Dirac R-matrix calculations

(electron-impact excitation/ionisation)

in support of tungsten plasma diagnostics

Connor Ballance

(Queen's University of Belfast)

Collaborators : Nicole Dunleavy, Ryan Smyth, Stuart Loch, Curtis Johnson, David Ennis and M O'Mullane

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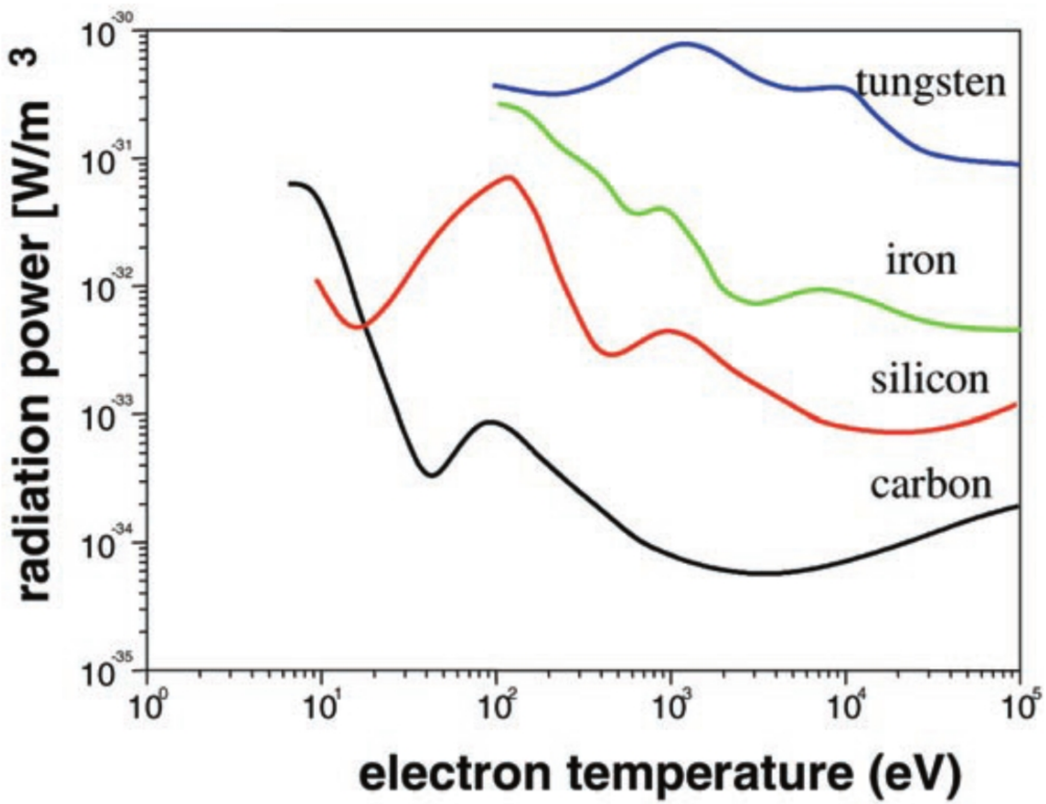
Overview

- Motivation : Provide the atomic structure, electron-impact excitation/ionisation rates used for temperature and density diagnostics (+ impurity influx) for W I and W II
- Method : Quick description of relativistic R-matrix theory : excitation
  : ionisation
  : Collisional-radiative modelling
  : SXB
- W I, W II (NEW) : excitation
- W I : ionisation (ground and excited state)
- Conclusions , uncertainty, future directions

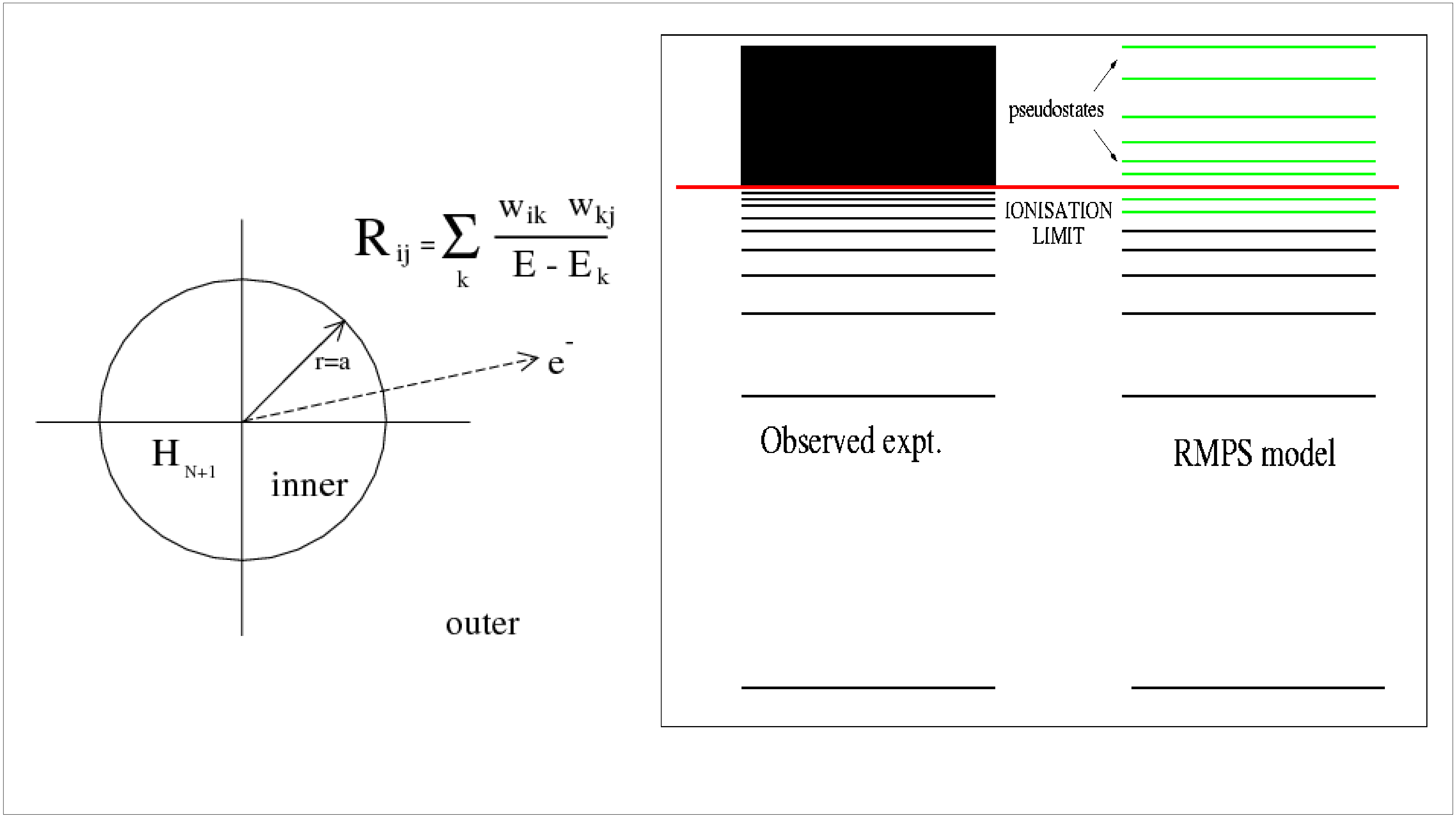
High Z materials are leading candidates for first wall materials, especially divertor region

