Breit-Pauli/Dirac R-matrix calculations

(electron-impact excitation/ionisation/recombination)

in support of fusion plasma diagnostics

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Decennial IAEA Technical Meeting on Atomic, Molecular and Plasma–Material Interaction Data for Fusion Science and Technology. (Helsinki Jul 15-19 2024)

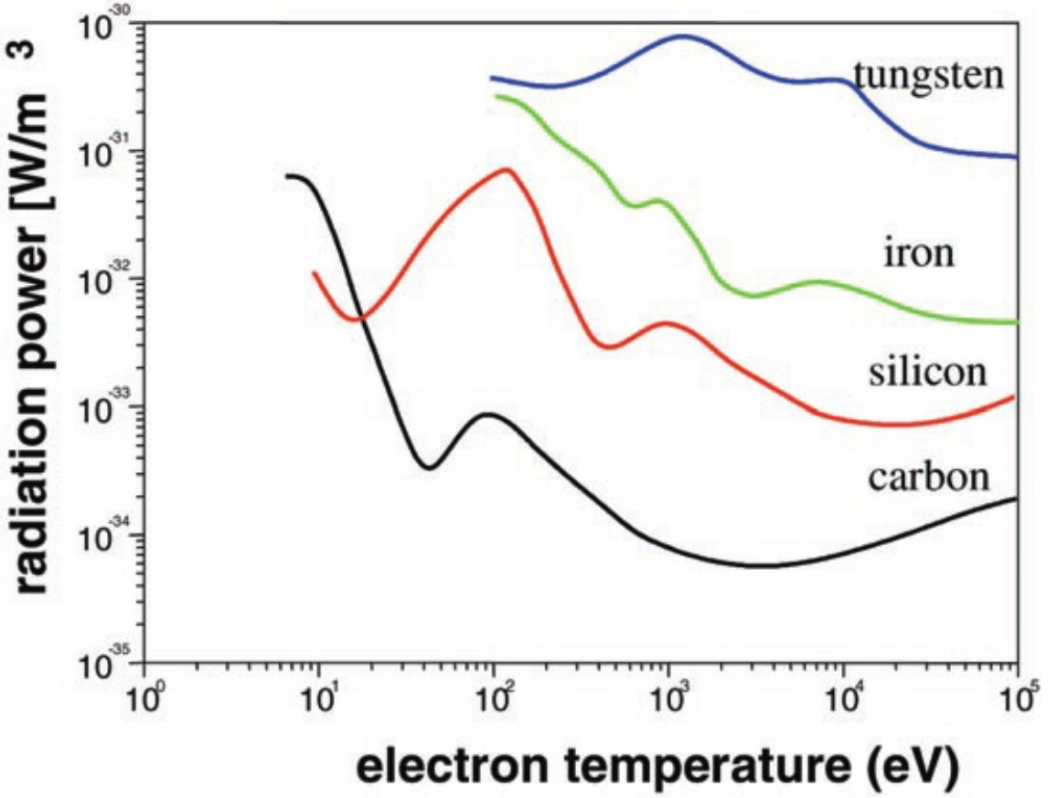
Funded in part by the UK STFC consolidated astrophysics grant to QUB, Auburn/QUB subcontract to QUB and ERC 'Heavy Metal' grant

Talk Overview

- Motivation for studying tungsten
- R-matrix (RMPS) methodology and how we scale-up for heavy systems. Terminology used throughout.
- Electron-impact excitation of Tungsten W I-III and how we compare with the CTH (Auburn)experiments
- Electron-impact ionisation of W III and assessing the impact of ground and metastable RMPS ionisation on impurity influx determination (SXB).
- Electron-impact excitation of Ar II by three different R-matrix methods with an attempt to constrain uncertainty.

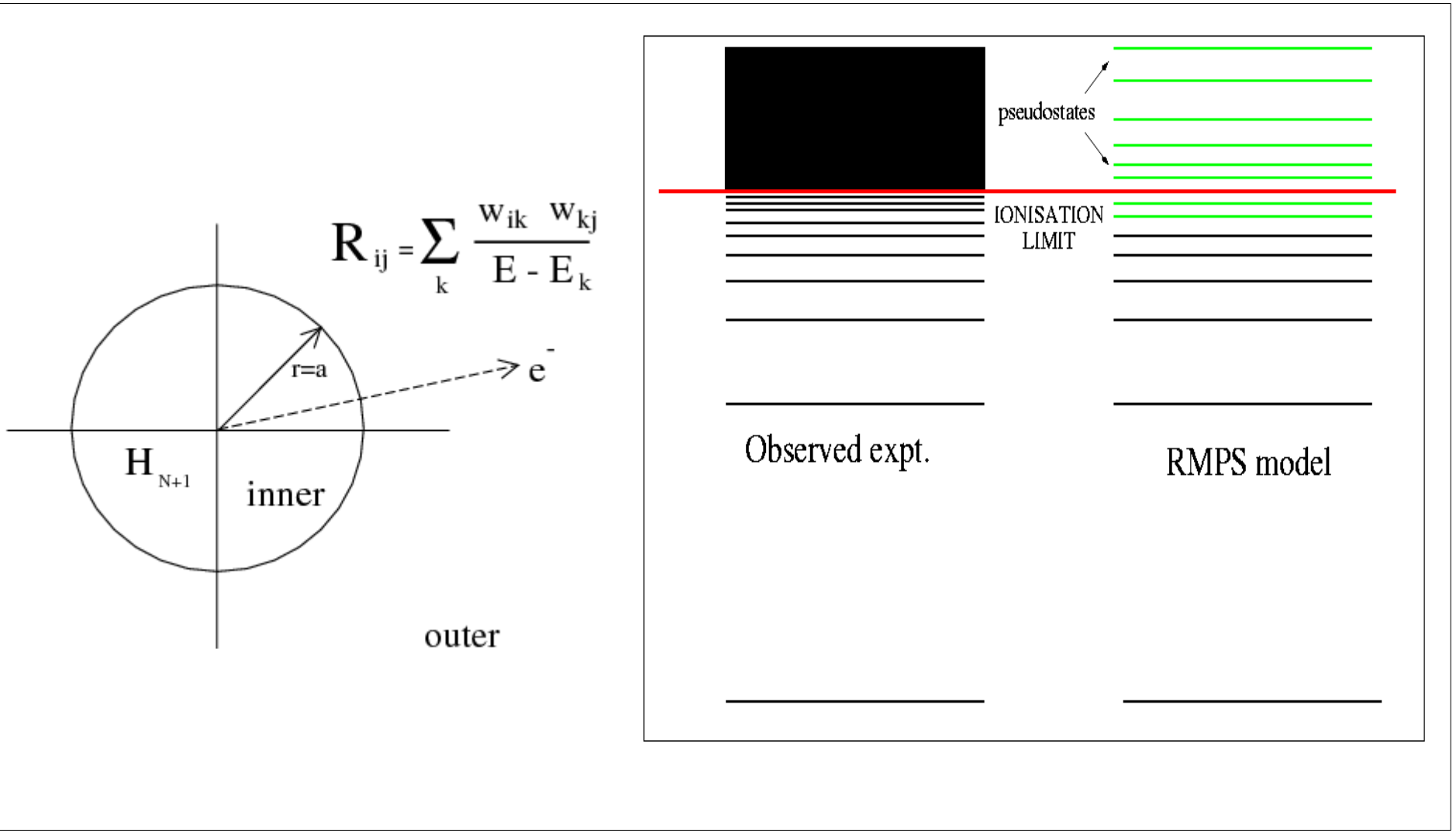
Tungsten is still one of the leading candidates for PFCs(plasma facing components), i.e. divertor

- ***Allowable impurity concentration lower for high-Z materials***
  - High-Z materials radiate much more than previously used materials
  - Radiation significant enough to denigrate plasma performance
    - Concentration needs to be less than ~1E-4 (Putterich)
  - Need to accurately quantify and minimize erosion of PFC.



Although unwanted, the impuity influx must be categorized, which is modelled by an SXB ratio, which is in turn dependent on electron impact excitation and effective ionisation rates.

One slide R-matrix/RMPS overview



$$\Psi_k(x_1 \ldots x_{N+1}) = A \sum_{ij} c_{ijk} \bar{\Phi}_i(x_1 \ldots x_N, \hat{r}_{N+1}\sigma_{N+1}) u_{ij}(r_{N+1}) + \sum_j d_{jk} \phi_j(x_1 \ldots x_{N+1})$$

Quantifying Wall Erosion impurity influx : SXB ratio, underpinned by accurate atomic structure, excitation & ionisati

- The intensity of a spectral line can be related to its influx rate [Behringer PPCF 31 2059 (1989)]
- The number of ionizations per photon (S/XB) is directly proportional to the impurity influx

$$\Gamma = \int_0^\infty N_e N^z S^{z\to z+1}\,dx = \int_0^\infty N_e \frac{S^{z\to z+1}}{A_{i\to j}\frac{N_i}{N^z}}\left(A_{i\to j}\frac{N_j}{N^z}\right)N^z\,dx$$

$$= \int_0^\infty N_e SXB^z_{i\to j}\left(A_{i\to j}\frac{N_j}{N^z}\right)N^z\,dx$$

where $SXB^z_{i\to j} = \frac{S^{z\to z+1}(N_e,T_e)}{A_{i\to j}\frac{N_i}{N^z}(N_e,T_e)}$

Note electron temperature and density dependence

Electron-impact excitation using
parallel DARC code.

- Why it is difficult ? (next slide)
- What has been done
  overcome these difficulties? (end of section)
- From a structure perspective (the core of
  a collisional model) we now can shift
  to known NIST/experimental values before
  oscillator strength determination.

