

# Effective one-electron approach to dressed carbon-ion collisions with atomic hydrogen

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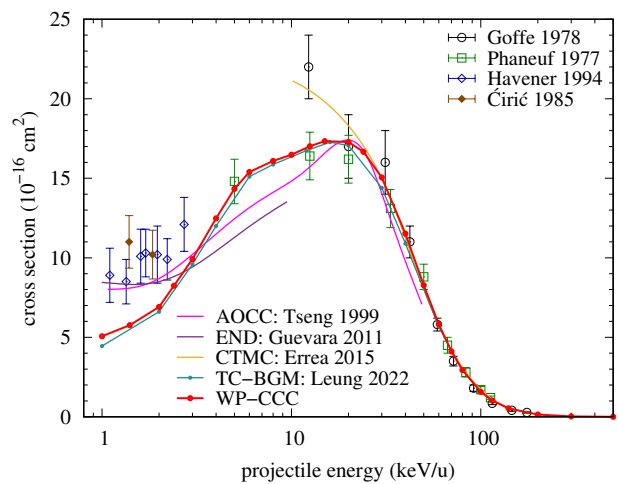
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**Synopsis** The two-centre wave-packet convergent close-coupling approach is extended to model dressed ion collisions. This is done by reducing the problem to an effective three-body system and using a model potential to approximate the interactions between the projectile-ion core with the target. We apply this method to partially stripped carbon-ion collisions with atomic hydrogen. The total cross sections for all single-electron processes are calculated in the energy region between 1 keV/u to 1 MeV/u, where coupling between the channels is important.

Collisions involving dressed ions is important for many applications such as fusion plasma modelling, analysing X-ray spectra from comets and hadron therapy of cancer. From a theoretical perspective, modelling collisions which involve more than two electrons in a completely *ab initio* manner is a challenging problem. We employ an effective potential to treat the interactions with the multi-electron projectile ion in a spherically symmetric manner. This reduces the scattering problem of dressed-ion collisions with atomic hydrogen to an effective three-body problem. We have incorporated this potential into the two-centre wave-packet convergent close-coupling (WP-CCC) formalism to study dressed carbon-ion collisions with atomic hydrogen. Calculations have been performed in the projectile energy range between 1 keV/u to 1 MeV/u, where electron capture, target excitation and ionisation are equally likely.

In Fig. 1 we show the projectile energy dependence of the total electron-capture cross section for  $C^{3+}$  collisions with  $H(1s)$ . For energies above 5 keV/u, we find excellent agreement with available measurements [1, 2]. At lower energies we note a discrepancy between our results and the experimental data. A possible reason for this is the two-electron processes that our method, at this stage, does not take into account. Here, we have presented results for  $C^{3+}$ -H collisions as an example, however, all charge states of carbon colliding with H have been considered.



**Figure 1.** Total electron-capture cross section in  $C^{3+}$ -H(1s) collisions. The WP-CCC results are compared with experimental measurements [1, 2, 3, 4] and theoretical calculations [5, 6, 7, 8].

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# Ion impact induced fragmentation dynamics of $C_2H_2^{2+}$ and $C_2H_2^{3+}$

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**Synopsis** In this abstract we will discuss about the fragmentation of  $C_2H_2^{2+}$  into  $(H^+ + C_2H^+)$  and  $(CH^+ + CH^+)$  and  $C_2H_2^{3+}$  into  $(H^+ + C^+ + CH^+)$  and  $(H^+ + H^+ + C_2^+)$  produced by electron capture upon collision between Kr projectile beam and supersonically cooled  $C_2H_2$  molecules.

$C_2H_2$  is a linear tetratomic system which has been studied from the perspective of fundamental physics in various earlier reports. The three body decay and isomerization of  $C_2H_2^{3+}$  by ultrashort laser was studied in by A. Hishikawa et al. [1]. Angular and energy distribution of various two-body fragmentation channels of  $C_2H_2^{2+}$  using 39 eV photons were report by M. Alagia et al. [2].

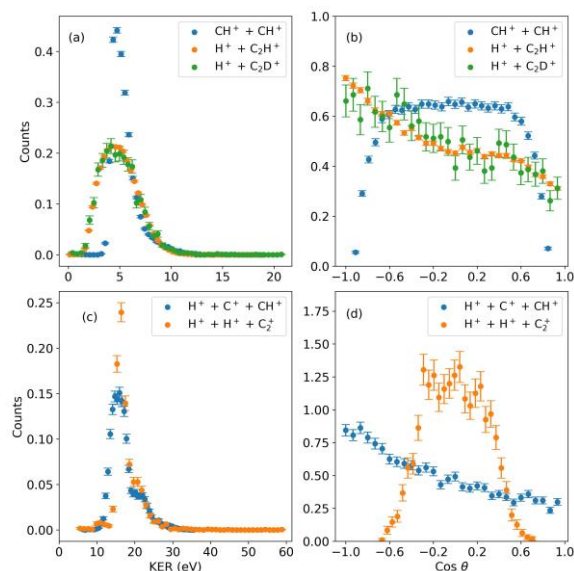
In this present work, we have presented the two and three body fragmentation channels of  $C_2H_2^{2+}$  and  $C_2H_2^{3+}$ , respectively, upon impact with 330 keV  $Kr^{11+}$  projectiles using COLTRIMS setup.

We detected all the recoil ions in coincidence with the projectile ion. In our data, we also observed the Duterium substituted acetylene (HCCD) and have done the analysis for the same also. In Figure (1) we have plotted the KER and angular distributions of various channels of the two and three body breakup. In Figure (1a) the KER distribution for  $CH^+ + CH^+$  channel has a sharp peak, while those for other two body channels have a relatively broader peak.

We observed in case of  $H^+ + C_2H^+$  channel that there is an anisotropy in angular distribution of the fragments. From Figure (1b) we infer that  $H^+$  ions have an orientation dependence on the angular distribution. Since the angular distribution of  $H^+$  ions is plotted with respect the projectile beam, the  $H^+$  recoil ion prefer to eject in the opposite direction of the projectile beam. The angular distribution for  $CH^+ + CH^+$  channel is isotropic.

The KER spectrum for three body fragmentation channels  $(H^+ + C^+ + CH^+)$  and  $(H^+ + H^+ + C_2^+)$  in Figure (1c) has a sharp peak at around 18 eV and a shoulder like structure at around 22 eV. Figure (1d) shows the angular distribution of the  $H^+$  ions for the two channels. Clearly, there is an anisotropy in case of  $(H^+ + C^+ + CH^+)$  channel, also, the distribution of

$H^+$  ions for  $(H^+ + H^+ + C_2^+)$  channel is narrow. Ideally the spectrum should lie between -1 and +1, but because of the dead time of the detector, two  $H^+$  ions flying at  $0^\circ$  and  $180^\circ$  have time-of-flight difference less than the dead time, this is why they are missing from the spectrum.



