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THERMAL AND ELECTROSTATIC CONTROL OF ATOMIC EMISSION, SPECTRAL CONTRAST, AND SELF-ABSORPTION IN ULTRAFAST PICOSECOND LIBS OF COPPER

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Laser-induced breakdown spectroscopy (LIBS) is a versatile technique for elemental analysis; however, its analytical performance is often constrained by plasma–radiation coupling effects such as continuum background and spectral line self-absorption. These challenges are particularly pronounced in ultrafast (picosecond) LIBS, where dense, transient plasmas are formed, and the emitted radiation is highly sensitive to charge transport and collisional–radiative balance.

This work presents an integrated plasma-control strategy that combines **target preheating** with a **static external electric field** to modulate atomic emission and spectral contrast in air. Building on recent advances in enhancement methods for LIBS, we focus on how thermal and electrostatic boundary conditions reshape the near-surface sheath and influence the redistribution of charged species within the expanding plume. Preheating increases the ablated mass flux and plume density, leading to stronger line emission while often enhancing the continuum contribution. In contrast, an external static bias primarily governs charge separation and ion–electron drift through sheath-driven transport and ambipolar fields, enabling plume reshaping without inducing substantial changes in electron temperature.

A key outcome of this approach is the polarity-dependent decoupling between net line intensity and signal-to-noise ratio behaviour. By tuning the electric-field polarity, the electron density and radiative transfer pathways can be selectively controlled, allowing for the independent optimization of emission strength (sensitivity) and spectral contrast (measurement robustness). This provides a practical route to mitigate self-absorption while preserving strong analytical signals—an essential requirement for quantitative LIBS of conductive targets and trace-level detection.

The proposed framework links field-assisted plasma dynamics with atomic emission formation and radiative processes, and is broadly applicable to ultrafast LIBS diagnostics, including multi-element analysis in complex matrices and real-time monitoring scenarios. A related experimental implementation in picosecond LIBS of copper is currently under review.

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P02

Development of a Framework for Modelling Reaction Systems in Fusion Plasmas

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The atomic and molecular processes play crucial role in the edge region of tokamak plasmas, as experimentally evidenced at magnetic confinement fusion devices, e.g., MAST-U [1], JET, AUG [2] and Alcator C-Mod [3]. A robust simulation capability with accounting for such processes is essential for analysis and planning of experiments and for design of the future fusion devices. As the number of the involved levels of atomic and molecular species may reach hundreds and even thousands (see, e.g., a system with rovibrationally resolved molecular hydrogen [4]), a brute-force inclusion in fluid codes for plasma edge simulations is extremely computationally prohibitive. To account for the atomic and molecular effects while attaining reasonable computational costs, the reduced (effective) models can be used instead.

A new framework for modelling reaction systems in fusion plasmas is currently under development at UKAEA, with a goal of providing a comprehensive toolset for analysis, modelling and reduction of plasma chemical kinetics to the scientific community. The framework is being developed with an emphasis on the best modern software development practices, and with an outlook for provenance and metadata tracking. The present capabilities include import of ADAS adf04 files [5], reduction methods for linear problems (quasi-steady-state assumption and a method by Greenland [6], i.e., classic collisional-radiative modelling), automatic identification of reduced models [6], solution of full and reduced systems, a solver for non-linear system, and synthetic spectrum generation. The reaction systems can be parametrized with scanning and automatic differentiation (using JAX library [7] for Python) capabilities allowing for tabulation of effective rates/cross-coupling coefficients. The planned future work includes implementation of uncertainty quantification and of reduction techniques for non-linear problems, such as Intrinsic Low-Dimensional Manifold [8] and Computational Singular Perturbation [9].

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P03

Electron impact total and partial ionization cross sections for $W(CO)_6$ and $Fe(CO)_5$

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Tungsten hexacarbonyl, $W(CO)_6$, and iron pentacarbonyl, $Fe(CO)_5$, are widely used volatile precursors in electron/ion driven and plasma-assisted processes such as focused electron beam induced deposition (FEBID), chemical vapor deposition, and plasma-enhanced thin-film growth. In these environments, low-to-intermediate energy electrons initiate ionization and dissociative ionization, controlling precursor depletion, fragment formation (e.g., sequential CO loss), and ultimately the composition and purity of deposited W- and Fe-containing films. Despite this practical importance, comprehensive electron-impact ionization cross sections, particularly partial (channel-resolved) ionization data, remain scarce over the broad energy range needed for plasma kinetics and electron-transport modeling [1]. In this work, we report total ionization cross sections (TICS) and partial ionization cross sections (PICS) for $W(CO)_6$ and $Fe(CO)_5$ from the ionization threshold up to 10 keV using the Binary-Encounter-Bethe (BEB) framework [2]. Orbital-resolved BEB inputs, such as binding energies, kinetic energies, and occupation numbers, are obtained from quantum-chemistry calculations, and the total cross section is constructed by summing contributions from all occupied orbitals. Where experimental ionization thresholds are available, they are used to anchor the low-energy onset; otherwise, the threshold is estimated from the HOMO energy (Koopmans-like approximation). Partial ionization cross sections are provided in two complementary forms: (i) subshell/orbital-resolved ionization and (ii) dissociative ionization channel-resolved yields derived from mass-spectrometric branching information; when complete branching data are unavailable, we employ physically motivated, energy-dependent branching schemes to generate continuous PICS across the full energy range. The resulting cross-section set is intended to support plasma chemistry, FEBID modeling, and Monte Carlo electron-transport simulations involving metal–carbonyl precursors.

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P04

A Novel Diagnostic Probe for the Direct Detection of Runaway Electrons in ADITYA-U Tokamak

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Runaway electrons (REs), with energies ranging from a few keV to several MeV, are generated in ADITYA-U tokamak discharges under high loop voltage and low-density conditions. These energetic particles can degrade plasma performance, may damage plasma-facing components (PFCs), or cause structural harm [1], while also serve as diagnostic probes of particle magnetic confinement and instability dynamics. To explore this dual role, a new RE flux probe has been designed, developed, and calibrated for ADITYA-U tokamak [2]. It directly comes into contact with the confined REs and measures their flux deposited on the probe area and functions as an energy analyzer, enabling quantitative evaluation of RE effects on PFCs and detailed studies of their behavior during instabilities. The probe head shape made up from Graphite material is specifically designed to distribute heat flux impinging from plasma over a large area and to optimize heat load, it is insertable into the edge plasma up to ~3 cm through scrap-off layer using the fast-reversed drive system, it employs three Ceriumdoped Lutetium Yttrium Silicate (LYSO:Ce), a high-performance scintillator crystals, with Stainless Steel (SS-304L) filters inside a Graphite shield for detection and subtraction of background Hard Xray signal from RE flux signal. The probe materials and their thickness are carefully designed using a Monte-carlo code PHITS to optimize for its functionality during the measurement namely, the Graphite layer reduces backscattering less than 6% and the Graphite housing restricts detection to REs below1 MeV. The first crystal records REs above this threshold, the second crystal selects REs exceeding 3 MeV via additional SS filtering, and the third measures only Hard X-Rays background, blocked from the direct incidence of REs by optimized thickness of SS shielding. Experimental performance assessment and calibration are performed in the energy range from 1–10 MeV monochromatic electron beam and compared with PHITS simulations.

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P05

Spectral Narrowing in Highly Charged Tin Ions

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The unique emission spectrum of tin ions in charge states Sn^{8+}–Sn^{14+} produces radiation in a narrow region around 13.5 nm which is used for print patterns silicon wafers to make computer chips. To efficiently print narrower features, future shorter-wavelength printing techniques would benefit from a similarly narrow emission spectrum. The experimentally observed narrow spectrum is only reproduced theoretically when configuration interaction is included. To predict other element–charge-state combinations that may exhibit this effect, we investigate the physical origin of spectral narrowing induced by configuration interaction.

The Hamiltonian matrix elements $H_{bb'}$ are sums of products of radial integrals and angular factors. The radial integrals include the electrostatic (Coulomb) direct integrals F^k, the exchange integrals G^k, and the spin–orbit parameter ζ, all obtained by numerical integration. The angular coefficients arise due to the coupling between subshells and depend on the quantum numbers l and m_l of the interacting basis states b and b'. The Hamiltonian matrix elements are constructed following Cowan [1], Eq. (12.47).

$$H_{bb'} = \delta_{bb'} E_{\mathrm{av}} + \sum_{l_i,\, l_j,\, k} f_k^{bb'}(l_i l_j)\, F^k(l_i l_j) + d_j^{bb'}\, \zeta_j + g_k^{bb'}(l_i l_j)\, G^k(l_i l_j) \tag{1}$$

The calculation of the energy levels contributing to the emission spectrum requires assembling and diagonalising a large sparse Hamiltonian matrix. Inclusion of triply, quadruply, and quintuply excited configurations is necessary [2, 3] but can increase the matrix dimension substantially (exceeding 10^6 is within the scope of this project). To address this computational challenge, we aim to perform the diagonalization on graphical processing units (GPUs) to achieve a speed-up of up to a factor fifty [4]. Ultimately, this large-scale atomic-structure modelling is aimed at isolating the physical mechanism by which configuration interaction leads to spectral narrowing.