- ***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 wall



V. Philipps

R-matrix/RMPS in a nutshell



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

$$+ \sum_j d_{jk} \phi_j(x_1 \ldots x_{N+1})$$

Electron-impact excitation of neutral tungsten

PHYSICAL REVIEW A
covering atomic, molecular, and optical physics and quantum information

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

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.

Snapshot of W I

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

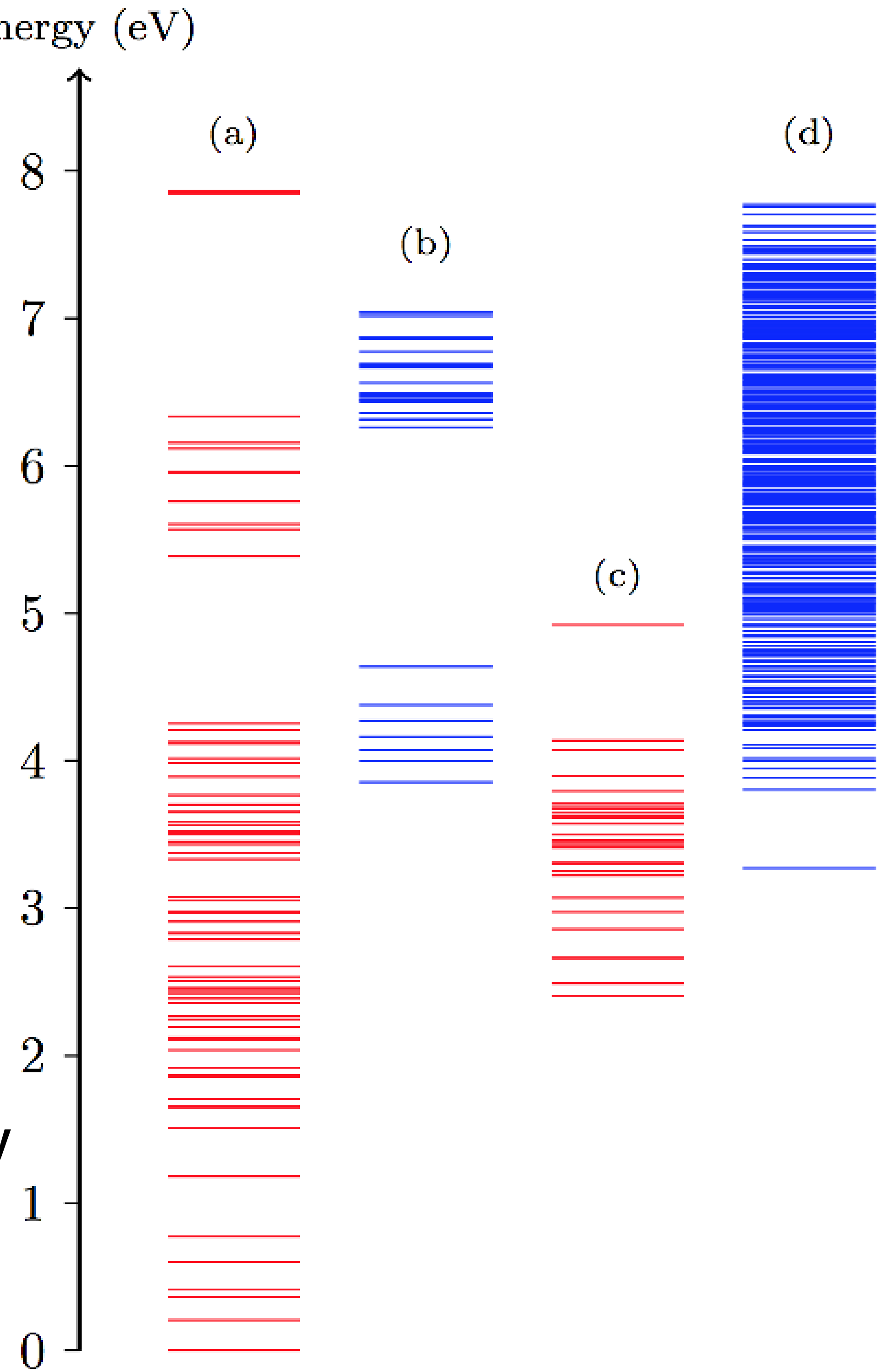
Method : GRASP0 structure groundstate
+ 24 excited state configurations
(~7500 levels)

