A Generalized DARC RMPS Approach for the Electron-Impact Ionization and Excitation of C I from Ground and Excited States

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Abstract

Within magnetically confined fusion plasmas, the rate of ionization is often dominated by ionization from excited states. For this to be modelled realistically, the ionization data needs to be coupled with accurate excitation data. We have calculated new electron-impact ionization and excitation data for the lowest lying 42 levels of neutral carbon (C I) using a generalized DARC R-matrix with Pseudostates (DRMPS) approach, which we have developed. The DRMPS approach allows for both ionization and excitation rates to be calculated from the same initial structure model, and makes excited state ionization calculations more readily available for non-hydrogenic systems. There is good agreement in both the ionization and excitation data with available measurements and other theoretical calculations. With this new data set we show, through collisional-radiative modelling, that the ionization contributions from excited levels will have a non-trivial effect on the effective ionization rate coefficients of C I within magnetically confined plasmas.

Why Carbon?

Carbon is an important species when considering tokamaks due to its presence as an impurity species, and its role as a material in plasma facing components.

Figure 1: The Interior of the Mega Amp Spherical Tokamak (MAST) Upgrade. The plasma facing components are constructed of carbon. *Credit: UKAEA*

Impurities of only 0.1% can quench the fusion reaction.

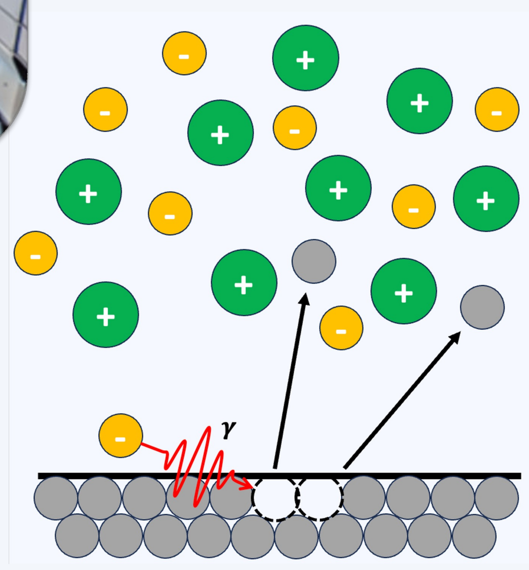

Figure 2: The erosion of impurities from the plasma facing components will mix with the plasma reactants.

DRMPS Methodology

Our C I target structure is developed using the General-purpose Relativistic Atomic Structure Package (GRASP[0]). This acts as our starting point for the *R*-matrix calculations. The *R*-matrix approach is performed using the Dirac Atomic *R*-matrix Codes (DARC).

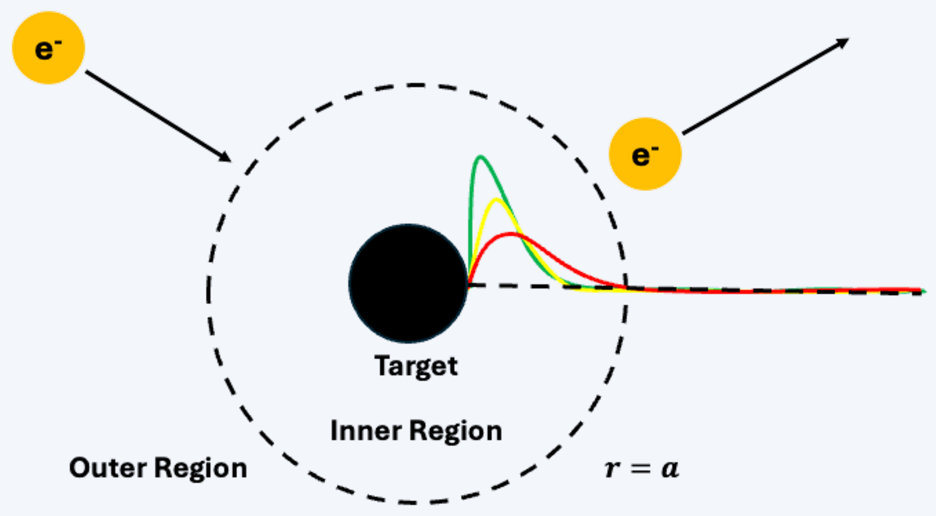

Figure 3: Schematic representation of the R-matrix approach.

Pseudostates are included in our structure to represent the continuum above the ionization potential (I_0).