Snapshot of W I

Groundstate : 4f^14 5d^4 6s^2

Method : GRASP0 structure groundstate

+ 24 excited state configurations

(~7500 levels)

: Dirac R-matrix calculation

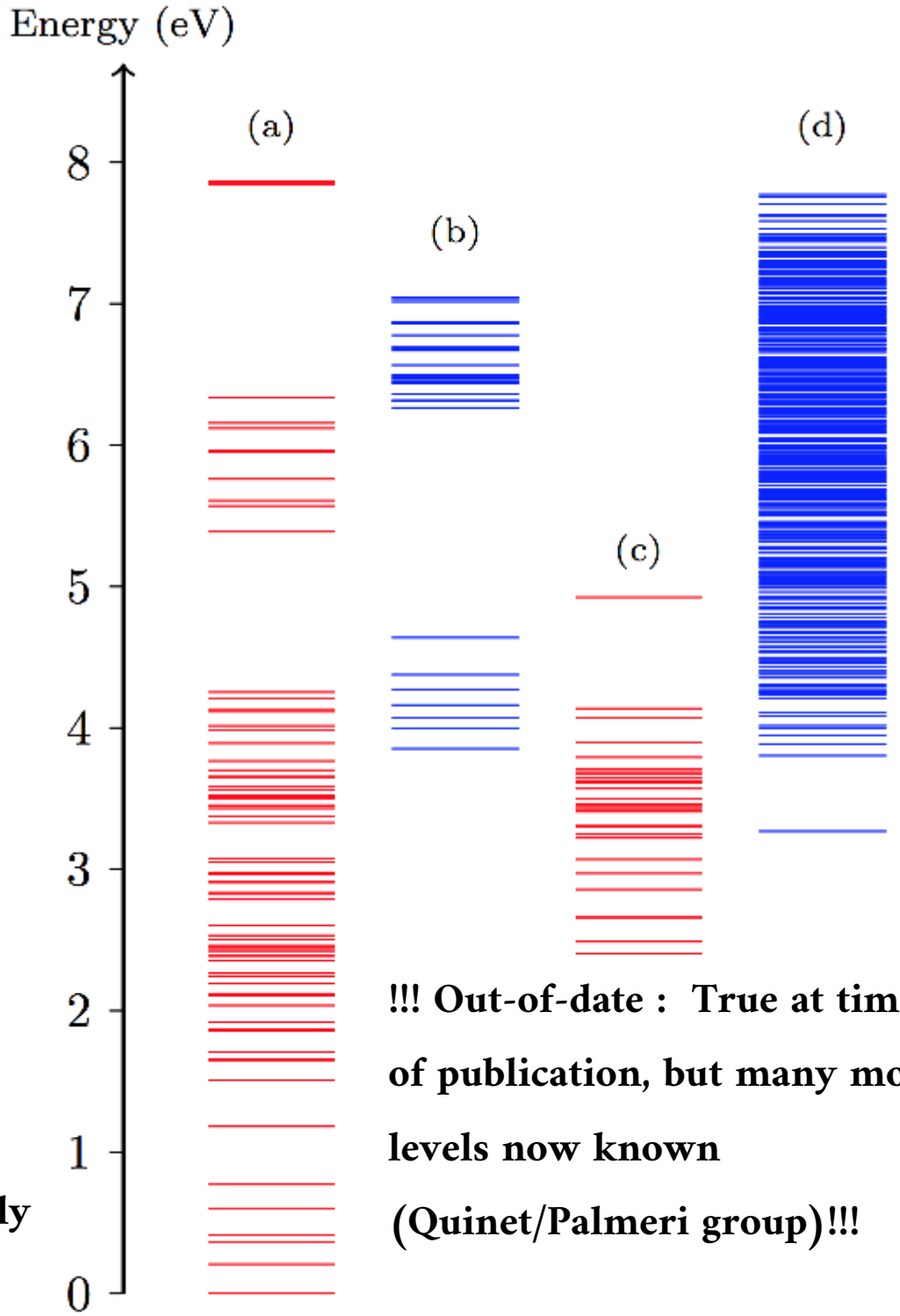
keeps 250 levels in the

close-coupling expansion

(a) Known (NIST/literature) even levels

(b) Known (NIST/literature) odd levels

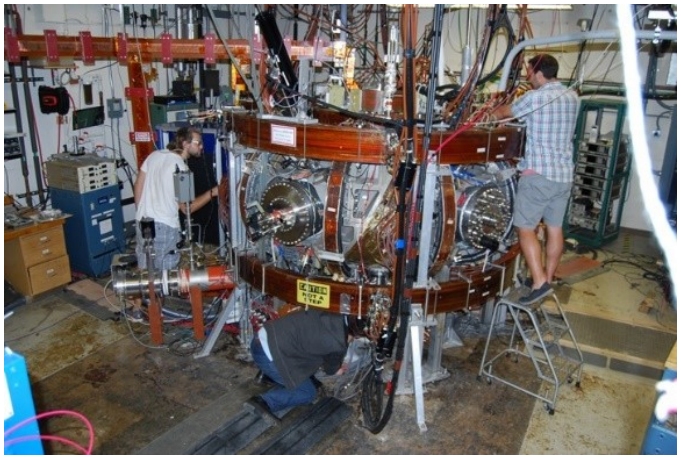
(c) & (d) unknown or at least only partially designated even and odd levels

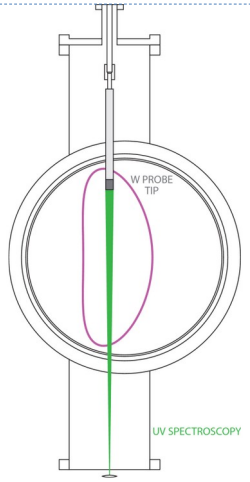


!!! Out-of-date : True at time of publication, but many more levels now known (Quinet/Palmeri group)!!!

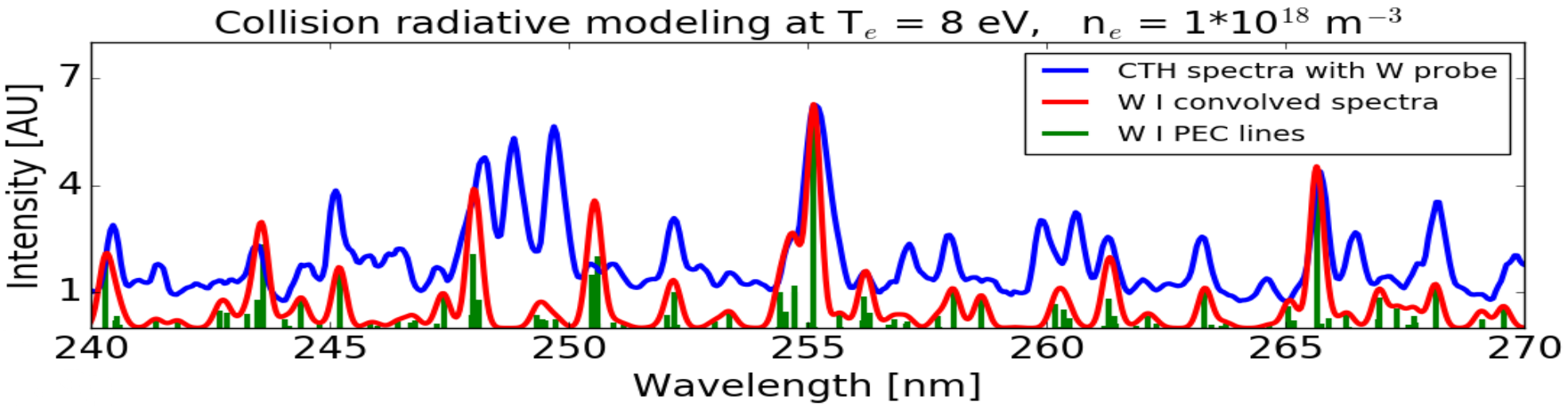
Compact Toroidal Hybrid (CTH) has been an invaluable test of the electron-impact excitation dataset

- The emission was indeed strongest in the UV!
- We identified 30 new tungsten spectral emission lines.
- Results in Johnson et al., Plasma Physics and Controlled Fusion, Volume **61**, 095006 (2019).