: 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

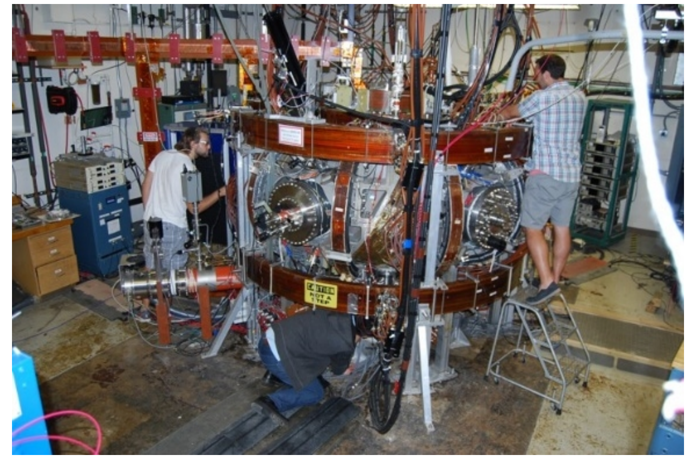


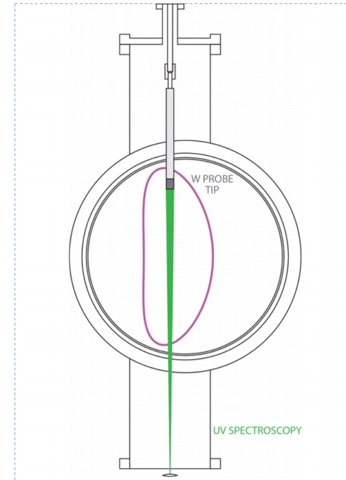
We must exploit High Performance Computing resources

- Electron-impact calculations involves hundreds of level-resolved target states and thousands of close-coupled channels $\rightarrow$ large Hamiltonian matrices.
- Huge effort goes into the parallel construction of hundreds of Hamiltonians, which require diagonalisation (now employing GPU accel.)

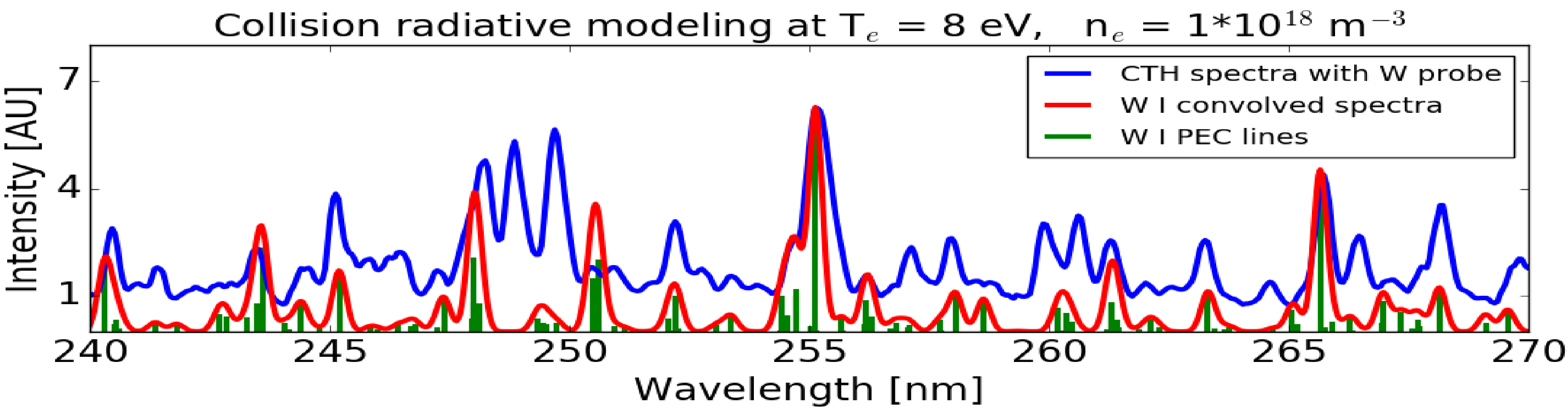
Compact Toroidal Hybrid (CTH) has been an invaluable test of the electron-impact excitation dataset

- 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).