By resolving how extensive configuration mixing redistributes line strength in highly charged tin ions, we seek general criteria that explain why narrowing occurs in Sn^{8+}–Sn^{14+} and to identify other element–charge-state combinations that may exhibit similarly favourable emission characteristics for future shorter-wavelength lithography.

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P06

Synchrotron calibration of a transmission grating spectrometer for broadband EUV measurements

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Laser-produced plasma (LPP) of tin is used as the light source in the latest generation extreme ultraviolet (EUV) nanolithography applications. The plasma dominantly emits light in the spectral range around 13.5 nm [1]. In addition to 13.5 nm band, emission in other spectral ranges, including vacuum and deep ultraviolet (DUV) ranges are also present in the spectra. The longer wavelength emission may cause creation of secondary hydrogen plasma, hence interacting with the surfaces of the scanner [2]. A broadband characterization of the EUV emitting LPP is therefore necessary. Using a transmission grating spectrometer (TGS) [3] is found to be useful in such broadband characterization due to ease of alignment in using different gratings for covering different spectral ranges. Besides the gratings, the TGS consists of filters, slits, a photodiode and a charge-coupled device. These components have different spectral efficiencies needing individual calibrations for interpreting the plasma emission spectra.

Here, we present the calibration of the TGS that has been performed at Elettra synchrotron facility in Trieste, Italy. The calibration covers the 5-400 nm range such that absolute intensity measurements of EUV light sources can be done in the needed EUV to DUV range.

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P07

A Python-based Hybrid Atomic Structure Collisional-Radiative Model for Spectroscopic Plasma Diagnostics and Equation-of-state Computations

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Collisional-radiative modelling is a powerful predictive utility for diagnosing the physical parameters of plasmas. The accuracy of a collisional-radiative model relies on the *detail* (of the energy levels and their level refinement) and *completeness* (of the excited state levels and the processes coupling them) of the atomic data underpinning the collisional-radiative processes. These components are inherently competitive; achieving statistical completeness with highly detailed atomic data requires tracking an exceedingly large number of energy levels that rapidly become computationally intractable in, for example, mid-to-high Z elements. Efforts to balance the detail, completeness, and tractability of an atomic model have shown promise when employing "hybrid" level averaging techniques [1-3], which selectively blend highly detailed levels with ensemble-averaged level arrays that can comprise hundreds of detailed states in a single array. A hybrid structure collisional-radiative atomic model [4] has been developed for diagnostic application to plasma experiments and equation-of-state tabulation at the U.S. Naval Research Laboratory. The model blends sets of atomic data calculated with varying degree of detail using the Flexible Atomic Code [5] to achieve high-fidelity predictions of plasma ionization and x-ray radiation, while maintaining computational tractability through selective implementation of statistical averaging techniques to the energy level data. The coupled collisional-radiative rates problem is solved using a mixture of detailed and ensemble-averaged energy levels in collisional-radiative (steady-state) equilibrium to generate level population densities. Radiative emissivities and synthetic spectra are computed from the population solution, while key equation-of-state parameters are derived from the combined populations and emissivities, including charge state distribution, K- and L-shell radiative powers, and line opacities – determined from an iterative probability-of-escape formalism [6]. Theoretical validation is carried out against the state-of-the-art spectroscopic collisional-radiative model SCRAM [2], which also employs a hybrid structure technique for the collisional-radiative problem. Comparison between the two hybrid models is performed for argon and krypton elements, looking at predictions of ionization balance, average ion charge, fractional ion abundance, L- and K-shell synthetic spectra, and probability-of-escape factors.

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P08

A New Approach for Ground and Excited State Electron-Impact Ionization of C I within Magnetically Confined Plasmas

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In magnetically-confined plasmas the temperatures and densities are such that the effective ionization rate may be dominated by the contributions from the metastable ionization rates rather than the ground state [1]. Sophisticated approaches, such as Convergent Close-Coupling (CC) and Time-Dependent Close-Coupling (TDCC), have often focused on the comparison of ground state ionization with experimental data [2, 3], in contrast to comprehensive ionization from all excited states required for collisional-radiative modelling. We update the electron-impact ionization and excitation data available for neutral carbon (C I). Carbon embodies many favourable characteristics required by Plasma Facing Components within tokamaks, in terms of erosion, redeposition, H retention and neutron damages [4]. This is due to its simple electron structure and excellent temperature characteristics relative to its low atomic number [5].

We expand upon the R-matrix with Pseudostates (RMPS) methodology and incorporate it more generally into the Dirac Atomic R-matrix Codes (DARC) [6], to allow both ionization and excitation rates to be calculated from the same initial target structure. This is a generalization of the work of Badnell (2008) [7] which considered only a neutral hydrogen system. The cross sections from two distinct C I targets show good agreement with experimental data and other theoretical calculations for the C I ground level. However, this is not our primary focus, given the agreement of previous calculations with existing experimental data [8]. Rather, the DARC R-matrix with Psuedostates (DRMPS) method allows for the first level-resolved excited state ionization cross sections to be calculated. In addition, our level-resolved excitation collision strengths are also in alignment with other theoretical calculations.

The availability of both electron-impact excitation and ionization rates allows for the determination of effective ionization rates through collisional radiative calculations. We show that for the temperatures and densities applicable in magnetically confined plasmas, the ionization contributions from metastable levels have a non-trivial effect on the effective ionization rate coefficients of C I. These results provide confidence in our new DRMPS approach, which will now make ionization cross sections, both ground and excited, more readily available for non-hydrogenic systems.

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P09

Modeling Atomic Processes in Fusion Plasmas

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Abstract: Understanding atomic processes is essential for accurately describing the behavior of magnetically confined fusion plasmas. In this work, we investigate key atomic interactions—including excitation, ionization, recombination, and radiation emission—under conditions relevant to fusion devices. Using state-of-the-art theoretical models and available atomic databases, we aim to improve the reliability of collisional-radiative descriptions and spectral diagnostics for high-temperature plasmas. The study focuses on the role of atomic rate coefficients, population modelling, and spectral line formation, with particular emphasis on their impact on plasma parameters such as electron density, temperature, and charge-state distributions. The results contribute to developing more accurate modelling tools that support the interpretation of spectroscopic measurements in fusion experiments. This work forms an essential part of my PhD research on the modelling of atomic processes in fusion plasma and aims to advance our understanding of atomic-level mechanisms that govern plasma behavior in fusion-relevant environments.

P10

The Challenge of Accurate Recombination Data for Lanthanides and Actinides

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Interpreting kilonova spectra from neutron-star mergers requires accurate atomic data for the heavy r-process elements synthesized in these events. From a plasma-physics perspective, this problem is closely connected to population modelling and collisional–radiative (CR) modelling in complex, low-density, transient plasmas, where departures from local thermodynamic equilibrium (LTE) are significant. Reliable modelling therefore demands self-consistent non-LTE level populations, ionization balance, and emissivities derived from detailed atomic data rather than equilibrium assumptions. These requirements pose a major challenge for lanthanides and actinides, whose open f-shell configurations produce extremely dense level structures and strong sensitivity to atomic structure approximations. Such ions represent some of the most complex species encountered in CR modelling, with atomic data uncertainties propagating directly into predicted charge-state distributions and spectral modelling. I present recent progress in the production and benchmarking of non-LTE atomic data for key heavy f-shell elements, with a focus on neodymium (Nd), uranium (U), and related species. New atomic-structure calculations are used to compute radiative and dielectronic recombination rates, as well as direct excitation data, suitable for population and CR modelling under kilonova ejecta conditions. For open f-shell ions, the resulting atomic structure is found to be highly sensitive to the choice of orbital scaling parameters, with even minor variations leading to significant changes in level ordering and transition probabilities. This sensitivity is particularly evident in the determination of ground configurations and terms. As a case study, Nd VI exhibits extreme sensitivity: two competing ground-state configurations reported in the literature [1] can both be reproduced within AUTOSTRUCTURE [2] by adjusting scaling parameters at the level of the third decimal place. Small structural differences translate into substantial spreads in predicted recombination rates, with direct consequences for CR population modelling and non-LTE spectral synthesis. These results highlight both the challenges and the necessity of robust atomic data for heavy f-shell elements, not only for interpreting kilonova spectra but also for advancing plasma population modelling in regimes where atomic complexity and non-equilibrium effects dominate.