**Figure 1.** (a) KER of three two body fragmentation channels (b) angular distribution of the first ion in two body fragmentation of  $C_2H_2^{2+}$ , (c) KER of the three fragments and (d) angular distribution of the first ion for three body fragmentation channels.

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# Energy and angular distributions of electrons produced in intermediate-energy proton-helium collisions

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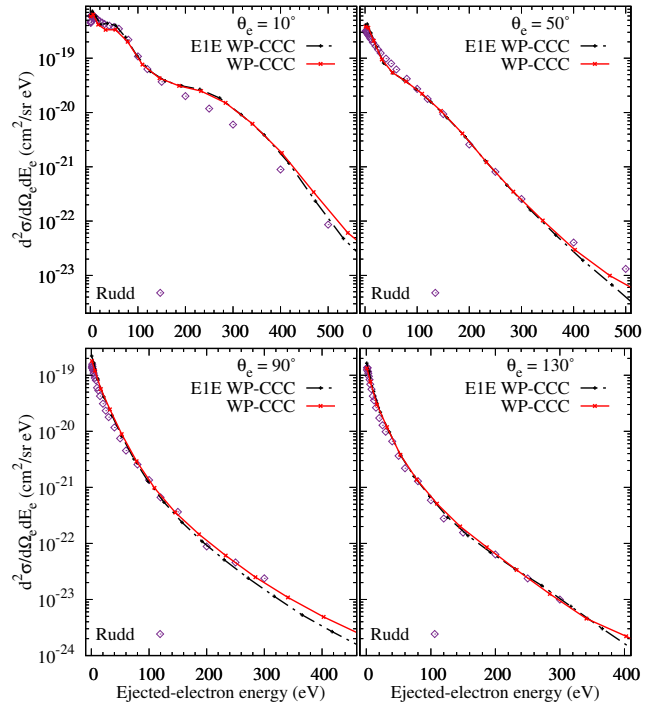
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**Synopsis** The wave-packet convergent close-coupling approach is applied to differential ionization in proton-helium collisions. The approach employs a correlated two-electron description of the helium atom. The doubly differential cross section as a function of the energy and angle of the emitted electron is calculated for incident proton energies in the intermediate range. Results are in excellent agreement with experimental data.

Modelling ionization in ion-atom collisions is a challenging problem requiring two-center effects to be accounted for. Here, we investigate single ionization of helium atoms by protons using the wave-packet convergent close-coupling (WP-CCC) approach. This method uses a correlated two-electron wave function to describe the helium target and discretizes the continuum using wave-packet pseudostates. We also apply an alternative, simpler approach that reduces the target to an effective single-electron (E1E) system. Previously, we have calculated integrated [1] and singly differential [2] cross sections, and the results displayed excellent agreement with respective experimental measurements. This work represents the first study of doubly differential ionization in a nonperturbative manner. The doubly differential cross section (DDCS) is calculated in the intermediate energy (50–300 keV) region.

A sample of the calculated DDCS is shown in Fig. 1 at an incident-proton energy of 150 keV. Results from both the E1E and two-electron WP-CCC methods agree very well with experimental data. At an ejection angle of  $10^\circ$ , the low-energy peak followed by the wider shoulder is perfectly captured by the present calculations. However, at this ejection angle, results from both approaches slightly overestimate the shoulder believed to be due to the binary-encounter mechanism. At the three larger ejection angles shown, perfect agreement between the experiment and WP-CCC data is seen. No other theoretical cal-

culations are available for comparison at this collision energy.



**Figure 1.** DDCS for ionization of helium by 150 keV protons as a function of ejected-electron energy at ejection angles of  $10^\circ$ ,  $50^\circ$ ,  $90^\circ$ , and  $130^\circ$ . Experimental data are by Rudd and Jorgensen [3].

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# Energy distribution of electrons emitted in proton-helium collisions as a function of projectile angle

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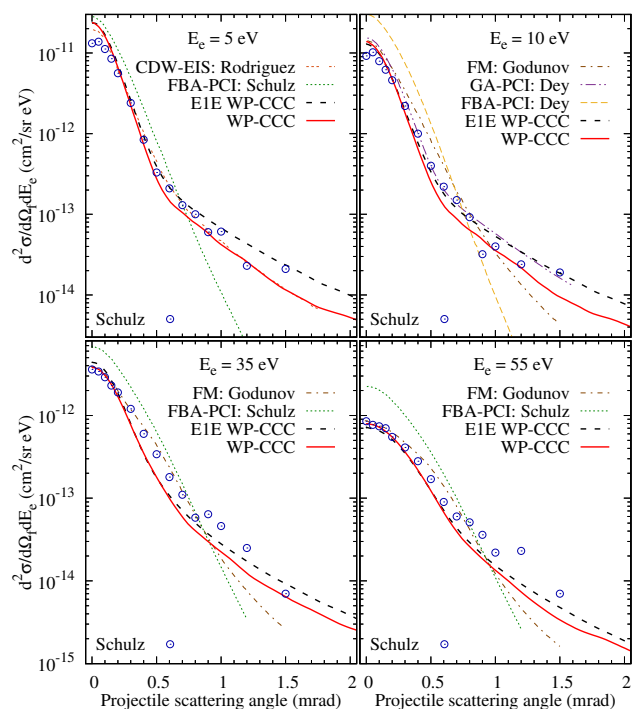
**Synopsis** The doubly differential cross section as a function of ejected-electron energy and projectile scattering angle for ionization in proton-helium collisions is calculated using the wave-packet convergent close-coupling approach. This method employs a correlated two-electron description of the helium atom. The obtained results are in very good agreement with experimental data where available.

Differential ionization in intermediate-energy proton collisions with helium remains a challenging problem. This is because of two-center effects that need to be accounted for. We investigate single ionization using the wave-packet convergent close-coupling (WP-CCC) approach. This method uses a correlated two-electron wave function to describe the helium target and discretizes the continuum using wave-packet pseudostates. We also apply an alternative, simpler approach that reduces the target to an effective single-electron (E1E) system. Calculations of the doubly differential cross section (DDCS) differential in the solid angle of the projectile and the energy of the emitted electron are performed for intermediate-energy (50–300 keV) collisions. In previous works, we have calculated integrated [1] and singly differential [2] cross sections. The results displayed excellent agreement with respective experimental measurements. This work represents the first study of the DDCS for ionization of helium in a nonperturbative manner.