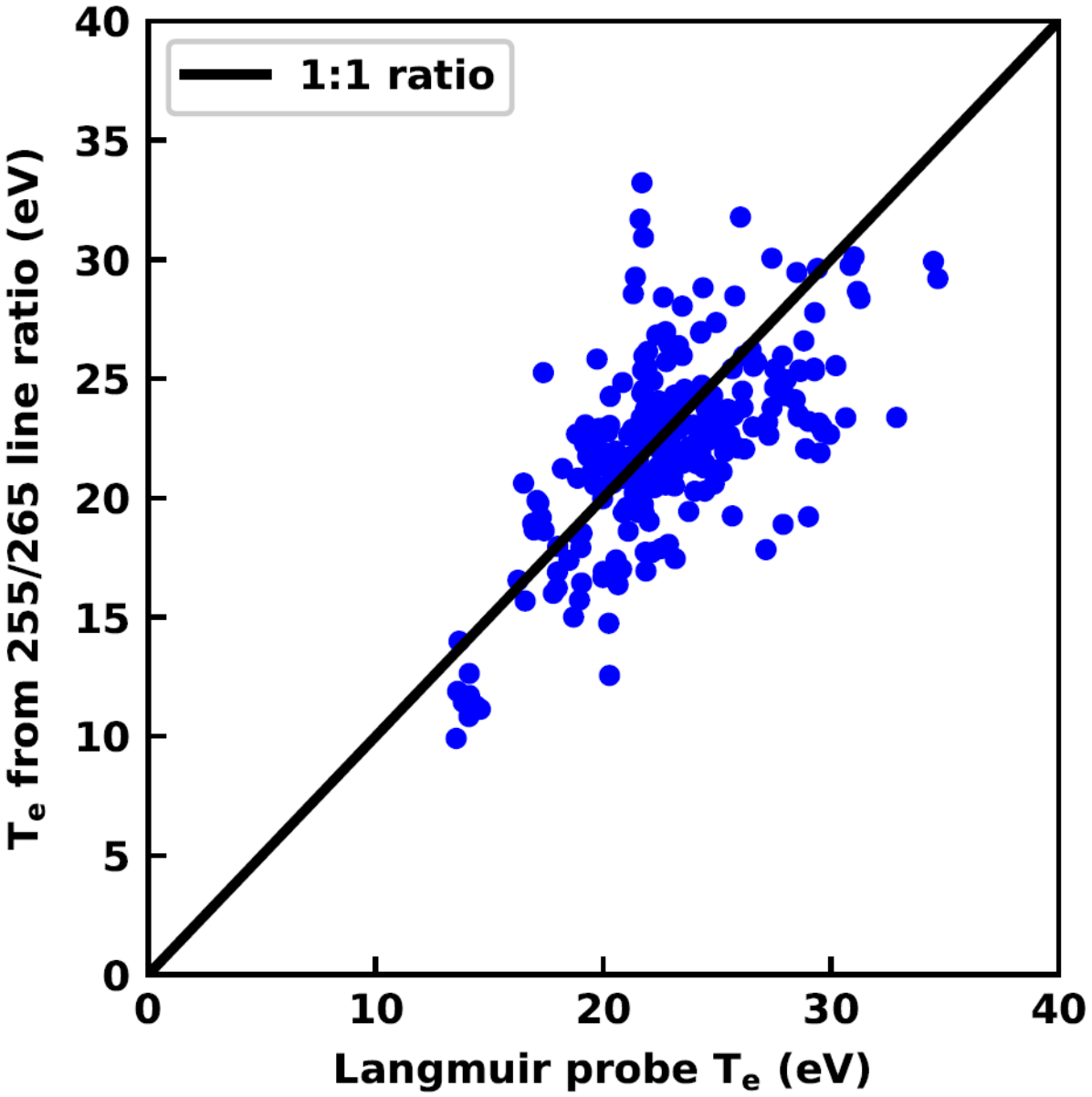




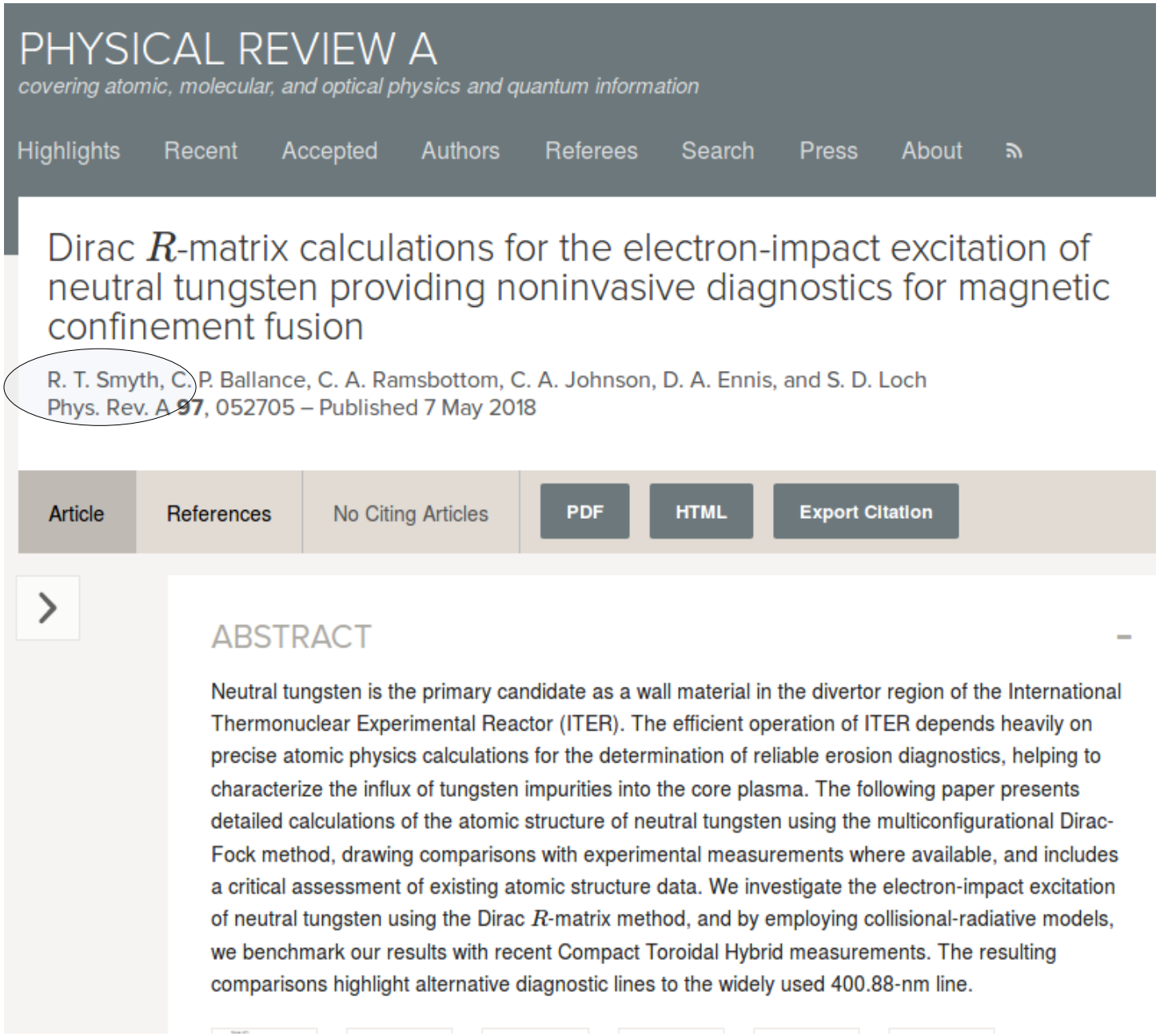
CTH cross section with probe and UV spectrometer line of sight



Temperature derived from lines within R Smyth W I adf04 file and those measured with a Langmuir probe on the Auburn CTH experiment.



Electron-impact excitation of neutral tungsten



PHYSICAL REVIEW A
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Dirac R-matrix calculations for the electron-impact excitation of neutral tungsten providing noninvasive diagnostics for magnetic confinement fusion

R. T. Smyth, C. P. Ballance, C. A. Ramsbottom, C. A. Johnson, D. A. Ennis, and S. D. Loch
Phys. Rev. A **97**, 052705 – Published 7 May 2018

Article References No Citing Articles PDF HTML Export Citation

ABSTRACT

Neutral tungsten is the primary candidate as a wall material in the divertor region of the International Thermonuclear Experimental Reactor (ITER). The efficient operation of ITER depends heavily on precise atomic physics calculations for the determination of reliable erosion diagnostics, helping to characterize the influx of tungsten impurities into the core plasma. The following paper presents detailed calculations of the atomic structure of neutral tungsten using the multiconfigurational Dirac-Fock method, drawing comparisons with experimental measurements where available, and includes a critical assessment of existing atomic structure data. We investigate the electron-impact excitation of neutral tungsten using the Dirac R-matrix method, and by employing collisional-radiative models, we benchmark our results with recent Compact Toroidal Hybrid measurements. The resulting comparisons highlight alternative diagnostic lines to the widely used 400.88-nm line.

W II : Dirac R-matrix calculation

J. Phys. B: At. Mol. Opt. Phys. **55** (2022) 175002 (15pp) https://doi.org/10.1088/1361-6455/ac8089

A Dirac *R*-matrix calculation for the electron-impact excitation of W^+

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Received 30 March 2022, revised 29 June 2022
Accepted for publication 11 July 2022
Published 11 August 2022

Abstract

Aims: tungsten has been chosen for use as a plasma facing component in the divertor for the ITER experiment, and is currently being used on existing tokamaks such as JET. W^+ plays an integral role in assessing the impurity influx from plasma facing component of tokamaks and subsequent redeposition. Together with previously calculated a neutral tungsten electron-impact dataset this study allows us to determine neighbouring spectral lines in the same wavelength window of the spectrometer, and detect if there is strong blending of overlapping lines between these two ion stages as well as providing ionisation per photon ratios for both species. The new data is to be used for tungsten erosion/redeposition diagnostics. *Methods*: a significantly modified version of the GRASP0 atomic structure code in conjunction with DARC (Dirac Atomic *R*-matrix Code) are used to calculate the Einstein *A* coefficients and collisional rates used to generate a synthetic W II spectrum. The W II spectrum is compared against tungsten spectral emission experiments. *Results*: this study is used to model the spectrum of W II, providing the predictive capability of identifying spectral lines from recent experiments. These results provide an integral part of impurity influx and redeposition determination, as the ionisation rates may be used to calculate S/XB ratios.