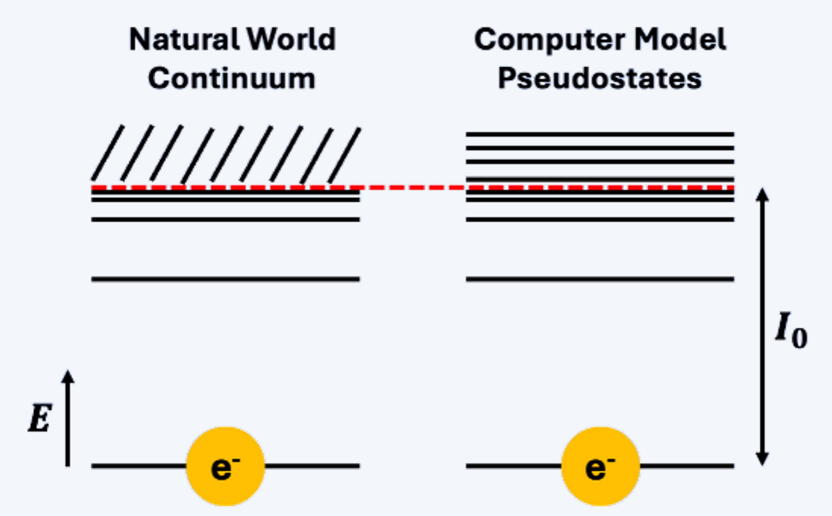

Figure 4: The incorporation of pseudostates into the R-matrix calculation.

We have generalized the DRMPS approach to allow for calculations of non-hydrogenic systems.

Advantages of DRMPS

- ✓ Can perform both ionization and excitation calculations from the same target structure.
- ✓ Can easily scale up to more computationally intensive calculations.
- ✓ Makes excited state ionization calculations more readily available for non-hydrogenic species.

C I Ionization

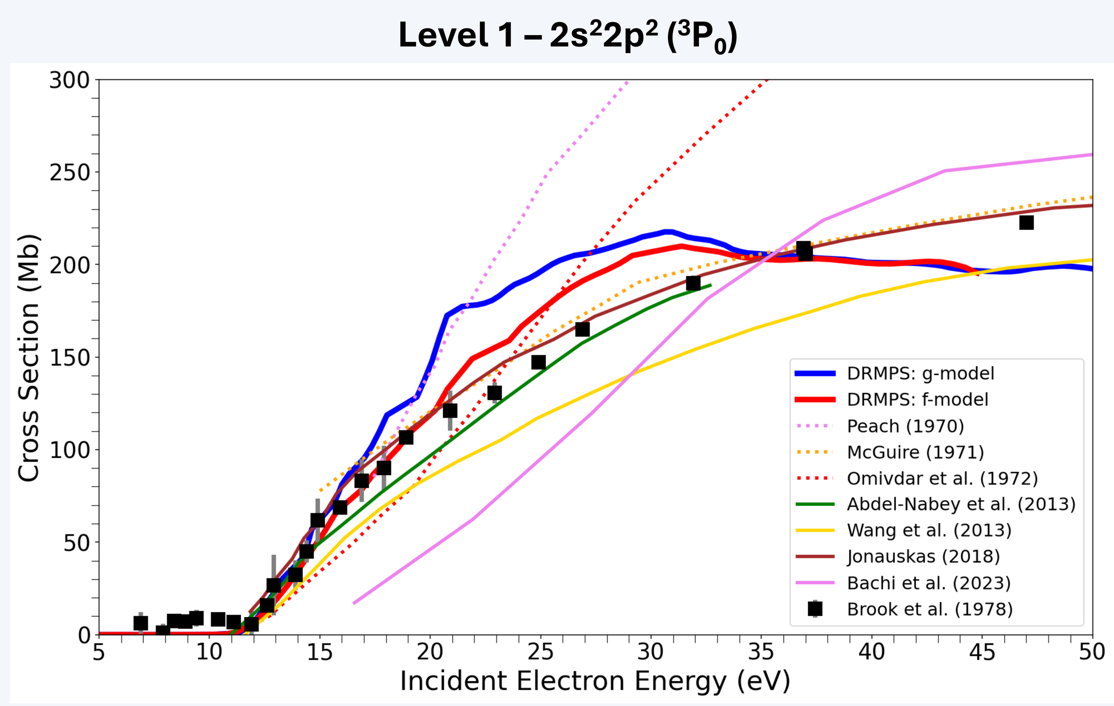

Figure 5: The ionization cross sections of C I from the ground level.

Our cross sections for the ground state of C I are in good agreement with the available experimental and theoretical data.

