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P01

Cross Sections and Spectral Models for Charge Exchange Between Bare Ne and Atomic H and He at Solar Wind Velocities

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Charge exchange between highly charged ions and neutrals introduces a problematic background for every x-ray observation [1], including comets [2], supernovae remnants [3], and a plethora of other environments [4]. For H-like ions produced by charge exchange with bare ions, the ℓ states within each n shell are degenerate. The majority of charge exchange spectral models rely on calculated n-resolved cross sections, and the unknown distribution of ℓ states is assumed to follow one of several analytical expressions. With few laboratory measurements available for benchmarking at the relevant solar wind velocities (300 - 1000 km/s, $\sim$0.5 – 5 keV/amu), comparison to $n\ell$-resolved cross sections can be used to mitigate inaccuracies introduced by the use of analytical ℓ-distributions. We report explicit calculations of $n\ell$-resolved CX cross sections using the time dependent close coupling method [5] for Ne^{10+} incident on atomic H and He at 1 - 5 keV/amu. We incorporated the cross sections into a radiative cascade model and investigated the influence of n- and $n\ell$-resolved cross sections on important line ratios. Comparison of the ℓ-distribution extracted from the new cross sections to the 4 available analytical distributions shows similarities to the statistical ℓ-distribution for the majority of the possible ion-neutral-energy combinations considered. Similar agreements are observed in Lyman and Balmer line ratios for collisions involving atomic H, and disagreements for the Ne^{10+}-He collision system are discussed. Possible line ratio diagnostics are explored, and data needs related to molecular targets are identified.

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P02

The effect of electron correlation on trielectronic recombination rate coefficients for Be-like argon

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Abstract

The merged-beam rate coefficients of dielectronic and trielectronic recombinations (DR and TR) within $\Delta N = 0$ channels for Be-like Ar^{14+} were measured by Huang *et al.* [Astrophy. J. Supp. Ser. 235, 2 (2018)] with the cooler storage ring at Lanzhou, China. Meanwhile, theoretical data are calculated with Autostructure code for comparison with the measured resonance spectrum. However, TR resonance strengths are significantly underestimated by Autostructure calculations in most cases. In the present work, we find that the electron correlation between DR and TR resonance states with different captured electron principal quantum numbers n can lead to a obvious increase in TR resonance strengths for $n = 6, 7$. Previous theoretical calculations for this system did not include this form of electron correlation. Considering additionally it could account for most of the discrepancy between existed theoretical calculations and experimental results. Understanding electron correlation and their consequences is of great importance for obtaining the accurate total rate coefficients that are extremely useful for plasma modeling and diagnostics.

Resonance energies

The low resonance energies are calculated with the relativistic second-order many-body perturbation theory (RMBPT) implemented in the FAC. In RMBPT calculations, the Hilbert space of the system is divided into two subspaces, including a model space M and an orthogonal space N. By means of solving the eigenvalue problem of a non–Hermitian effective Hamiltonian in the space M, we can get the true eigenvalues of the Dirac–Coulomb–Breit Hamiltonian. The configuration interaction effects in the M space is exactly considered, and the interaction of the spaces M and N is accounted for with the many-body perturbation theory up to the second order. Through the single and double virtual excitations of the states spanning the *M* space, all states are contained in the space *N*.

The high-n resonance positions can be estimated by the hydrogenic formula

$$E_{nl} = E_{\rm exc} - R(\frac{z}{n-\mu_l})^2, \tag{1}$$

where E_{nl} is resonance energy for a given nl state, $E_{\rm exc}$ is core-excitation energy of recombining ion, z is the charge state of recombining ion, and R is the Rydberg energy.