Overview of W II

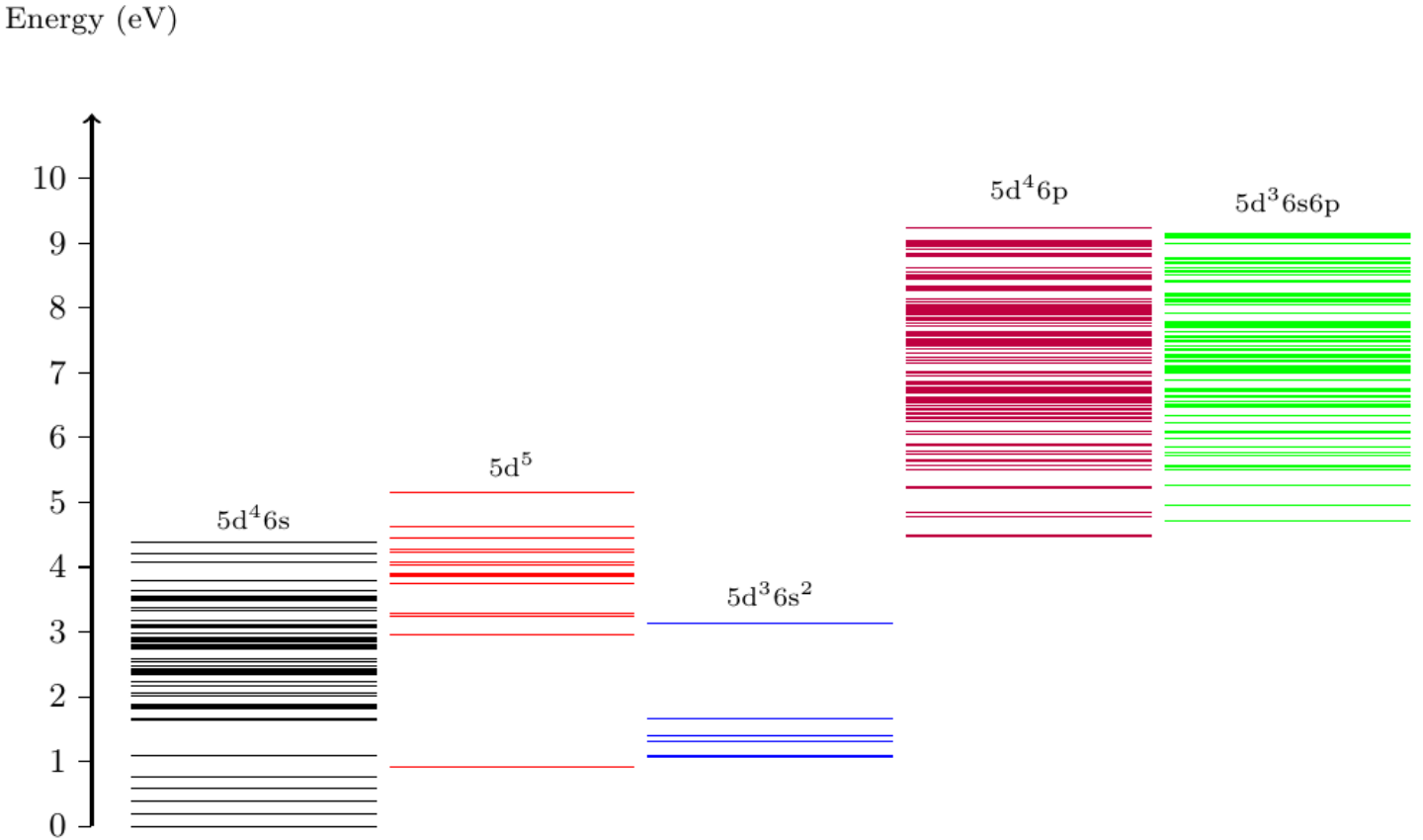
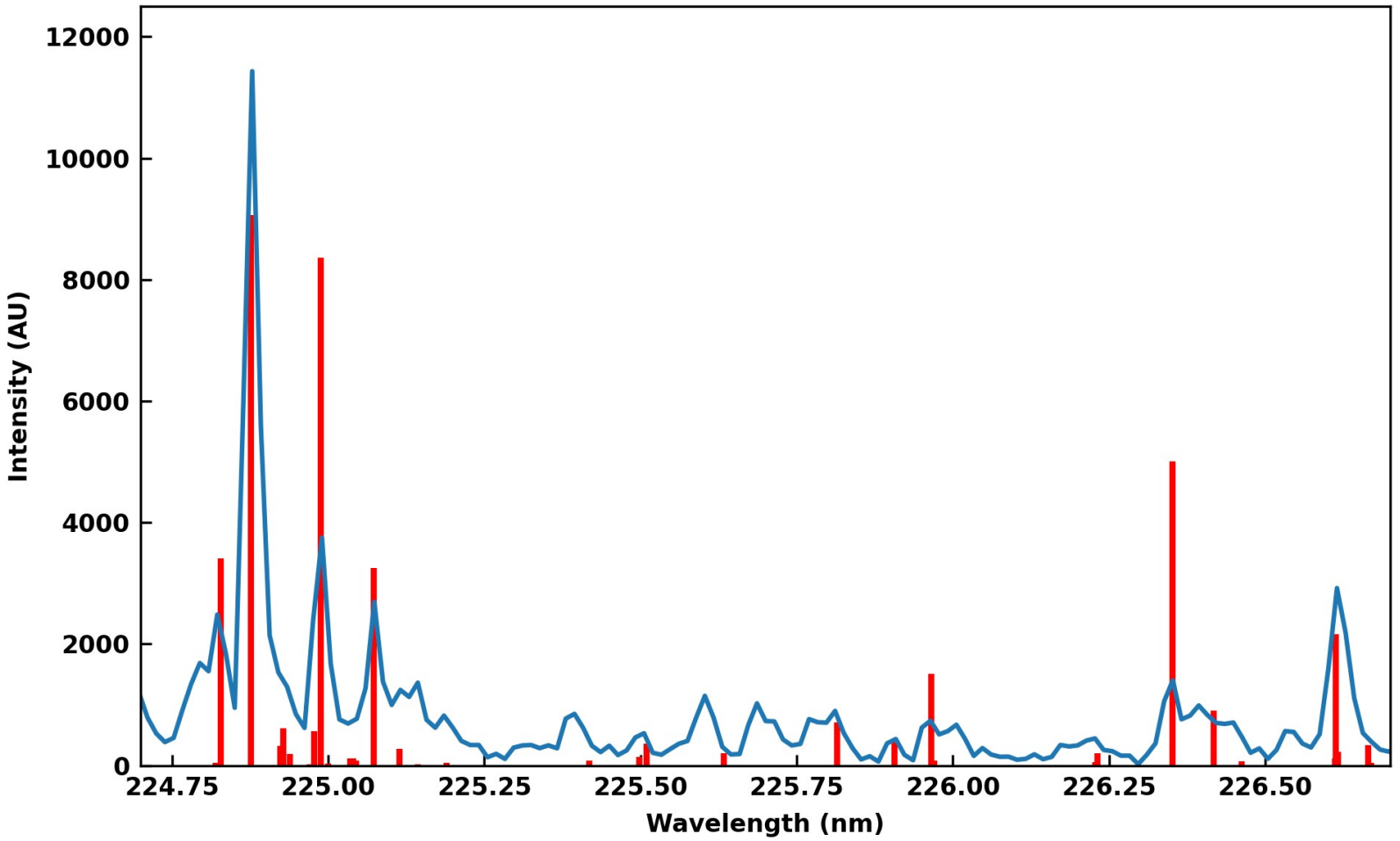


Figure 1. Energy level spectrum of W II organised by electronic configuration (For the first 5 configurations which contribute to the lowest-lying levels). Each horizontal line designates a specific fine structure level (taken from the NIST database).

To assure spectroscopic wavelengths, pre-diagonalisation of Hamiltonian, energy levelsare shifted to experimental values. Easy for low levels , not so for excited states.

W II calculation, currently being tested against CTH spectra at 30 eV and and a density of 1e+12 cm^-3.



W III calculation
(Dr M McCann: submitted J Phys B)

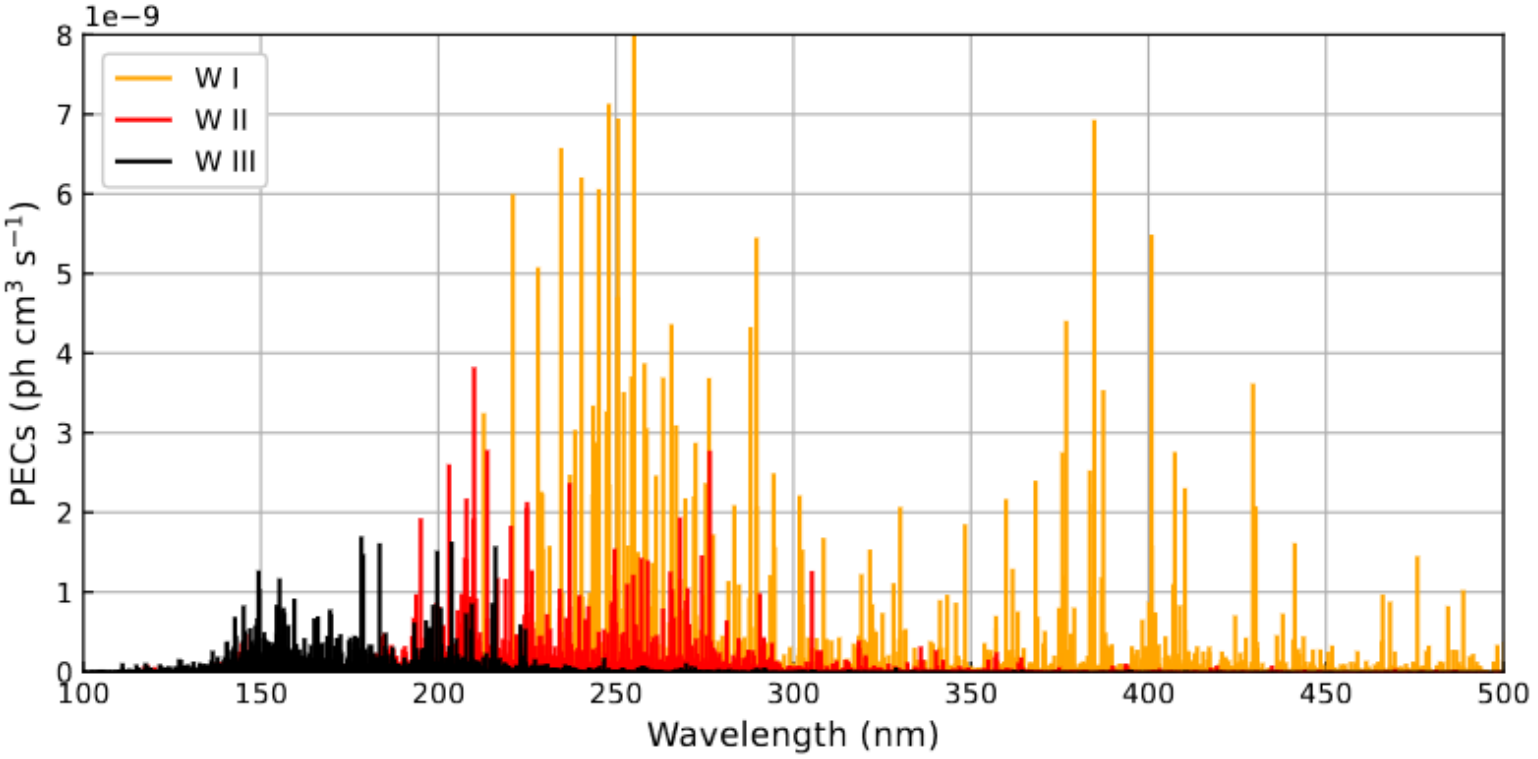


Figure 4. Tungsten synthetic spectra of W I (orange), W II (red), and W III (black), for an electron temperature of 25 eV and a density of 1×10^{12} cm^{-3}. The spectra for each of these charge states of tungsten were calculated independently, therefore the relative line heights between charge states should not be compared.