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P11

Atomic and Molecular Opacity in Low-Temperature Plasmas: Quantifying Uncertainty in Atomic and Plasma Physics Models

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ABSTRACT

Radiative properties of heated air species are vital ingredients in detecting, modeling, and characterizing transport. This information can be utilized to describe the radiative energy transfer, collisional-radiative, radiation-hydrodynamic, and plasma kinetic models which are utilized to model spectra, energy transfer, and bulk-plasma transport in media such as the atmosphere. Ambient air at sea-level is composed primarily of N_2 and O_2, at 78% and 21%, respectively, with contributions from H_20, Ar, CO_2, Ne, He, CH_4, Kr, and N_20. The composition of air can change when heated into a mixture of molecular and atomic species. Historically, the ATOMIC opacity software package developed at Los Alamos National Laboratory has implemented efficient approximations to the atomic physics (intermediate-coupling), plasma physics, and atomic-plasma interactions appropriate for high-temperature and high-density regimes used to generate the OPLIB tables.[1] These approximations breakdown for low-temperature plasmas containing neutral and near-neutral species. To address this we use improved atomic electronic structure with a selective-CI approach[2] and a semi-empirical 'sum-over-states' approach for the atom-electron scattering for improved line-broadening.[3] The error in gray-mean opacities are reported and the improved opacities are tested on a benchmark 1-D radiation hydrodynamics simulation.

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P12

Temporal and Spatial evolution of the ion temperature in the WEST tokamak

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Ion temperature a crucial parameter for achieving fusion

The WEST tokamak is a device in which D-D plasmas are being produced to investigate various aspects related to the operation of future devices[1].
The typical plasma density and temperature reachable on this device is $n_e = 10^{19}$-10^{20} m^{-3} and T_e = 3 to 8 KeV.

The ability to measure spatial and temporal variations in the ion temperature is crucial for:

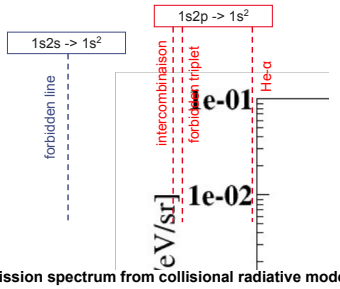
- improving **plasma confinement**
- optimizing **fusion reactions**.

Photo of the WEST tokamak

How to measure the temporal and spatial evolution of the plasma ion temperature ?

He-like argon impurity emission suitable for determining ion temperature

☐ **Spectral range from 3100 to 3150 eV is convenient to clearly distinguish the He-like lines of argon.**



Argon He-like emission spectrum from collisional radiative model for $n_e = 10^{20} m^{-3}$ and T_e=1500 eV [3].

☐ **Line FWHM is directly related to Ion temperature.**

Natural Broadening

Doppler Broadening

$$\frac{\Delta E_{FWHM}}{E_0} \sim \sqrt{\frac{8\ln 2\ kT_i}{m_i c^2}}$$

with :

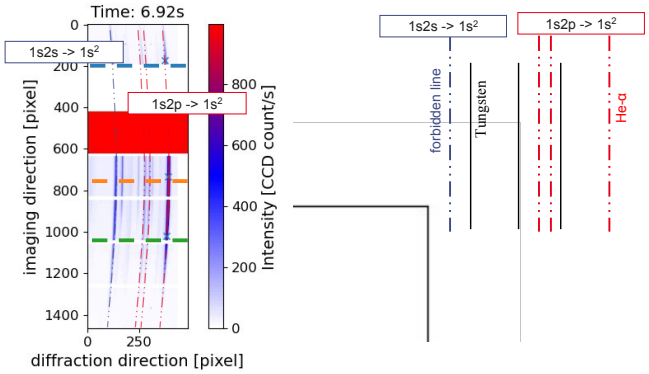
- kT_i the Ion temperature.
- ΔE_{FWHM} the Full Width at Half Maximum of the spectral line
- E_0 the central wavelengh of the spectral line
- m_i the ion mass

The X-ray Imaging Crystal Spectrometer designed for retrieving the ion temperature

☐ **A Spherical Bragg crystal in Johann configuration to obtain the spectral resolution as well as spatial resolution [4].**

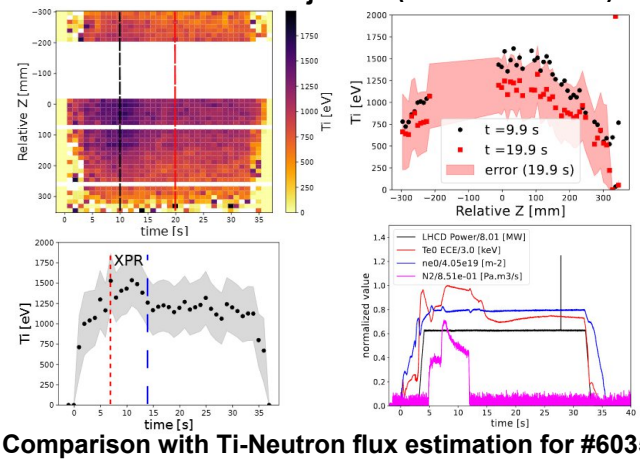
Johann configuration imaging the collected photon on poloidal plan (top) and diffract them on the toroidal plan by Bragg law (bottom).

☐ **2d map of the collected photon emitted by the plasma reveal Kα spectral lines (shot #61530)**



Intensity map of a WEST shot (#61530) (left). Spectra obtained at 3 relative Z positions (left).

☐ **Temporal and spatial evolution of the ion temperature give valuable information on the plasma evolution i.e. increase of Ti while N2 injection (X-Point Radiator).**



☐ **Comparison with Ti-Neutron flux estimation for #60359.**

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P13

Theoretical study of electron-molecule collisions for plasma simulations

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The development of low-power electric propulsion thrusters [1] is a crucial step to respond to the growing demand for small satellite technology. In this context, iodine is a promising candidate to replace the currently used propellants (e.g. xenon), for both technological and economic reasons [2]. Indeed, in 2019 the first satellite propelled by iodine was launched into space [3].

However, the physics and the chemistry of iodine low-temperature plasma generated in the thruster are not well understood, due to the lack of data on the elementary electronic processes occurring. Moreover, electron impact collisional processes, and their associated reaction cross sections, are critical inputs required for plasma modeling. In this context, we have studied the electronic processes in electron-iodine molecule collisions up to 100 eV using the R-matrix method [4] combined with Effective Core Potentials [5] for the description of the core electrons.

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P14

Dirac R-matrix electron-impact excitation of Ni I for the interpretation of magnetically-confinded/astrophysical plasmas

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Interpreting the spectra from magnetially-confined/astrophysical plasmas involves generating synthetic spectra from collisional-radiative models at required densities and temperatures. These models are underpinned by accurate atomic and collisional rates, ideally employing the same atomic structure. For example, within an astrophysical context, near-neutral ion stages of Nickel (Ni) are required for non-local thermodynamic equilibrium of the nebular phase of supernovae [1].

Collisional rates for near neutral targets, benefit from non-perturbative approaches such as the Dirac R-matrix (DARC) or Dirac R-Matrix with Pseudo-states approach (DRMPS). Initially, relativistic atomic orbitals are calculated within a Multi-Configuration-Dirac-Fock (MCDF) approximation employing a modified version of the General Relativistic Atomic Structure Package (Grasp0). Where available, Energy levels and A-values were compared with experimental values and in general found good agreement. Subsequently, a relativistic electron-impact excitation was then performed (DARC) [2] producing collision strengths that have been Maxwellian convolved for implementation within collisional-radiative codes. Some of our results shall be presented.

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P15

Effect of pulsed neutral gas injection on heat flux scrape-off layer (SOL) width in ADITYA-U tokamak

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Handling the extremely high heat fluxes, often reaching ~10 MW m^{-2}, on plasma-facing components is a major challenge for future tokamak reactors. The heat-flux scrape-off layer width, λ_q, represents how rapidly the parallel heat flux decays radially in the SOL and is a key parameter that determines divertor and limiter heat loads. When λ_q is very narrow, the power is deposited over a small area, leading to severe localized thermal stress. Plasma detachment produced by impurity seeding is a widely used method to reduce divertor heat flux, but it often comes at the cost of degraded core confinement [1]. Achieving a detached edge while simultaneously maintaining or improving core performance is therefore essential for reactor-relevant operation. Experiments on devices such as TCV, ASDEX Upgrade, and DIII-D have previously investigated this challenge using advanced divertor configurations [2] and real-time impurity-seeding control techniques [3,4].

