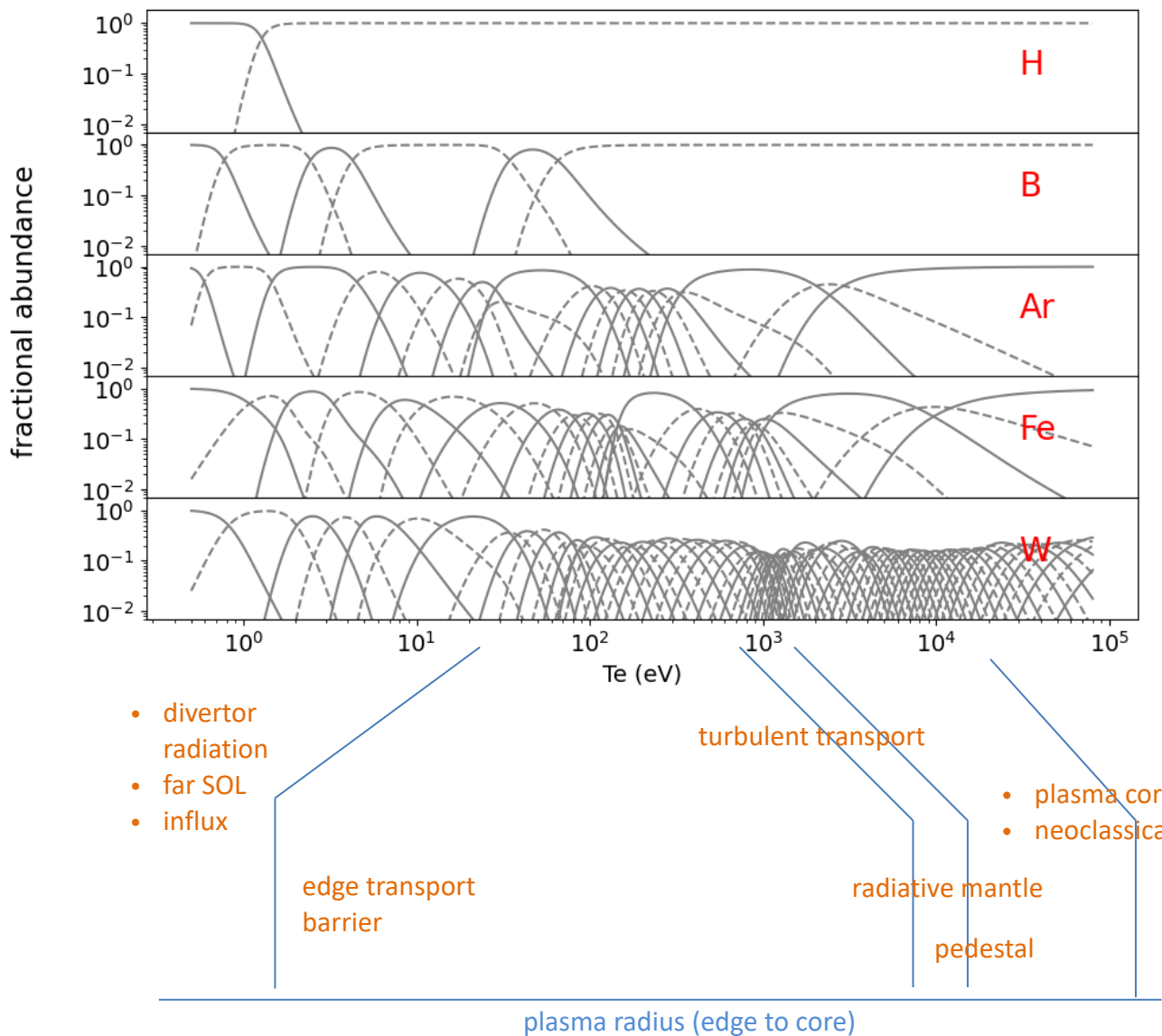# Update on atomic data and population models for hydrogen and tungsten