Computational challenges

(a) For heavier systems, the code must be refactored to build large Hamiltonians that recognise which elements interact and farm these out to processors in a manner that achieves load-balancing (computationally and I/O) .... easier said than achieved

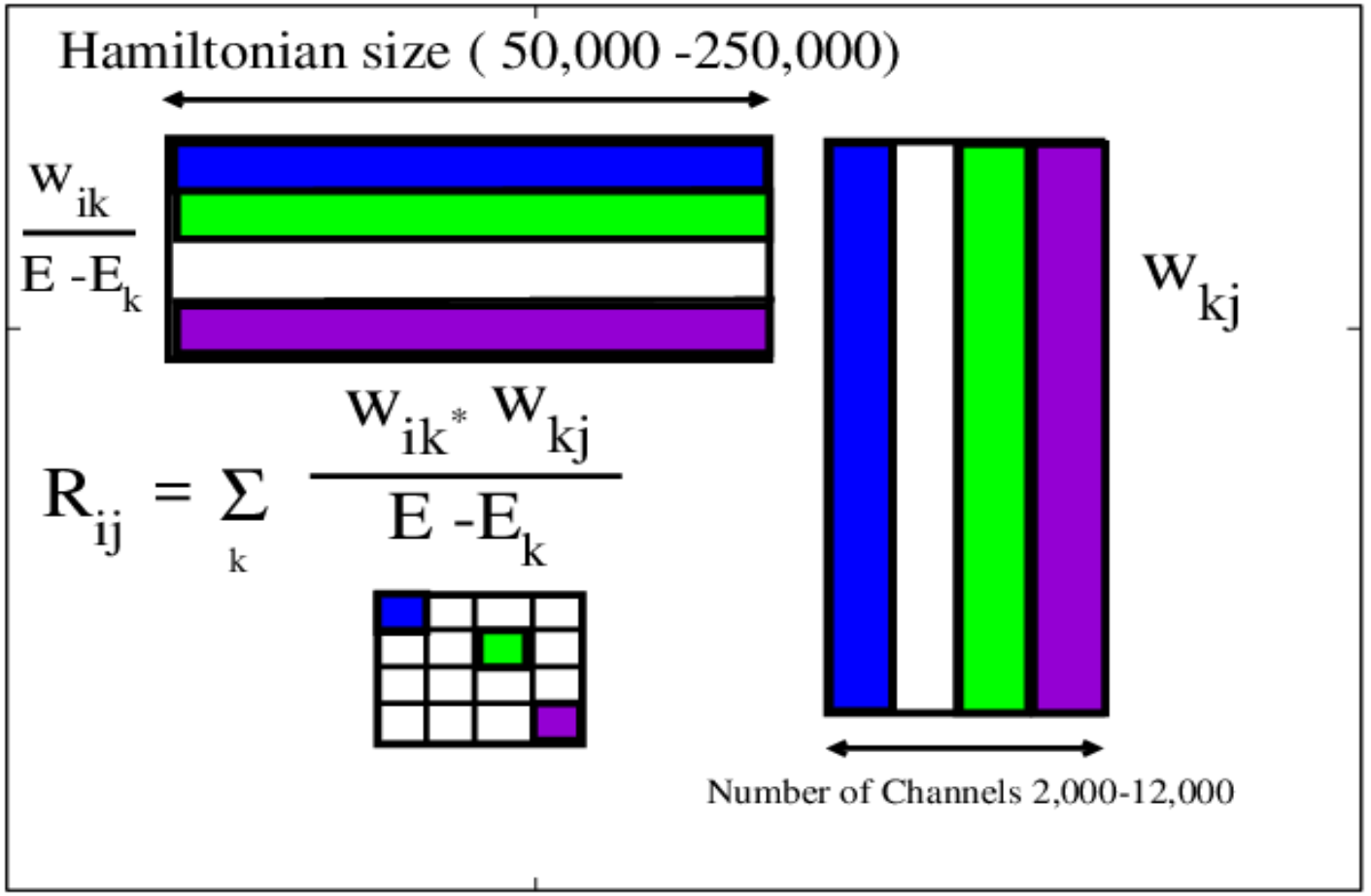
(This has been achieved for the LS/Breit-Pauli codes)

(b) We need to adapt to the hardware opportunities that GPUs (graphical processor unit) offer. R-matrix has many dense matrix operations and these must be offloaded to GPUS --→ 20-30K channel case.

You have mentioned 10,000 channels and matrices exceeding 100 K by 100 K, but does not the R-matrix have to be calculated for every energy ?

10,000*10,000*100,000= 10^13 operations ….. and modern CPUs only are of the order 10^9 operations per sec. Do you wait an hour per energy point ?

No fortunately, we can employ GPUs (Graphical Processing Units) for the dense matrix multiplies



Excitation Summary

- W I (published , Ryan Smyth et al 2018)
  adf04 (Maxwellian averaged collision strength)
  10.1103/PhysRevA.97.052705

- W II (work completed)Nicole Dunleavy
  J. Phys. B: At. Mol. Opt. Phys. 55 175002
- W III (submitted to J Phys B)Michael McCann
- W IV (Ballance et al, adf04 available,2013)
  DOI: 10.1088/0953-4075/46/5/055202)

We can improve the DARC (Dirac R-matrix) calculations in two ways

- Firstly, as the number of levels included in a close coupling expansion expands, dense Hamiltonians need constructed in parallel (code development)
- Exploitation of the DRMPS method for the DARC code. L-spinors instead of associated Laguerre polynomials for pseudo-states. (Hydrogen Badnell 2008)

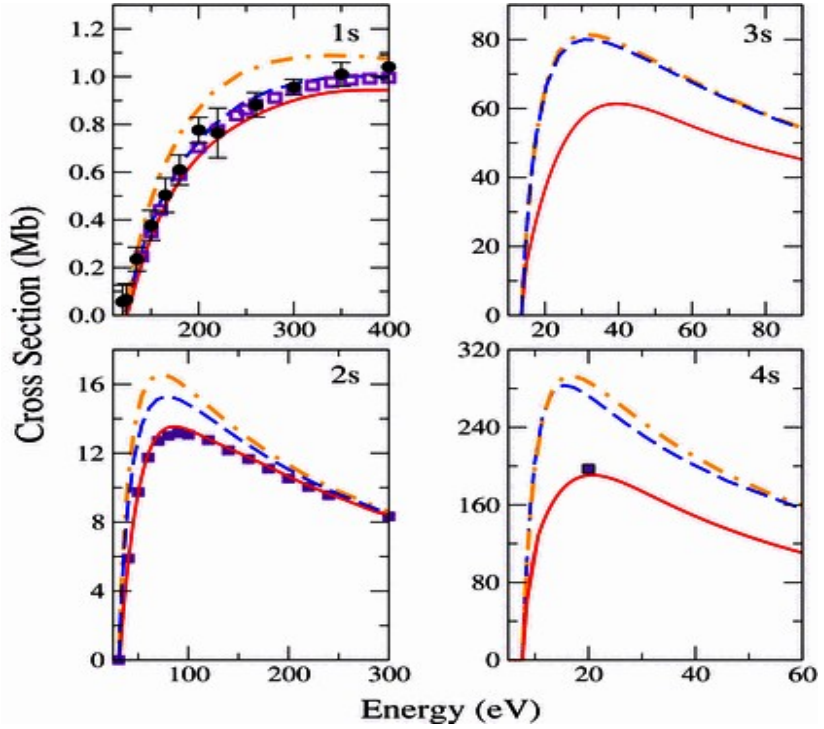
Ionisation : LS/BP developments

If we first consider the ground and meta-stable ionisation for the simpler cases of hydrogen and lithium, what uncertainties should we expect as a function of principal quantum number ?

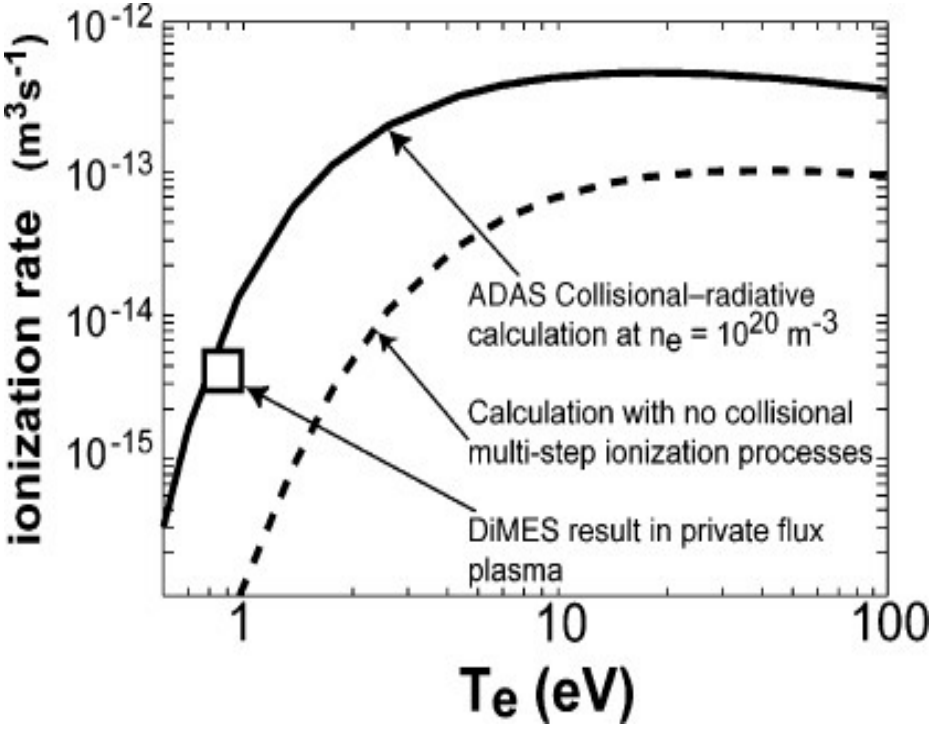
RMPS : ionisation

It is the accuracy of the excited states that can prove problematic

Neutral Hydrogen



Neutral Lithium Effective Ionisation



Ionisation: Increase in complexity

- Unlike ‘one-electron’ systems the ground-state of W I : 4f^14 5d^4 6s^2 requires direct ionisation of 6s and 5d ionisation

