (with a wavelength $\lambda = 1.08$ μm) from a gas discharge helium lamp. As a result of collisions between spin-oriented metastable helium atoms and rubidium atoms, the rubidium atoms were polarized. The detection of rubidium atom polarization was implemented by the change in light absorption by helium atoms when the spin polarization of rubidium atoms was broken by exciting an magnetic resonance (MR).

MR signals for the two rubidium isotopes little differ from each other in amplitude but are significantly (almost by two orders of magnitude) less in the amplitude than the MR signal for helium atoms. To explain the effect we used a theoretical approach used for the interpretation of the results in the case of the Cs–He pair [2]. The main factors determining the observed anomaly are the following:

1. Effect of the nuclear spin magnitude:

The redistribution of electronic angular momentum between the ensembles of metastable helium atoms and rubidium atoms in collisions of optically oriented He(2^3S_1) with unpolarized Rb is a result of the ionization and the spin exchange proportionally to the electronic spins. Before the next collision with a He (23 S1) atom, the spin orientation of the Rb atom is redistributed between the electron and the nucleus.

2. Effect of spin exchange between rubidium isotopes on magnitudes of observed signal:

In the absorption chamber containing a mixture of rubidium isotopes, atoms of different rubidium isotopes can collide with each other.

3. The role of various quenching processes in a gas discharge:

Given the high probability of other relaxation processes in the gas discharge (spin exchange with nonoriented Rb atoms, relaxation in collisions with the electrons, metastable singlet and other excited He atoms, as well as in collisions with molecules, photons, the absorption cell walls, etc.).

The contributions from each of these processes were calculated to explain the results.

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Transfer ionization cross sections in $A^{+q} + He$ collisions

Abdelmalek Taoutioui[1], Bin He[2], Károly Tőkési[1]
[1]*Institute for Nuclear Research, Debrecen, 4026, Hungary*
[2]*Institute of Applied Physics and Computational Mathematics, Beijing, China*
Abdelmalek.taoutioui@atomki.hu

We present a nonperturbative study of the total and differential cross-sections of the transfer ionization (TI) process in collisions between helium atom and bare ions A^{q+} (q = 1 - 3) from intermediate to high impact energies (10 keV-1 MeV). We used the 4-body classical trajectory Monte Carlo (CTMC) method.

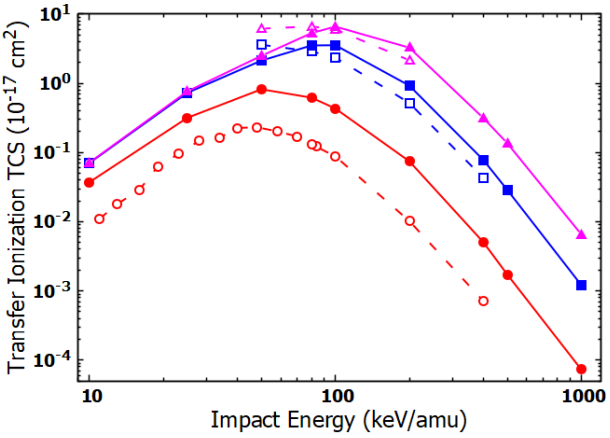

Figure 1: Total cross sections for transfer ionization as a function of projectile impact energy using the 4-body CTMC method. Experimental data of Shah et al. [1, 2] H^+: open-circles, He^{2+}: open-squares and Li^{3+}: open-triangles. Present 4-body CTMC method H^+: filled-circles, He^{2+}: filled-squares and Li^{3+}: filled-triangles.

In Fig. 1 we show TI total cross sections obtained by using the CTMC method for collisions between H^+, He^{2+} and Li^{3+} and the ground state helium atom. According to Fig. 1, the total cross sections of TI in case of H^+ projectile show a remarkable discrepancy between our data and the experimental observation which may improve it including correction term in the Hamiltonian taking into account the Heisenberg principle via model potential [3]. At the same time the agreement between our data and the experimental data is reasonable for He^{2+} and Li^{3+} ions. For deeper understanding of the collision dynamics, we also present angular and energy differential cross sections.

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Neonization method to calculate multiple ionization cross sections of water molecules by ion impact

Mariel E Galassi[1], Verónica B. Tessaro[1,2], Benoit Gervais[3] and Michael Beuve[2]

[1]*Grupo de Física Biomédica, Instituto de Física de Rosario (CONICET-UNR) and Facultad de Ciencias Exactas, Ingeniería y Agrimensura, Universidad Nacional de Rosario, Argentina.*
[2]*Université de Lyon 1, CNRS/IN2P3, Institut de Physique des 2 Infinis de Lyon, France.*
[3]*Centre de Recherche sur les Ions, les Matériaux et la Photonique, CIMAP-CIRIL-Ganil, CEA/CNRS/ENSICAEN/Université de Caen-Basse Normandie UCBN, France*
galassi@fceia.unr.edu.ar

In the present work, multiple ionization cross sections of water molecules by proton and light ion impact are calculated in the framework of the Independent Electron Model (IEM). To keep the model as simple as possible, the impact parameter single-particle ionization probabilities, required by the IEM, are described by means of decreasing exponential functions. The parameters of these functions are obtained from total net ionization cross sections for each molecular orbital, calculated by applying the Continuum Distorted Wave-Eikonal Initial State approximation [1]. The contribution of Auger and Coster-Kronig electron emission to multiple ionization cross sections is included by using the Ne post-collisional emission probabilities [2], considering that H_2O and Ne are isoelectronic. This post-collisional treatment offers a simple alternative to the much more complex evaluation of the molecular post-collisional relaxation. The results are in close agreement with experimental data for proton and other light ions, as shown in Figure 1.

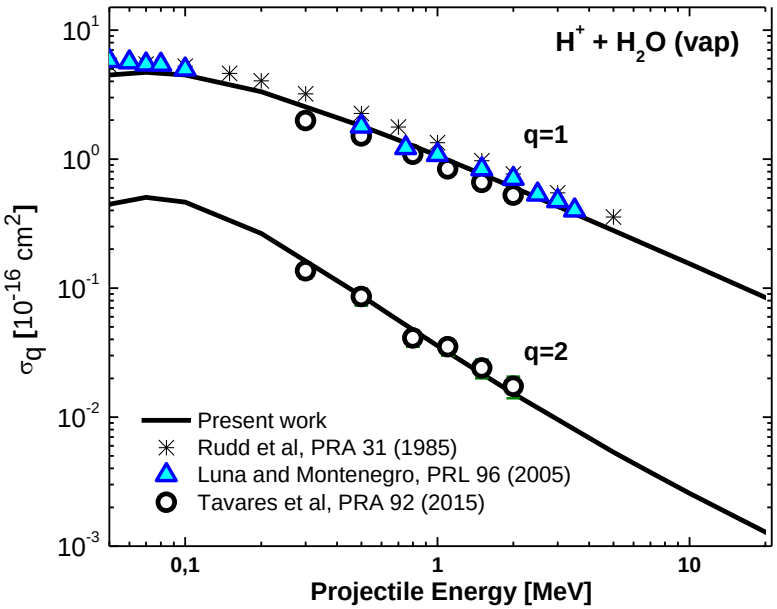

Figure 1: Single and double ionization of water molecules by proton impact. Solid line: present work. Scatters: experimental values.

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Multi-electron effects in collisions of swift ions and atoms

A. Dubois[1], S. Passalidis[1], E. P. Benis[2], T. J. M . Zouros[3]

Laboratoire de Chimie Physique-Matière et Rayonnement, Sorbonne Université - CNRS, 75005 Paris France
[2] Department of Physics, University of Ioannina, GR-45110 Ioannina, Greece
[3] Department of Physics, University of Crete, GR-70013 Heraklion, Greece

Synopsis State-to-state charge exchange cross sections are presented for ion-atom collision systems involving several active electrons. Focused in the intermediate and high impact energy regions, the results stem from a semiclassical close-coupling treatment taking into account dynamically several electrons and are compared with monoelectronic approximations.

Semiclassical close-coupling approaches within the molecular and asymptotic representations have been widely used with great success for one- or quasi-one-active electron ion-atom collisions [1]. For multielectronic systems and for the intermediate energy domain the situation is more complex and a majority of investigations have been performed using the independent electron, independent event approximations and/or frozen core approximation [2]. Much less non perturbative calculations taking into account the dynamics of several electrons have been done in the past due to the important computer resources they require. They often presented a limited control of convergence with respect to the number of states included in the basis sets employed.

In the symposium a recently developped approach based on a semiclassical multi-electron close coupling treatment will be presented. The solution of the time dependent Schrödinger equation is performed within a full configuration interaction (CI) approach by expanding the scattering wavefunction on a basis of multielectronic states centred on target, projectile and both. These states are augmented by electron translational factors to ensure Galilean invariance of the results and to remove spurious dipolar coupling terms in the final equations to be solved [1]. The states are obtained by using a set of Gaussian type orbitals and their products, keeping all possible spin states for the different (charged) species involved in the collision, for a given, conserved, total spin.

We shall present cross sections from this approach, showing, its limits and also its advantages by comparison with results based on similar close coupling treatments but taking into account a single active electron and using independent electrons or frozen core approximations.

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* mailto: alain.dubois@sorbonne-universite.fr

Underlying scaling rules for the ionization of molecules

Alejandra M. P. Mendez , Claudia C. Montanari, Jorge E. Miraglia
Instituto de Astronomía y Física del Espacio, Buenos Aires, Argentina
alemendez@iafe.uba.ar

Modeling the ionization of molecules with biological interest by multicharged ions is a challenging task with critical implications. In the last decade, many comprehensible yet straightforward ab initio models have been proposed to obtain reliable values for several DNA and RNA bases. In recent work [1], we combined a continuum distorted wave (CDW) method with a simple molecular stoichiometric model (SSM) to compute the ionization cross sections of over a hundred biologically relevant collisional systems. Further analysis of these results led us to propose three scaling rules [2]. First, we considered the molecular description of the target by taking into account the number of active electrons per molecule, n_e. Then, we reduced the nature of the projectile by scaling the cross section with the ion charge, Z^α, as a function of the reduced impact energy $E/Z^{2-\alpha}$, with $\alpha = 1.2$. Finally, we propose a two-folded rule by combining the n_e-scaling with the Z^α-reduction of the cross section. Figure 1 shows the implementation of this scaling on CDW-SSM calculations for five different charged ions in eighteen targets and on the available experimental data. The generality of the scaling proposed is proved to be valid within 35% in a wide energy range by considering a significant number of experimental data sets for other collisional systems.