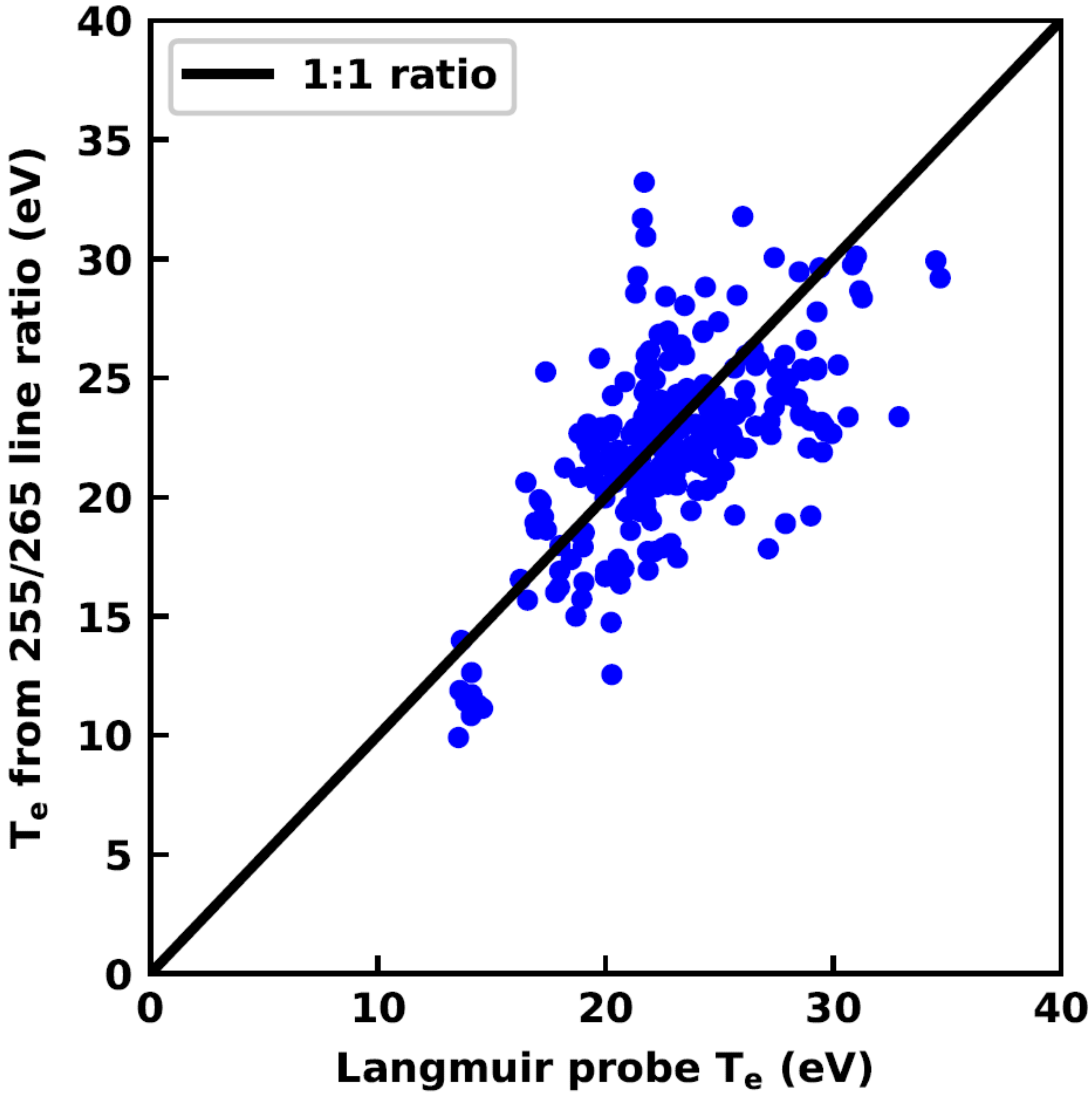




CTH cross section with probe and UV spectrometer line of sight



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



Overview of W II

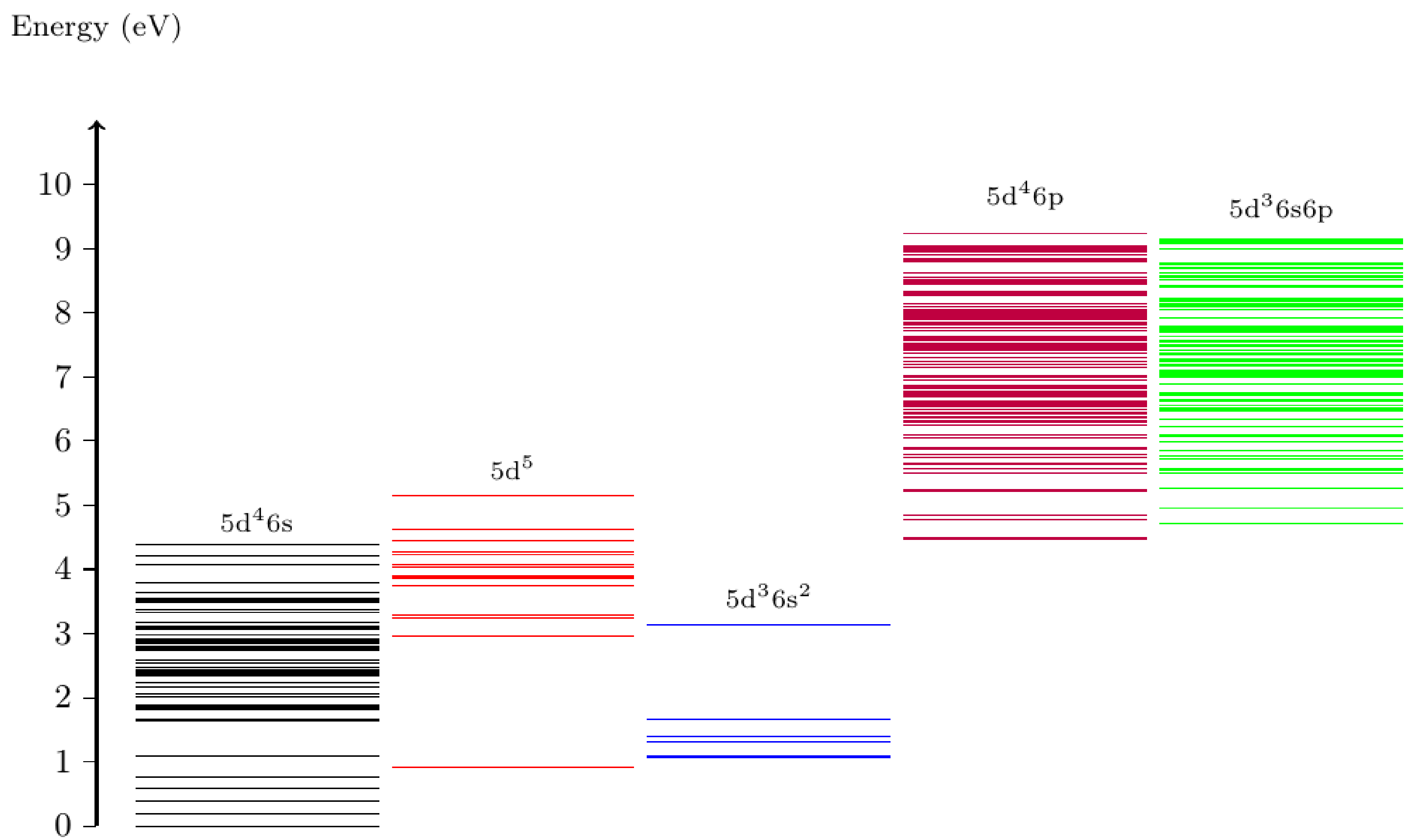
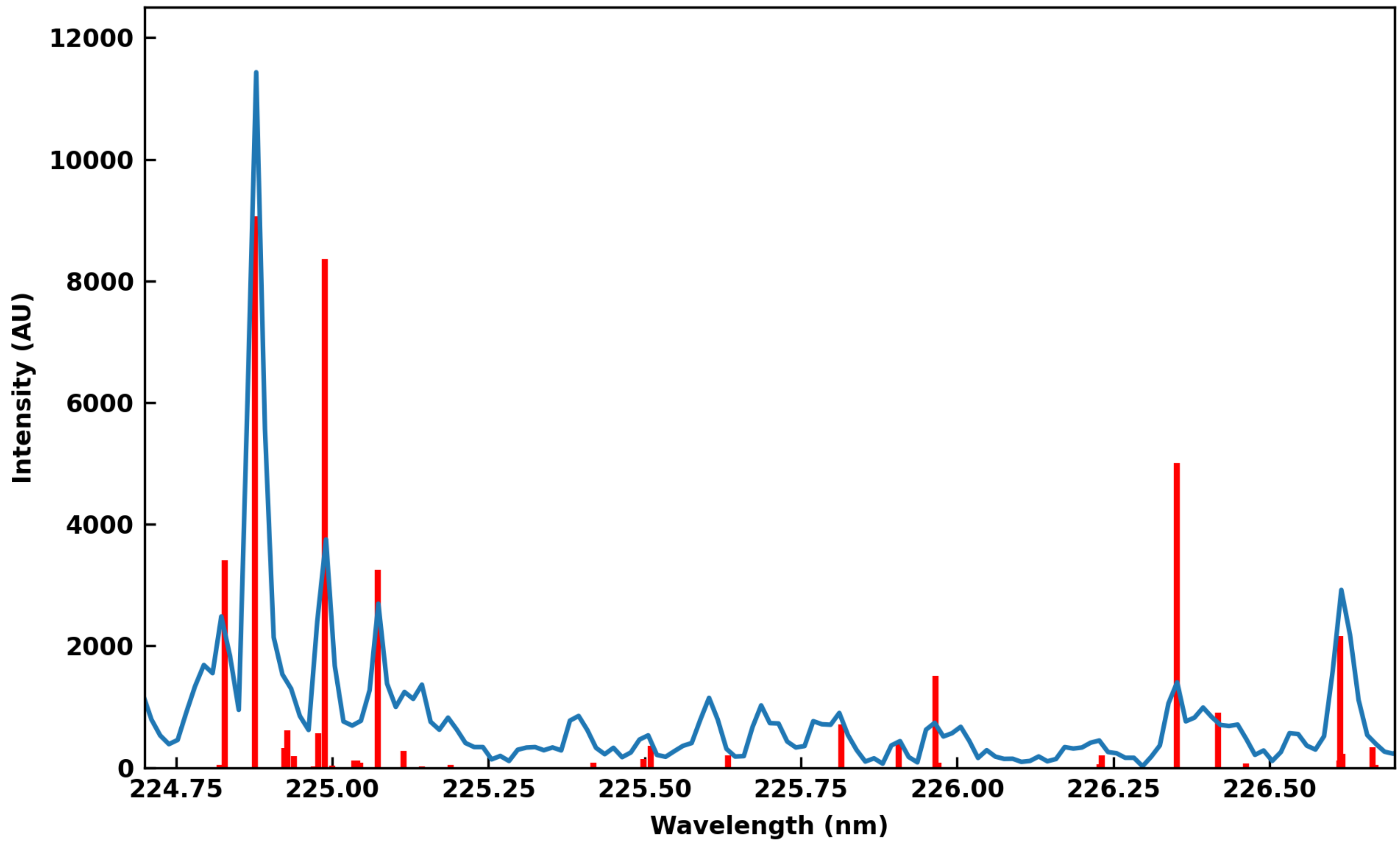