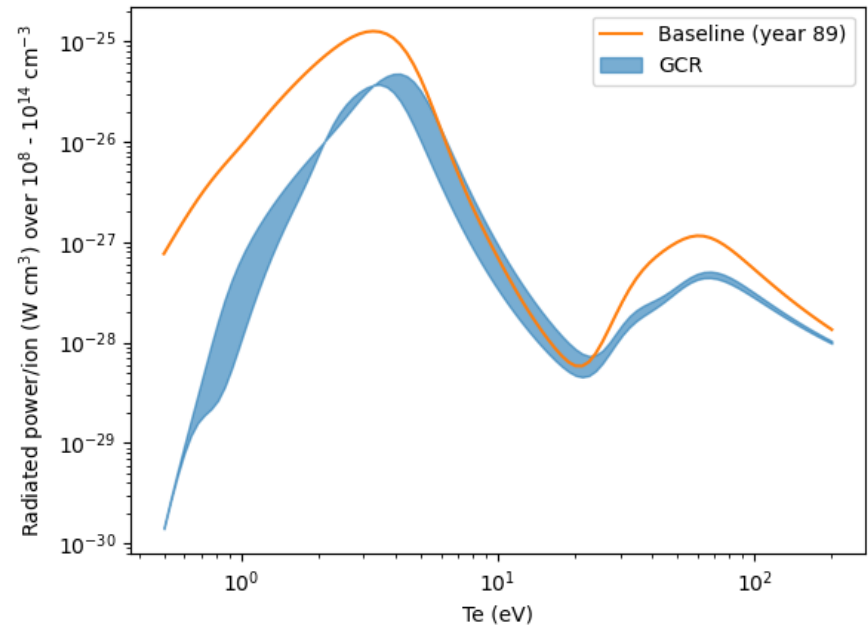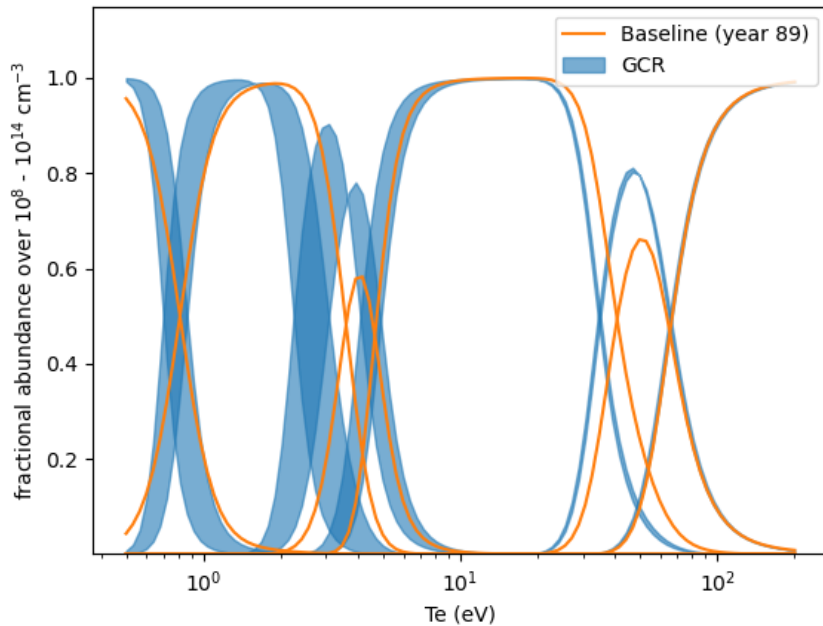**Martin O'Mullane** and ADAS contributors

Te-dependence of abundances

Equilibrium balance
- effective rate coefficients for ionisation balance
- All fundamental atomic data calculated by ADAS group and close collaborators (adf04, adf09, adf48, adf23)

- divertor radiation
- far SOL
- influx

turbulent transport

- plasma core
- neoclassical accumulation

edge transport barrier

radiative mantle

pedestal

plasma radius (edge to core)

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A quick detour to boron

- New data exists, based on R-matrix excitation data from QUB with ionization and recombination from ADAS codes.
- Simple equilibrium balance – no thermal CX.
- The variation with density (from the CR model) may be larger than any uncertainties in the fundamental data.