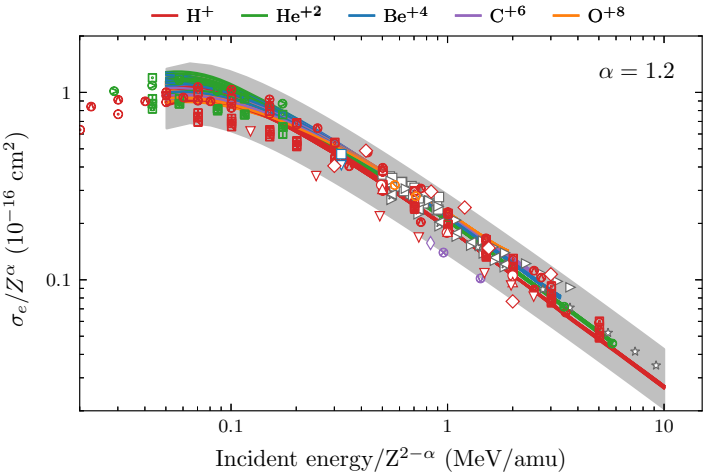

Figure 1: Ionization cross section reduced with the ion charge Z and scaled with number of active electrons per molecule n_e with $\alpha = 1.2$. Curves: CDW-SSM theoretical results from [1]. Symbols: experimental data (see Refs. in [2])

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Hydrogen Migration in the Dissociation of Hydrocarbon Dications

Yu Zhang[1], Baihui Ren[2], Chuan-Lu Yang[3], Long Wei[2], Bo Wang[2], Jie Han[2], Wandong Yu[2], Yueying Qi[1], Yaming Zou[2], Li Chen[2], Enliang Wang[4] and Baoren Wei[2]
[1]*School of Mathematics, Physics and Information Engineering, Jiaxing University, Jiaxing, 314001, China*
[2]*Key Laboratory of Nuclear Physics and Ion-beam Application (MOE), Institute of Modern Physics, Fudan University, Shanghai, 200433, China*
[3]*School of Physics and Optoelectronics Engineering, Ludong University, Yantai, 264025, China*
[4]*Affiliation J. R. Macdonald Laboratory, Physics Department, Kansas State University, Manhattan, KS 66506, USA*
brwei@fudan.edu.cn

Hydrogen migration plays an important role in the chemistry of hydrocarbons which considerably influences their chemical functions. The migration of one or more hydrogen atoms occurring in hydrocarbon cations has an opportunity to produce the simplest polyatomic molecule, i.e. H_3^+ and isomerization channels. Here we present a combined experimental and theoretical study of hydrogen migration in those channels from small hydrocarbon dications [1, 2]. The experiments are performed by 300-eV electron and 3-keV/u Ar^{8+} collisions with hydrocarbons using the cold target recoil ion momentum spectroscopy (COLTRIMS). The kinetic energy releases (KERs) and relative yields of corresponding hydrogen migration channels are determined. On the theoretical side, quantum chemistry calculations including reaction path calculation and *ab initio* molecular dynamics simulation are carried out. Also, theoretical KERs are extracted and compared with experimental ones.

Taking the dissociation of ethane dication for example, the calculations show that the H_3^+ formation channel can be opened on the ground-state potential energy surface of ethane dication via transition state and roaming mechanisms. The ab initio molecular dynamics simulation shows that the H_3^+ can be generated in a wide time range from 70 to 500 fs. Qualitatively, the trajectories of the fast dissociation follow the intrinsic reaction coordinate predicted by the conventional transition state theory. The roaming mechanism, compared to the transition state, occurs within a much longer timescale accompanied by nuclear motion of larger amplitude. In addition, the hydrogen-migration-induced isomerization is found responsible for both the symmetric and asymmetric C-C bond breakup channels.

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Shell Effects on Electron Capture to the Continuum in MeV/u Collisions of Deuteron Ions with Multielectron Targets

S. Nanos[1,2], I. Madesis[2,3], A. Laoutaris[2,3], T.J.M. Zouros[3], J.M. Monti[4], R.D. Rivarola[4], and E.P. Benis[1]

[1]*Department of Physics, University of Ioannina, GR-45110 Ioannina, Greece*

[2]*Tandem Accelerator Laboratory, INPP, NCSR "Demokritos", GR-15310 Ag. Paraskevi, Greece*

[3]*Department of Physics, University of Crete, GR-70013 Heraklion, Greece*

[4]*Laboratorio de Colisiones Atómicas, FCEIA, IFIR, Universidad Nacional de Rosario, Avenida Pellegrini 250, Rosario 2000, Argentina*

nanos@inp.demokritos.gr

The capture of a target electron into the projectile continuum (ECC) in collisions of 1.25-6.0 MeV deuteron ions with multielectron gas targets is studied both experimentally and theoretically. The double differential cross sections (DDCS), $d^2\sigma/d\Omega dE$, of the cusp shape electron peak for the gas targets of He, Ne and Ar were measured at zero degrees with respect to the ion beam, using the electron spectroscopy setup operating at the 5.5 MV Tandem Van der Graaff accelerator of NCSR "Demokritos" [1]. Theoretical DDCSs were obtained using continuum distorted wave-eikonal initial state (CDW-EIS) and CDW model calculations [2] and compared to the measurements. Multielectron targets provide stringent tests for theories exposing shell effects owed to the role of the inner shell electrons. Such an effect is the DDCS crossing for Ne and Ar targets observed around the energy of 0.8 MeV/u [3] as seen in Fig. 1.

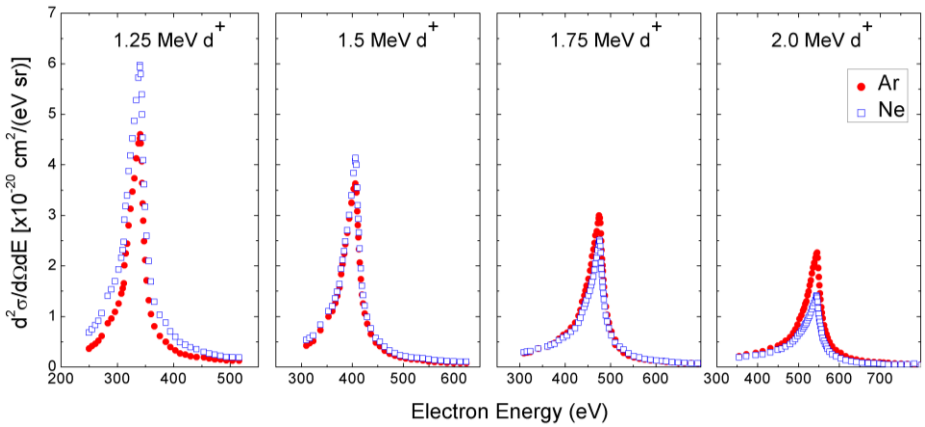

Figure 1: ECC cusp peak measurements for Ne and Ar targets showing the crossing in the DDCSs.

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First Observation of RDEC for $F^{9,8+}$ Ions on Graphene†

D. S. La Mantia[1], P. M. Niraula[2], R. Jayathissa[2], K. Bhatt[2], A. Kayani[2], and J. A. Tanis[2]
[1]*Department of Physics & Astronomy, Clemson University, Clemson, SC 29634 USA*
[2]*Department of Physics, Western Michigan University, Kalamazoo, MI 49008 USA*
dlamant@clemson.edu

Radiative double electron capture (RDEC) is a fundamental atomic collision process wherein two electrons are captured from a target to bound states in the projectile simultaneous with emission of a single photon [1]. RDEC is considered the inverse of double photoionization for ion-atom collisions. Preliminary RDEC results for 2.11 MeV/u (40 MeV) $F^{9,8+}$ ions on single-layer graphene are presented.

This work was performed using the tandem Van de Graaff facility at Western Michigan University. The incident beam was directed toward a ∼0.35 nm thick graphene sample mounted on a 200 nm thick silicon nitride grid with ∼6400 holes of 2 μm diameter on a 200 μm thick silicon substrate (commercially purchased, see Fig. 1 [2]). A Si(Li) x-ray detector at 90° to the beamline collected photons, with outgoing charged-particles collected by individual silicon surface-barrier detectors following magnetic separation. Event-mode acquisition assigned coincidences between x rays and charge-changed particles.

Fig. 2 shows preliminary x-ray gated particle spectra obtained for F^{9+} ions on the graphene target (left side) compared with the same spectra for thin-foil carbon. Similarities and differences are seen, with the data for the graphene showing up in all three outgoing charge states. Previous studies for 2.11 MeV/u F^{9+} on C [3] showed similar results due to multiple-collision effects with the q-2 and q-1 channels being dominant, whereas the present results attributed to single collisions because of the thinness of the graphene occur primarily in the q-1 channel. For F^{8+} the graphene counts were dominant in the q channel by about a factor of four, in contrast to thin-foil carbon [3] where the counts were split about equally between channels q-1 and q. Previous work for gas targets of N_2 and Ne [4] showed all events to occur as expected in the q-2 channel. †Supported in part by NSF Grant 1707467.

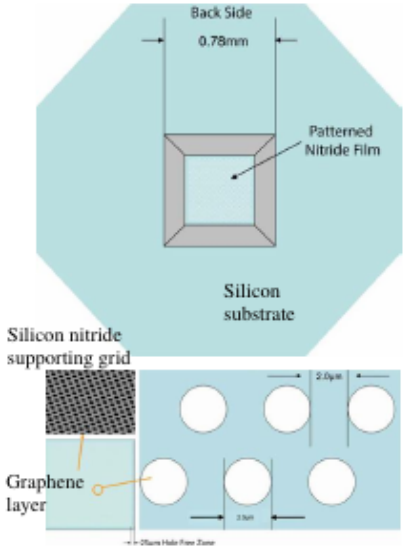

Fig. 1 Schematic of the graphene assembly used as the target in the RDEC measurements.

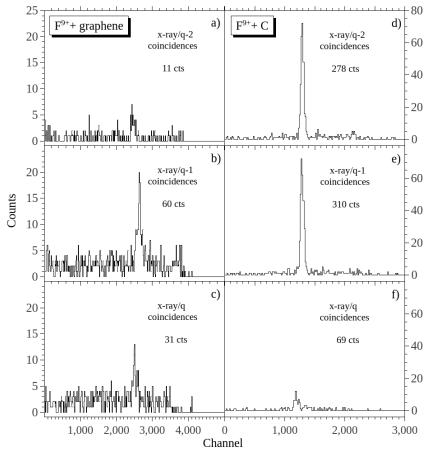

Fig. 2 Doubly- (q-2), singly- (q), and no (q) charge changed particle spectra associated with RDEC events for 2.11 MeV/u F^{9+}+ graphene (left panel, preliminary) and thin-foil C (right panel). The numbers on the graphs are the totals after background subtraction.