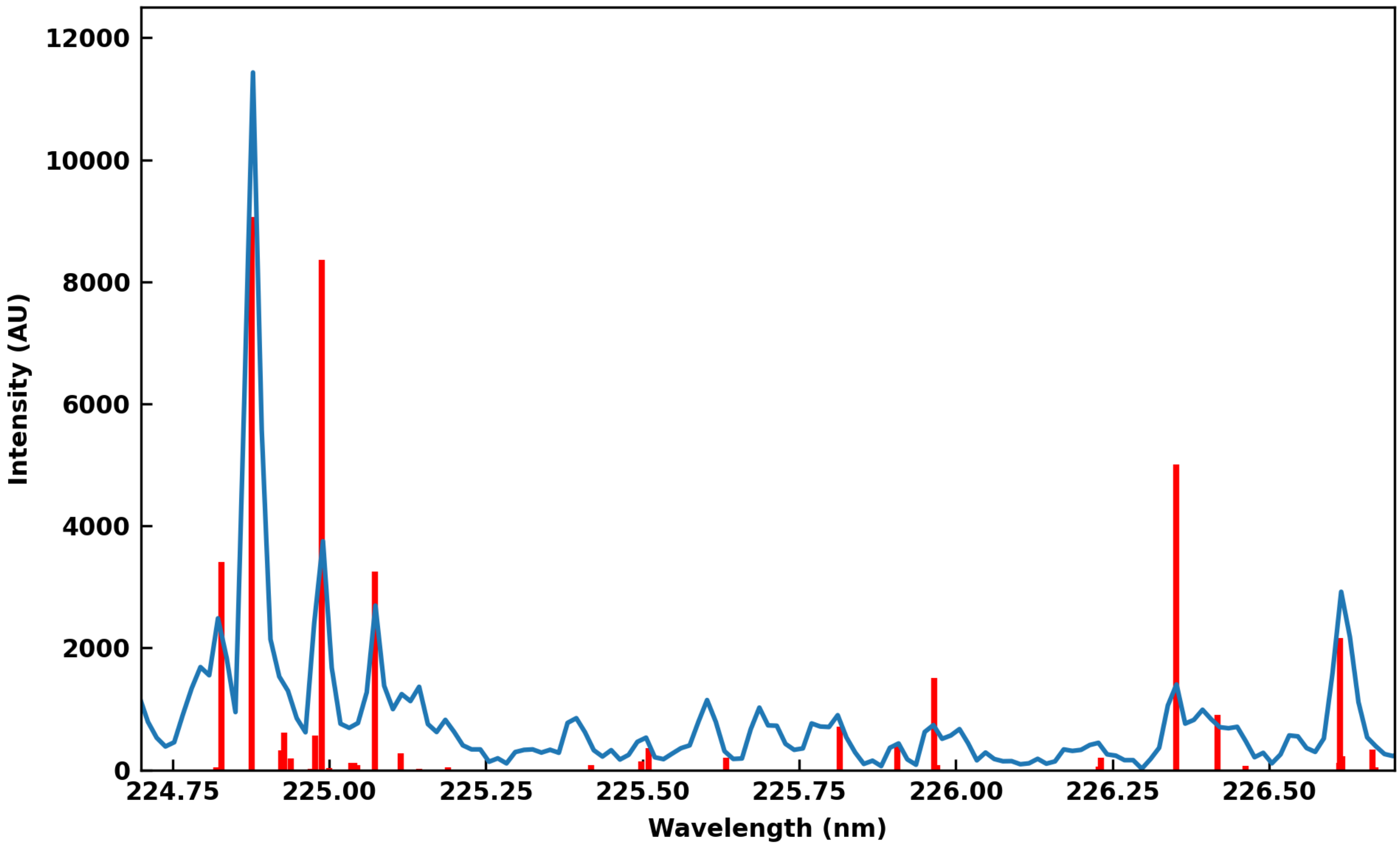
Figure 1. Energy level spectrum of W II organised by electronic configuration (For the first 5 configurations which contribute to the lowest-lying levels). Each horizontal line designates a specific fine structure level (taken from the NIST database).