A sample of the DDCS as a function of projectile scattering angle at selected ejected-electron energies for a projectile energy of 75 keV is shown in Fig. 1. Results from both methods are in very good agreement with experimental data and with each other. The CDW-EIS [4] and GA-PCI [5] calculations agree well with the present WP-CCC results. At the same time, the FBA-PCI [3, 5] and FM [6] calculations appear to disagree with the experimental DDCS.

For completeness, we will also present the DDCS as a function of projectile and ejected-electron solid angles. No experimental measurements or theoretical calculations have been per-

formed for this cross section.



**Figure 1.** DDCS for ionization of helium by 75 keV protons as a function of the projectile scattering angle at ejected-electron energies of 5, 10, 35, and 55 eV. Experimental data are by Schulz *et al.* [3]. Other theoretical data are obtained using the FBA-PCI [3], the CDW-EIS [4], the FBA-PCI and GA-PCI [5], and the FM [6] methods.

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# Role of different electron capture mechanisms in fragmentation of $\text{CO}_2^{3+}$ ions into $\text{O}^+ + \text{C}^+ + \text{O}^+$

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**Synopsis** In this abstract we will discuss about the fragmentation of  $\text{CO}_2^{3+}$  into  $\text{O}^+ + \text{C}^+ + \text{O}^+$  produced by electron capture upon collision between Ar beams of three different charges and different velocities and supersonically cooled  $\text{CO}_2$  molecules.

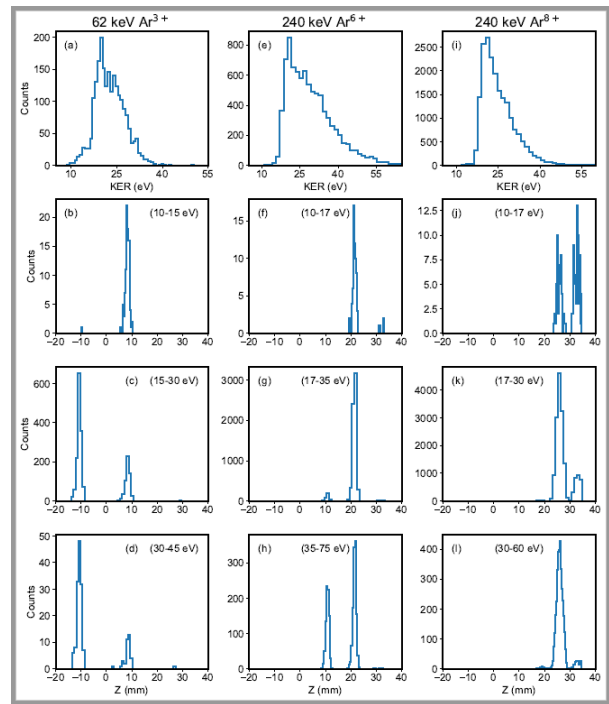
$\text{CO}_2$  being a linear triatomic system has attracted a lot of attraction from the point of view of fundamental physics involved. Three body fragmentation of  $\text{CO}_2^{3+}$  into  $\text{O}^+ + \text{C}^+ + \text{O}^+$  has been studied extensively by ion collision [1], Intense femtosecond laser induced ionization [2] and electron impact induced ionization [3], to name a few. Different pathways of fragmentation, i.e. sequential, where two C-O bonds break in a sequential manner, and concerted, in which both bonds break simultaneously, have been reported in the literature.

In present work, we studied roles of different electron capture mechanisms to produce  $\text{CO}_2^{3+}$  ion upon impact by 62 keV  $\text{Ar}^{3+}$ , 240 keV  $\text{Ar}^{6+}$  and 240 keV  $\text{Ar}^{8+}$  projectiles. These beams were produced by 14.5 GHz ECR ion source and supersonically cooled  $\text{CO}_2$  molecules were crossed inside COLTRIMS setup. Post collision projectile ions hit the MCP which gave the start signal for the data acquisition. The projectile MCP is used to construct post interaction charge altered projectile image which we used to separate different capture positions.

In Figure (1) we have plotted the vertical projection of projectile image for different KER ranges. We saw interesting variation across different beams. For  $\text{Ar}^{3+}$ , as we go towards higher KER, the contribution of second capture starts decreasing and that of third capture increases, i.e. pure triple capture (PTC) strengthens and single ionization double capture (SIDC) weakens as we go towards higher KER.

A similar variation was observed in case of  $\text{Ar}^{6+}$ . While in case of high KER, for  $\text{Ar}^{3+}$  PTC became dominant channel, but in case of  $\text{Ar}^{6+}$  although contribution of PTC becomes stronger but SIDC still prevails. In case of  $\text{Ar}^{8+}$ , We did not observe any contribution from PTC, and as we go towards high-

er KER, autoionizing triple capture (ATC) becomes stronger than triple capture with projectile double autoionization (TCDDPAI).



**Figure 1.** Histograms showing projectile vertical projection of the post collision charge altered projectile image for different kinetic energy release (KER) ranges.

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# Nuclear stopping power of protons and antiprotons

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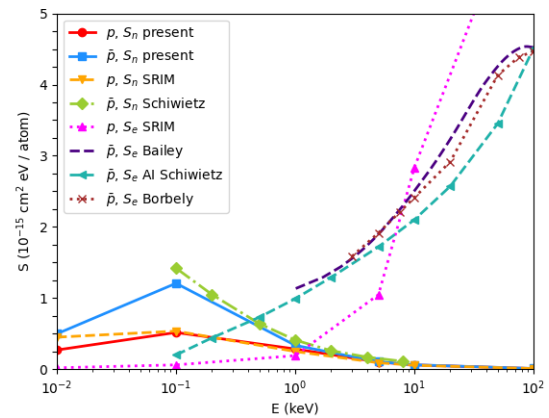
**Synopsis** We have calculated the nuclear stopping cross sections of protons and antiprotons in different gaseous and solid materials and have investigated its dependence on the atom-projectile potential and on the charge sign of the projectile.

The interaction of fast charged particles with matter have attracted much interest since a century. The stopping of ions in matter has important applications in medical treatment, astrophysics and material science. The slowing down of antiprotons to thermal energies is important for antihydrogen atom production.

High energy (above 1 keV) projectiles lose energy mainly because of inelastic collisions resulting in ionization or excitation of the target, this is the electronic stopping. But at lower energy also the nuclear stopping, occurring as a result of elastic scattering on the target atoms, becomes important.