Resonance strengths

The resonance capture strength are related to autoionization rates by the detailed balance. It can be written as

$$S_{ij}^{\rm cap} = \frac{g_j}{2g_i}\frac{\pi^2\hbar^3}{m_e E_{ij}} A_{ji}^a, \tag{2}$$

where m_e denotes the electron mass, g_j and g_i represent respectively the statistical weights of j and i, E_{ij} is the resonance energy.
The DR (TR) resonance strength is given by

$$S_{ij} = S_{ij}^{\rm cap} B_j^r, \tag{3}$$

where B^r indicates radiative branching ratio. It can be defined iteratively as

$$B_j^r = \frac{\sum_f A_{jf}^r + \sum_{j'} A_{jj'}^r B_{j'}^r}{\sum_k A_{jk}^a + \sum_f A_{jf}^r + \sum_{j'} A_{jj'}^r}, \tag{4}$$

here A_{jf}^r is radiative decay rate from j to f, the final states f lie below the ionization limit, j' is the low-lying autoionizing levels. $B_{j'}^r$ is the radiative branching ratio for radiative stabilization of j'.

Results

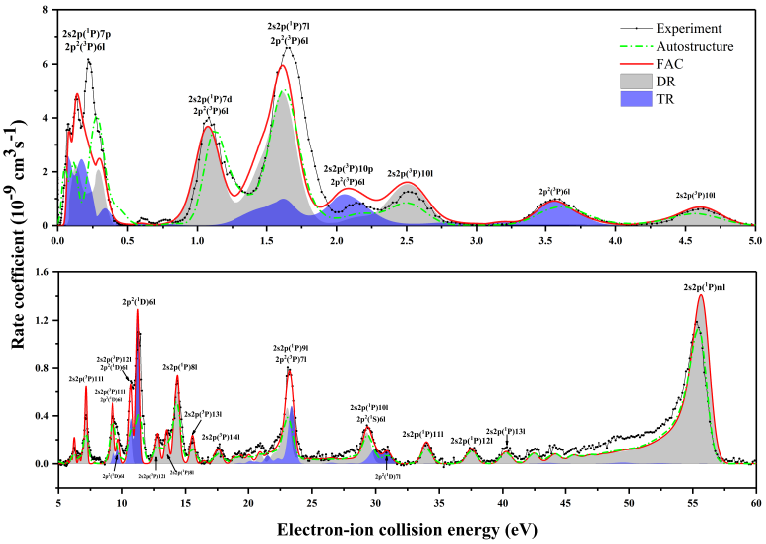

Fig.1 Comparison of the present merged-beam rate coefficients (red solid line) with the measured recombination spectrum (black data points). The present DR and TR parts are shown by the gray shaded areas and the blue shaded areas, respectively. The Autostructure calculations are presented by the green dash dot line.

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P03

Direct Simulation Monte Carlo simulations of laser-produced plasma expansion using SPARTA

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In laser machining, when the incident pulsed laser is strong enough to remove layers from the material target, a laser-produced plasma (LPP) forms, which is widely applied from material characterization to thin film deposition. LPP has been used in pulsed laser deposition to grow complex films with good stoichiometry [1]. A good model of the plasma expansion dynamics allows us to better predict the thickness distribution of the resulting film, especially considering the inherently narrow angular distribution of typical LPPs.

We model the LPP expansion using Direct Simulation Monte Carlo method [2], which treats the plasma constituents as representative particles and evaluates the particle interactions stochastically–in contrast with the deterministic modelling in molecular dynamics. We used SPARTA (Stochastic Parallel Rarefied-gas Time-accurate Analyzer) [3], which is an open-source code, to implement the expansion of the LPP from a copper target to a model substrate. The ablation is assumed to be caused by a nanosecond pulsed laser with a rectangular beam spot, and the particle emission input for SPARTA consists of copper atoms with a shifted Maxwellian velocity distribution [4].

We validated the model by demonstrating the flip-over effect, which is known as the apparent rotation of the plume aspect ratio as it propagates away from the target. By assuming the particle flux over a plane as representative of the film thickness distribution, we demonstrated the 90° flipping of the film distribution. This effect has also been experimentally observed in numerous studies and is considered a qualitative validation of LPP expansion models [5–6]. Modelling of LPP with DSMC paves the way for a facile and low-cost optimization of pulsed laser deposition, such as using mechanical filters of various geometries and exploring different deposition geometries, towards a more uniform film thickness distribution.