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

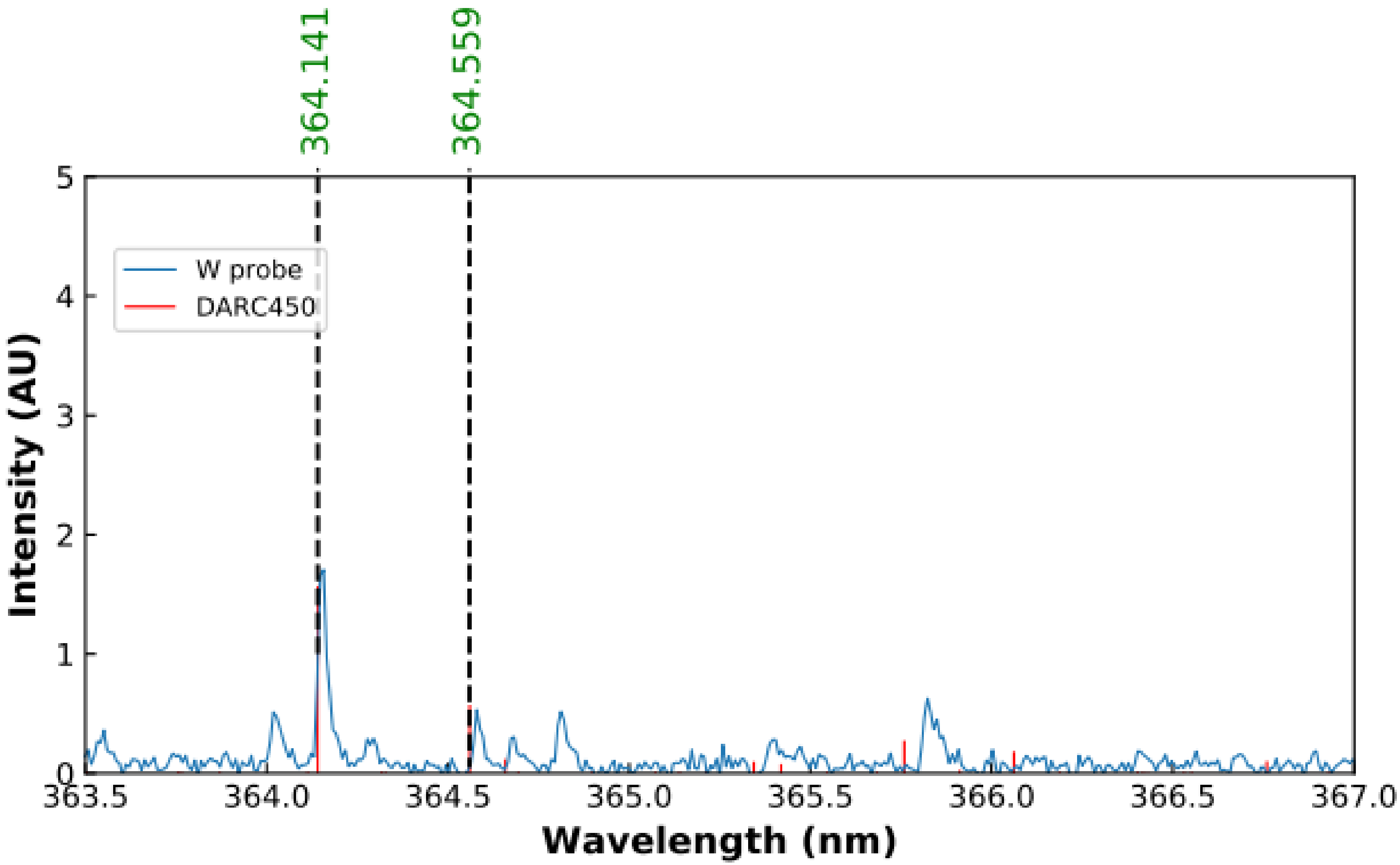
W II calculation (NEW) , currently being tested against CTH spectra at 30 eV and and a density of 1e+12 cm^-3.



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



W II calculation (NEW) , currently being tested against CTH spectra at 30 eV and and a density of 1e+12 cm^-3, but at higher wavelengths



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

  adf04 under testing)

- W III (To be done !)