Most of the work dedicated to the slowing down of charged particles in matter focuses on electronic stopping. Beside the great number of experimental data and theoretical calculations, many codes are available for calculating the stopping cross sections for ions, one example is the SRIM [1]. In the last decades is an increasing interest for antiproton stopping, and several calculations were published [2,3,4,5].

In the present work we have calculated the nuclear stopping cross sections for protons and antiprotons impacting on different atoms. The elastic scattering of the projectile on the target is treated classically. The only variable in the model is the interaction potential between the atom and the projectile. We have performed the calculations first assuming a frozen electron cloud (more appropriate for fast projectiles), and then an adiabatic potential, accounting for the static influence of the projectile on the atom.



**Figure 1.** Stopping cross sections for protons and antiprotons incident on helium as a function of the projectile energy. The present calculations for nuclear cross sections are compared with the calculations using the SRIM code [1] and the results published by Schiwietz [2], Bailey [3] and Borbély [4].

Figure 1 represents our calculation results for the nuclear stopping cross sections  $S_n$  for protons and antiprotons incident on helium as a function of projectile energy compared with other calculations of nuclear and electronic ( $S_e$ ) stopping cross sections. Nuclear stopping is dominant at low energies, especially for antiprotons.

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# Theoretical and experimental developments in atomic physics for the study of ion-ion collisions in the 1 - 140 keV energy range

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**Synopsis** Electronic processes during ion-matter interaction play a crucial role in various research fields, including plasma physics, fusion research, and hadrontherapy. In the low-energy regime, some charge-exchange cross-section data are available [1] for light Z ion-ion collisions. Here we propose to investigate how atomic levels are populated following electronic processes occurring during medium to high Z symmetric ion-ion collisions at both low and medium energies - collision regimes where data are still lacking.

We present here the current state of theoretical and experimental developments on the study of electronic processes in multicharged ion-ion collisions, as we aim to both compute and measure the corresponding cross sections.

Theoretically we use a semi-classical approximation to describe coupled channel electronic processes. In this approach, the relative motion between target and projectile ions is described classically, while the dynamics of the electrons are treated by solving the time-dependent Schrödinger equation non-perturbatively using a spectral method [2]. The code developed for this purpose can model systems and processes with up to four active electrons. Initially, as a benchmark, we focused on studying systems involving a single electron, including  $C^{6+} + H$  and  $N^{7+} + He^+$ , with energies varying between 0.1 and 100 keV/u. The results show that at low energy (0.1 to 10 keV/u) the capture process,  $C^{6+} + H(1s) \rightarrow C^{5+}(n\ell) + H^+$ , occurs mainly in  $n = 4, 5$  states. At higher energies (50 to 100 keV/u) the  $n = 6$  state is also populated but ionization becomes the dominant process. The cross section values obtained correctly replicate previous results from the literature [3][4][5]. Computations with two electrons are now being successfully conducted for  $N^{6+} + He^+$  and  $N^{7+} + He$  collisions. Computations of cross sections for electron capture as well as excitation and ionization will be presented and compared to independent theoretical

data when available in the literature.

To perform experiments on ion-ion collisions, we have developed a novel setup consisting of an ECR ion source connected to a beam line, followed by three custom-built devices to clean the beam in terms of charge states [6], achieve the collisions (in UHV conditions) and analyze the collision products. This platform will be connected to the SIMPA (Source d'Ions Multichargés de Paris) facility to conduct ion-ion collisions in the keV/u regime. We will thus be able to acquire precise information on the population of atomic levels of the collision products by measuring in coincidence the ion charge state and the X-rays emitted during the collision using a new generation silicon drift detector.

Conclusions from tests performed in november 2021 [7] and june 2023 at the ARIBE beamline (GANIL, Caen) on two successive versions of the ion spectrometer will be discussed as well.

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# A versatile 3D transmission setup for ion-solid interaction studies using keV ion energies at Uppsala University

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**Synopsis** The capability of our highly configurable scattering setup at Uppsala University is presented with a focus on the trajectory dependence of ion-solid interaction in the keV energy regime.

The renewed and broadened interest in the medium energy ion scattering (MEIS) technique with increasing focus on single crystalline targets and 2D materials, combined with much better technology for high-speed, position-sensitive detectors with improved lateral resolution, motivated the development of time-of-flight MEIS systems (TOF-MEIS) at Uppsala University, Sweden [1]. The highly configurable character of our setup makes it a powerful experimental research tool with particular focus on *in-situ* studies as well as for studying ion-solid interactions in several dimensions with the possibility to employ coincidence measurements.

The velocity of keV ions as projectiles being comparable to the one of electrons in the target valence and conduction bands renders the interactions highly dynamic and strongly trajectory dependent [2]. Several charge exchange processes including Auger neutralization and collision-induced reionization as well as electron promotion due to creation of molecular orbitals lead to an oscillatory alternation of the projectile charge and directly affect the specific energy loss. Ion transmission through self-supporting crystalline targets was shown to be an excellent model system to study the trajectory dependence of the ion-solid interactions.

Understanding energy deposition and electronic excitation by energetic charged particles in matter is imperative for prediction of ion-induced materials modification, as in semiconductor doping or extreme environments like e.g. fusion devices. Such understanding also forms the basis for analytical tools based on ion beams and can yield a well-defined test scenario for theoretical models, which aim to predict equilibrium [DFT] and non-equilibrium conditions [TD-DFT] in solids.

In this contribution, we showcase a set of experiments revealing the broad applicability of our instrumentation for studying ion-solid interaction:

- Analysis of primary ions transmitted through thin self-supporting foils allows for mapping of intensity and different energy loss moments [3,4].
- A deflection unit allows for studying the equilibrium charge distributions of the transmitted projectiles [5].
- Other energy transfer channels i.e. electron and photon emission can be addressed in coincidence detection with the transmitted projectiles [6,7].
- By employing heavier projectiles, recoils can be detected with high sensitivity for light elements and surface structure [8].
- TOF approach allows for studying ion-induced surface sputtering and desorption [9].

The most recent upgrade to the system comprises of a versatile *in-situ* preparation chamber. This extension enables extended control over target quality and allows for *in-situ* material modifications, also enabling more complex systems to be investigated.