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Radiolysis of Valine by keV electrons

Cíntia A. P. da Costa and Enio F. da Silveira
Physics Department, Pontifícia Universidade Católica do Rio de Janeiro, Rua Marquês de São Vicente 225, 22451-900, Rio de Janeiro, RJ, Brazil.
cintia-apc@hotmail.com

The detection of amino acids in meteorites and comets [1,2] brought discussions about how they are produced in such inhospitable environments as the interstellar medium (ISM). As they are exposed to radiation on those locations, knowledge on their radioresistance is fundamental to predict their half-lives, and they also might have an important role, combined with other extraterrestrial molecules, concerning studies about origins of life on early Earth.

The radiolysis of L-valine by keV electron beams is analyzed in laboratory, at 10 and 300 K. The column density evolutions during the irradiation are measured via infrared spectroscopy and destruction cross sections are extracted [3]. Data show that, in general, destruction cross sections depend on projectile energy, sample thickness, temperature and fluence. Beside this, a model is proposed for describing the valine destruction as a function of sample depth and fluence; predictions are compared with experimental results. As shown in Figures 1 (a) and (b), for thin films (< 60 nm), a good agreement is found for the precursor column density evolution with fluence, with projectile energy and with sample thickness. For thick films, Fig. 1 (c), the model overestimates the sample degradation, suggesting that the sample was grown with a distinct amorphyzation. The model uses CASINO code [4] output to determine the deposited energy distribution in the sample. As astrophysical implications, the radiolysis of valine dissolved in H_2O ice and shielded by a CO_2 layer is predicted, as an attempt to analyze the degradation of realistic materials by keV electrons.

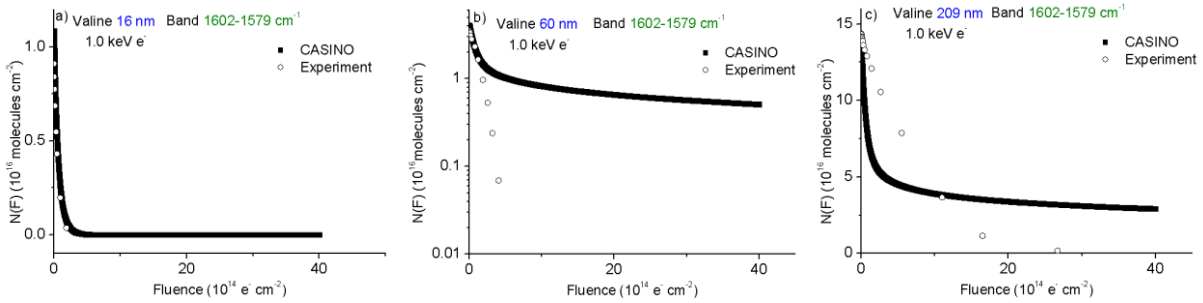

Figure 1: Column density evolutions with fluence for experimental results and the predictions of the CASINO-based model of (a) 16, (b) 60, and (c) 209 nm thick valine.

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Energy loss of relativistic charged particles in 2D materials, using the oscillator model

Silvina Segui[1], Juana L. Gervasoni [1,2], Nestor R. Arista[2], Zoran L. Miskovic[3]
[1]*Centro Atomico Bariloche, Comision Nacional de Energia Atomica. Av. Bustillo 9500, 8400 S.C. de Bariloche, Argentina.*
[2] *Instituto Balseiro, Universidad Nacional de Cuyo. Av. Bustillo 9500, 8400 S.C. de Bariloche, Argentina.*
Juana.gervasoni@gmail.com
[3]*Department of Applied Mathematics, and the Waterloo Institute for Nanotechnology, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1.*

In this work we present a fully relativistic formulation for the energy loss of an external charged particle interacting with a 2D material.

We model this material as a monolayer of atoms represented by harmonic oscillators, with isotropic or anisotropic electronic vibration modes.

Adapting the oscillator model from [1] to a mono-atomic layer, we derive relativistic analytical expressions as a function of the relevant parameters of the process.

We develop the model for a wide range of incident energies and considering both parallel and perpendicular trajectories. We obtain several useful analytical expressions for the energy loss considering isotropic and anisotropic in-plane oscillators, for parallel and perpendicular trajectories of the particle.

The results shown for stopping power and energy loss are analyzed for generic materials by the use of adequate normalization factors, absorbing the dependencies on the specific properties of the material, namely the oscillator's areal density η and their resonant frequency ω. In the perpendicular case the total energy loss $E_{perpendicular}$ depends on the value of the frequency ω due to the adiabatic behaviour at large distances.

We notice that in an anisotropic 2D-oscillators system, the energy loss due to single oscillator (and therefore the integrated quantities as stopping power and total energy loss) presents a reduction with respect to the isotropic case, especially in the parallel trajectory. We ascribe this effect to the lower availability of oscillation modes, and hence to a reduction of the interaction channels.

Finally, we remark that the present model stands out for its generality, and provides a direct evaluation of the energy loss processes in a generic 2D material.

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Electronic Sputtering from SiO_2 Targets

R. Martinez[1], A. Domaracka[2], M.E. Palumbo[3], G. Strazzulla[3], P. Boduch[2], H. Rothard[2], E.F. da Silveira[4]

[1] *Departamento de Física, Universidade Federal do Amapá, Brazil*
[2] *Centre de Recherche sur les Ions, les Matériaux et la Photonique CIMAP Normandie Univ, ENSICAEN, UNICAEN, CEA, CNRS, 14000 Caen, France*
[3] *INAF-Osservatorio Astrofisico di Catania, Italy*
[4] *Departamento de Física, Pontifícia Universidade Católica do Rio de Janeiro, Brazil*

[*] *rafael.mr@unifap.br*

Silicates are among the dominant materials in space; they occur in grains in the Interstellar Medium (ISM) and in several bodies in the Solar System (SS), like the moon, planets, asteroids and comets. Particularly, SiO_2 has been detected in protoplanetary disks, in amorphous and crystalline states, in the Mars Gale crater and in Mercury. For instance, observations of Mercury's surface indicate a heterogeneous surface composition with SiO_2 content ranging from 39 to 57 wt% [1]. All those surfaces in the ISM and SS are exposed to radiation from galactic cosmic rays, solar wind and/or energetic coronal ions, inducing several processes, among them, sputtering. As a laboratory approach, sputtering yields of SiO_2 were measured using the PDMS-TOF-MS technique (time-of-flight plasma desorption mass spectrometry), under high vacuum. Energetic (MeV/u) and highly charged ions, fission fragments produced by a ^{252}Cf source, were used as projectiles to irradiate silicon targets. Mass spectra of positive and negative ions were obtained at two temperatures, 300 and 330 K. The mass spectra of positive ions are characterized by the hydrogen peaks (H^+, H_2^+ and H_3^+) that obviously represent an unavoidable contamination and small peaks of Si^+ and Si_2^+. Higher yields of negative secondary ions are observed, mainly $(SiO_2)_n^-$ (n=1-3), $(SiO_2)_nO^-$ and $(SiO_2)_nOH^-$ (n=1-5) clusters. This is unexpected, since due to the prompt secondary electron emission, anion emission is expected to be less intense and softer than cation emission, being therefore more informative on crystalline structures. The current results show, however, similar positive and negative ion yields: $Y_{i,pos}$ = 0.05 ions/impact and $Y_{i,neg}$ = 0.06 ions/impact. This is probably due to relatively low secondary electron emission and/or due to high electron capture by Si containing molecules. For low electronic stopping power (S_e), the Total Ion Yield (Y) of different materials produced by heavy ions are expected to follow a power law as a function of S_e: $Y = \xi (S_e)^n$, where n ~ 3 [2]. Assuming that this law also holds for high S_e values (S_e = *850 eV/Å for FF)* and considering the experimental results for Y, the ξ value for SiO_2 is determined as being 1.7E-10 (Å/eV)^3. The ξ value for other silicates are also measured; anorthite: 1.5E-10, jadeite: 2.0E-10 and nepheline: 2.2E-10 (Å/eV)^3. Thus, ξ values for silicates are approximately the same; for comparison, the ξ value for H_2O ice is 3.0E-8 (Å/eV)^3, two orders of magnitude higher [2].

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Stopping power in heavy atoms, the role of $4f$ electrons

Claudia C. Montanari, Alejandra M. P. Mendez, Darío M. Mitnik, Jorge E. Miraglia
Instituto de Astronomía y Física del Espacio, Buenos Aires, Argentina
mclaudia@iafe.uba.ar

We present recent theoretical calculations for the stopping power of protons in solid Hf, Ta, and Pt. We compute the stopping power of these heavy post-lanthanide metals considering three different methods. First, we use a non-perturbative description for the energy loss in the FEG [1] based on the screening potential and the value of r_S. The second model employs the dielectric formalism [2] for the stopping of the FEG in the energy region where plasmon excitations are important. The third method considers a detailed description of the electronic structure of the bound electrons –wave functions and binding energies– using relativistic solutions of the Dirac equation. The stopping of bound electrons ($1s$-$4f$) is calculated using these structure calculations and the shellwise local plasma approximation (SLPA) [3, 4]. We modified the SLPA to include inter-shell screening ($5p$-$4f$) and a local Mermin dielectric function [2]. Present results and the comparison with available experimental data and with SRIM 2013 are displayed in Figure 1. The differences with SRIM predictions are noticeable.