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P04

Correlation of Hydrogen Emission and Electron Properties in Low Temperature Plasma Conditions Close to Divertor-like Materials

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Understanding the behaviour of atoms and molecules in tokamak divertor plasmas is vital in order to gain information about the key processes that result in divertor detachment, crucial for the successful operation of future fusion devices [Krasheninnikov 2016].

The aim of this research is to understand atomic and molecular emission of hydrogen in a controlled low-temperature plasma environment close to divertor-like materials. The study combines electron property measurements, made using Langmuir probes, with plasma emission measurements, in an ICP discharge source. A sample heater was used to insert carbon and tungsten surfaces into the plasma. This allows the material temperature and surface conditions to be varied, while the discharge ICP environment allows the plasma conditions to be varied in a controlled way. Analysis of the set of measurements provides insight into how plasma and material conditions influence atomic and molecular emission.

For these experiments, the pressure and power were varied from 0 to 10 Pa and 10 to 300 W respectively, which provided a variety of electron properties, with densities of 10^{16} - 10^{18} m^{-3}, electron temperatures of 1 - 6 eV, and a range of electron energy distributions. Emission intensities were measured over a range of wavelengths, focusing on atomic emission of the H-alpha and H-beta lines and molecular emission in the Fulcher Band. The temperature of the carbon or tungsten surfaces was varied in the range of 100-1200C.

The experimental data was used to correlate hydrogen emission with plasma and surface conditions. These results will be compared with results from a 0-D collisional radiative model, and also used to inform emission measurements planned for the current MAST-U campaign in the Super-X divertor [J Harrison, 2019].

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P05

A Study of the Required Balmer-Lines for Integrated Data Analysis Systems in Tokamak Divertors

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Integrated data analysis (IDA) systems, based on Bayesian inference, offer the potential to describe entire divertor poloidal cross sections in terms of electron temperature, T_e, electron density, n_e, and neutral density, n_0 [1]. Such IDA systems rely heavily on heavily on multiple, wavelength-filtered, camera diagnostics owing to these diagnostics having a wide spatial coverage over the divertor. How accurately T_e, n_e and n_0 can be inferred depends on the combination of diagnostics included in the IDA. The complicated emission models of spectral lines, comprised of excitation and recombination emission (already simplified by provisionally ignoring plasma-molecule interactions), makes it challenging to decipher what information is held by different spectral line combinations in the IDA. To address that question, research has been performed to interrogate the information held by different Balmer-lines ($n \rightarrow 2$ Deuterium transitions) and so inform the lines required to be used in the IDA going forward.

Using SOLPS as a guide, different 'true' plasma conditions (that can be plausibly found in the MAST-U divertor: $(0.5 < T_e < 45)eV$; $(10^{18} < n_e < 3 \times 10^{21})m^{-3}$; $(10^{16} < n_0 < 10^{20})m^{-3}$) were used to simulate different data sets for Balmer line emissivities. The IDA, with different line combinations, was used to infer the maximum a posteriori (MAP) estimation of T_e, n_e and n_0 for each data set and these MAP estimations were compared to the 'true' plasma conditions that were used to make that data set. To quantify how much information is held by a combination of lines, an inference metric, ϵ_D^P, has been defined to be the percentage of, plausible, plasma conditions for which a MAP estimate of within 30% of the 'true' plasma value was achieved. Here, P is the inferred parameter and D is the diagnostics used.