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# Vibrationally resolved inner-shell photoexcitation of the molecular anion $C_2^-$

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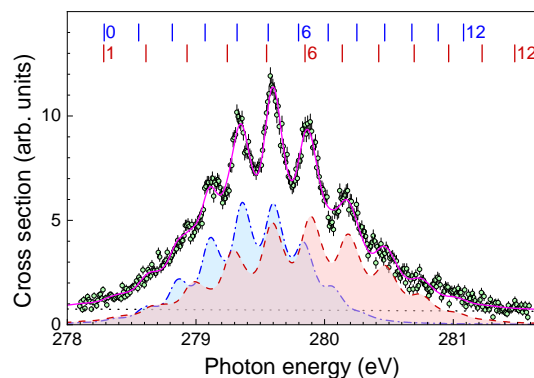
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**Synopsis** Carbon  $1s$  core-hole excitation of the  $C_2^-$  anion has been experimentally studied at high resolution by employing the photon-ion merged-beams technique at a synchrotron light source. The experimental cross section for photo-double-detachment shows a pronounced vibrational structure associated with  $1\sigma_u \rightarrow 3\sigma_g$  and  $1\sigma_g \rightarrow 1\pi_u$  core excitations of the  $C_2^-$  ground level and the first excited level, respectively. A detailed Franck-Condon analysis provides the spectroscopic parameters of the associated core-excited levels.

Carbon  $1s$  core-hole excitation of the dicarbon anion  $C_2^-$  has been experimentally studied at high resolution [1] by employing the photon-ion merged-beams technique as implemented at the PIPE end-station [2] at beamline P04 of the PETRA III synchrotron light source operated by DESY in Hamburg, Germany. As in our previous work with atomic  $C^-$  anions [3], we used a Cs-sputter ion source, here, for the production of a  $C_2^-$  ion beam. The experimental cross section for photo-double-detachment (PDD) of the  $^{12}C^{12}C^-$  anion shows a pronounced vibrational structure associated with  $1\sigma_u \rightarrow 3\sigma_g$  and  $1\sigma_g \rightarrow 1\pi_u$  core excitations of the  $X^2\Sigma_g$  ground level and of the  $A^2\Pi_u$  first excited level, respectively (Fig. 1).

A detailed Franck-Condon analysis, which involves the numerical calculation of the Franck-Condon factors between two displaced Morse potentials [4], reveals a strong contraction of the  $C_2^-$  anion by  $0.2 \text{ \AA}$  upon this core photoexcitation. This is a much stronger contraction as observed for the isoelectronic  $N_2^+$  ion [5]. The associated change of the molecule's moment of inertia leads to a noticeable rotational broadening of the observed vibrational spectral features. This broadening is accounted for in the present analysis, which provides the spectroscopic parameters of the  $C_2^-$   $1\sigma_u^{-1}3\sigma_g^2^2\Sigma_u^+$  and  $1\sigma_g^{-1}3\sigma_g^2^2\Sigma_g^+$  core-excited levels. In principle, the present results should be useful for the identification of  $C_2^-$  anions in the interstellar medium and other cosmic objects.

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**Figure 1.** Experimental cross section for PDD of  $C_2^-$  (symbols) and Franck-Condon fit (pink full curve) [1]. The experimental photon-energy spread was 50 meV. The blue dashed-dotted and red dashed shaded curves represent contributions by the  $X^2\Sigma_g(v=0)$  ground level and the by the first excited  $A^2\Pi_u(v=0)$  metastable level, respectively. The vertical bars mark the energies of the respective core-excited vibrational levels. They are labeled with the associated vibrational quantum numbers  $v'$ . The dotted line represents the continuous cross section for direct ionization.

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# ErUM-FSP APPA: BMBF Collaborative Research Center at FAIR

S Schippers<sup>1,2\*</sup> and T. Stöhlker<sup>3,4,5†</sup> for the APPA collaborations

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**Synopsis** The collaborative research center ErUM-FSP APPA joins the German university groups who contribute to the scientific instrumentation and to the scientific research at the international heavy-ion research facility FAIR under the umbrella of research pillar APPA (Atomic, Plasma Physics and Applications). It is funded by the German Ministry for Education and Research (BMBF). We will briefly present the individual projects of the current funding period 2021–2024.

The BMBF collaborative research center ErUM-FSP APPA [1] joins the German university groups (Figure 1), who have set out to perform scientific research at the future international accelerator complex FAIR under the umbrella of APPA (Atomic, Plasma Physics and Applications [2]). The FAIR installations are currently under construction at the site of the GSI Helmholtz Center for Heavy Ion Research in Darmstadt, Germany. APPA is one of the four research pillars of FAIR comprising the international research collaborations BIOMAT (biophysics and materials science [3]), FLAIR (low-energy antiprotons), HED@FAIR (plasma physics [4]), and SPARC (atomic physics [5]) who focus on investigations of (anti)matter under extreme conditions (strong fields, high densities, high pressures, and high temperatures).

The collaborative research center ErUM-FSP APP pursues coordinated research projects in the area of accelerator based experiments with heavy ions at the future FAIR-installation. Central issues are:

- Further development of the the experimental infrastructure, in particular, research and development for enhancing the scientific capabilities of the existing installations and of the future accelerator and detector systems including the respective base technologies.
- Set-up of the APPA experiments of the modules 0-3 of the modularized start version of FAIR.

- Realization of the APPA research program during the current FAIR Phase-0.



**Figure 1.** Map showing the locations of German university groups with APPA-related scientific activities.

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# Interaction of Protons with Noble Gas Atoms: Total and Differential Ionisation Cross Sections

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**Synopsis** We present total and differential cross sections for single ionisation in the collision of protons with Ne, Ar, Kr and Xe. We used the Garvey model potential and the classical trajectories Monte Carlo (CTMC) method to model the collision system. We present the total ionisation cross sections in the energy range between 10 keV and 100 MeV and the ionisation differential cross sections for an impact energy of 35 keV.

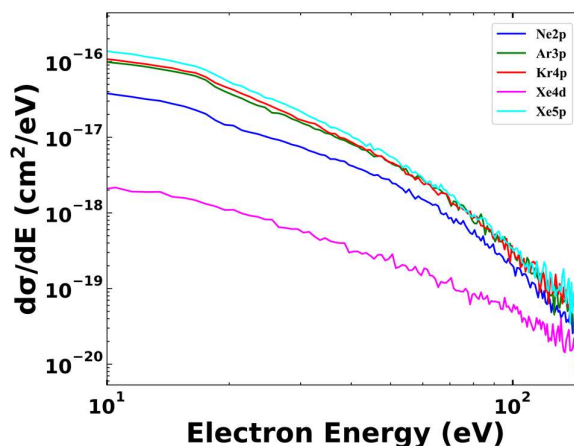
Electron processes have a crucial impact on various fields of study, such as radiation physics, atomic and molecular structures, and fusion plasma research. In the context of tokamaks, neutral atom beams are used as diagnostic tools[1].

The aim of our present work is to provide total and differential cross sections for single ionisation in collisions between  $H^+$  with Ne(2p), Ar(3p), Kr(4p), Xe(4d) and Xe(5p).