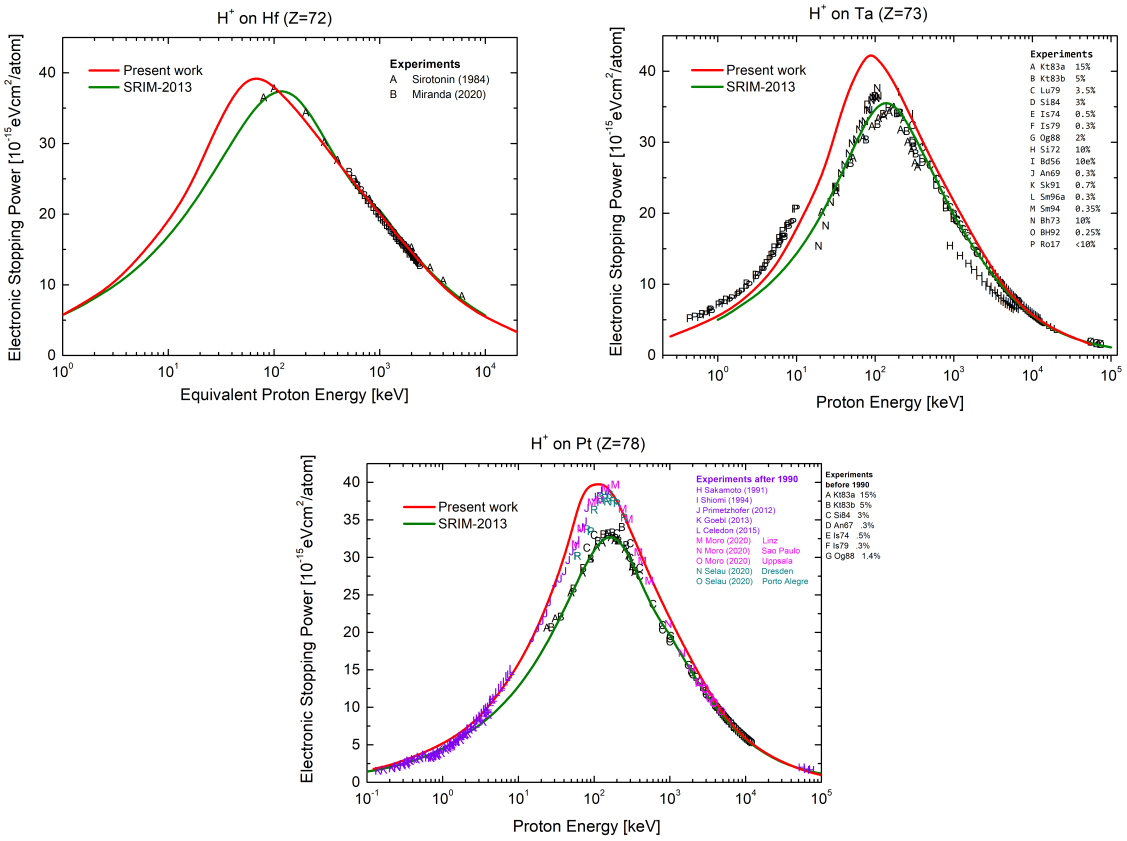

Figure 1: Stopping power of protons in Hf, Ta and Pt. Curves and symbols detailed inside the figures.

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Planned Laboratory Studies of N_2 reacting with H_3^+ Isotopologues

D. Schury[1], C. Bu[1], P.-M. Hillenbrand[2], X. Urbain[3], and D. W. Savin[1]
[1]*Columbia Astrophysics Laboratory, Columbia University, New York, NY 10027, USA*
[2]*GSI Helmholtzzentrum, Darmstadt, 64291, Germany*
[2]*Université catholique de Louvain, Louvain-la-Neuve, 1348, Belgium*
daniel.schury@physik.uni-giessen.de
savin@astro.columbia.edu

Deuterated molecules are used to infer the temperature, chemistry, and thermal history of cosmic objects such as prestellar cores and protoplanetary disks [1]. In the very dense cold regions found in prestellar cores and the outer mid-plane of protoplanetary disks, most molecules beside hydrogen freeze onto dust grains, leaving HD as the primary deuterium reservoir in the gas phase. The HD can react with H_3^+ to form deuterated isotopologues of the ion. Subsequent ion-neutral reactions pass on the deuteration to other gas-phase species. Of particular importance is the abundance ratio for N_2D^+ and N_2H^+. Their formation occurs near the N_2 snow line of prestellar cores and protoplanetary disks and they are commonly used to trace the properties of these objects. However, to reliably interpret observations of these ions, an accurate understanding of their formation process is needed. We will use our dual-source, ion-neutral, merged-fast-beams apparatus [2, 3], shown in figure 1, to measure the integral cross sections of the reaction of N_2 with H_3^+ and its isotopologues, to an accuracy of about 15%. From these results, we will derive the thermal rate coefficients used in astrochemical models. In addition, our results will help the astrophysics community to determine the validity of the commonly assumed scaling of available kinetics data for H-bearing reactions to deuterated isotopologues and also of the assumed statistical branching ratios used for the relative fractions of H-bearing and D-bearing daughter products.

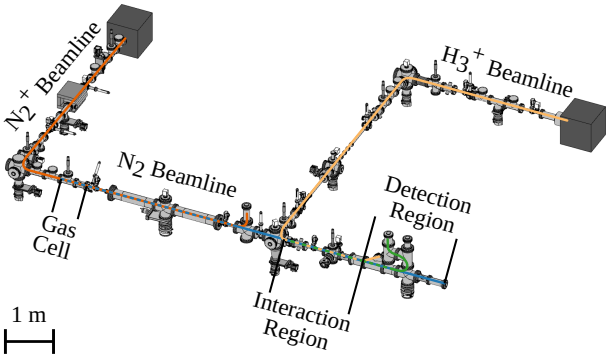

Figure 1: Schematic of the experimental setup with particle beam trajectories indicated. The initial N_2^+ beam (dark orange) neutralizes in the gas cell and forms N_2 (blue). In the interaction region, it reacts with the superimposed H_3^+ beam (light orange) and N_2H^+ is created (green). All initial and product beams are collected in Faraday cups and particle detectors.

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MDM-Ion Monte Carlo code: swift ion tracks in water to study physical parameters of interest in hadrontherapy

Verónica B. Tessaro[1,2], Benoit Gervais[3], Floriane Poignant[1,2], Michael Beuve[2], Mariel E Galassi[1]

[1]*Grupo de Física Biomédica, Instituto de Física de Rosario (CONICET-UNR) and FCEIyA, Universidad Nacional de Rosario (UNR), C.P.2000 Rosario, Argentina.*

[2] *Université Lyon, Université Claude Bernard Lyon 1, CNRS/IN2P3, IP2I Lyon, 69622 Villeurbanne, France.*

[3] *CIMAP, unité mixte CEA-CNRS-ENSICAEN-UCBN 6252 BP 5133, 14070 Caen Cedex 05, France*

verotessaro@gmail.com

Monte Carlo particle transport codes are important computational tools with the ability to simulate all the physical interactions involved by the projectile as it passes through biological matter, and all the secondaries generated. They are widely used in the field of radiation physics to study the energy deposition in different media. In this work, a new branch of the MDM Monte Carlo code, called MDM-Ion, is presented for ion projectiles in water. The original transport code MDM was developed to simulate electrons and photons trace, contemplating various heterogeneous domains (MDM for MeDiuM). Thus, it has been employed to study the influence of gold nanoparticles in water on nano dosimetry and chemical species production [1] and *W*-values for electron impact in water [2], among others topics.

The aim of the MDM-Ion is to study some physical parameters of interest in reference dosimetry for ion radiation therapy (called protontherapy or hadrontherapy). These parameters are the stopping power ratio of liquid water to air and the *W*-values in air, defined as the average energy required to generate an ion-electron pair by the incident particle and all the secondary generated. The relevance in their study is because they are the ones that contribute the most to uncertainties in the dose determination [3].

We present a detailed description of the MDM-Ion code and results for proton and carbon ion projectiles in water. Due to the energy range covered in hadrontherapy (from 200 MeV/u to 450 MeV/u approximately), relativistic approximations (RA) are included in the kinetic energy of the ion projectile. We also studied the contribution of post-collisional Auger electron emission to the calculation of *W*-values. The electronic stopping powers calculated with the MDM-Ion are in excellent agreement with the recommended data [4]. The W values are complex parameters, since all inelastic processes between the ion and the medium, including all secondary electrons (produced by ionization and post-collision Auger emission), must be taken into account. The results show the relevance of considering relativistic effects and multi-electronic emission. This parameter seems to be independent of the ion charge and energy, as it is assumed in reference dosimetry for hadrontherapy due to the lack of experimental data. Future work will extend the studies to other gaseous media of relevance in dosimetry, and other projectiles currently used in hadrontherapy.

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Interaction of C^{5+} ions with hydrogen atoms

Saed J. Al Atawneh[1, 2] and K Tőkési[1]

[1]*Institute for Nuclear Research (ATOMKI), 4026 Debrecen Bem tér 18/c, Hungary*
[2] *Doctoral School of Physics, Faculty of Science and Technology, University of Debrecen, P.O.400, Debrecen, Hungary*

tokesi@atomki.hu

Collisions between multiply charged ions and atomic hydrogen are important in determining the radiation losses and neutral beam heating efficiencies in tokamak plasmas [1]. In this work, a 4-body Classical Trajectory Monte Carlo (CTMC) and a 4-body Quasi-classical Monte Carlo (QCTMC-KW) model of the Kirschbaum and Wilets were used to calculate the cross sections in C^{5+} and H collisions. We present the ionization and capture cross sections in the projectile energy range between 20 keV and 10 MeV and compared them with previously obtained theoretical and experimental results. According to our knowledge, this is the first time to present cross section data using the QTMC-KW method for this collision system. Figure 1. shows the projectile capture cross sections in a collision between C^{5+} ion with H atom as a function of impact energy. According to the expectation, the QCTMC-KW method improved the cross section data compared with the results of the standard CTMC method. We found a reasonably good agreement between the experimental data and our results obtained by QCTMC-KW method.

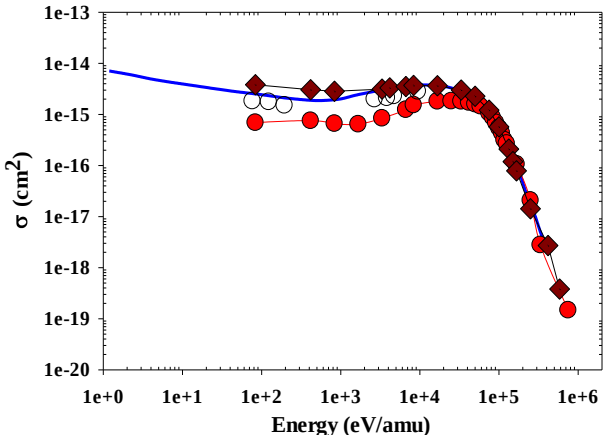

Figure 1: Electron Capture cross sections of the projectile as a function of impact energy in a collision between C^{5+} ion with H atom. Red solid-circles: presents 4-body CTMC results, brown solid-diamonds: presents 4-body QCTMC-KW results, open circles: experimental data by Crandall et a1 [3], blue solid line: 3-body CTMC calculation by R K Janev et al [2].