First comprehensive set of level-resolved excited state ionization cross sections for C I

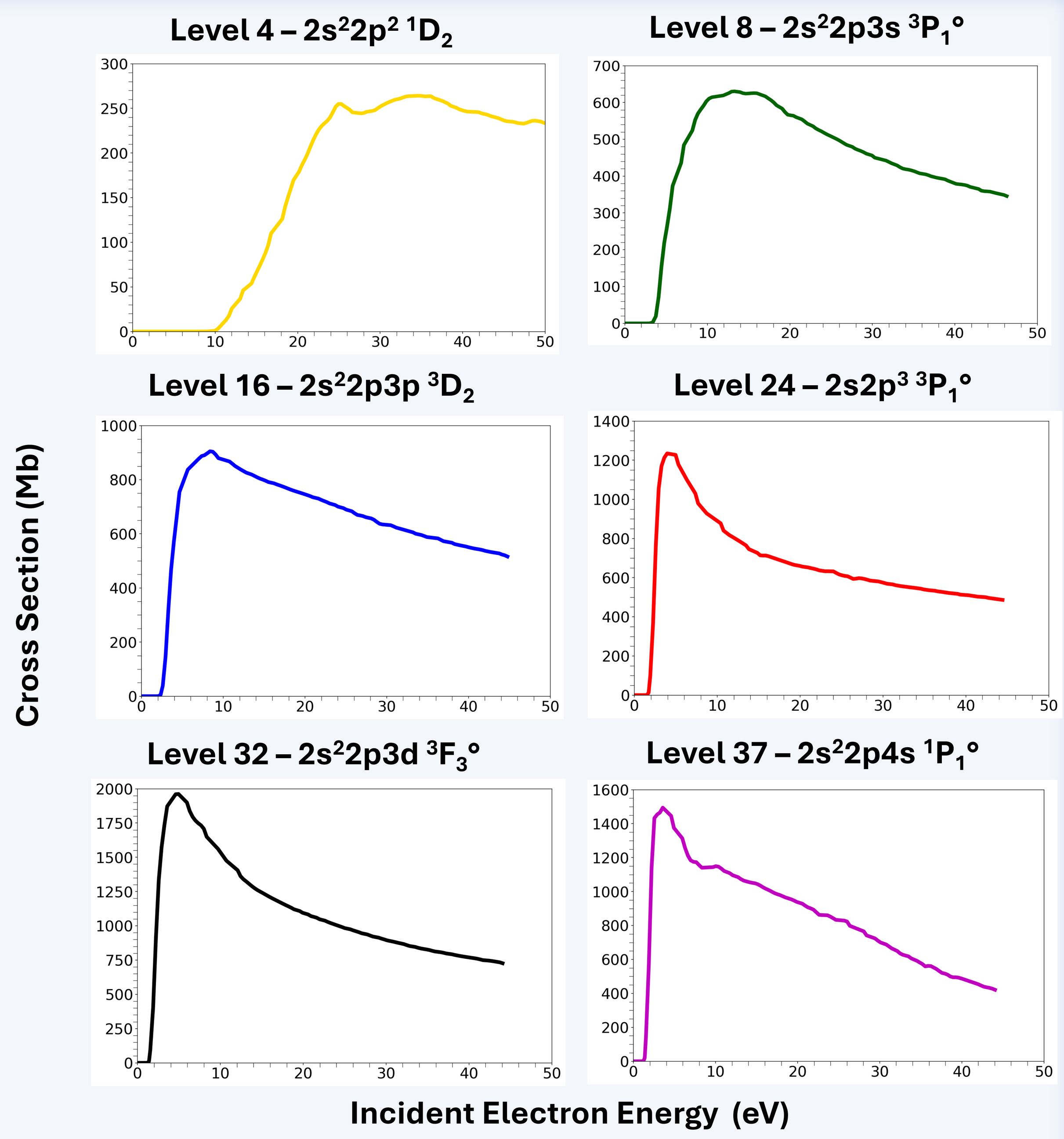

Figure 6: The ionization cross sections of C I from a selection of excited levels