To model our collision systems we used the 3-body classical trajectory Monte Carlo technique. The interactions among the particles are taken into account with the Garvey model potential [2]. The target was split into a single active electron and the target core consisting of the nucleus and remaining non-active electrons. The projectile  $H^+$  was the third particle. This model potential takes into account the effective charge of the target, incorporating the screening effect of non-active electrons. The classical equation of motions were solved numerically using the adaptive Runge-Kutta method, the step size depends on the initial parameters of all particles [3]. We present results both for the charge transfer and ionisation total cross section as a function of the impact energy. Moreover, we also present single (SDCS) and the double (DDCS) differential cross sections as functions of the ejected electron energies and angles at an impact energy of 35 keV.

We compared our cross sections with the existing experimental data, and with the previous theoretical data like first Born approximation (FBA), Oppenheimer-Brinkman-Kramers (OBK) approximation, and the results of the

two-state two-centre atomic expansion model [4].



**Figure 1.** Single differential cross section (SDCS) as a function of the ejected electron energies at impact energy 35 keV.

## Acknowledgements

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# Classical description of the ionization of carbon by electron impact

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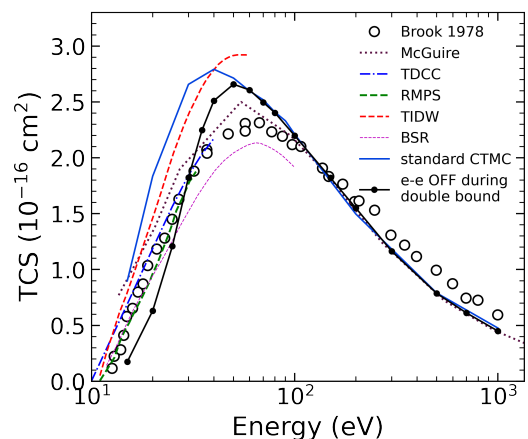
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**Synopsis** A theoretical description of the ionization process in collisions between electrons and carbon atoms is presented using the classical trajectory Monte Carlo method. At impact energies greater than about 100 eV, the present methodology is in very good agreement with the reported experimental data. In contrast, the ionization cross section is overestimated at lower impact energies. We show that this behavior can be related to the formation of a transient system of two bound electrons and introduce a dynamical strategy that compensates the effect.

In this work, we calculate the total ionization cross sections of carbon atoms by 10 to 1000 eV electron impact using a three-body classical trajectory Monte Carlo (CTMC) method. The present calculations are restricted to the L-shell due to the large difference in the ionization potentials of the K-shell electrons, whose ionization cross sections are negligible in the energy range explored. Results obtained by means of the simple addition rule of the C(2s) and C(2p) orbitals are shown in Figure 1 and compared to the experimental data of Brook *et al* [1], and to the theoretical predictions of the generalized oscillator strength formulation of the Born approximation [2], the time-dependent close coupling (TDCC), the R-matrix-with-pseudo-states (RMPS), the time-independent distorted wave method (TIDW) and the B-spline R-matrix-with-pseudostates (BSR) [3, 4]. Good agreement is obtained with the data at impact energies greater than about 100 eV. In contrast, electron emission as the threshold region is approached seems to be overestimated.

A closer inspection of the classical dynamics at low impact energies reveals the formation of a transient double bound electron system [5]. It is well known that classical two-electron systems are unstable and their resulting dynamics are not expected to be accurately reproduced. In a first approach to the problem, we analyze the results obtained by switching-off the e-e interaction during the transient double bound state. Results are

included in Figure 1 and clearly evidence an improvement with respect to the standard CTMC description at the time they highlight the need of further studies.



**Figure 1.** Total ionization cross section as a function of the impact energy for electron-carbon collisions. Expt. data from Ref. [1]. Theories as stated in the text.

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# Impact Parameter and Kinematic Information for Differential Ionization of Argon by 1 keV Positrons and Electrons

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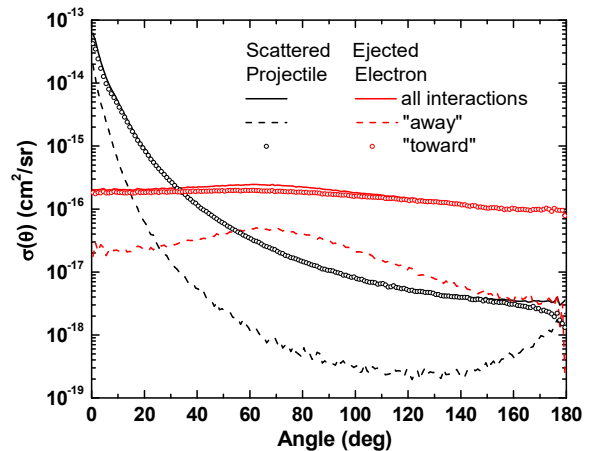
**Synopsis** CTMC calculations for ionization of Ar(3p) by 1 keV positrons show that for positron impact the projectile is predominantly scattered away from the central core and the target electron is primarily ejected toward the core. Also, the “away” interactions occur at a smaller impact parameter than the “toward” interactions.

It is well known that the reversal of directions of the Coulomb field for positron and electron impact ionization produces trajectory changes for the projectile. This results in a larger impact parameter for positron impact with respect to that for electron impact. In addition, post-collision effects between the post-collision particles introduce additional trajectory effects. In order to test various theoretical models for ionization, comparisons on the differential level are used. For electron impact, a large amount of experimental information, ranging from singly to fully differential, is available whereas for positron impact, relatively few differential studies have been performed. Also, unlike the case for heavy ion impact where impact parameter information can be obtained, post-collision effects effectively prohibit such studies for lepton impact.

However, the Classical Trajectory Monte Carlo method allows us to investigate such kinematic effects and also to obtain information as a function of impact parameter. As an initial study, such information for ionization of argon 3p electrons by 1 keV positrons and electrons is presented. Similar to that used by Sparrow and Olson [1], the argon atom was modeled as a single 3p electron and a central core potential and interactions between all particle pairs are taken into account. Unlike previous studies, the present study also provides information about the impact parameter and the scattering and ejection directions, not just the angles but also whether the directions are “positive” or “negative”, i.e., toward, or away from the central core.