  → 5d^4 6s nl where n=7-14, l=0-6

  → 5d^3 6s^2 n’l’ where n=7-14, l=0-6

  which amounts to several thousand TERMS in a close coupling expansion and Hamiltonians in excess of 500,000 by 500,000
- W^2+ completed … 5803 terms, 22,000 channels + expt.
- Plan is to move from W^{2+} → W (easier structure)

The standard techniques, DW , Cowan HFR, configuration average TDCC , RMPS work for the groundstate .... but for excited states ....

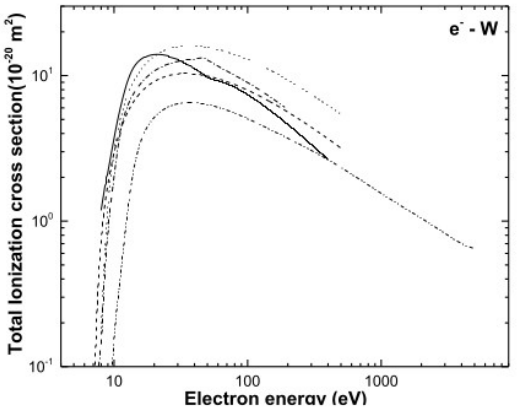


Fig. 1 Total ionization cross sections of W atoms plotted as a function of incident electron energy, solid curve: present DWA results in HULLAC [19], dashed and dotted curves: present DWA results in Cowan formalism with fine-structure and configuration mode; dash-dotted curve: results of [12] and dash-dot-dotted curve: results of [11].

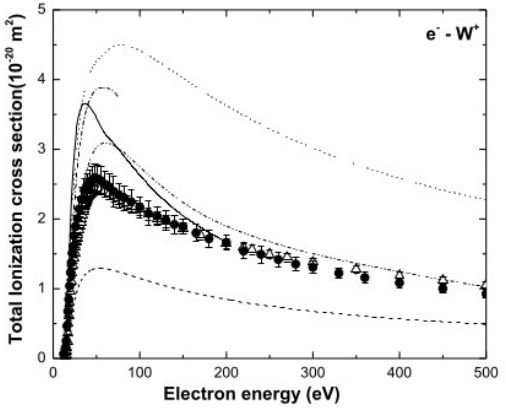
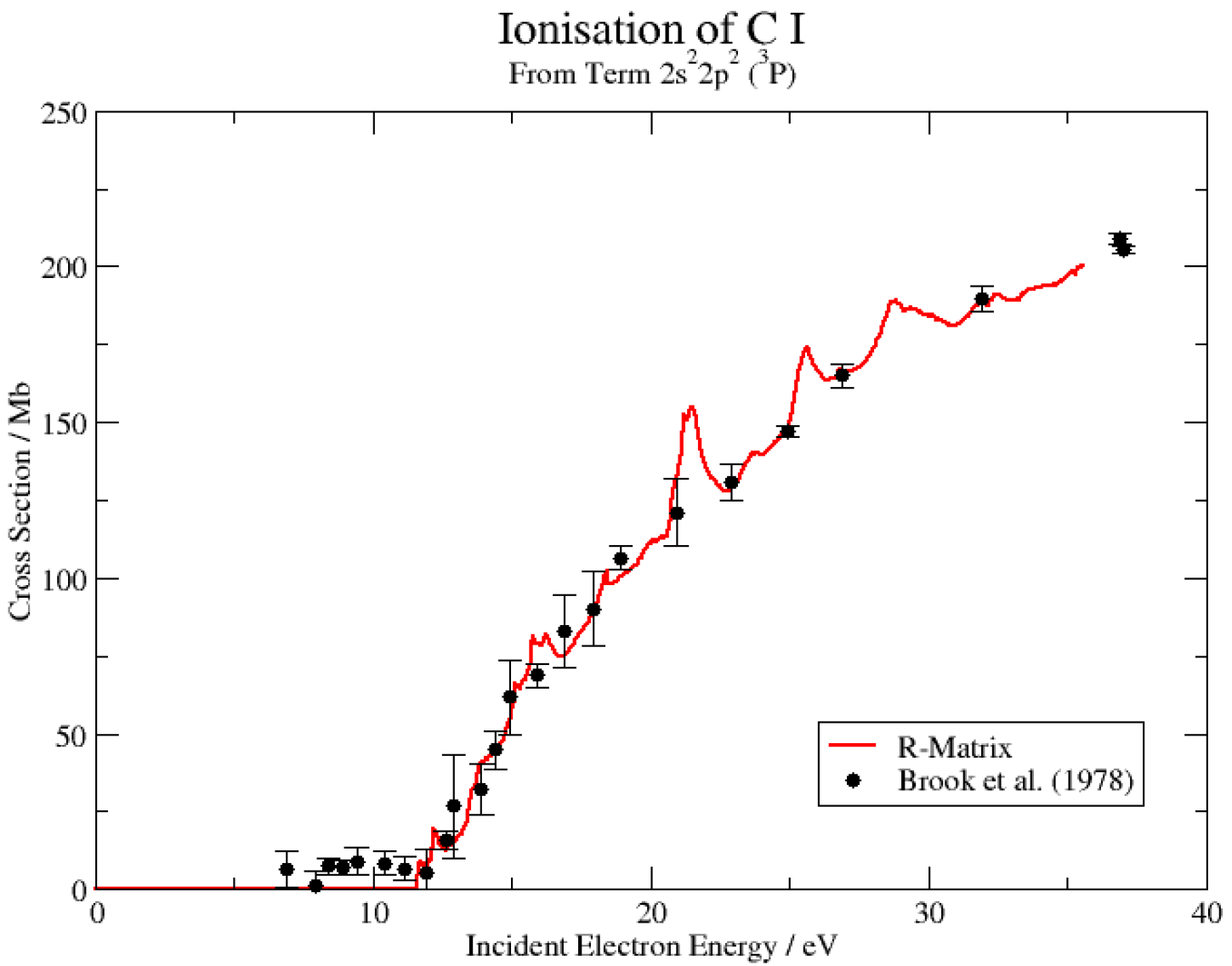
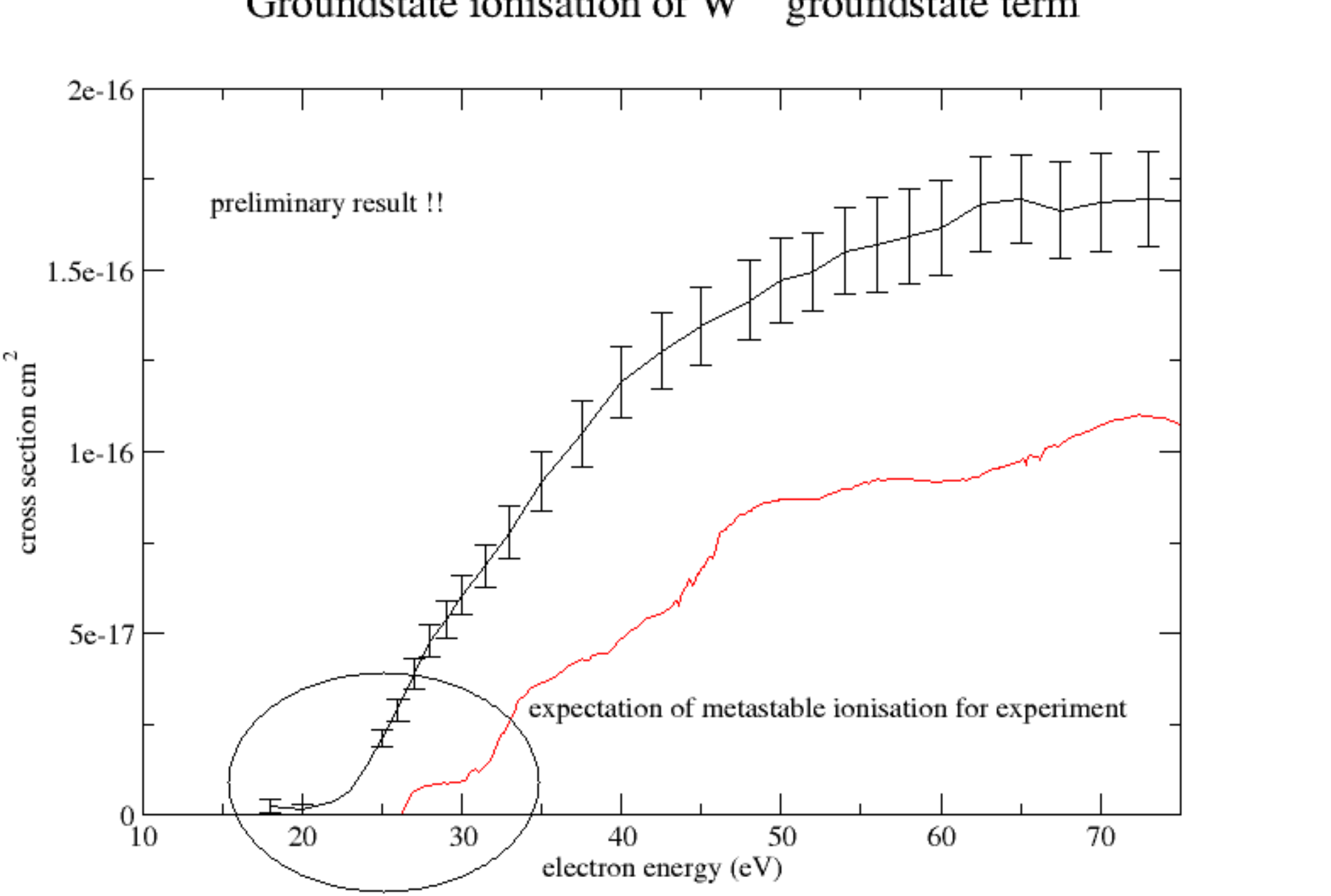


Fig. 3 Total ionization cross sections of W^+ ions plotted as a function of incident electron energy, dash-dot-dotted curve: results of [10]; dash-dotted curve: results of [8]; solid circles and hollow triangles: measurements [14] and [13]; other curves are the same as Fig. 1.