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Double-to-single ionization ratio for a PAH molecule coronene ($C_{24}H_{12}$) in fast ion impact

Chandan Bagdia[1], Deepankar Misra[1], Abhijeet Bhogale[1], Lokesh C Tribedi[1]
[1] *Tata Institute of Fundamental Research, Mumbai, 400005, India*
lokesh@tifr.res.in, chandanbagdia@gmail.com

The polycyclic aromatic hydrocarbons (PAH) have attracted a lot of attention in recent times owing to their presence in the interstellar medium (ISM) [1-2]. PAHs are in general planar molecule having delocalized π-electron cloud, which also provides the stability to these molecules in the harsh interstellar environment. The interstellar environment is largely ionized and it has highly charged ions. In order to understand the interaction with these radiations photo-ionization and photo-fragmentation study of PAHs have been studied extensively. However, ion impact studies are relatively scarce [3-4]. The collective excitation state resulting from the strong e^-- e^- correlations that is also known as giant dipole plasmon resonance (GDPR) is predicted for the PAHs. Hence, the studies on the PAH molecules are also important from fundamental molecular physics. In case of ion collisions, the collision dynamics are governed by the projectile charge state (q_p) and velocity (v_p) representing the perturbation strength.

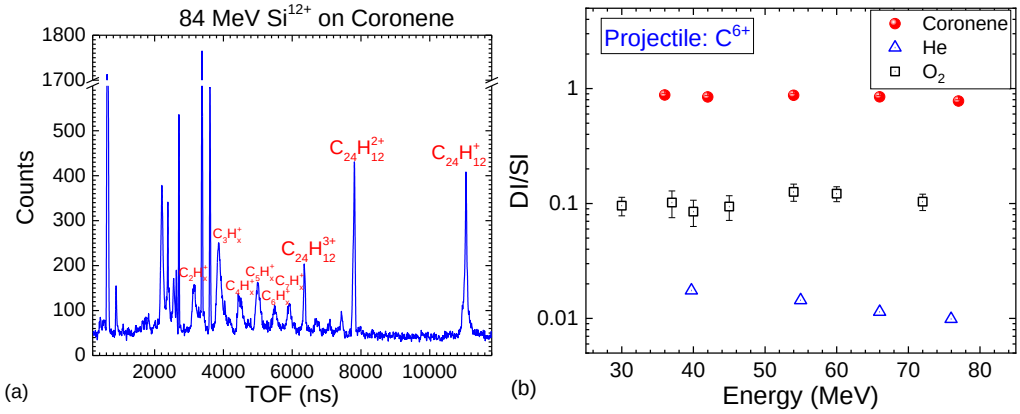

Figure 1: (a) Typical time of flight spectrum, (b) DI to SI ratio for coronene, He and O_2

We have studied the ionization and fragmentation of the coronene ($C_{24}H_{12}$) molecules in collisions with swift C, O, and Si ions as a function projectile charge state and velocity. The ion beams are obtained from the 14 MV Pelletron accelerator at TIFR, Mumbai. The recoil ions produced upon interaction with the effusive jet of coronene are analyzed using the double field time-of-flight (TOF) spectrometer. The typical TOF spectrum is shown in Fig. 1 (a). The various fragmentation products are identified from the TOF spectrum. The ratio of double ionization (DI) to single ionization (SI) has been found to be quite large (~0.8-0.9) in case of coronene as compared to He (0.018-0.02) and O_2 (0.085-0.12) [see Fig 1(b)]. The apparently large ratios in case of coronene indicates the effect of strong e^--e^- correlation among the electrons and hence collective plasmon excitation in such PAH molecules. Similar studies on relatively smaller PAH molecules-fluorene, will also be presented.

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Two electron processes in relaxation of Rydberg hollow atoms

Ł Jabłoński[1], D Banaś[1], P Jagodziński[1], A Kubala-Kukuś[1], D Sobota[1], I Stabrawa[1], K Szary[1], M Pajek[1]
[1]*Institute of Physics, Jan Kochanowski University, 25-406 Kielce, Poland*
l.jablonski@ujk.edu.pl
m.pajek@ujk.edu.pl

The M-X-rays emitted from Rydberg (n~30) hollow atoms (RHA) created in collisions of highly charged Xe^{q+} ions (q=23-36) with Be surface were measured and interpreted in terms of the MCDF calculations [1] as a cascade of nf-3d electric dipole X-ray transitions, including their M-shell hypersatellites. The measured X-ray spectra indicate the importance of two-electron processes, in particular the Internal Dielectronic Excitation (IDE) [2] and Two-Electron One-Photon (TEOP) transitions, in relaxation of studied RHA. In fact, the observed M-X-rays for Xe^{26+} ions (see Fig. 1), that have no initial vacancies in 3d subshell, result from filling 3d vacancies formed exclusively by the IDE. We found a sharp cut-off for X-ray cascade at n~10-20, which supports the idea that for higher n-states the relaxation proceeds via the Interatomic Coulombic Decay (ICD) [3]. Consequently, these observations explain why the relaxation of RHA can proceed in the ultrafast timescale.

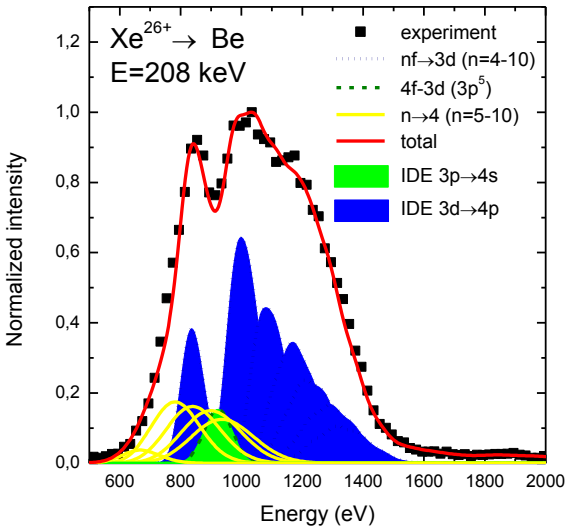

Figure 1: Measured spectrum of X-rays for 208 keV Xe^{26+} ions colliding with Be foil.

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Calculation of differential cross sections in proton-hydrogen collisions

C T Plowman, K H Spicer, I B Abdurakhmanov, A S Kadyrov, and I Bray
Curtin Institute for Computation and Department of Physics and Astronomy, Curtin University, GPO Box U1987, Perth, WA 6845, Australia
corey.plowman@postgrad.curtin.edu.au

Proton scattering on atomic hydrogen is a fundamental three-body Coulomb problem where all interactions between the particles and the two-body bound-state wave functions in the reaction channels are analytically known, making it an ideal testing ground for theoretical models. Many theoretical approaches to ion-atom collisions have been developed, but most have only been applied to calculate integrated cross sections. We used the wave-packet convergent close-coupling (WP-CCC) approach [1] to calculate singly differential cross sections for all binary and breakup reaction channels in the p+H collision system, including coupling between the channels.

Angular and energy differential cross sections for ionisation are shown in Fig. 1 in comparison with experiment and other calculations, for an incident energy of 20 keV. The WP-CCC results display excellent agreement with experiment. The CTMC and CDW-EIS calculations by Kerby *et al.* [2] fail to consistently replicate the experiment in both ejection angle (a) and ejection energy (b). The FHBS calculations by Reading *et al.* [3] overestimate experiment in angle (a) and become inaccurate with increasing energy (b).

Our approach provides good agreement with experiment for direct scattering, electron capture, and ionisation processes simultaneously, offering improvement over previous theoretical studies. For other processes and incident energies see Ref. [1].

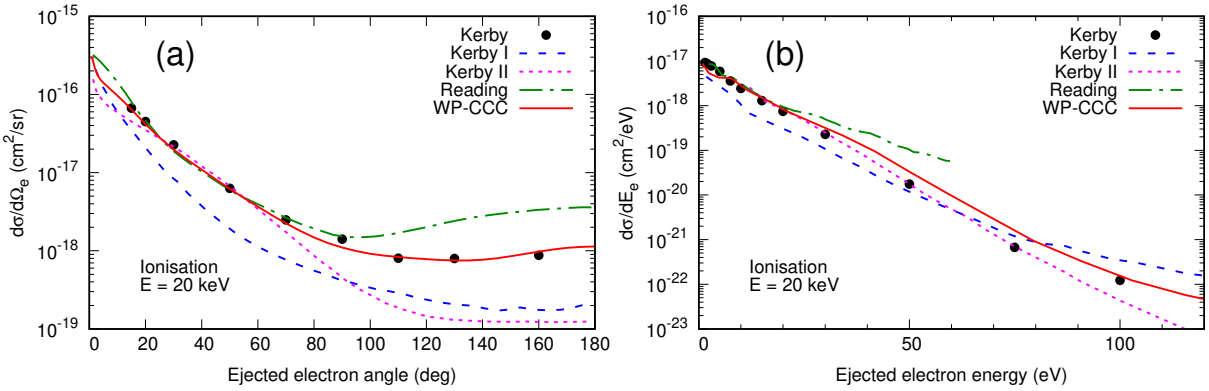

Figure 1: Angular (a) and energy (b) differential cross sections for ionisation in p+H collisions at an incident energy of 20 keV. Experiment data, CTMC (I) and CDW-EIS (II) calculations by Kerby *et al.* [2]; FHBS calculations by Reading *et al.* [3].

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Absolute total single- and double-electron capture in O^{6+} + (CO_2, CH_4, H_2 and N_2) collisions

L. Wei[1], J. Han[1], B. Ren[1], B. Wang[1], W. Yu[1], Y. Zhang[2], Y. Zou[1], L. Chen[1], J. Xiao[1], and B. Wei[1*]

[1] *Institute of Modern Physics, Key Laboratory of Nuclear Physics and Ion-Beam Application (MOE), Fudan University, Shanghai 200433, China*

[2] *College of Data Science, Jiaxing University, Jiaxing 314001, China*

brwei@fudan.edu.cn

Synopsis The absolute electron capture cross sections for single and double charge exchanges between the highly charged ions $^{16}O^{6+}$ and CO_2, CH_4, H_2, N_2, the dominant collision processes in the solar wind, have been measured in the energy from 2.63 keV/u to 19.5 keV/u. These measurements were carried out in the new experimental instrument set up at Fudan University. The measured data are useful for simulation of ion-neutral processes in astrophysical environments and contribute to advance the present theoretical model of fundamental atomic processes.