- W IV (Ballance et al, adf04 available,2013)

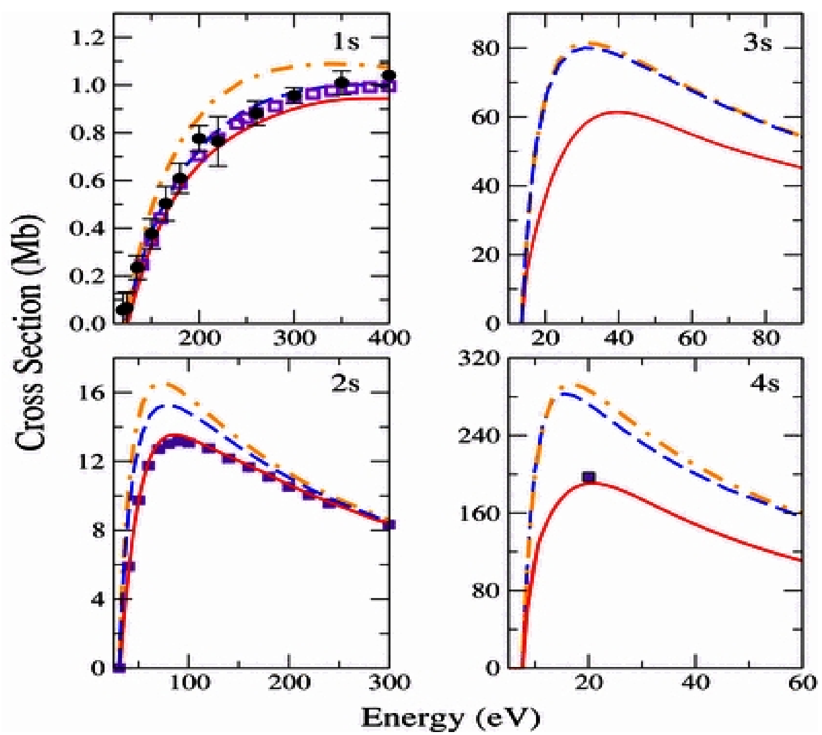
  DOI: 10.1088/0953-4075/46/5/055202)

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.

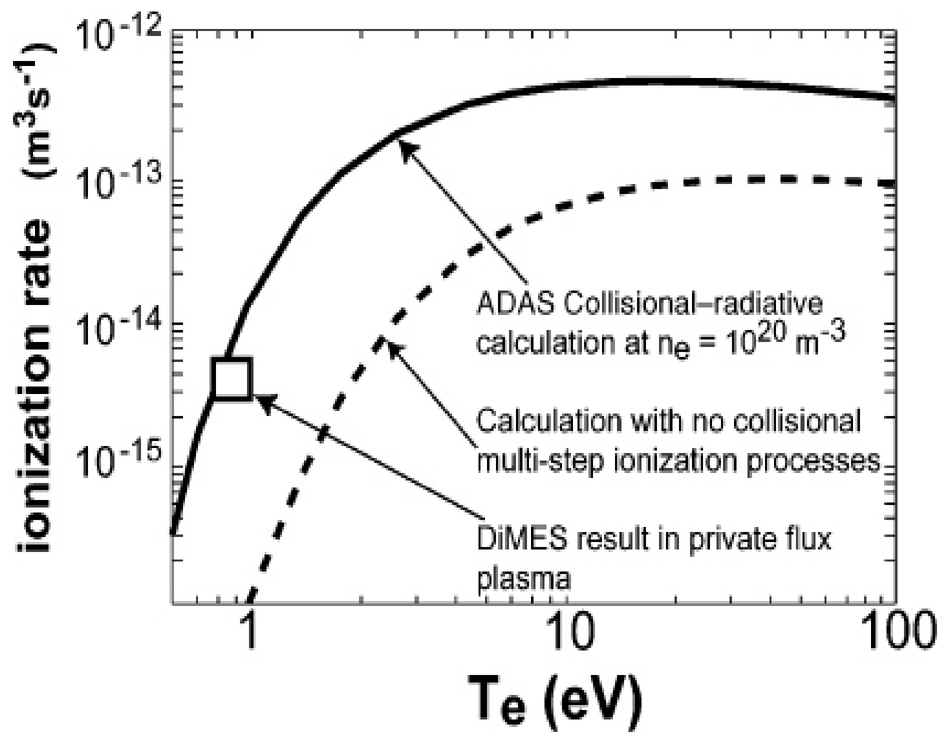
RMPS : ionisation

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 hundred TERMS in

  a close coupling expansion and Hamiltonians in excess of 360,000 by 360,000

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

Plasma and Fusion Research: Regular Articles Volume 13, 3401026 (2018)

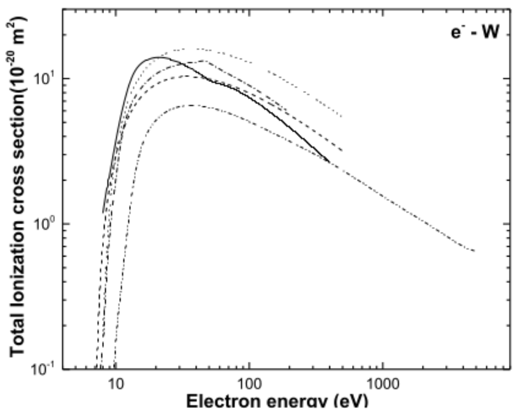


Fig. 1 Total ionization cross sections of W atoms plotted as a function of incident electron energy, solid curve: present DWA results in HULLAC [19], dashed and dotted curves: present DWA results in Cowan formalism with fine-structure and configuration mode; dash-dotted curve: results of [12] and dash-dot-dotted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

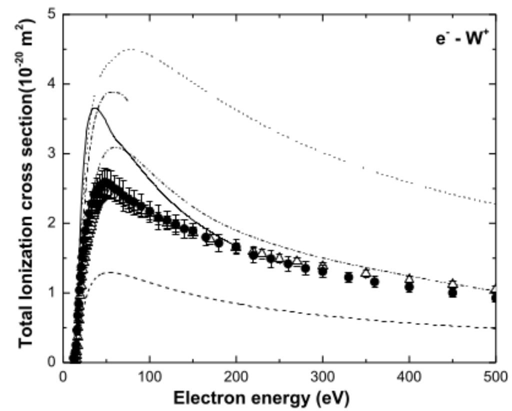


Fig. 3 Total ionization cross sections of W^+ ions plotted as a function of incident electron energy, dash-dot-dotted curve: results of [10]; dash-dotted curve: results of [8]; solid circles and hollow triangles: measurements [14] and [13]; other curves are the same as Fig. 1.