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Outline

Restrict to the atomic domain – molecules and molecular models cover extensively in other presentations

- Hydrogen behaviour at low-Te.
- e-impact processes at n>1 for hydrogen.
- p-impact processes for hydrogen and UQ considerations.
- Update on fundamental atomic data for tungsten.
- Spectroscopy and modelling of tungsten.

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Low Te recombination rate for hydrogen
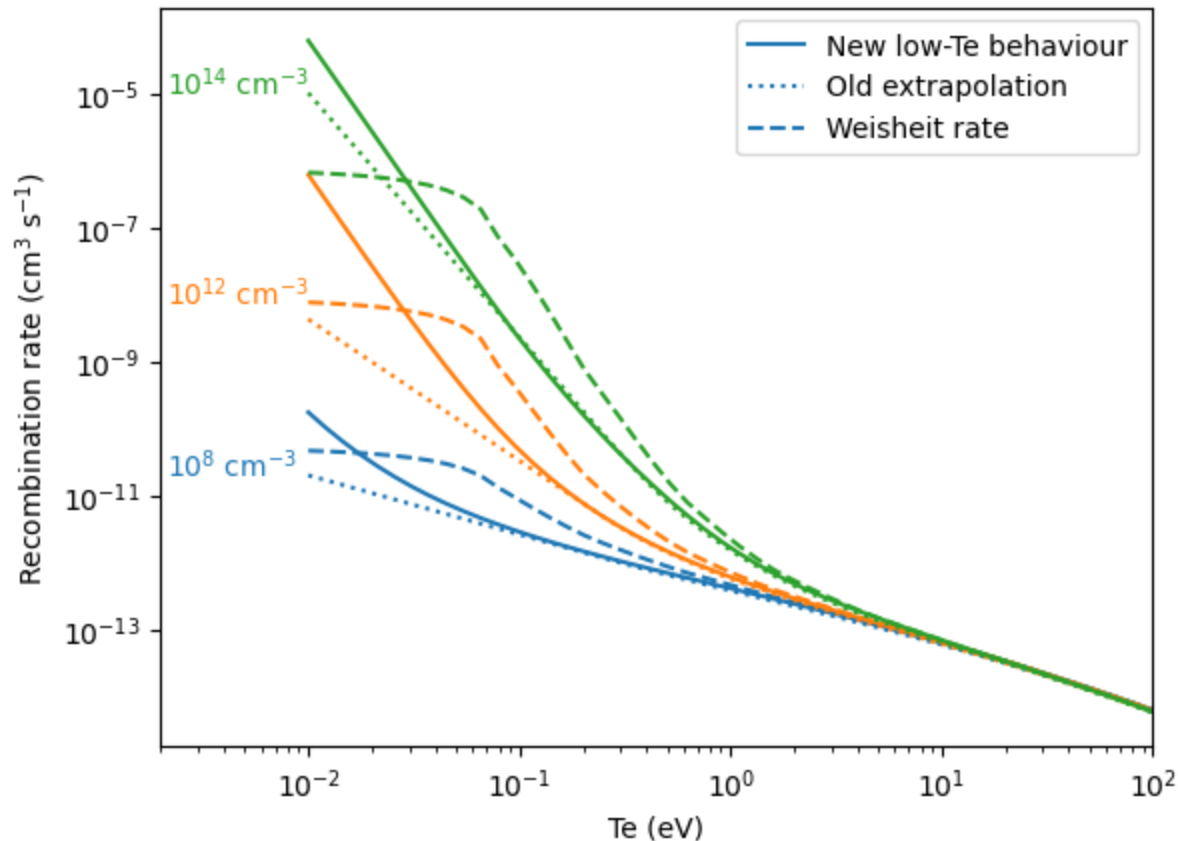
- Te=0.2eV was the lower limit in ADAS adf11 data for hydrogen (acd12_h.dat).
- Extrapolation to lower Te assumed a constant slope – reasonable but not when 3-body becomes important.
- Weisheit (J Phys B, 1975, vol 8, p2556) data used in B2.5 branch of solps irrespective of what is requested in the input file.