In this study, we present results showing that short neutral gas-pulse injection can simultaneously broaden the heat-flux SOL width, reduce edge heat loads, and improve core confinement. A comparative analysis further reveals that pulsed fuelling is significantly more effective than continuous gas fuelling in increasing λ_q, reducing edge power deposition, and enhancing core density and temperature. An analytical model is developed to explain how ionization and recombination of neutrals in the ADITYA-U edge region influence the heat-flux width λ_q. Further, simulations with UEDGE code reproduce the key transport features as predicted through analytical model. These findings suggest that short neutral gas-pulse injection provides an effective approach to reducing and broadening heat loads on the limiter or divertor, while simultaneously maintaining or even improving core confinement in fusion plasmas.

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P16

Theoretical Advances in Electron Molecular-ion Scattering, Method Benchmarking and Connecting Collisional and Photofragmentation Resonances

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Electron scattering off of molecular ions is an important and complicated topic for plasma chemistry studies, especially when talking about plasma neutralization which is dominated by dissociative recombination both in astrochemical (interstellar medium) and plasma reactor (fusion edge plasma) scenarios. In the past few years we've seen a substantial evolution in the theoretical methodology describing these processes.
We present here mainly the methodological improvements of the energy dependent frame transformation (EDFT) method [1, 2] which can now handle the branching ratios of individual dissociation channels as well as rotational degrees of freedom (neglected in most previous EDFT studies). We show several benchmarks, using a simplified model of Hydrogen and comparing with both more "brute force" solutions [3] and other contemporary frame transformation methods such as the step-wise multichannel quantum defect theory [4].
We also show our latest developments [5] coupling the scattering to photofragmentation and how the resonant features in the cross sections compare between the processes.

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P17

Mechanisms of Plasma–Matrix Interactions and Their Compensation Strategies in ICP-MS

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In this work, plasma–matrix interaction mechanisms in radio-frequency inductively coupled plasma (ICP) were investigated with emphasis on the physical processes governing ion formation, ionization equilibrium, and ion transport in ICP-MS under the presence of complex biological matrices. The study focuses on how matrix-induced perturbations of plasma energetics affect ionization efficiency and mass-spectrometric signal formation.

Spectral interferences were shown to originate predominantly from plasma-driven formation of polyatomic, molecular, and isobaric ions, reflecting ion–molecule and charge-transfer reactions occurring in high-temperature RF plasma. Non-spectral matrix effects arise from the interaction of organic components, salt residues, and acid-derived species with the plasma energy balance, leading to modifications of electron heating efficiency, ionization kinetics, and ion extraction conditions.

Isotopes of Mg, Ni, Cu, Zn, Ga, As, Se, Sb, Pt, and Pb were examined to evaluate plasma-induced distortions of ion populations. Pronounced spectral interference was observed for specific isotopes, such as ^{63}Cu and ^{69}Ga, due to enhanced formation of overlapping plasma-generated species. Selection of alternative isotopes with reduced sensitivity to plasma-driven interference significantly stabilized ion signals under optimized plasma conditions.

Non-spectral matrix effects were found to correlate strongly with elemental ionization potentials and shifts in ionization equilibrium within the plasma. Variation of RF generator power demonstrated its central role in controlling electron heating and ionization efficiency: reduced RF power suppressed analyte ionization, whereas excessive power enhanced the formation of doubly charged ions, leading to altered mass-to-charge distributions. An optimal RF power of 1430 W provided a stable compromise between ionization efficiency and suppression of multi-charged ion formation.

Optimization of nebulizer gas flow (1.00 L min^{-1}) and sampling depth (8 mm) revealed the influence of the axial zonal structure of the ICP on ion formation and transport. Additional optimization of sample uptake rate and ion-optical extraction potentials resulted in enhanced ion transmission efficiency.

The results demonstrate that effective compensation of biological matrix effects in ICP-MS requires plasma-physics-guided optimization of RF plasma parameters, enabling controlled ionization conditions and stable ion transport for reliable mass-spectrometric detection.

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P18

Irradiation-driven fragmentation of $W(CO)_6$ in gas phase: Analysis of scaling behaviour

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Irradiation-Driven Molecular Dynamics (IDMD)[1] is an emerging multiscale simulation methodology that bridges quantum chemistry, molecular dynamics, and radiation physics to study how energetic particles interact with complex molecular systems. Unlike conventional MD approaches, IDMD incorporates stochastic irradiation events—such as bond cleavage, ionization, and secondary electron generation—directly into the dynamical evolution of molecules and materials. And one of the promising applications of this methodology is focused electron beam induced deposition (FEBID)[2], a direct-write nanofabrication technique under different irradiation conditions. This makes it uniquely suited for investigating processes where radiation plays a decisive role, including the fragmentation of organometallic precursors, radiation damage in biomolecules, and the formation of clusters or nanoparticles. Implemented in the advanced computational platform, MBN Explorer[3], IDMD enables the integration of experimental cross-section data with large-scale simulations to offer mechanistic perspectives on both atomistic and mesoscopic levels. In this upcoming school, the scaling dependencies on the fragmentation process of $W(CO)_6$ molecules in the gas phase under different irradiation conditions will be presented. The outcome of the work is expected to deepen our understanding of radiation-driven chemistry and open avenues for predictive modelling of nanostructure growth, offering direct relevance to nanofabrication, materials science, and radiation biology.

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P19

Spectroscopic Time-of-Flight Spatial Distribution Measurements of Mono- and Polycrystalline W with Varying Surface Properties in Ne and Ar Plasma at the Linear Plasma Device PSI-2

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Tungsten (W) is the plasma-facing material (PFM) for future fusion reactors, such as ITER. Its erosion by the plasma and subsequent lifetime is of great interest. Additionally, this sputtered W can enter the plasma and cool it through radiation losses. The quantity and spatial distribution of sputtered W from PFMs therefore has a direct impact on reactor performance: The erosion can be modelled by spectroscopic investigation of W and W^+ or re-deposition processes [1]. Therefore, monitoring the W flux is necessary for operating the reactor, and utilising optical spectroscopy is an important tool to do so. For energy impacts in the keV range, the sputtered W atoms follow a cosine angular distribution [2]. For lower energies, as typically exist in the divertor region, experimental data shows a discrepancy to existing models [3]. This can be investigated at the linear plasma device PSI-2. Low-temperature plasmas in the eV range can be studied with densities up to $n_e \approx 10^{18}$ m^{-3}.

In this experiment, polished poly- and monocrystalline (100, 111) W is exposed to a linear Neon and Argon plasma at kinetic energies of about 100 eV. Additionally, W fuzz on a polycrystalline substrate is examined. The W atoms sputtered into the Ne/Ar plasma column allow for the acquisition of line shapes in a spectroscopic time-of-flight (ToF) measurement; multiple lines can be acquired due to further excitations in the plasma beam. The total sputtering yield can be deduced from multiple acquisitions. In this ToF measurement it is possible to differentiate between angular distributions of sputtered W flux, while all other experimental parameters stay fixed. Multiple spectral lines are investigated for cross-reference in the 400-500 nm region.

These new experimental results show deviations in angular distributions between lattice structures and can be used to support modelling of low temperature plasma-wall interactions. In addition, the surface nanostructure impacts photon reflectivity of the PFM and angular distribution of sputtered atoms.

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P20

Observation of Non-Conventional Electron Dynamics and Temperature Scaling Driven by Relativistic Brunel Heating

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We investigate hot-electron temperature scaling in relativistic laser–plasma interactions using two-dimensional particle-in-cell (PIC) simulations. Electron angular distributions extracted from the simulations are integrated to generate energy–electron-number spectra, from which hot-electron temperatures [1] are obtained. A systematic parameter scan is performed over a broad range of laser amplitudes (a_0) and plasma density scale lengths.
The simulation results reveal electron dynamics that differ markedly from classical Brunel heating [2] and the conventional j × B mechanism. Under ultra-intense laser irradiation combined with steep plasma density gradients, two clearly separated electron bunches appear. In this regime, relativistic gyromotion confines electrons near the target surface, which in turn restricts their ability to gain kinetic energy. Such electron dynamics are not captured by classical heating models. Analysis of the corresponding angular and energy distributions shows that, at high intensities and sharp gradients, the resulting hot-electron temperature falls to less than half of the value predicted by the widely used Wilks scaling. This pronounced reduction in temperature indicates the onset of a relativistic Brunel–dominated heating regime.
The distinct temperature evolution exhibited by the two electron populations provides valuable insight into how dominant energy-absorption mechanisms change with laser intensity and plasma scale length. These findings refine the current understanding of hot-electron generation in relativistic laser–matter interactions and help clarify the physical processes governing energy absorption at steep plasma interfaces.