Electron capture processes play a central role in understanding astro-physical plasma environments and treatment of thermonuclear fusion plasmas [1]. As X-ray emission from solar wind (SW) heavy ions interacting with cometary and planetary atmospheres, the observations and model analyses on the X-ray spectrum of comets, Jupiter and Jovian planets, and outer heliosphere, such as supernova remnants, starburst galaxies have been successively carried out, further confirming that the charge exchange (CE) process has an important influence on the cosmic X-ray. Due to the complex many-body dynamics process involved, such reaction faces great challenges in theoretical description. The availability of atomic data for CE is usually insufficient, thus hindering the completeness and validity of present model, and more experimental data are necessary as a theoretical benchmark.

As the most abundant heavy-ion constituents in the SW, oxygen in the form of O^{6+} ions, single and double electron capture (EC) cross sections from 2.63 keV/u to 19.5 keV/u for $^{16}O^{6+}$ colliding with abundant cometary and planetary species CO_2, CH_4, H_2, N_2 are accurately measured. which will fill the gap in the data of EC cross sections for highly charged ions (HCIs) in the energy range of 10 keV/u-100 keV/u.

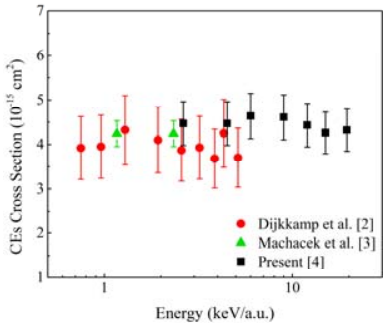

Figure 1: Single EC cross sections as a function of impact energy for O^{6+} colliding with H_2.

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Interactions and quantum effects on molecular ions' microsolvation process

R. Yanes-Rodríguez[a], R. Rodríguez-Segundo[a], P. Villareal[a] and R. Prosmiti[a]

[a] *Institute of Fundamental Physics (IFF, CSIC), Madrid, Spain*

The investigation of helium nanodroplets has received a great deal of attention during the last few years, being a challenge for both theoreticians and experimentalists. Such nanodroplets have emerged as a new and exciting medium for studying the isolation of otherwise hardly accessible molecules, allowing detailed study of a wide variety of molecular dopants, neutral or charged. In this context, alkali ions have attracted particular attention because of their strong binding to helium.

The main focus of this work is to analyse thermal and nuclear quantum effects in various He_N-A_2^+ clusters, with A=Li-Cs, as the size of the system changes, and their effect on the molecular ions' microsolvation process, related with slow mobility of such ions observed experimentally in ultra-cold He-droplets [1]. For this purpose, pure helium clusters containing up to 100 atoms and doped with an alkali dimer cation have been studied through thermostatted PIMD (Path Integral Molecular Dynamics) simulations in the NVT canonical ensemble, at a low temperature of 2K, using the open i-PI code [2]. The description of the total interaction between the A_2^+ cation and the He atoms is based on a sum-of-potentials approach containing accurate three-body *ab initio* terms, plus two-body He-He interactions [3,4]. The most stable structures, as a function of the number of solvent He atoms, were determined by employing an evolutionary algorithm [3]. New insights into energetics, that control the stabilization of specific compact-structure conformers from such quantum simulations will be discussed.

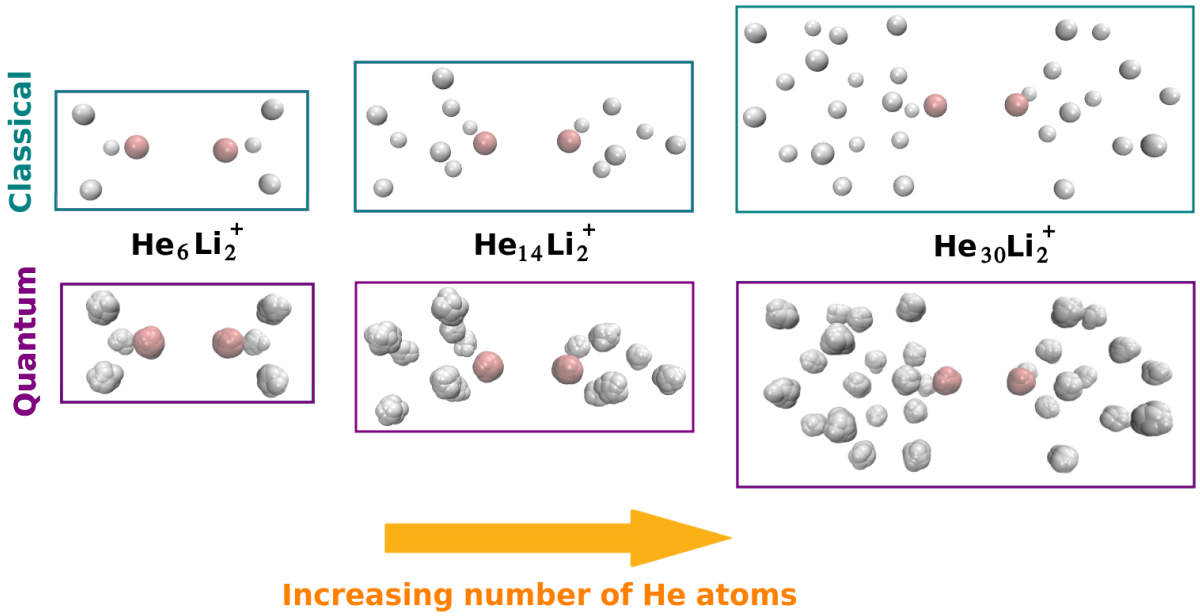

Figure 1. Minimum energy clusters arrangement as a function of the number of He atoms.

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Effective single-electron treatment of ion collisions with multielectron atomic targets

I. B. Abdurakhmanov, C. T. Plowman, A. S. Kadyrov and I. Bray
Curtin Institute for Computation and Department of Physics and Astronomy, Curtin University, GPO Box U1987, Perth, WA 6845, Australia
ilkhom.abdurakhmanov@curtin.edu.au

Ion-atom collisions involving one- or two-electron targets can be dealt with in an *ab initio* manner without significant approximations. However, as the number of target electrons increases it becomes unavoidable to introduce approximations. Usually, processes involving the outer-shell and inner-shell electrons are treated using an independent-event model. However, the independent-event model becomes impractical when the number of shells is more than two. We develop an effective single-electron approach to ion collisions with multielectron atomic targets that overcomes this difficulty by treating all the atomic electrons on an equal footing [1]. The ground state wave function for the target atom obtained in the Hartree-Fock approximation is used to calculate the probability density for the whole atom. The latter is then averaged over the spatial coordinates and spin variables of all of the target electrons except for the position of one electron from the nucleus. The obtained single-electron probability density is then used to derive a pseudopotential describing the interaction of one electron with an effective field produced by the target nucleus and the other electrons. The procedure reduces the many-body Schrödinger equation effectively into a three-body one.

We have calculated the total cross section for single-electron capture and single ionisation in proton collisions with alkali atoms of Li, Na and K. For single electron capture the results are in excellent agreement with all the available measurements. For single ionization our results are also in good agreement with the experimental measurements where available.

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[1] Abdurakhmanov I B *et al* 2021, submitted

Interaction of electrons and positrons with protons aligned in one-dimension line

M Al-Ajaleen[1], K Tőkési[2]
[1]*Institute of Nuclear Research (ATOMKI), Debrecen, 4026, Hungary*
[2]*Doctoral School of Physics, University of Debrecen, Debrecen, 4032, Hungary*
tokesi@atomki.hu

We present theoretical studies of electron and positron interaction with protons aligned in one-dimension line. The periodic proton line generated artificially where the individual protons are fixed in a certain position. The electron and positron trajectories passing through these periodic multiple scattering object are calculated using a Classical Trajectory Monte Carlo method [1]. The purpose of our present work is twofold. At first the results obtained from this model calculations will help us to go further studying more complicated systems such as two-dimensional materials like graphene. Secondly, these calculations also help us to mimic the interference effect even classically [2].
In our CTMC approach, Newton's classical non-relativistic equations of motions for a many-body system are solved numerically for a large number of trajectories. We present results for three different systems: when the target consists of a) one proton, b) two protons and c) 10 protons. The protons were fixed and have separation of 3 au. The initial kinetic energies of the projectiles were 500 and 1000 eV.
We found characteristic periodic peak structure after the proton line (see Fig. 1). We analyze and discuss this behavior as a function of the distance between the protons.

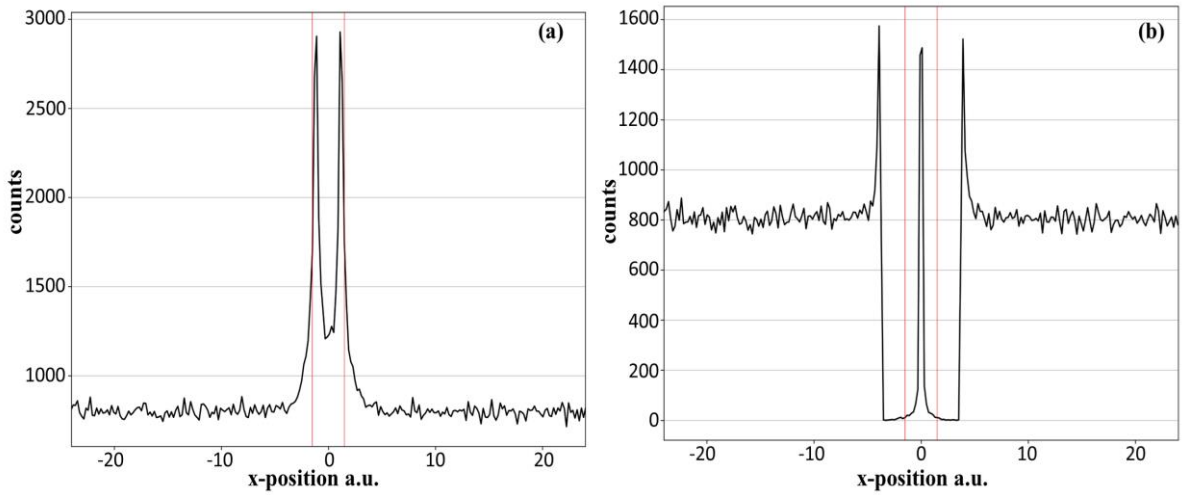

Figure 1: Electron (a), and positron (b) intensities at 40 au. from the proton line after they passed the proton line at 1000 eV primary energy. Red lines show the positions of the protons.