Unfortunately, the effective ionisation rates are completely dominated by excited state ionisation !

Validate code with C I ionisation




Groundstate ionisation of W2+ groundstate term
preliminary result !!
expectation of metastable ionisation for experiment
cross section cm2
electron energy (eV)
2e-16
1.5e-16
1e-16
5e-17
0
10
20
30
40
50
60
70

- Constraining uncertainty on plasma diagnostics

Ar II : Constraining uncertainty

- Ar II chosen as a benchmark case, as LS/Breit/Pauli, intermediate-coupling frame transformation (ICFT) and DARC codes are all applicable
- Do the different choices in atomic structure (autostructure/grasp0) or code usage

  affect magnetic fusion diagnostics ?
- Also completes Ar sequence, therefore ADAS

  will have level-resolved GCR coefficients !

Results

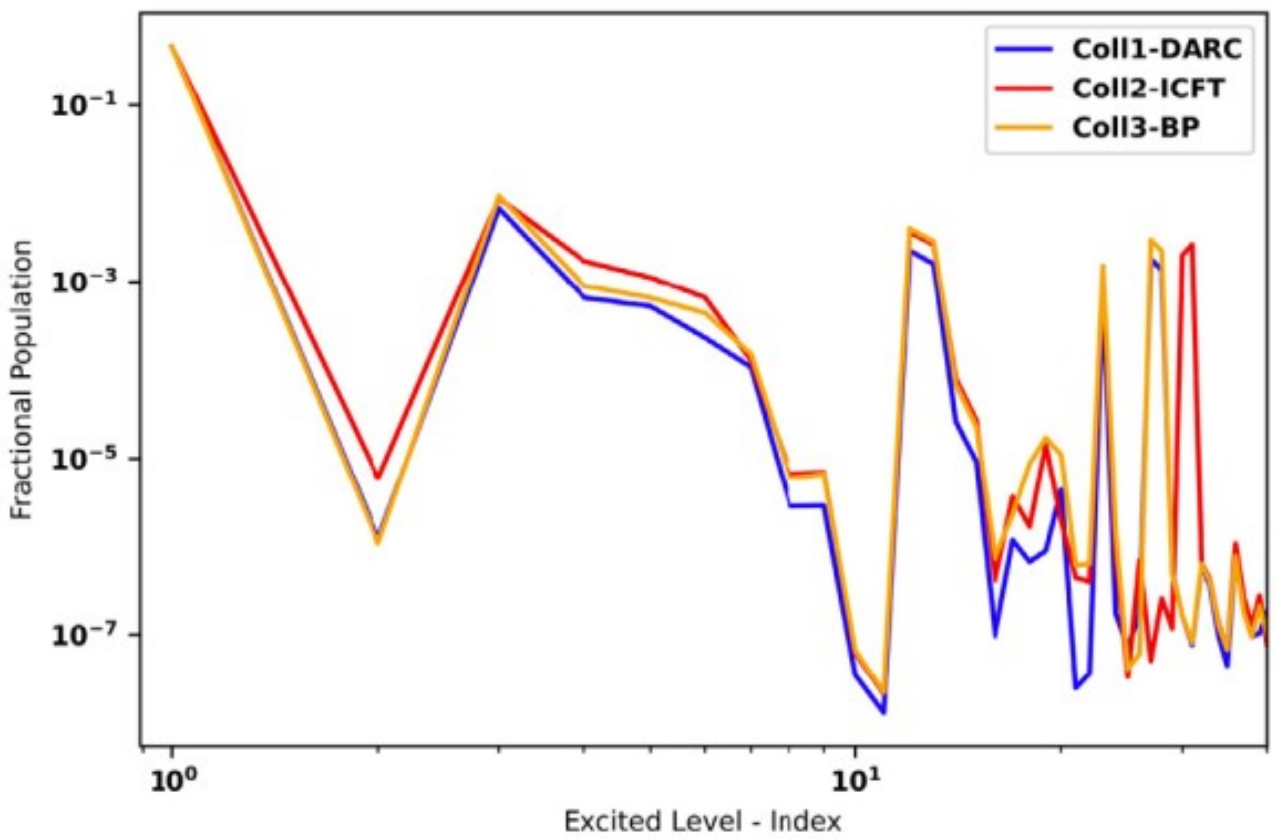
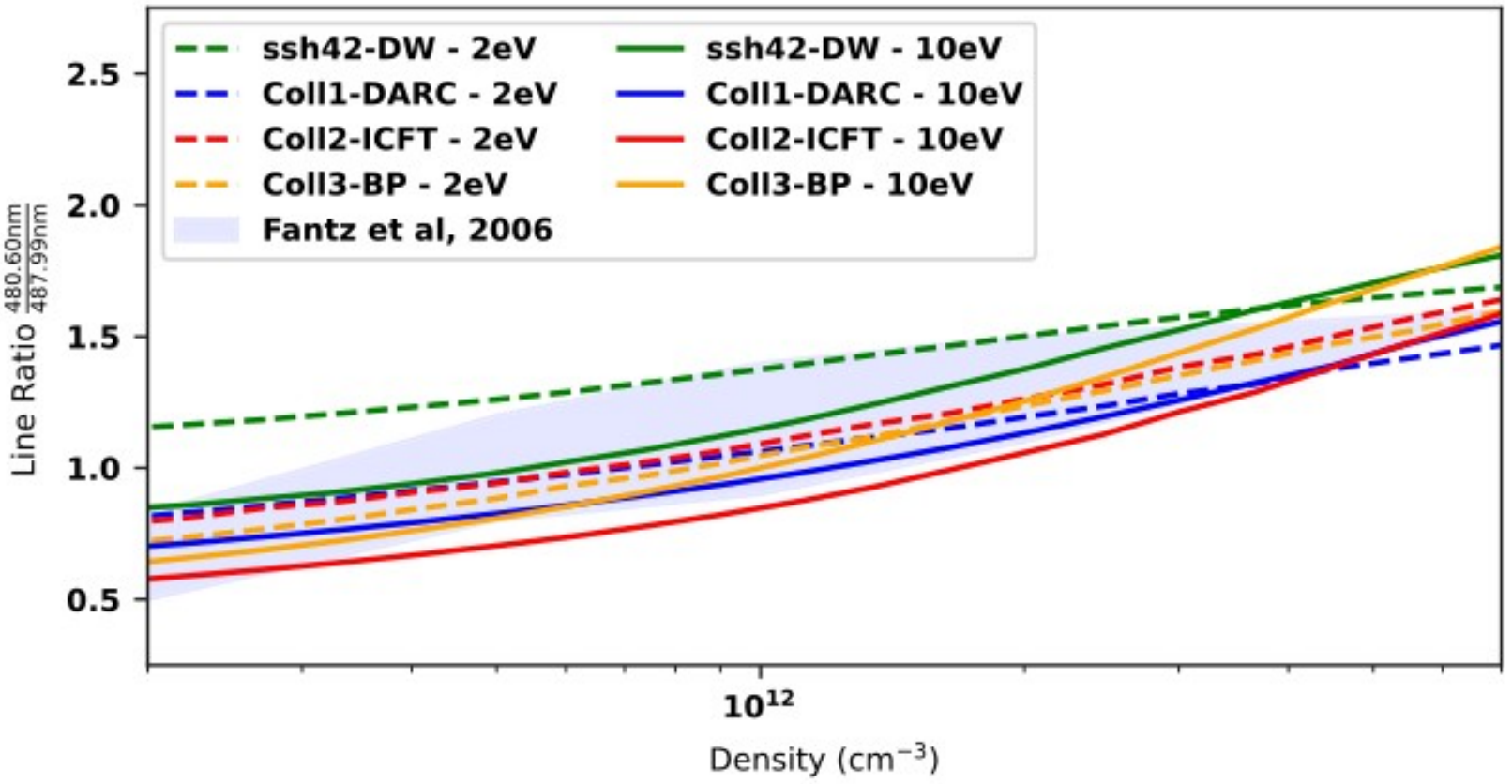


Fig. 5. Calculated fractional populations in a quasi-static collisional radiative calculation for the first 40 Excited states for each collisional calculation, at T_e = 7eV and n_e = 10^{11} cm^{-3}, with first excited state at index 1.