It has been found that Balmer lines held more information on T_e ($\epsilon^{T_e}_{D_\alpha,D_\beta,D_\gamma,D_\delta,D_\varepsilon} \sim 92\%$) and n_e ($\epsilon^{n_e}_{D_\alpha,D_\beta,D_\gamma,D_\delta,D_\varepsilon} \sim 100\%$) than for n_0 ($\epsilon^{n_0}_{D_\alpha,D_\beta,D_\gamma,D_\delta,D_\varepsilon} \sim 27\%$). It was also found that the Balmer lines held more information for T_e in plasma existing in recombination-majority regions ($\epsilon^{T_e}_{D_\alpha,D_\beta,D_\gamma,D_\delta,D_\varepsilon} \sim 100\%$) than plasma existing in excitation-majority regions ($\epsilon^{T_e}_{D_\alpha,D_\beta,D_\gamma,D_\delta,D_\varepsilon} \sim 89\%$). This is deemed due to the excitation emission depending on n_0 and so n_0's inaccurate inference permits a range of possible excitation emissions and so reduces the information held on T_e in excitation-majority regions. With just two lines used in the IDA, it was found that in recombination-majority regions an $n < 5$ Balmer line is required to be used with an $n > 5$ Balmer line to provide the most information for all inferred parameters ($\epsilon^{T_e}_{D_\alpha,D_\varepsilon} \sim 80\% > \epsilon^{T_e}_{D_\delta,D_\varepsilon} \sim 40\%$). This is likely due to the IDA's tendency to assume all emission in a recombination majority region is from recombination alone (vice versa for excitation). $n < 5$ Balmer lines have a greater relative excitation contribution to their emission than for $n > 5$ Balmer lines [2] and so the provision of a line that has more excitation emission in a recombination-majority environment prevents the assumption of all emission being from recombination and so increases the information held on T_e and n_e (and vice-versa for the excitation-majority region).

Consequently, for adequate inference of T_e and n_e across the entire divertor region, minimally the D_α line and an $n > 5$ Balmer line is required. Further, additional information is required to accurately infer n_0. This is likely to become increasingly important when plasma-molecule effects are added to the emission models.

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P06

The Next Generation of Collisional Radiative Modelling for Tokamak Plasmas

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Collisional Radiative (CR) modelling has been of interest to the plasma physics community for decades, and provides a powerful tool for predicting the spectral emission and state population behaviour of plasmas in various regimes. The ITER project will require sophisticated CR codes to provide predictive capability across all modes of operation, as well as during periods of instability, especially during tokamak disruption events, wherein runaway electron populations can form and threaten the integrity of the tokamak machine. Herein we present a cursory summary of the motivation for development of robust CR models, provide a surface level summary of some of the physics included in contemporary codes, and provide simulations of ionic populations in relevant plasma regimes using one contemporary CR package, FLYCHK. We further explore the limitations present in these simulations, and examine where improvement is required in the next generation of CR models to provide sufficient predictive power for the ITER project. We conclude by providing recommendations for the inclusion of improved atomic and scattering data, semi-empirical models of Runaway Electron population formation, and the development of alternative models of the time-evolution of tokamak plasmas.

P07

Spectroscopic Analysis of Reactive Species in a Non-equilibrium Cold-Plasma Based Plasma Activated Water

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Non-equilibrium cold plasmas produced in the laboratories have demonstrated the synthesis of radicals which are thought to arise from the reactive oxygen species (ROS) and reactive nitrogen species (RNS), collectively referred to as RONS. Plasma activated water (PAW) generated from cold plasma received much attention now a days in the field of Medicine, Food, Agriculture, and Environment [1]. To increase PAW's bactericidal effectiveness, it is necessary to understand how cold plasma forms the essential reactive species in both short- and long-term water interactions. Controlling the RONS chemistry in PAW can provide potential of designing the best RONS chemistry for various purposes (e.g., fruits and vegetables decontamination, functionalization of various food products, medication of chronic wounds, achieving rapid seed germination, development of optimal plants and other various applications in biology and agriculture, etc.). In this study, UV-VIS technique has been utilized to precisely quantify the changes in the concentrations of these RON in PAW. The PAW is generated through indigenously developed large volume surface dielectric barrier discharge based cold plasma and narrow cold plasma Jet. To tailor the PAW to achieve specific biological response UV-VIS spectroscopy is the most widely used technology for characterization of cold plasma [2]. The repeated measurements during plasma activation have been demonstrated as the significant benefit of UV-VIS spectroscopy. For this the absorption spectra of RONS in PAW recorded from 200 to 800 nm has been analysed. Efforts are underway to demonstrate that the plasma spectroscopy, which focuses on the atomic and molecular emission spectroscopy of low temperature plasma, would be an extremely strong diagnostic technique in a non-equilibrium cold-plasma based Plasma Activated Water. The results of these efforts will be presented.