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P21

First principles optical constants of water ice: geometry effects and vibrational contributions

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In plasmas, atmospheres, and interstellar environments, the relevant material is often inaccessible to direct in situ measurements. Instead, spectroscopy and scattering measurements provide our main insight into the composition, density, and thermodynamic state. Radiative transfer calculations that model these observations reduce to knowing, as a function of frequency, how strongly electromagnetic radiation is attenuated and redistributed by the medium. In practice, this requires specifying the radiative properties for each constituent in the medium, from atomic and molecular opacities to the optical constants of condensed phases.

A substantial fraction of the potential required inputs is now supported by community databases and curated tables. For gas-phase atmospheres, spectroscopic databases such as HITRAN and GEISA provide line and cross-section data that underpin predictive calculations of transmission and emission spectra [1, 2]. At higher temperatures, dominated by ionized particles, opacity tables computed from atomic structure and radiation models provide an analogous foundation; the LANL ATOMIC framework, and the associated OPLIB tables, are a representative example used widely in radiation-transport and astrophysical modeling [3, 4]. These resources are powerful, but they do not address larger particles and condensed phases such as dust, aerosols, and ice, which require knowledge of their complex optical constants.

Hexagonal ice (ice Ih) is a particularly consequential condensed phase because it appears in atmospheric clouds and snow/ice surfaces, and as mantles or solid phases in cold astrophysical environments. Widely used optical-constant datasets for ice—notably the Warren and Brandt compilation [5]—aggregate and interpolate heterogeneous measurements across preparation methods, temperatures, and morphologies. Calculating optical constants from first-principles would allow for internal consistency and yield insight into temperature, interface, and size dependence.

Here we use density functional theory calculations to compute the complex dielectric response of ice Ih and the corresponding complex refractive index. We treat electronic and ionic (vibrational) contributions separately and complement our bulk calculations with surface (slab) calculations to assess how the interface modifies absorption. We benchmark the results against the Warren and Brandt compilation [5] of heterogeneous "hexagonal" ice measurements. From this comparison, we identify regions where more complex computational techniques are required, establishing a workflow for other phases of ice and other large particles and condensed phases essential for atmospheric and astrophysical modeling.

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P22

Analysis of carbon ion temperatures using an upgraded multichannel Doppler spectroscopic diagnostic in NBI-heated TJ-II plasmas

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Understanding the dynamics of impurity ions in magnetically confined fusion (MCF) plasmas is essential to optimize the performance of future fusion reactors. Impurities affect plasma radiation and stability, requiring precise monitoring. Spectroscopic techniques, particularly the Doppler Effect analysis of spectral line broadening, are used to determine ion temperature (T_i), related to ion thermal motion.

This work reports Doppler spectroscopic measurements of C^{+4} ion temperatures using an enhanced system: a Spec10 CCD with a 400 × 1340-pixel matrix coupled to a 1 m focal length spectrometer. Unlike previous TJ-II setups with 9 lenses and fibers, the new system orients 400 pixels along the wavelength dispersion and uses 1340 pixels across the plasma diameter, with binning during readout, achieving 72 points per profile (up from 9) and improving signal by ~25%. Calibration with Hg pen lamps ensures alignment precision and reliable spectroscopic parameter extraction.

Experiments with 150 neutral beam injection (NBI) heated discharges across various plasma conditions, including H isotopes, reveal T_i dependence on density and absorbed NBI power. Notably, T_i is higher during counter-injection than co-injection. These findings will be compared with neoclassical transport simulations and radial electric field measurements to analyze T_i profiles. The results contribute to understanding impurity transport in stellarators and provide a basis for studying fast NBI-driven ion interactions with impurities in MCF plasmas.

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P23

Laser-collision induced fluorescence for measurement of collision rate coefficients in helium plasmas

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Optical emission spectroscopy (OES) techniques are widely used to infer electron density (n_e) and temperature (T_e) in plasma devices. The interpretation of spectral line intensities relies on collisional-radiative models (CRMs) to retrieve plasma parameters. The accuracy of OES diagnostics is currently limited by uncertainties in the atomic data used within the CRMs. The cross-sections for electron impact (de)excitation (EIE/EID) in particular often carry large or poorly defined uncertainties that propagate all the way into results from OES diagnostics [1].
To address this issue, we propose to measure EIE/EID rates using laser-collision induced fluorescence (LCIF). The principle of LCIF is to pump an excited atomic state with a laser. A portion of this excited population transitions to a neighboring state through electron collisions, before radiatively decaying at a different wavelength. The intensity and temporal evolution of the LCIF signal depend on EIE/EID rates, themselves function of n_e and T_e. Using available EIE/EID rates from databases, LCIF has been applied to locally measure n_e and T_e [2-4] and is planned to be deployed on the ITER and T-15MD tokamak divertors [5,6]. In contrast, we plan to probe the EIE/EID rates by measuring n_e and T_e independently with Thomson scattering (TS).
This work presents proof of concept measurements of LCIF signals in helium plasmas. Experiments are performed on the Resonant Antenna Ion Device (RAID) [7], a linear helicon plasma source, where both LCIF and TS diagnostics are installed. RAID can sustain helium plasmas at densities up to $n_e \leq 6 \cdot 10^{19}$ m^{-3} in steady state operation, allowing for high sensitivity measurements. The plasma reaches temperatures up to $T_e \leq 7$ eV, relevant to tokamak divertors [8]. To pump different atomic transitions, we use a pulsed laser, continuously tunable between 190 nm and 2000 nm. The 28 ps pulse duration allows for a clear separation of timescale between the excitation and decay processes. We use an ICCD with a 0.5 ns gate duration to measure the fluorescence.
We show experimental measurements of LCIF signals in different pumping schemes and discuss the extraction of EIE/EID rates based on previous works [9].

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P24

ELECTRON-INDUCED VIBRATIONAL TRANSITIONS AND DISSOCIATIVE RECOMBINATION OF H_2^+ AND BH^+

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Hydrogen molecular ions and their isotopologues play a central role in the edge plasmas of magnetic fusion devices, as they originate from the fuel species hydrogen, deuterium, and tritium interacting with plasma-facing components. In particular, H_2^+ and its isotopologues (D_2^+, HD^+) are of primary importance for dissociative recombination and ro-vibrational excitation processes governing plasma kinetics.

In this poster, we present recent and ongoing calculations of electron-induced dissociative recombination and vibrational transitions for BH^+ and H_2^+, focusing on effective cross sections and rate coefficients. Results are presented for H_2^+ at high electron energies ($E > 3$ eV), following the MQDT methodology previously developed for BeH^+ [1], as well as for D_2^+ at low electron energies ($E < 1$ eV), where rotationally resolved calculations are applicable, extending recent studies on H_2^+ and HD^+ [2].

The molecular structure data for H_2^+ and BH^+ are computed by the quantum chemistry methods as we did for BeH^+ [3] and continuously improved using the Halium code [3]. These data, including potential energy curves and electronic couplings, are then used in dynamical calculations to obtain dissociative recombination and vibrational transition cross sections and rate coefficients.

More recently, boronized tungsten walls have been considered as plasma-facing materials in fusion devices, leading to the presence of boron hydride ions in the edge plasma. Consequently, BH^+ has emerged as a species of growing interest. In this context, we investigate electron–BH^+ collisions using the Multichannel Quantum Defect Theory (MQDT).

The presented results provide valuable theoretical support for spectroscopic diagnostics and plasma modeling of edge fusion plasmas, while ongoing developments in molecular structure calculations ensure increasingly accurate descriptions of electron–molecule interactions.

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P25

Construction of atomic collisional radiative models for use in solar atmospheric modelling

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For the solar atmosphere the most important atomic transitions originate from hydrogen and helium atoms which compose over 98% of the Sun by mass. Recently, several new collisional radiative models have been produced for helium and its ion [1,2]. These models aimed to address shortcomings in the He recombination spectra and collisional excitation rates present in previous models through the use of more accurate atomic data. Between the present and previous models differences were found to be far above the target accuracy of 1% for predicted emissivity. Following from these models, similar models for atomic hydrogen are to be constructed, but for inclusion into Radiative Transfer/MHD codes reduced models are being built, also considering the evolution of the populations with time dependence. Thereafter, these models will also be modified for inclusion into the Solar Atomic Modelling Suite (SAMS) project [3]. The models will have wide-ranging applications in astrophysics and laboratory plasmas.