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Low Te recombination PECs for hydrogen

H0 emissivity for n= 3 - 2
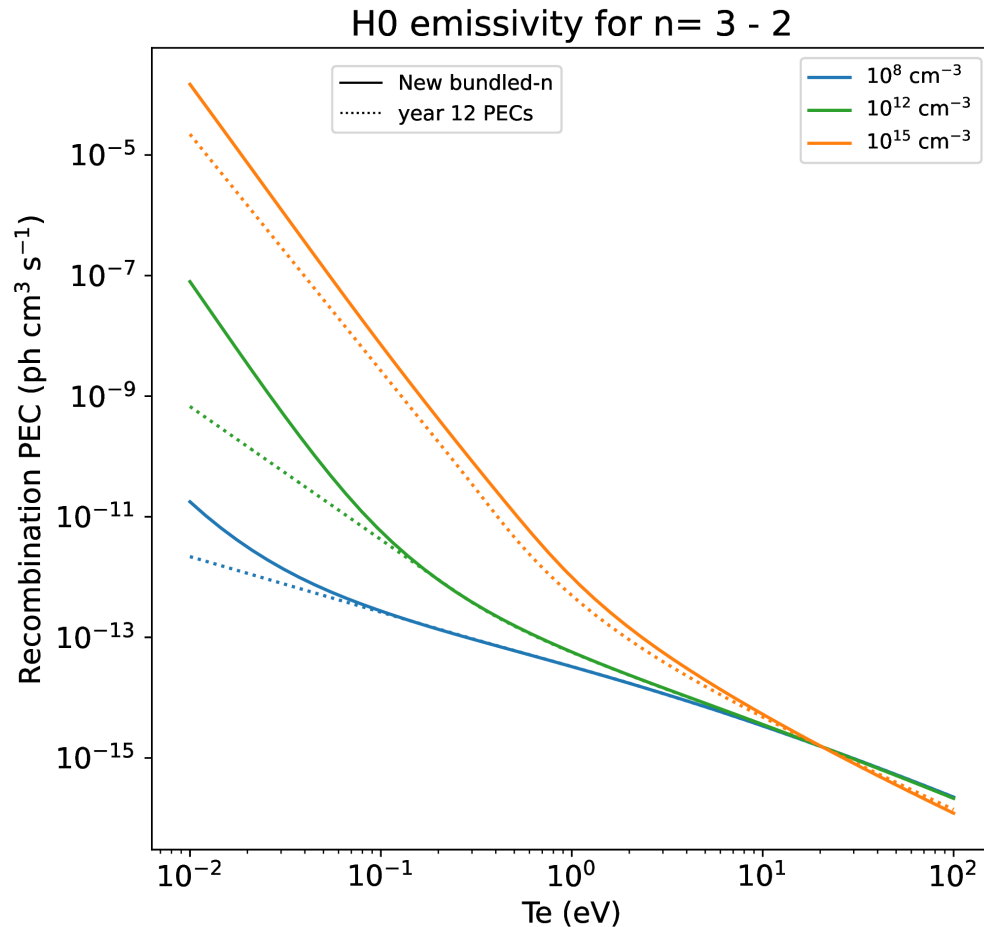
- Alter the representation of the population enables extension to 100K.
- Effect is also seen in the photon emissivity coefficients.