Figure 1 shows angular distributions for the scattered and ejected particles for 1 keV positron impact. The solid curves are the “normal”

singly differential cross sections, i.e., for all interactions, whereas the dashed and open circle curves are for interactions restricted to scattering toward and away from the central core. As seen, rather than being scattered symmetrically with respect to their initial direction, positrons predominantly are scattered away from the central core. This results in the target electron primarily being ejected toward the central core. As seen, the relative probability for these kinematics varies with observation angle. Not shown is impact parameter information. The bP(b) curves differ, with scattering away (towards) being centered at  $\sim 0.8$  ( $\sim 1.8$ ) a.u. As a final note, for electron impact the preferred scattering and emission directions are reversed from those shown.



**Figure 1.** SDCS  $s(q)$  for 1 keV  $e^+-\text{Ar}(3p)$  ionization. See text for explanation of curves.

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# Energy loss straggling of $p$ and $\bar{p}$ in He: electron correlation effects.

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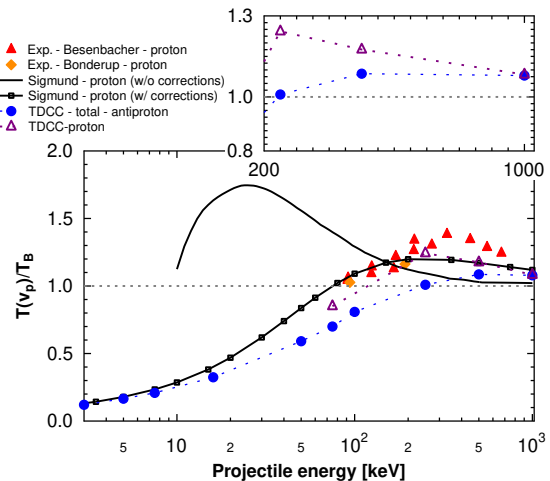
**Synopsis** The energy loss straggling cross section, the second order moment of the energy transfer differential cross section, is studied based on *ab initio* calculations for the proton and antiproton projectiles interacting with the He target. At high projectile velocities we found that regardless of the projectile the straggling cross section converges to a constant value, which exceeds the asymptotic value established by Bohr due to the electron correlation effects.

The energy transfer process between a charged projectile and a target is fully described by the differential energy transfer cross section (DETCS). In applications, instead of the DETCS, the stopping and the straggling cross sections are used, which are the first and second order moments of the DETCS.

The investigation of these integrated quantities dates back to the early work of Bohr [1], who showed with the help of a simple classical model that the straggling cross section converges toward a constant value for large projectile velocities. This value of the straggling cross section remains valid also for elaborate quantum mechanical models which treat the energy transfer between the target and the projectile on the basis of single-active electron approximations. This Bohr straggling cross section ( $T_B = 4\pi Z_p^2 Z_T$ ) is widely used at high projectile velocities.

Employing the binary collision theory of Sigmund [2] it was shown that by including screening and shell corrections (i.e. multi electron correlation effects) the high energy limit exceeds the Bohr straggling. This prediction was recently confirmed by us [3] for the case of antiproton-He collision.

In this contribution we will present further stopping and straggling cross section data for antiproton and proton collision with the He target based on the direct numerical solution of the two-electron Schrödinger equation, obtained within the framework of the time-dependent close coupling (TDCC) model.



**Figure 1.** Straggling cross section as a function of projectile energy. The present TDCC results are compared to experimental data [4, 5] and to the binary collision theory predictions [2]. The cross sections are expressed in units of Bohr straggling.

Here we focus on the high velocity behavior of the straggling and stopping cross sections and on the investigation of the Barkas effect. In particular, we compare the TDCC data with the modified Bethe formula [6] and we study the effect of the different correction terms.

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# Photofragmentation of $CD_3^+$ Ions Driven by Ultrashort Laser Pulses

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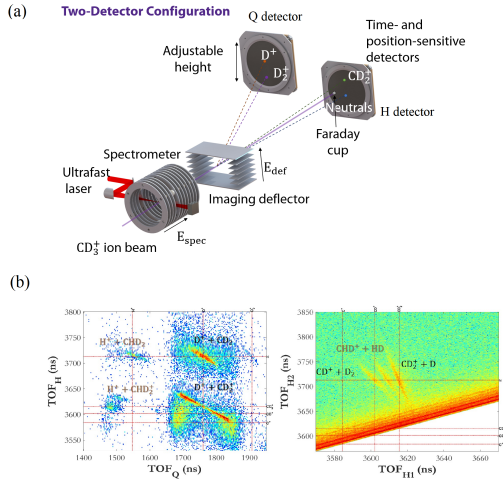
**Synopsis** We study the photofragmentation processes of  $CD_3^+$  ions induced by ultrafast strong laser fields using a fast (keV) ion beam as a target. Employing coincidence three-dimensional (3D) momentum imaging enables kinematically complete measurements of the  $CD_3^+$  dissociation, and provides details on the deprotonation, hydrogen-atom or -molecule elimination processes.

As one of the building blocks of many chemical reactions, the fragmentation processes of  $CD_n^+$  ions garners interest in the scientific community. We investigate the deprotonation, hydrogen elimination, and hydrogen-molecule elimination processes of  $CD_3^+$  in strong laser fields.

momenta of all photofragments measured in coincidence.

There is, however, a limitation to this one-detector configuration. When the mass-to-charge ratio of the heaviest and lightest mass fragments is too large, either the heaviest fragment would be blocked by the FC, or the lightest fragment would be deflected off the detector. As a solution, we use a second detector to measure the lighter fragments. We observe deprotonation channels for both  $CD_3^+$  and  $CD_3^{2+}$  parent ions in the left panel of Figure 1(b), and hydrogen elimination on the right.

When we generate the  $CD_3^+$  ions using deuterated methane in an ECR source, contaminant  $C_2D_6^{2+}$  fragments are also observed. We will discuss how these contaminant contributions are identified and subtracted. Once subtracted, the strong-field photo-fragmentation branching-ratios of deprotonation, hydrogen elimination, and hydrogen-molecule elimination processes of  $CD_3^+$ , are retrieved.