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P26

Steady-State-Informed Latent Dynamics Surrogate Model for TD-NLTE Atomic Kinetics

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Time-dependent non-local thermodynamic equilibrium (TD-NLTE) atomic calculation plays a key role in plasma simulations across a wide range of applications, including inertial confinement fusion. Inline coupling of TD-NLTE calculation with radiation–hydrodynamic simulations enables more accurate modeling by reducing the gap between simulations and experiments, but its practical use remains limited by the high computational cost. We develop a physics-informed surrogate TD-NLTE model based on the Latent Space Dynamics Identification (LaSDI) framework [1], with the key novelty being the explicit incorporation of NLTE steady-state constraints. High-dimensional atomic population data generated by SCFLY [2] are compressed into a low-dimensional latent space using a nonlinear autoencoder with a mixed reconstruction loss that captures both microscopic population accuracy and macroscopic observables. The latent dynamics are identified using Sparse Identification of Nonlinear Dynamics with control (SINDyC) [3], driven by time-dependent temperature and density histories. To ensure physically meaningful long-term behavior, the analytically derived latent steady state is explicitly constrained to match reference NLTE steady-state solutions, in addition to enforcing Hurwitz stability. These preliminary results demonstrate the feasibility of a steady-state–constrained latent dynamics approach for efficient and physically consistent TD-NLTE modeling, paving the way toward practical inline coupling with radiation–hydrodynamic simulations.

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P27

Effective cross sections and rates coefficients derived from collision-induced rotational excitation of $HCl^+(X^2\Pi)$ with $He(^1S)$: Isotopic effects

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In this work, we studied the helium-induced collisional excitation of the radical ion HCl^+. Our work focuses on calculating three-dimensional potential energy surfaces (PES) to study the interaction due to the collision between HCl^+ and He, and on analyzing the influence of the isotopic effect on cross sections and collision rates. For *Ab initio* calculations of PES $^2A'$ and $^2A''$ of $HCl^+(X^2\Pi)$-He complex, we used the RCCSD(T)-F12 method with cc-pVQZ-F12 basis sets. These surfaces have been fitted using the Reproducing Kernel Hilbert Space (RKHS) method and were submitted to the close-coupling approach in order to work out the inelastic integral cross sections. Collision cross sections taking into account the fine structures of HCl^+ have been performed for kinetic energies up to 3500 cm^{-1} and the thermal excitation rates for kinetic temperatures from 0K to 400 K. It appears that the difference in the cross section and collisional rate cofficients for the $H^{35}Cl^+$ and $H^{37}Cl^+$ colliding with He was found to be negligeable. In contrast, a significant difference in effective cross-sections and collision rates between HCl^+-He and DCl^+-He was observed to the extent that it is impossible to make estimation of collision rates of deuterated species from those of the hydrogenated species.

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Absolute calibration of various crystal types and geometries for National Ignition Facility x-ray spectrometers

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Absolute calibration of crystals within x-ray spectrometers fielded at the National Ignition Facility (NIF) is critical to understand the plasma source properties that they aim to diagnose. The spectrometer calibration station (SCS) located at the Lawrence Livermore National Laboratory was established in recent years to perform integrated spectrometer throughput measurements in order to fully characterize a given crystal's response. Full NIF spectrometer or duplicate surrogate hardware is placed in a vacuum chamber adjacent to the x-ray source chamber, such that the crystal-to-source standoff can be adjusted to its actual position from a target in the NIF. We use a steerable electron beam to bombard an anode foil as our x-ray source. The anode foil is housed in a rotatable turret, allowing for an easy selection of various elements without breaking vacuum. This combined with a voltage of up to 30 kV, for the electron beam power supply, allows for x-ray line emission of up to 30 keV photon energies. The crystal response is determined by taking a ratio of the crystal diffracted signal to the source emission spectrum for a given set of x-ray lines within the spectrometer's bandwidth. We use an absolutely calibrated Amptek silicon drift detector to infer the source emission signal. The SCS further characterizes crystal attributes by illuminating any spectral warping or defects that can only be seen with x-rays. Spectral dispersion is also mapped so that theoretical design can be vetted. Here we present the calibration data from various NIF x-ray spectrometers of different geometries and crystal types. We show that often each crystal is unique and requires individual calibration, regardless of identical design and fabrication specifications.

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P29

Near-Surface Hydrogen Inventory Response to Picosecond Laser Pulses in Tungsten

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Tungsten is the leading candidate for plasma-facing components in fusion devices. In future fusion reactors, neutron irradiation creates material defects that trap hydrogen isotopes, including the fusion fuel tritium and deuterium. Monitoring the hydrogen inventory is mandatory for nuclear safety and important for the efficient use of fuel. Laser-based diagnostic methods such as Laser-Induced Breakdown Spectroscopy (LIBS) and Laser-Induced Ablation with detection of volatile species by Quadrupole Mass Spectrometry (LIA-QMS) provide quantitative, depth-resolved assessments of the local fuel inventory and release. They are offering a controlled measurement of near-surface retention on short time scales for in-situ and ex-situ applications

To describe the effect of transient material heating on fuel release beyond the ablated layer, a one-dimensional modelling framework is developed in FEniCS/FESTIM for picosecond laser pulse trains. The simulations address depths below 1 mm. Transient heat conduction with temperature-dependent properties is coupled to a minimal near-surface trapping-detrapping scheme. Initial near-surface fuel fractions are in the percent to sub-percent range. Coarse ablation is represented by removing a thin surface layer tens of nanometers thick at the start of each pulse, which updates both the thermal and hydrogen-isotope boundary conditions. Per-pulse release is obtained by integrating the simulated desorption flux. Evolution over fuel release is analyzed for tens to hundreds of pulses.

Here in this modelling approach, the initial fuel distribution is taken from NRA depth profiles measured on proton-irradiated and self-damaged, deuterium-decorated tungsten samples which act as reference.

Results show that heating-induced release dominates over the contribution attributable to the imposed ablation layer release. Early pulses are characterized by rapid mobilization of the near-surface fuel reservoir, leading to pronounced, prompt desorption transients. Consequently, when ablation is applied at the start of subsequent pulses, it largely removes a layer already partially depleted by prior heating. With a simple defect-annealing term, model predictions are compared to LIA-QMS-derived depth reconstructions, yielding reasonable agreement.

The modelling framework supports the interpretation of LIA-QMS data for self- or proton damaged tungsten as proxy for neutron-damaged tungest and clarifies the respective roles of fast heating and material ablation in pulse-train experiments with ps-laser systems.

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Optical Emission Spectroscopy in Helium plasmas for validation of collisional-radiative model on the Resonant Antenna Ion Device

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Helium (He) is an important element in plasma physics due to its abundance in space and laboratory plasmas, as well as its relative simplicity in atomic structure. Optical Emission Spectroscopy (OES), combined with collisional radiative models (CRMs) can be used to determine the electron density n_e and temperature T_e. However the relation between plasma parameters and spectral line intensity is complex and present CRMs have been found to break down under certain conditions, particularly at low temperatures in tokamak divertors, which emphasizes the further need for development and validation of He CRMs [1].
The intensity of a given spectral line is proportional to both the density n_i of the emitting state and the Einstein coefficient A_{ij}, i.e $\varepsilon_{ij} \propto n_i A_{ij}$. The distribution of the excited states is described by the CRM as a function of the plasma parameters, accounting for both radiative and collisional processes. Development of an accurate CRM is challenging and requires an exact description of the atomic structure, inclusion of all relevant processes, availability of precise reaction rates, as well as a correct treatment of transport processes, such as opacity.

We are currently investigating He plasmas on the Resonant Antenna Ion Device (RAID) [2] for validation of the CRM CoRa-He [3] developed at SPC, EPFL. RAID produces steady-state plasmas with $n_e \approx 0.3 - 5 \cdot 10^{19}$ m^{-3}, $T_e \lesssim 5$ eV, relevant for tokamak divertor physics. Plasma emission is collected through an optical fibers bundle and guided to an Isoplane SCT 320 spectrometer (f = 320 mm, λ: 200-1300 nm, 150 l/mm grating) to obtain radial emission profiles, which are then interpreted using CoRa-He, accounting for the plasma's environment and opacity effects. Complementary diagnostics, particularly RAID's high resolution Thomson scattering (TS) system, provides precise and independent characterization of the plasma parameters, used as input to the CRM.

We present OES measurements of He plasmas in RAID alongside CRM simulations and discuss the influence of opacity and transports on these measurements. Future work on the CRM will include several updates, such as the addition of higher level ($n > 4$ for He I), level-mixing between singlet and triplet states [4] as well as the development of a more complex opacity model. Furthermore, the laser induced fluorescence (LCIF) diagnostic implemented on RAID offers another powerful tool to validate the CRM when the plasma is perturbed out of its equilibrium state [5].