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Differential cross section of emitted electrons from acenapthene under fast H-like Si ion impact

Debasmita Chakroborty[1], S Phatak[1], C. Bagdia[1], A. Bhogale[1], L. Gulyas[2] and L. C. Tribedi[1]

[1]*Tata Institute of Fundamental Research, Colaba, Mumbai 400005, India*
[2] *Inst of Nucl Res of Hungarian Academy of Sciences, Debrecen H-4001, Hungary*
debasmita.chakraborty@tifr.res.in, lokesh@tifr.res.in

Atomic collisions involving polycyclic aromatic hydrocarbons (PAH) are subject of strong interest in contemporary research because of their technological as well as astrophysical importance. The studies involving the PAH molecules provide rich information regarding mechanisms of electron emission . This will have implication in the study of the astrochemistry of the interstellar medium and planetary atmosphere in which the PAH molecules have substantial presence. The giant plasmon resonance is shown to be a strong source of e-emission for large PAH molecule such as coronene. It may be of interest to investigate such resonance lines in case of PAH molecules of smaller size, such as, acenapthene ($C_{12}H_{10}$).

We present the measurement of energy and angular dependence of double differential electron emission cross section (DDCS) for acenapthene under collisions with 94 MeV fast Si^{13+} ion.obtained from the Pelletron accelerator at TIFR, Mumbai. An electrostatic hemispherical analyzer equipped with a CEM was used. Fig. 1 displays an example of the energy distribution of the DDCS for the ejection angle $\theta = 45^{\circ}$. New calculation based on the CDW-EIS model has been applied for the PAH molecules for the first time, which provides a reasonable agreement for most of the angles. The C-KLL-Auger peak is observed at around 240 eV. This Auger electron emission cross section was used for absolute normalization. The forward backward angular asymmetry was deduced which indicates the existence of a plasmon peak at around 17 eV, as predicted.

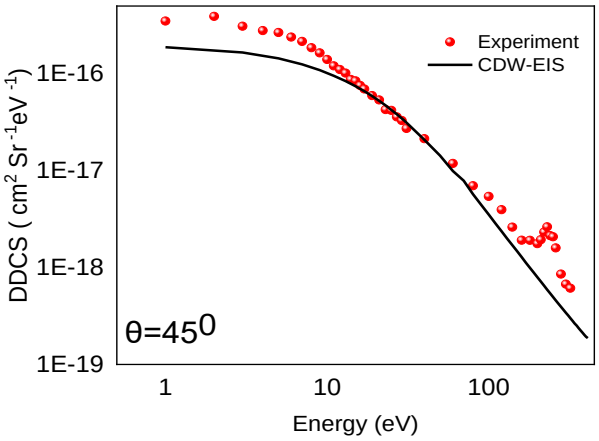

Figure 1: Energy distribution of absolute DDCS of acenapthene

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Adsorption energy of Hydrogen and Nitrogen in Tungsten

Sergio Beneitez[1], Juana L. Gervasoni[1,2], Jorge G. Gallardo[1]
[1]*Centro Atomico Bariloche, Comision Nacional de Energia Atomica. Av. Bustillo 9500, 8400 S.C. de Bariloche, Argentina.*
2 Instituto Balseiro, Universidad Nacional de Cuyo. Av. Bustillo 9500, 8400 S.C. de Bariloche, Argentina.
Juana.gervasoni@gmail.com

In this work we analyze the interaction of hydrogen, nitrogen (and their isotopes) with tungsten. This material is candidate to form the divertor wall of fusion reactors (ITER, [1]), and these atoms have a very sensitive (desired and unwanted) interaction with it. For this purpose, we study the effects and electronic state densities of atomic hydrogen and nitrogen in pure tungsten, in order to analyze some important properties such as the density of states of the system.

Focusing on this application, this work is a preliminary study of the behavior of atoms of hydrogen and nitrogen, on a surface of tungsten on the three sites of the cell: top, hollow and bridge. We use a program simulation based on the DFT (density functional theory) implemented in the Open-Source Code Quantum Espresso [2], in order to obtain the adsorption energy and the density of states of the systems. Considering E_{ads} as the parameter to be stabilized, we take a slab of 10 atomic layers in the direction (001) with a lattice of 74 atoms. The same size is taken in the perpendicular directions (010), and (100), as shown in Fig. 1. In each of the three crystallographic directions of tungsten, we study different sites and angular dependence. We focus to determine the process of adsorption in order to explain the existence of NH3 in the divertor of the fusion reactor. This development began with the simulation of ion implantation experiments, validated against existing laboratory experimental results [3]. The findings and challenges of developing a 3-D predictive capability for ammonia transport in a Tungsten divertor wall are under way.

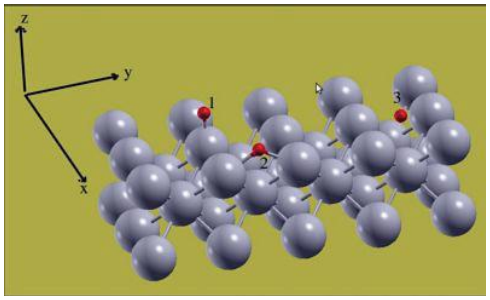

Figure 1: Scheme of the considered system W-atom: (1) top interaction site, (2) bridge interaction site, (3) hollow interaction sites.

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Photon polarizations in two-photon $2s \to 1s$ transitions in one-electron ions

V. A. Knyazeva[1],K. N. Lyashchenko[2], O. Yu. Andreev[1,3]
[1]*St. Petersburg State University, 7/9 Universitetskaya nab., St. Petersburg, 199034, Russia*
[2]*Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China*
[3]*Petersburg Nuclear Physics Institute named by B.P. Konstantinov of National Research Centre "Kurchatov Institute", Gatchina, Leningrad District 188300, Russia*
viknyazeva16@gmail.com

The two-photon transitions represent one of the fundamental processes in the atomic physics. The two- photon transition is the dominant decay channel of the $2s$ state for light and middle Z one-electron ions, where Z is the atomic number. The probabilities of one- and two-photon transitions become comparable for $Z \sim 40$. For larger Z, the decay occurs mainly via one-photon emission.

In this study, the differential transition probability for two-photon $2s \to 1s$ decay with respect to the polarization of the emitted photons was investigated. The angular distribution of the emitted photons is determined by the dominant E1E1 transitions, which gives $1+\cos^2\theta$ distribution, where θ is the angle between the momenta of the emitted photons. The deviation from this distribution was investigated in the nonrelativistic limit in [1].

We investigated the asymmetry of the angular distribution for both unpolarized and polarized emitted photons for all one-electron ions including the superheavy elements. We found that the differential transition probability can be approximated by two parameters: the total two-photon transition probability and the asymmetry factor. The difference between our relativistic calculation of the asymmetry and the calculation [1] reaches three times for the superheavy elements. In the case of light ions, the asymmetry is small, but important for evaluating the nonresonant corrections [2].

Using this approximation we investigated the emission of photons with linear and circular polarizations. We also investigated the transition probabilities for the polarized initial and final electron states.

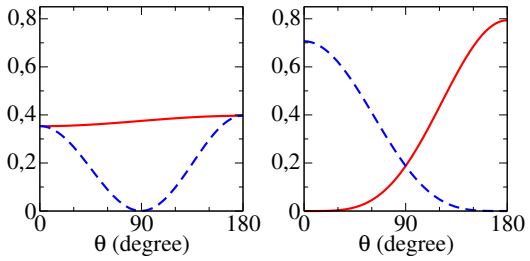

Fig. 1: The normalized differential transition probabilities as a function of the angle (θ) between the momenta of the emitted photons (k_1 and k_2, respectively) for the photons with equal energies. In the left graph,the linear polarization is concidered, the red solid line represents angular dependence of the differential transition probability for the photon polarization vectors placed in the (k_1,k_2)-plane, the blue dashed line represents angular dependence of the differential transition probability for the photon polarization vectors orthogonal to the (k_1,k_2)-plane. In the right graph, the red solid line represents the equal circular polarizations of the photons, the blue dashed line represents the different circular polarizations of the photons. The data are presented for uranium.

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Unusual overproduction of excited hydrogen atoms identified in the H_3^+ collisions with tetrahydrofuran

Tomasz J. Wasowicz[1]
[1]*Department of Physics of Electronic Phenomena, Gdańsk University of Technology, ul. G. Narutowicza 11/12, 80-233 Gdańsk, Poland*
tomasz.wasowicz1@pg.edu.pl

Ion-molecule collisions occur in natural and technical processes. For instance, they are the fundamental reactions underlying cosmochemistry. They are highly relevant to understand the lesions induced in ion therapies and evaluate the risk of the exposure of astronauts to cosmic rays. Ion-molecule collisions participate in the etching and deposition processes prompted by focused ion beams. In ion-molecule interactions, the heterocyclic molecules are essential since many take part in the life processes and form mixtures exploited in industry.

In this context, tetrahydrofuran (THF, C_4H_8O) is a prototypical heterocyclic molecule that is regarded as a simple analog to deoxyribose sugar and as a precursor to polymers. Therefore, interactions of the H_3^+ ions with the gas-phase tetrahydrofuran molecules have been investigated in the energy range of 20–1000 eV. The measurements have been carried out at the University of Gdańsk exploiting collision-induced emission spectroscopy [1]-[4]. Such ionic bombardment may lead to excitation, ionization, and fragmentation of THF. The charged dissociation products are easily probed using mass spectrometry (see, e.g. [5]). However, fragmentation into neutral fragments is more puzzling to detect experimentally. If the species are formed in the excited states, they decay by emission of characteristic light [1], [2]. Thus, we focus our attention on photon emission arising during THF fragmentation triggered by H_3^+ ion impact. Optical spectra display prominent fluorescence of the hydrogen Balmer series and weak bands of vibrationally and rotationally excited diatomic CH fragments (see Fig. 1a). The measured relative emission cross-sections of the excited fragments show the highest yields for the production of hydrogen atoms whose intensities rapidly decrease with an increasing principal quantum number. Depopulation factors of hydrogen excited states are determined at each impact energy from the H(n = 4–7) intensity ratios (Fig. 1b), and possible collisional mechanisms leading to enhanced production of the hydrogen atoms are suggested.