C I Excitation

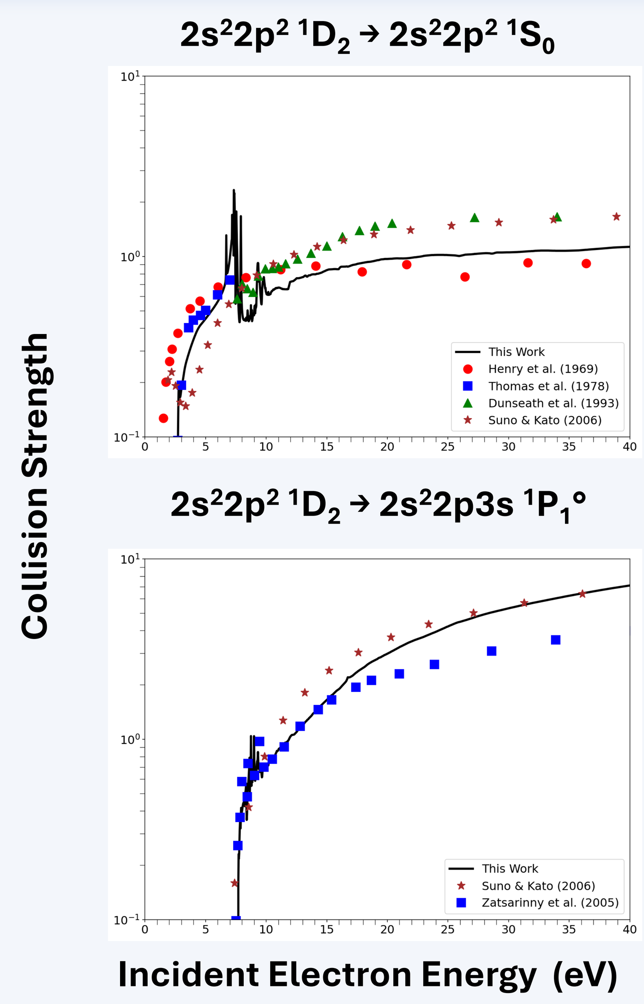

Figure 7: A comparison of the C I electron-impact collision strengths between our DRMPS calculations and other theoretical calculations.

We have calculated accurate electron-impact ionization and excitation data for the lowest lying 42 levels of C I.

Effective Ionization

Using our new data set, we explored the extent to which excited state ionization contributes to the effective ionization rate coefficients (SCDs) for magnetically confined plasmas. This was performed using COLRADPY.

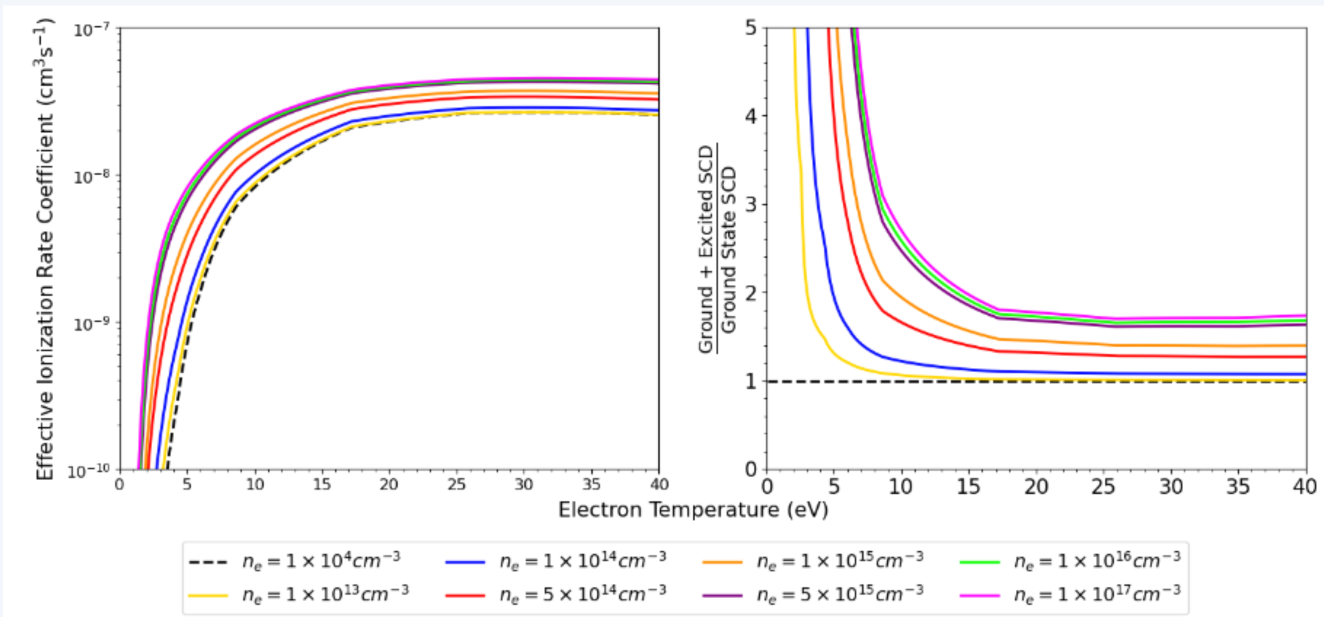

Figure 8: The SCDs of C I using the electron-impact ionization and excitation data calculated in this work.

Excited state ionization is making a non-trivial contribution to the SCDs within magnetically confined plasmas

Conclusions

- ➢ Newly developed generalized DRMPS approach for non-hydrogenic systems.
- ➢ Electron-impact ionization and excitation rates for C I from the same target structure.
- ➢ DRMPS allows level-resolved excited state ionization rates to be calculated.
- ➢ Excited state ionization makes a non-trivial contribution to the total ionization of carbon within magnetically confined plasmas.

View our paper

Ionization calculations for neutral tungsten (W I) are ongoing