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P31

Interparticle Coulombic electron capture beyond the virtual photon approximation

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Interparticle Coulombic electron capture (ICEC) is an environment-enabled electron capture process where the excess energy is released by ionization or excitation of a neighboring particle. Both the capturing particle and the neighbor can be atoms, molecules, or ions. It is one of the plethora of electron capture (or electron attachment) processes that are relevant to astrophysics [1] and plasma physics [2]. ICEC was theoretically predicted in 2009 [3, 4] and is expected to be significantly more efficient than the competing photorecombination. To date, it has been studied using analytical approximations [5], theoretical models [6], and *ab initio* calculations [7]. It has yet to be experimentally observed.

The asymptotic approximation derived in [4] has been shown to severely underestimate the ICEC cross section when the distance between the two particles is comparable to their size. It treats the process as two independent events: virtual photorecombination at the capturing particle and virtual photoionization of the neighbor. They are linked by the transfer of the excess energy. It therefore neglects the correlation between the electrons of the two particles and, most importantly, the possibility of electron transfer from the neighbor to the capturing particle. We have improved on the asymptotic approximation by proposing an analytical model of the electron transfer mechanism of ICEC. We have benchmarked it with *ab initio* R-matrix scattering calculations for several systems [8].

In comparison to the original asymptotic approximation, our model improved the agreement with the *ab initio* results at relevant inter-particle distances while keeping its simplicity. The model ICEC cross sections can be evaluated with a simple analytical formula using tabulated properties of the participating particles.

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P32

Full-dimensional quantum dynamic study for the H atom scattering from graphene surface

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The adsorption of hydrogen atoms on graphene has received significant attention due to its importance in astrophysics, hydrogen storage, and semiconductor technologies. A full-dimensional potential energy surface (PES) for a periodic graphene surface containing 24 carbon atoms and one hydrogen atom was recently developed [1,2]. Based on this PES, classical molecular dynamics (MD) simulations were used to study hydrogen atom scattering from graphene. However, for certain collision conditions, discrepancies were observed between experimental results and MD predictions.

To clarify these differences, full-dimensional quantum dynamics (QD) simulations were performed. The original neural-network PES was refitted into a sum-of-products representation using the Monte-Carlo Canonical Polyadic Decomposition (MCCPD) method [3]. The nuclear wave function was then propagated using the multilayer multiconfiguration time-dependent Hartree (ML-MCTDH) method [4,5,6], with a multilayer tree optimized through hierarchical clustering [7]. Sticking probabilities and scattering distributions were obtained using quantum flux-based approaches.

The comparison between QD and MD simulations showed very good agreement [8,9], demonstrating that classical dynamics captures much of the essential physics. Importantly, the analysis revealed that remaining discrepancies with experimental observations arise primarily from PES limitations and genuine quantum effects, such as zero-point energy and resonance phenomena. Furthermore, phonon-resolved analysis highlighted the key role of longitudinal graphene phonons in the collision and adsorption mechanisms.

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P33

Relativistic Calculations Of Transition Parameters Of Doubly Ionized Argon

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Atomic structure parameters for inert gas ions are of significant importance due to their wide uses in fusion plasma modeling and diagnostics. In fusion devices, inert gases can exist in various charge states therefore, reliable atomic data are essential to support ongoing projects focused on the design and development of fusion reactors.

Limited data are available for the transition parameters of doubly ionized argon (Ar^{2+}). To address this gap, we have carried out detailed calculations of energy levels and transition parameters, including wavelengths, weighted oscillator strengths, transition probabilities, and line strengths, for electric dipole (E1) and magnetic dipole (M1) transitions. The computations were performed using the fully relativistic multiconfiguration Dirac–Hartree–Fock method implemented in GRASP2018 [2], which incorporates both Breit interaction and quantum electrodynamics effects. These calculations were conducted for the lowest 230 fine-structure levels of sulphur-like Ar^{2+}, arising from the configurations $3s^23p^4$,$3p^6$, $3s^23p^34\ell$ (ℓ = s, p, d, f), $3s3p^5$, $3s^23p^33d$, and $3p^53d$.

Our calculated energy levels show excellent agreement with the 125 experimentally measured [1,3] levels reported in the NIST database. Furthermore, good consistency is observed between the published line strength data and our calculated results. To further validate the accuracy of our calculations, we compared the line strengths obtained in both the length and velocity gauges, which also exhibit strong agreement.

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P34

Photoionization, Rayleigh, and Raman scattering cross sections for the hydrogen molecule

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Photon scattering cross sections have proved essential in many applications, such as calculating opacities, modeling plasma and radiative transport, analyzing planetary atmospheres, and Raman spectroscopy. In particular, Raman spectroscopy of H_2 plays an important in analyzing hydrogen storage techniques, monitoring ortho-to-para conversion, and monitoring nuclear waste. Atomic and molecular hydrogen are abundant in the interstellar medium. Hence, photon scattering cross sections for H_2 and its ion are of particular interest in astrophysics.

Photon–molecule scattering processes have been well understood to second order in perturbation theory since the development of the Kramers–Heisenberg–Waller (KHW) matrix element [1, 2] in the mid-1920s. The convergent close-coupling method, which has previously been used to study electron scattering from atoms and molecules as well as single and double photoionization [3], has been applied to photoionization and radiative association of the hydrogen molecule. We have calculated rovibrationally-resolved photoionization cross sections for the ground electronic state of H_2. Rayleigh and Raman scattering cross sections have been calculated for transitions between all rovibrational levels of the $X\,^1\Sigma_g^+$ ground electronic state of H_2, resulting in a total of 9582 Rayleigh and Raman cross sections [4]. This work represents the most comprehensive study of photon scattering on molecular hydrogen. Thermally-averaged photoionization, Rayleigh, and Raman scattering cross sections have been produced for a system in local thermodynamic equilibrium.

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GEOSH: Chemical Equilibrium Calculations of Ideal Gas Mixtures

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Understanding the relative abundances of atoms, molecules, and ions in a gaseous mixture at equilibrium is necessary when modeling gaseous mixtures in a wide range of applications such as planetary and stellar atmospheres. To simplify the problem, we apply the law of mass action and Saha-Langmuir equations to express the chemical species in terms of the atomic species present in the system. By normalizing chemical species and eliminating electron capture and ionization degrees of freedom, we reduce the problem to a set of non-linear equa- tions describing the conservation of each atomic nuclei and charge species. We introduce GEOSH, a code designed to solve for the relative concentrations of chemical species by solving a system of non-linear equations using a Newton- Raphson solver while determining the thermodynamic quantities of the system in equilibrium.

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Vibrationally resolved core excitation of the CN^+ molecular ion

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Near-edge x-ray absorption fine structure spectroscopy (NEXAFS) is a powerful tool to probe electronic core excitations. We measured the electronic structure of the CN^+ ion vibrationally resolved to gain insights towards accurate descriptions of core-excited diatomic molecules. So far, there is no other experimental data on the CN^+ ion, consequently theoretical data is also scarce. First theoretical studies of the core excitation of the C atom of CN^+ were published only recently [1].
The experiment took place at the Photon Ion end station at PETRA III (PIPE) [2]. The PIPE setup is a permanently installed user facility at the XUV beamline (P04) of the PETRA III synchrotron radiation facility operated by DESY in Hamburg. The brilliant synchrotron light of PETRA III enables vibrationally resolved core-excitation spectroscopy and provides access to high resolution measurements. The production of CN^+ ions is quite challenging due to its toxicity and also due to its chemical characteristics. The CN^+ ions were produced in an electron cyclotron resonance ion source (ECR) from a mixture of CO and N_2 gases [3]. The ion beam was mass-over-charge analyzed with a dipole magnet and the CN^+ ions were selected and merged with the counter-propagating photon beam over a length of ca. 1.7 m. The collimated CN^+ ion current in the interaction region was 2 nA. The photon energy was scanned across the carbon and nitrogen K edges. CN^{2+} product ions resulting from the photon-ion interaction were separated from the ion beam with a demerging magnet and detected with a single particle detector. The measured ion yields as a function of photon energy exhibit vibrationally resolved resonances associated with the excitation of a $1s$ electron to unoccupied molecular levels. On our poster, we will present the current status of our data analysis.

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P37

Initial predictive modeling of plasma-wall interactions using ERO2.0 for W7-X with tungsten wall divertor

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Plasma-wall interaction (PWI) is a critical aspect of fusion device operation, influencing material lifetime, fuel retention, and overall plasma performance. In addition to interpretive modelling used to analyze and understand physics experiments, predictive modeling with validated codes like ERO2.0 becomes essential for anticipating system behavior and guiding design or operational decisions as required for an exchange of the wall material in Wendelstein 7-X (W7-X).