**Figure 1.** (a) Schematics of our two-detector coincidence 3D momentum imaging setup. (b) Two-body coincidence TOF with one hit on each detector (left), and both hits on the H detector (right)

In a single-detector configuration of our experiment, a 20 keV  $CD_3^+$  ion beam is crossed with ultrashort laser pulses within a spectrometer. Due to the beam velocity the resulting ionic and neutral fragments are detected using a time-and-position sensitive delay-line-detector (DLD). The  $CD_3^+$  beam is monitored by a Faraday cup (FC). Using the position and time-of-flight (TOF) information, we reconstruct the 3D

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# Dissociation of $\text{CD}_4^+$ molecular ions in laser fields

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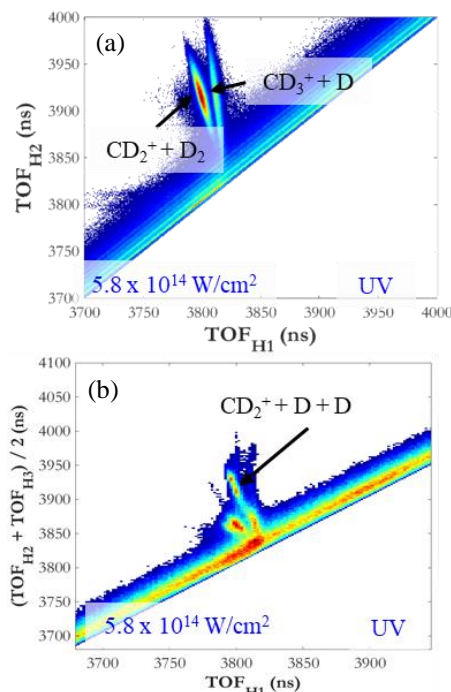
**Synopsis** Competition between various dissociation processes of  $\text{CD}_4^+$  molecular ions in a strong laser field is studied using a coincidence three-dimensional momentum imaging technique. Particularly, the hydrogen molecule elimination ( $\text{CD}_2^+ + \text{D}_2$ ) is distinguished from the elimination of two hydrogen atoms ( $\text{CD}_2^+ + \text{D} + \text{D}$ ).

Ionization and fragmentation of methane molecules in collisions with charged particles [1,2] and in intense laser fields have been studied extensively [3,4]. One of the interesting fragmentation channel is hydrogen-molecule elimination from the methane mono-cation. Hence, to understand the hydrogen-molecule elimination and its competition with other dissociation channels, we study the dissociation of a  $\text{CD}_4^+$  beam target in the presence of strong laser fields.

Our experiments are performed by focusing intense ultrashort laser pulses onto a fast (20 keV)  $\text{CD}_4^+$  ion beam target. The target  $\text{CD}_4^+$  ions are produced in an ECR ion source. A coincidence three-dimensional momentum imaging technique allows us to measure the charged and neutral photofragments.

One of our goals is to study the competition between different  $\text{CD}_4^+$  dissociation processes, specifically hydrogen elimination ( $\text{CD}_3^+ + \text{D}$ ), deprotonation ( $\text{CD}_3 + \text{D}^+$ ), and hydrogen-molecule elimination ( $\text{CD}_2^+ + \text{D}_2$ ). In addition, we observe a very weak molecular hydrogen ion elimination ( $\text{CD}_4^+ \rightarrow \text{CD}_2 + \text{D}_2^+$ ). Curiously, some branching ratios show strong wavelength dependence.

Undetected neutral fragments in traditional coincidence momentum imaging techniques like COLTRIMS, results in ambiguity about the final products in some of the channels. For example, hydrogen molecule elimination ( $\text{CD}_2^+ + \text{D}_2$ ) versus the elimination of two hydrogen atoms ( $\text{CD}_2^+ + \text{D} + \text{D}$ ). Our imaging technique allows us to distinguish between these two channels (see Fig.1), and also measured their relative branching ratios.



**Figure 1.** Coincidence time of flight for (a) two-body fragmentation showing the  $\text{CD}_2^+ + \text{D}_2$  channel, and (b) three-body fragmentation showing the competing  $\text{CD}_2^+ + \text{D} + \text{D}$  channel.

We will also discuss the kinetic energy release (KER) and angular distributions of these dissociation channels.

**Acknowledgements:** Supported by the Chemical Sciences, Geosciences, and Biosciences Division, Office of Basic Energy Sciences, Office of Science, U.S. Department of Energy under award number DE-FG02-86ER13491.

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# Interaction of Singly Charged Sodium Ion with Nitrogen Atom: Total and Differential Ionisation Cross Sections

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**Synopsis** We present total and differential cross sections for single ionization in collision between  $\text{Na}^+$  ions with  $\text{N}(2p)$  atom. We used the Garvey model potential and the classical trajectories Monte Carlo (CTMC) method to model the collision system. We present total ionisation cross sections in the energy range between 10 keV to 100 MeV and single/double differential cross sections for impact energies of 30, 40, 50 and 60 keV.

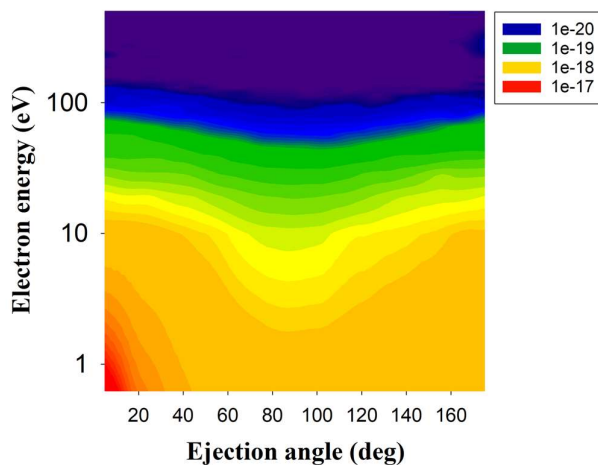
The electron processes play a significant role in radiation physics, the study of atomic and molecular structures, fusion plasma, and other research domains. In tokamak, atoms are used as a neutral diagnostic beams, such as helium and nitrogen [1].

In our work, we present total and differential cross sections for single ionization in collision between  $\text{Na}^+$  ions with  $\text{N}(2p)$  atom.

We modelled the collision system as a three body system using Garvey model potential [2]. The target is separated into a single active electron and nitrogen core (i.e., nitrogen nucleus and its remaining non-active electrons), the projectile  $\text{Na}^+$  with its electrons are considered as a single particle. This model potential invokes the effective charge for a given particle, hence, it considers the screening effect of the non-active electrons. The equations of motion of the collisions system are solved numerically using classical trajectories Monte Carlo CTMC method [3].

We present the total ionisation cross section as a function of the impact energy in the energy range between 10 keV to 100 MeV. Moreover, we present the single (SDCS) and double (DDCS) differential cross sections for impact energy range of 30-60 keV as a function of the ejected electron energies and angles.

We found that the dominant contribution of the Double Differential Cross Sections (DDCS) are achieved by electrons with energies below 10 eV and ejection angles under 20 degrees. Moreover, electrons ejected with energies larger than 20 eV have shown very small angular dependence [4].



**Figure 1.** Double differential cross section (DDCS) of the single ionization in collision between  $\text{Na}^+$  ions with  $\text{N}(2p)$  atom as a function of the ejected electron energies and ejection angles at impact energy of 30 keV.

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