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

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.

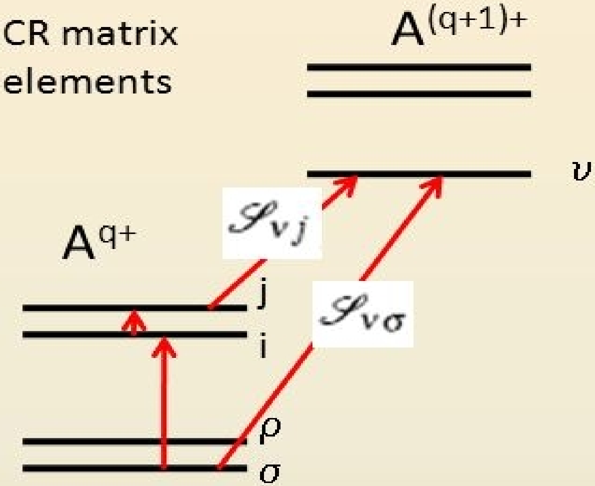
Generalized collisional-radiative (GCR) coefficients

- Effective ionization rates

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

Ionization rates

CR matrix elements



- Effective recombination rates

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

RR and DR rates

- Total Line Power Loss

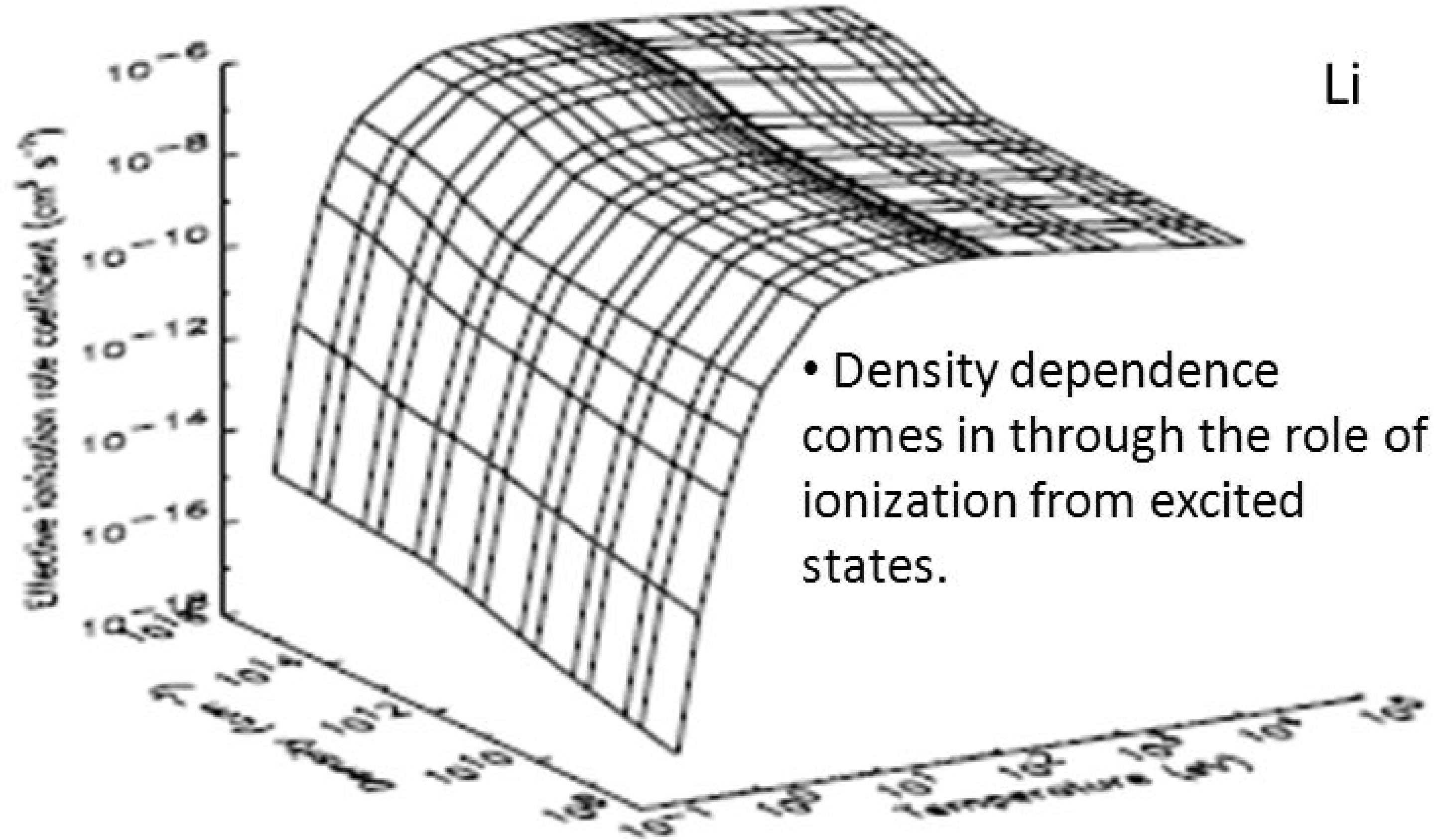
$$P_{LT,\sigma} = \sum_{k,j} \Delta E_{kj} A_{j\rightarrow k} F_{j\sigma}^{exc},$$

excitation rates

spontaneous emission rates

j->k transition energy

Effective ionization rate coefficient vs density and electron temperature



- Density dependence comes in through the role of ionization from excited states.

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)

Quantifying Wall Erosion impurity influx, culmination of collisional processes and their associated Uncertainty.

- 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

Conclusions/Future Directions

- Electron-Excitation : in reasonable shape, has predictive and diagnostic capability. Only W III remains for W I-IV to be complete
- Electron-impact ionisation : Difficult to achieve a sufficiently accurate representation of excited states. This is the dominant contribution to effective ionisation rate
- We hope to constrain the uncertainties in SXB ratios

Future Directions : Uncertainty propagation through models