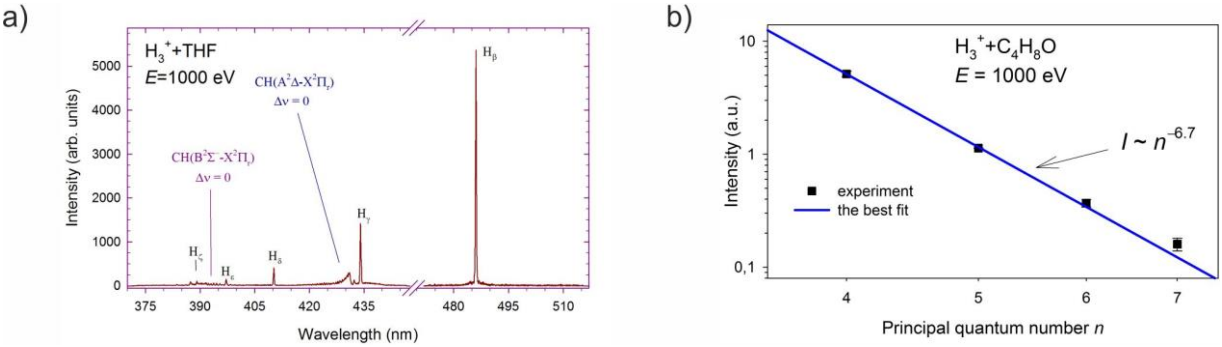

Figure 1: a) Emission fragmentation spectrum of THF. b) Intensities of the lines of the Balmer series as a function of the principal quantum number n. The solid line shows the best fit to the points.

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State selective charge exchange cross sections in Be^{4+}+H(1s) collisions

I Ziaeian[1,2], K Tőkési [1]
[1]*Institute for Nuclear Research (Atomki), 4026 Debrecen Bem tér 18/c, Hungary*
[2]*Doctoral School of Physics, Faculty of Science and Technology, University of Debrecen, P.O. Box 400, H-4002, Debrecen, Hungary*
tokesi@atomki.hu

Beryllium, as the first wall of the fusion reactor, is one of the impurities in the reactor chamber. Therefore the accurate knowledge of various cross sections when Be colliding with hydrogen atoms is essential. In this work, the state selective charge exchange cross sections are studied in the energy range between 1 keV/amu and 1000 keV/amu. We treat the collision dynamics classically using a four-body classical trajectory Monte Carlo (CTMC) [1] and a four-body quasi classical trajectory Monte Carlo (QCTMC) model [2,3] when the Heisenberg correction term is added to the standard CTMC model via model potential. Figure 1 shows the projectile energy dependent charge exchange cross sections into $Be^{3+}(n = 3)$ state. Due to lacking the experimental data for Be^{+4}+H collision system, we have compared our classical calculations with the previous results using quantum-mechanical approaches.

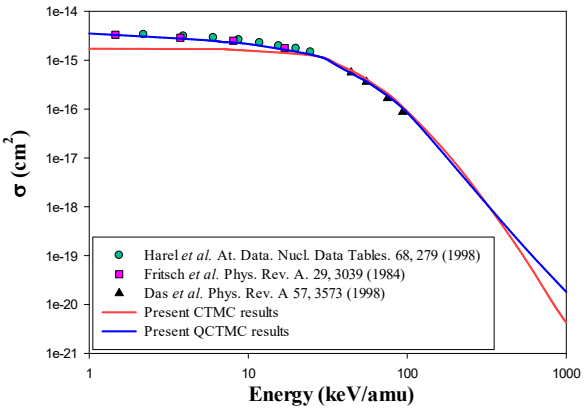

Figure 1. Projectile energy dependent charge exchange cross sections into Be^{3+} ($n = 3$) state.

We found that our QCTMC results are higher than the CTMC results, and they are in good agreement with the previously obtained quantum-mechanical results.

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Authors Index

A
Abdurakhmanov, I.B. 10, 24, 47, 50
Abril, I. 9
Ábrók, L. 26
Al Atawneh, S.J. 44
Al-Ajaleen, M. 51
Ali, E. 15
Alladustov, Sh.U. 24
Andreev, O.Yu. 54
Antonio, N.W. 10
Arista, N.R. 39

B
Bagdia, C. 19, 45, 52
Bagschik, K. 17
Banaś, D. 46
Bastola, S. 15
Beneitez, B. 53
Benis, E.P. 33, 36
Beuve, M. 32, 43
Bhatt, K. 37
Bhattacharya, D. 14
Bhogale, A. 19, 45, 52
Biri, S. 26
Bocan, G.A. 23
Boduch, P. 40
Bray, I. 10, 24, 47, 50
Breiss, H. 23
Brennecke, S. 17
Bu, C. 42

C
Cassimi, A. 16, 25, 28
Chakroborty, D. 52
Chen, L. 35, 48
Chesnel, J.-Y. 26
Chuluunbaatar, O. 17
Ciappina, M.F. 15
da Costa, C.A.P 38

D
Dapor, M. 9
Davis, J. 15
Demes, S. 26
Dhital, M. 15
Dmitriev, S. 30
Domaracka, A. 40
Dong, D. 16
Dörner, R. 17, 25
Dovator, N. 30
Dubois, A. 8, 33

E
Eckart, S. 17, 25
Eicke, N. 17

F
Fehre, K. 25
Feng, W. 16
Fischer, D. 25
Fléchard, X. 28
Frisco, L. 12
Fulvio, D. 21

G
Galassi, M.E. 32, 43
Gallardo, J.G. 53
Gao, J.W. 8
Gao, Y. 16
Garcia-Molina, R. 9
Gervais, B. 28, 32, 43
Gervasoni, J.L. 39, 53
Grande, P.L. 18
Gravielle, M.S. 12, 23
Grundmann, S. 17, 25
Guillous, S. 28
Gulyas, L. 52
Guo, D. 16

H
Hai, B. 16
Hailey, P.A. 20
Han, J. 35, 48
Hasan, A. 15
He, B. 31
Herczku, P. 20, 26
Hillenbrand, P.-M. 42
Holeňák, R. 18
Horbatsch, M. 19
Houamer, S. 17
Hu, X. 16

I
Ioppolo, S. 20

J
Jabłoński, Ł. 46
Jacob, A. 29
Jagodziński, P. 46
Jahnke, T. 17, 25
Jayathissa, R. 37
Jorge, A. 19
Juhász, Z. 20, 26

K
Kadyrov, A. 7
Kadyrov, A.S. 10, 24, 47, 50
Kaňuchová, Z. 20
Kartoshkin, V. 30
Kastirke, G. 25
Kayani, A. 37
Khemliche, H. 23
Kircher, M. 17, 25
Kirchner, T. 14, 19
Knyazeva, V.A. 54
Kovács, S.T.S. 20, 26
Kubala-Kukuś, A. 46
Kumar, V. 28

L
La Mantia, D.S. 37
Lalande, M. 28
Lamichhane, B.R. 15
Laoutaris, A. 36
Lein, M. 17
Lohmann, S. 18
Lomsadze, R.A. 15
Luna, H. 22
Lyashchenko, K.N. 54

M
Ma, X. 16
Madesis, I. 36
Madison, D.H. 15
Martinez, R. 21, 40
Mason, N.J. 20
McCullough, R.W. 20
Mendez, A.M.P. 34, 41
Méry, A. 28
Mery, A. 25
Mifsud, D.V. 20, 26
Miraglia, J.E. 34, 41
Miskovic, Z.L. 39
Misra, D. 45
Mitnik, D.M. 41
Momeni, A. 23
Montanari, C.C. 34, 41
Montenegro, E.C. 22
Monti, J.M. 19, 36
Moshammer, R. 25
Müller, C. 29

N
Nanos, S. 36
Niraula, P.M. 37

O
Oliveira, P.R.B. 21

P
Pajek, M. 46
Palumbo, M.E. 40
Paripás, B. 20
Passalidis, S. 33
Pedrielli, A. 9
Peng, Y. 16
Phatak, S. 52
Piancastelli, M.N. 17
Plowman, C.T. 10, 24, 47, 50
Poignant, F. 43
Popov, Y.V. 17
Primetzhofer, D 18
Prosmiti, R. 49

Q
Qi, Y. 35

R
Rácz, R. 26
Rangama, J. 25, 28
Ren, B. 35, 48
Rist, J. 17, 25
Rivarola, R.D. 19, 36
Rodríguez-Segundo, R. 49
Rothard, H. 40
Roy Choudhury, M. 19

S
Sánchez, E.A. 23
Savin, D.W. 42
Schmidt, L.Ph.H. 25
Schöffler, M.S. 17, 25
Schulz, M. 15, 25
Schury, D. 42

Segui, S. 39
Sens, N. 26
da Silveira, E.F. 21, 38, 40
Silvus, A. 15
Simonucci, S 9
Sisourat, N. 8, 13
Sobota, D. 46
Spicer, K.H. 24, 47
Stabrawa, I. 46
Staicu Casagrande, E.M. 23
Strazzulla, G. 40
Sulik, B. 20, 26
Szary, K. 46
Szilasi, S. 23

T

Taioli, S. 9
Tanis, J.A. 37
Taoutioui, A. 31
Tessaro, V.B. 32, 43
Tőkési, K. 31, 44, 51, 56
Trabert, D. 25
Traspas Muiña, A. 20
Trevisanutto, P.E. 9
Tribedi, L.C. 19, 27, 45, 52
Trinter, F. 17
Tsitsonis, D. 25

U

Ullrich, J. 25
Urbain, X. 42

V

Vela-Perez, I. 17, 25
de Vera, P. 9
Villareal, P. 49
Vizcaïno, V. 26
Voitkiv, A.B. 29
Volobuev, I.P. 17

W

Wang, B. 35, 48
Wang, E. 35
Wang, J. 16
Wang, J.G. 8
Wasowicz, T.J. 11, 55
Wei, B. 35, 48
Wei, L. 35, 48
Wolff, W. 22, 28
Wu, Y. 8, 16

X

Xiao, J. 48
Xu, J. 16

Y

Yan, S. 16
Yanes-Rodríguez, R. 49
Yang, C.-L. 35
Yu, W. 35, 48

Z

Zhang, S. 16
Zhang, Y. 35, 48
Zhang, Y.W. 8
Zhao, D. 16
Zhu, X. 16
Ziaeian, I. 56
Zou, Y. 35, 48
Zouros, T.J.M. 33, 36