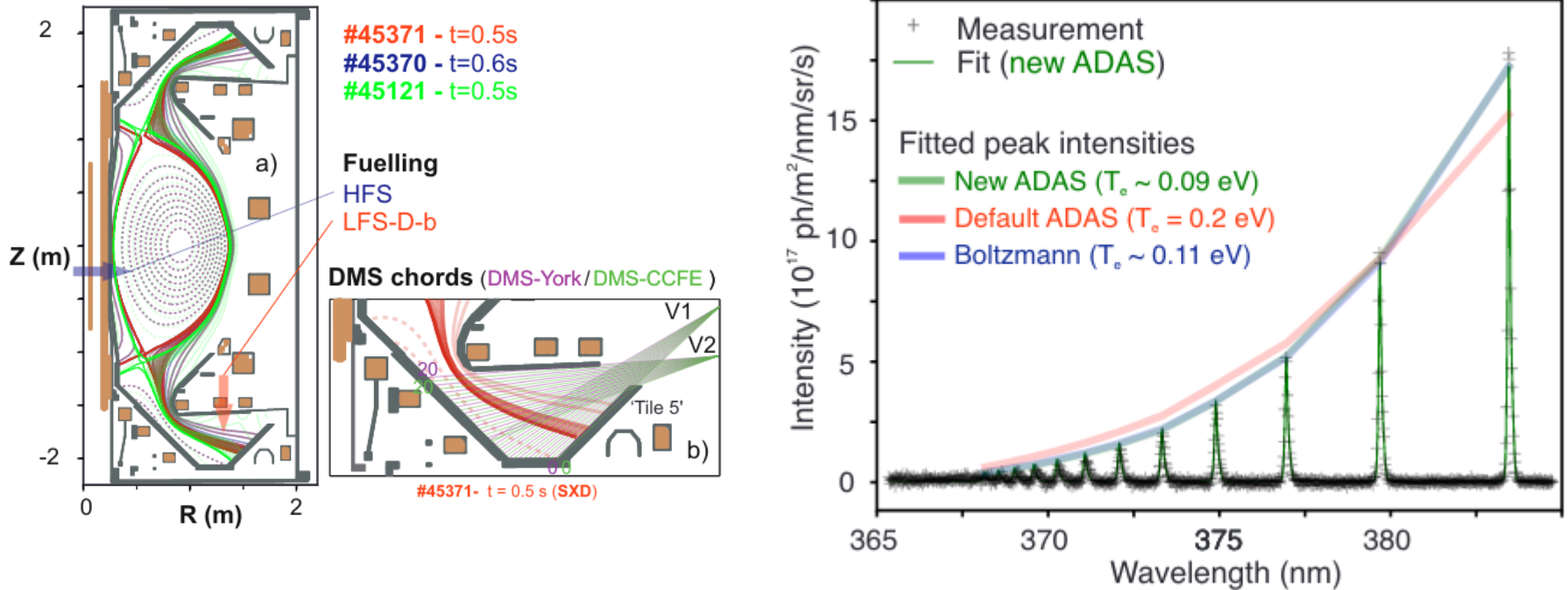University of Strathclyde Science

Fit to MAST-U Balmer series

Figure 12. High-n Balmer line spectra from # 45370 from line-of-sight 6 (see figure 2) at $t = 0.8$ s with example high-n Balmer line fit using new ADAS data that can go below 0.2 eV ($T_e = 0.09$ $(0.08 - 0.1)$ eV, $n_e = 3.5 \times 10^{18} m^{-3}$). High-n Balmer line fits using standard ADAS data ($T_e = 0.2$ eV, $n_e = 5.1 \times 10^{18} m^{-3}$) as well as a Boltzmann relation ($T_e = 0.11$ $(0.1 - 0.11)$ eV, $n_e = 3.7 \times 10^{18} m^{-3}$) have also been performed, but, for clarity, only peak intensities are shown in the figure rather than the full fit. The line of sight used is significantly downstream of the electron density bulk ($n_e \sim 1.4 \times 10^{19} m^{-3}$) at . Transparent lines are shown connecting the peaks of the various Balmer lines for the three different fits, showing an overlap between the Boltzmann fit and fit with new ADAS data and a mismatch between the measurement and the default ($T_e = 0.2$ eV) ADAS data.