Keywords: Non-equilibrium cold plasma, Reactive oxygen species (ROS), Reactive nitrogen species (RNS).

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P08

Energy levels, lifetimes, wavelengths, weighted oscillator strengths and transitions rates of He-like Zr

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In recent years, there have been extensive studies, both experimental and theoretical of helium isoelectronic sequence [1, 2, 3]. In this work, energy levels, wavelengths, weighted oscillator strengths, transitions rates, lifetimes have been calculated for the lowest 71 odd and even parity states arising from the $1s^2$ and $1snl$ $(n = 1 - 6, 0 \leq l \leq n - 1)$ configurations of He-like Zr. The calculations were performed using the Multiconfigurational Dirac-HartreeFock (MCDHF) [4], followed by the Relativistic Configuration Interaction (RCI) methods. For the accuracy of our results, we have implemented parallel calculations using a Flexible Atomic Code (FAC) [5] by introducing the Relativistic Many-Body Perturbation Theory (RMBPT) method. Transition probabilities are reported for all E1, E2, M1 and M2 transitions. Breit interactions and quantum electrodynamics effects were included in the RCI calculations.
Comparisons were made with other available theories reported in the literature [6, 7, 8, 9]. A good agreement between them has been found, which confirms the reliability of our results. The present complete and consistent results can be used to facilitate the identification of many observed spectral lines in astrophysical and plasma fusion.

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P09

MEASUREMENTS OF THE ABSOLUTE DENSITY OF GROUND STATE RO-VIBRATIONALLY EXCITED D_2 MOLECULES IN AN ECR-DRIVEN PLASMA BY MEANS OF SYNCHROTRON RADIATION

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The investigation of the production mechanisms of electronic $X^1\Sigma^+$ ground state ro-vibrationally excited molecules D_2*(v”>0,J”) on surface materials is relevant for fusion plasmas either for the plasma heating or for the divertor targets’ shielding [1]. In cold plasma physics, and particularly with regard to negative ion source development for neutral beam injection (NBI) systems, these excited molecules are of particular interest since they are one of the main reactants of the Dissociative Electron Attachment (DEA) reaction which is commonly accepted as the dominant path towards the production of negative ions in sources based on the volume production concept [1,2]. Electron cyclotron resonance (ECR) ones driven by dipolar plasma modules [3] are a representative example of this type of source. The production of the aforementioned excited molecules takes place in the plasma bulk but may also result from surface reactions. Among the most probable is the Recombinative Desorption reaction. Therefore it is worth exploring the influence of various plasma facing materials on their production, with the goal of determining a more efficient material. It is evident that an enhancing trend is accordingly reflected in the negative ion yield, which is highly desirable.

In this context, a deuterium plasma is studied in the ECR-driven source SCHEME II+ which is coupled to the VUV Fourier Transform Spectrometer at the DESIRS (Dichroïsme et Spectroscopie par Interaction avec le Rayonnement Synchrotron) beamline of the SOLEIL synchrotron (Saint-Aubin, France). Absorption spectra are recorded in different operational conditions, i.e. for pressures ranging from 1 – 36 mTorr, under constant microwave power (150 W). Both bare Quartz and material covered surfaces are considered. For the latter case, fresh in-situ magnetron sputtered thin films of tantalum (Ta) and tungsten (W) upon the Quartz surface are investigated. Preliminary observations do not indicate any difference as the material is changed. However, in a previous study [1] where commercially available foils of the same materials were placed in the interior surfaces of the same source, a drastic modification of the excited molecule population was clearly demonstrated. This may suggest that the structural properties of the sputtered surface influence the Recombinative Desorption mechanism and thus the production of the ro-vibrationally excited molecules. This subject is currently under scrutiny.