ERO2.0 is a fully kinetic Monte Carlo code dealing with PWI processes at the surface and incorporating phenomena such as drifts, ionization, and impurity-ion collisions in the plasma. While there have been multiple ERO2.0 studies of stellarators - including cases with some tungsten components - no systematic investigation exist for a fully metallic stellarator with a tungsten divertor.

In this work, PWI and impurity transport for the W7-X stellarator are studied with focus on the planned wall material exchange from a carbon wall to a tungsten wall. The influence of the resolution of existing 3D grids on the resulting PWI and impurity transport is analyzed.

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Machine Learning-Assisted Diagnostics of Laser-Induced Aluminium Plasma

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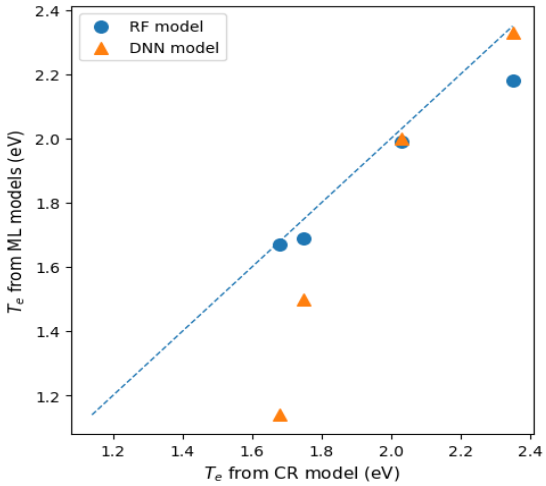
Laser-induced plasmas (LIPs) are gaining special attention nowadays due to their unique physical and chemical characteristics. These plasmas exhibit a transient nature with their properties varying with space and time. On one hand, where their versatile nature makes them suitable for a wide range of applications, at the same time this brings challenges in their accurate diagnostics [1]. The optimization of these plasmas for certain applications involves the correct determination of the plasma parameters. Techniques like laser induced breakdown spectroscopy (LIBS) when coupled with theoretical collisional-radiative (CR) modelling approach serves as a reliable way to diagnose these parameters accurately [2]. However, the real-time diagnostics is often infeasible with conventional CR modelling approach as these models are computationally intensive.

In light of this, people are approaching towards data driven methodologies namely machine learning (ML) for fast diagnostics of these plasmas [3, 4, 5, 6]. Due to the availability of open source softwares and resources and enhancement in data acquisition techniques, ML based approaches serves as efficient tools in the field of plasma spectroscopy. ML models once trained with CR model generated synthetic spectral intensity data can then be employed for rapid estimation of plasma parameters. In this context, we have developed two supervised learning based ML models namely – Random Forest (RF) and Deep Neural Network (DNN) for aluminium (Al) plasma. These models are trained and tested with CR model simulated spectral intensity data and then employed for predicting the electron temperature from experimental observables. Hyperparameter optimization is done using random search strategy to enhance predictive performance. The accuracy of these models is evaluated by measuring performance functions including MSE and R^2 values. The electron temperature values as predicted by CR model and ML models are compared showing reasonably good agreement also shown in the attached figure along with this abstract. Details of the models will be discussed in the poster presentation. Overall, this study highlights the potential of ML based methods as an effective way for real-time diagnostics of non-equilibrium plasmas.



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Abstract for Joint ICTP-IAEA School on Atomic and Molecular Process in Plasmas

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This document is the template for contributed abstracts (posters and/or talks) and gives the guidelines for preparing and submitting abstracts for the *Joint ICTP-IAEA School on Atomic and Molecular Processes in Plasmas* to be held online from *4 May 2026* to *8 May 2026*.

Time-resolved spectroscopy is a critical diagnostic for probing the evolution of plasma conditions in high-energy-density experiments [1]. The streaked visible spectroscopy (SVS) diagnostic at Sandia National Laboratories' Z Machine provides temporally and spatially resolved measurements of plasma emission, enabling inference of fundamental plasma parameters such as electron temperature and density. In this work, we analyze SVS data from the MagShockZ platform, which studies high-Mach-number quasi-perpendicular magnetized collisionless shocks. Using PrismSPECT, a collisional-radiative spectral analysis code, we model emission spectra across a range of electron temperatures and densities and compare the simulated spectra to the experimental measurements [2]. We present the first results of the electron temperature and density evolution of the background aluminum wire array plasma, and we compare the results to the MARZ campaign, which featured similar aluminum wire array plasmas.

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Title: Streaked Visible Spectroscopy Analysis for Laser-Driven Collisionless Shocks on Z

P40

Dielectronic Recombination Study on Sr^{4+}, Se^{4+}, Ga^{4+} and In^{4+} Ions

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Dielectronic recombination (DR) is a crucial process in astrophysical plasmas and laboratory fusion devices, directly regulating plasma ionization balance, energy transport, and radiative spectral properties[1]. Löbling et al.[2] analyzed ultraviolet spectra from the BD−22°3467 of a DAO-type white dwarf, and reported the first detection of spectral lines from trans-iron elements. The intense radiative field drives the extreme enrichment of these elements in the stellar atmosphere, and the DR processes of their ionized states play a crucial role in regulating the stellar atmosphere. Given the higher abundances of Sr, Se, Ga, and In, we calculated the DR cross sections of 4+ ions of these element.

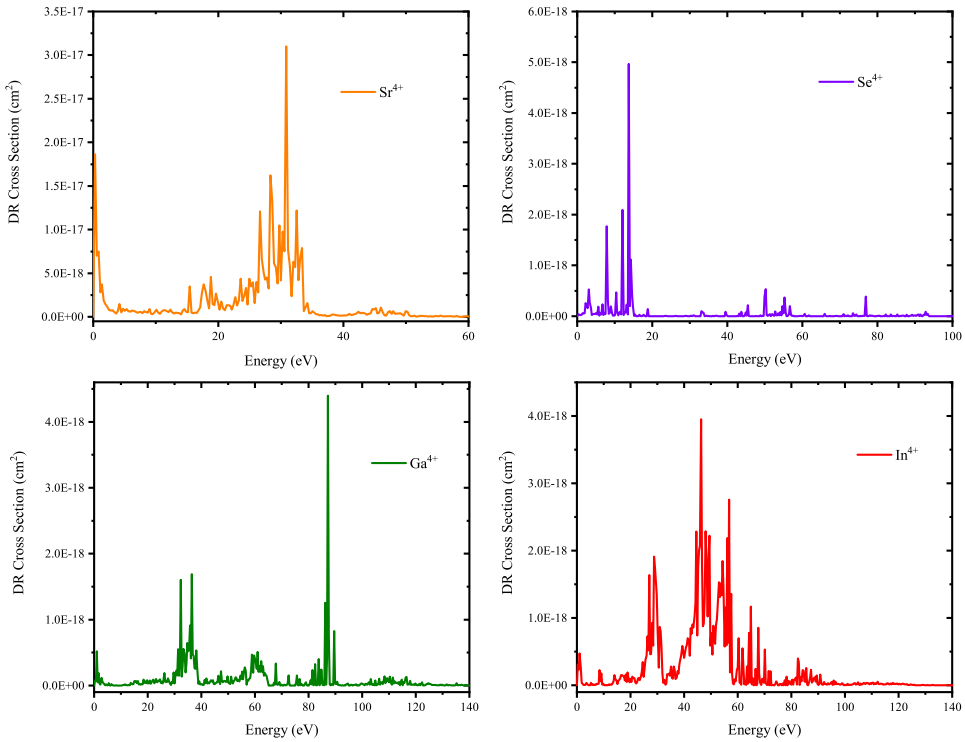

Figure 1: DR cross section for Sr^{4+}, Se^{4+}, Ga^{4+} and In^{4+}

Firstly, using the Flexible Atomic Code based on the Dirac-Fock-Slater method[3], we computed the energy levels, radiative transition rates, and autoionization rates for these four ions. Next, under the approximations of isolated resonance and independent processes, we calculated the DR cross sections with the Voigt profile, where the full width at half maximum (FWHM) of the Gaussian broadening was set to 10 meV.

Figure 1 shows the DR cross sections of these four ions. The DR cross section of Sr^{4+} is the largest (on the order of 10 $^{-17}$cm^2), while those of the other three ions are of the order of 10^{-18}cm^2. The DR cross section of each ion exhibits distinct density in different energy intervals; e.g., Sr^{4+} shows density in 20–35 eV and In^{4+} in 40–60 eV. Among them, the strong resonance peaks with large cross sections significantly enhance the intensity of recombination reactions in this energy segment, thereby increasing the occurrence probability of electron recombination processes within this energy interval. In subsequent work, we will calculate their DR rate coefficients and analyze their impacts on the plasma.

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