Note : ICFT Coll2 (unshifted to NIST) , others shifted to NIST values

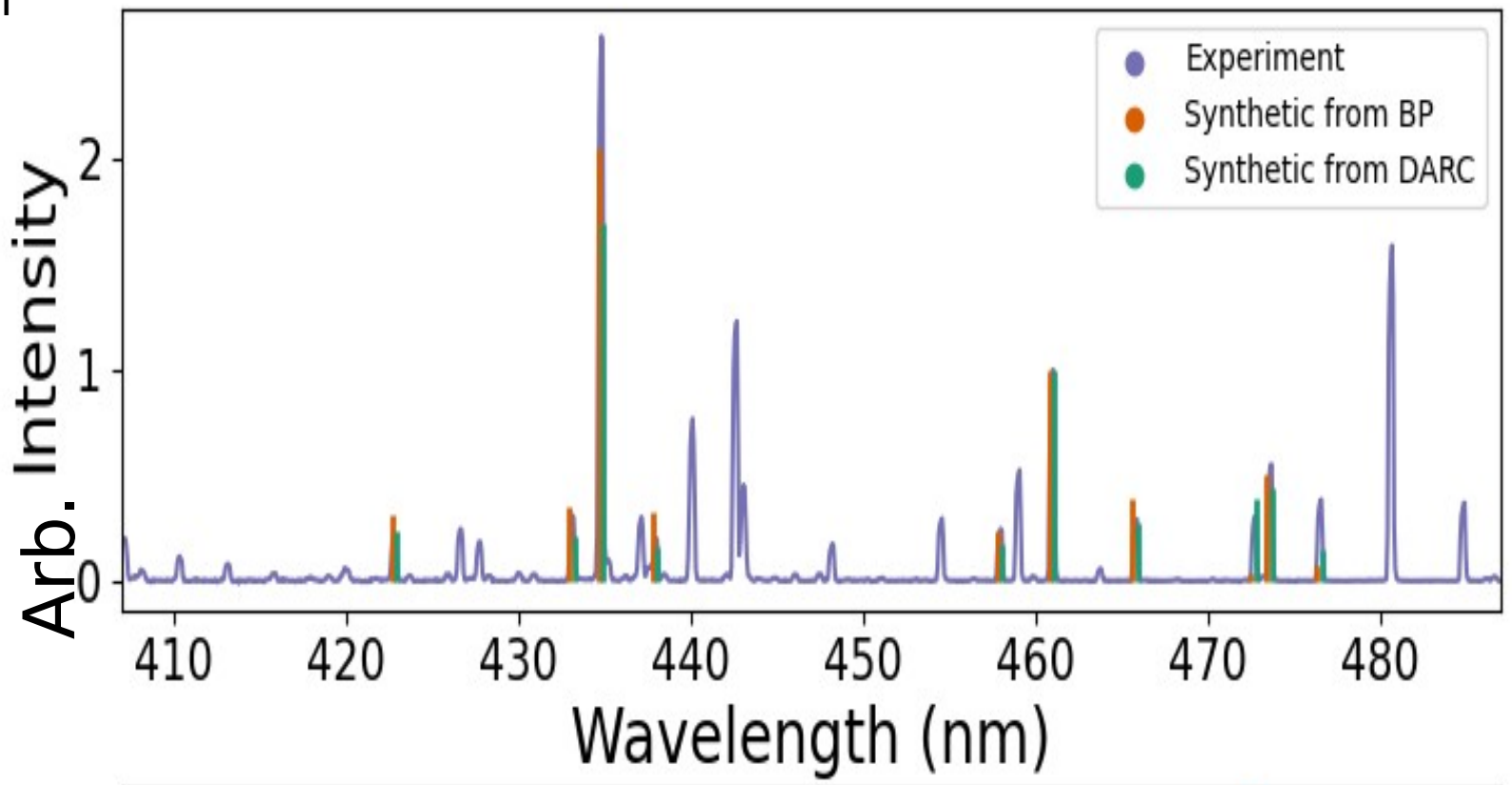
Line ratio constrained to tighter values over the earlier Fantz work.



Fantz distribution of results given by the grey shaded area. DW (Henderson) (green dashed) and ICFT (red solid) previously spanned a wider range.

- Generate Synthetic Spectra to compare against CTH
- Use as a benchmark of calculations

(purple : CTH will have other impurities as well as tungsten !)



Comparison of Two Ar II calculations against CTH Spectra.
Credit:Dr. E Williamson

Thanks for your attention, questions ?

Ultimately, the electron-impact excitation and ionisation rates are both required if we to produce Generalised Collisional Radiative (GCR) coefficients that are both temperature and density dependent.

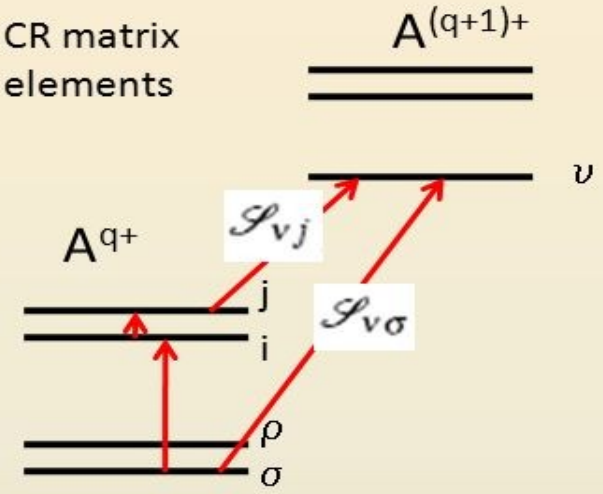
Generalized collisional-radiative (GCR) coefficients

- Effective ionization rates

$$S_{CD,\sigma\to\nu} = \mathscr{S}_{\nu\sigma} - \sum_{j=1}^{O} \mathscr{S}_{\nu j} \sum_{i=1}^{O} \mathscr{C}_{ji}^{-1} \mathscr{C}_{i\sigma}$$

Ionization rates

CR matrix elements



- Effective recombination rates

$$R_{CD,\nu\to\sigma} = \mathscr{R}_{\sigma\nu} + \sum_{j=1}^{O} \mathscr{C}_{\sigma j} \sum_{i=1}^{O} \mathscr{C}_{ji}^{-1} \mathscr{R}_{i\nu}$$

RR and DR rates

- Total Line Power Loss

$$P_{LT,\sigma} = \sum_{k,j} \Delta E_{kj} A_{j\to k} F_{j\sigma}^{exc},$$

excitation rates

spontaneous emission rates

j->k transition energy

Effective ionization rate coefficient vs density and electron temperature

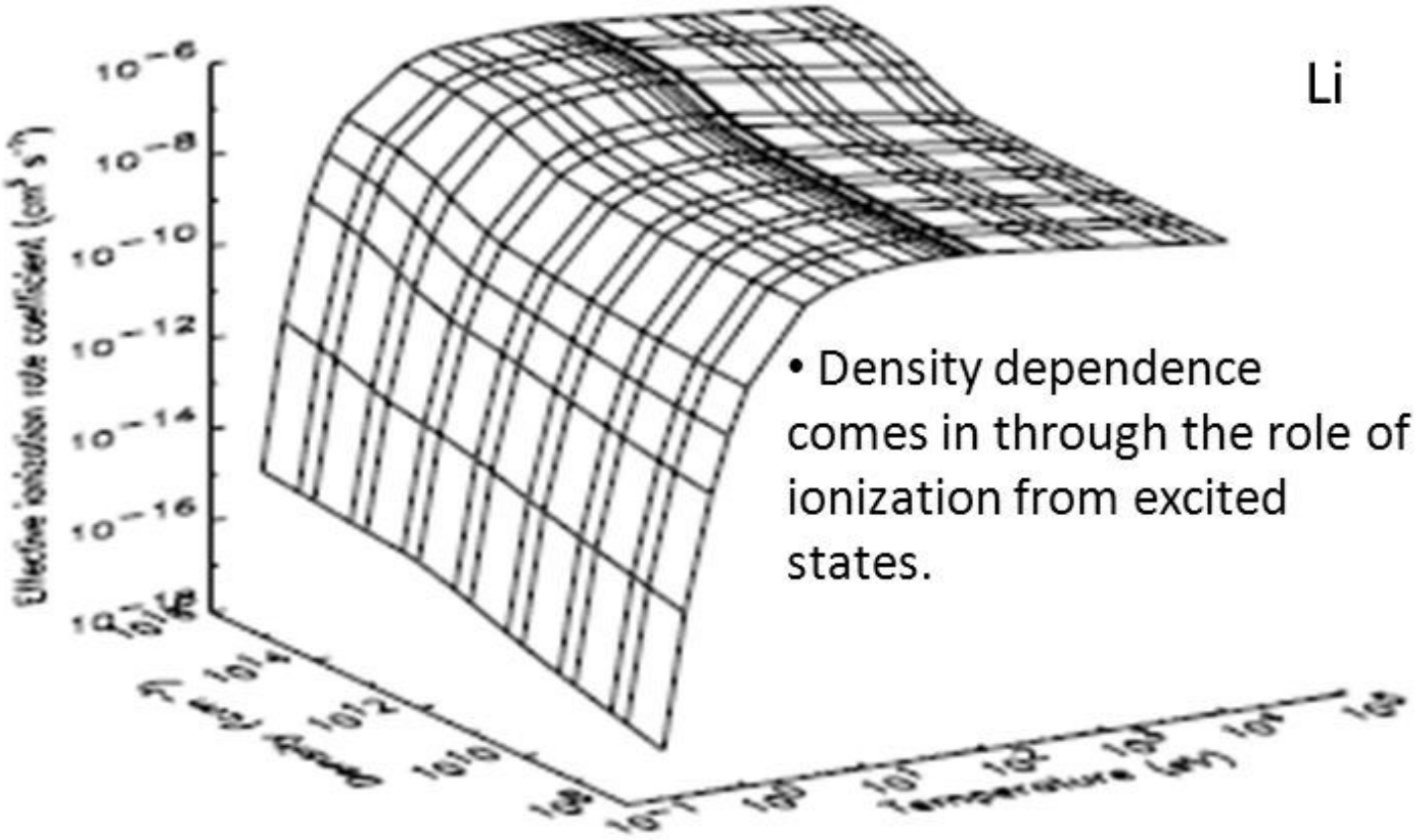


Fig. 8. Effective ionization rate coefficient for the ionization process $e + Li(1s^2\,2s\,^2S) \rightarrow Li^+(1s^2\,^2S) + 2e$ as a function of electron temperature and density. Note that the density dependence comes in through the role of ionization from excited states.

Loch et al., ADNDT, 92 813 (2006)