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P10

Study of Particle in Cell Method to Obtain Laser Thomson Scattering Spectrum to calculate Density in a plasma same as ITER plasma

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One of the most accurate diagnostic tools in Tokamak plasmas is Thomson scattering (TS) [1]. In this method a laser light passes through a plasma and undergoes Thomson scattering. By investigating the frequency spectrum of scattered light we can demonstrate plasma density and temperature. Here we simulate non- collective Thomson scattering that is related to single particle behavior of system from a plasma with ITER's parameters [2] by using Particle in cell method (PIC) [3] to study PIC ability for simulating non-statistical systems. For studying a system consists of particles it is necessary to solve the motion equation for every single particle, so for N particles N^2 equations should be solved that needs significant memory and processor resources. PIC is a simplifying method in computational plasma physics. It works based on statistical behavior of system. Super particles are considered in PIC method so that every super particle is composed of a number of system's real particles and the motion equations of particles will be solved for these super particles that way the number of motion equation will be reduced.
Here non- collective TS of a polarized laser light passing through a plasma with a density of $3.00 \times 10^{13}\ \mathrm{cm}^{-3}$ same as ITER plasma is simulated using 2D/3V PIC code (XOOPIC). Laser wavelength, intensity and FWHM are $\lambda_i = 0.8\ \mu\mathrm{m}$, $I_i = 5.00 \times 10^{15}\ \mathrm{W/cm}^2$ and 50.00 fs, respectively. Calculated scattered power predicts that the plasma density is about $2.64 \times 10^{13}\ \mathrm{cm}^{-3}$ which is in a good agreement with its real value. The properties of scattered power are dominated by non-collective effects and the polarization of the scattered wave is affected by the non-relativistic condition. Results show that PIC can simulate the non-collective TS so PIC ability to simulate a non-statistical system with a high accuracy is verified. The accuracy of TS as a diagnostic tool to measure the plasma features like density is reconfirmed as a secondary result.

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P11

Plasma Molecule Interactions and Their Influence on Detachment in Magnetically Confined Fusion Devices.

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Plasma detachment is considered essential for the successful operation of future fusion devices such as ITER and DEMO, as it can reduce the target heat flux by orders of magnitude. The reason for its necessity is the avoidance of unsustainable heat loads at the divertor. During detachment, atomic and molecular reactions induce simultaneous power, momentum, and particle losses, leading to a reduction in particle flux to the divertor plates in a tokamak [1].

Divertor spectroscopy is essential in diagnosing detachment. Plasma-atom and molecule interactions result in *excited hydrogen atoms*. Analysing the Balmer line series emitted by those atoms, yields important information about the conditions of hydrogen plasmas. Excited atoms from molecular break-up involving reactions with molecular ions play a significant role in Balmer line emission through chain processes and cannot be ignored in the diagnosis of detachment [1, 2, 3]. Molecules may play a very important role in the detachment process itself. Particle and power loss may occur through plasma-molecule reactions; and momentum and power transfer through collisions [1, 2]. Collisions between the plasma and the molecules can result in *excited molecules*, leading to emission of the Fulcher band from electronically excited molecules [4].

The aim of this PhD project is to perform a deep analysis of high-resolution Fulcher band data obtained by divertor spectroscopy in the MAST-U tokamak, in order to gain a better understanding of the role of molecules in detachment. Plans include Fulcher and Balmer line analysis and comparison of measurements with simulation data generated by synthetic diagnostics employed on SOLPS-ITER simulations. This approach requires modelling the Fulcher emission band, which would be useful tool for the community.

Such analysis is intended to provide input on the populations of the excited levels of the molecules. Monitoring those distributions is important as they have large model uncertainties whilst they have a strong impact on the various reaction rates between the plasma and the molecules. For example, it is known that the distribution of vibrational states in molecules has a significant effect on the formation of D_2^+ and D^-.

Ultimately, determining the utility of Fulcher emission measurements during plasma detachment is an important goal. It is explored whether the Fulcher emission brightness may be used as a temperature diagnostic; as there is a minimum electron energy required to excite molecules electronically.

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