K Verhaegh et al. Nuc. Fus., 126023 (2023)

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Hydrogen excitation and ionization
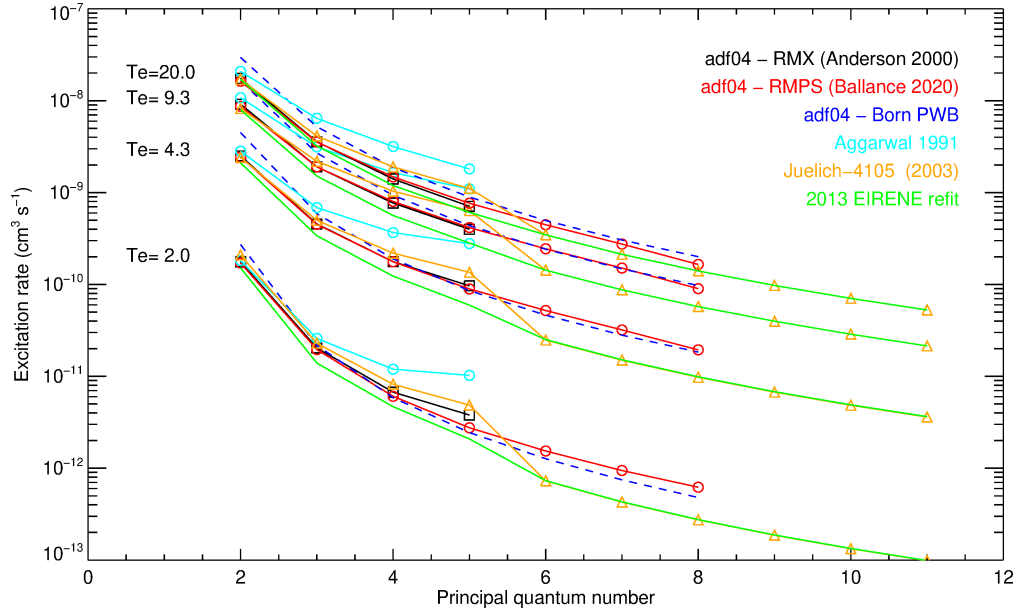
- R-matrix excitation up to n=8 with RMPS approach.
- Can we say the scaling to higher n is established?
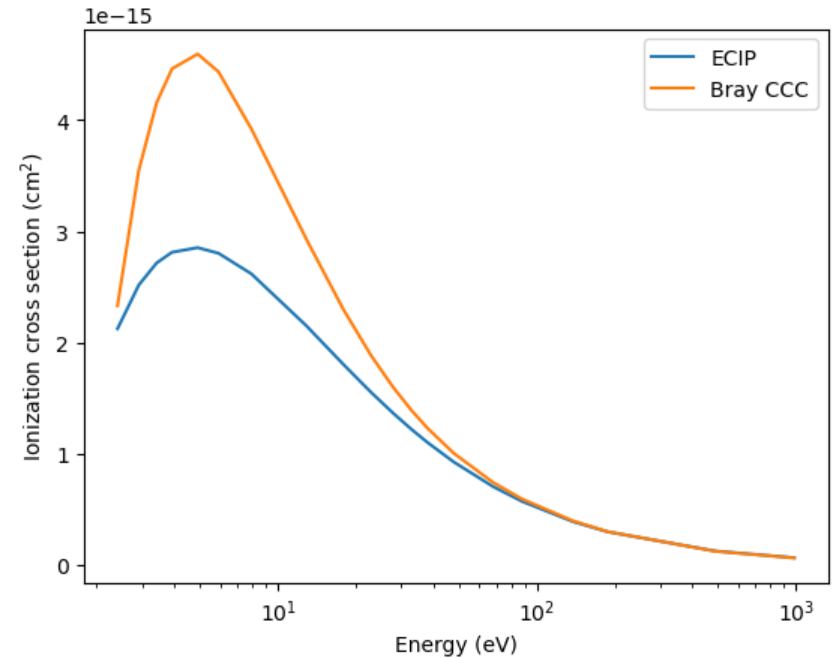
- ECIP vs CCC for ionization from n=3 excited level.
- Does this scale?

To Do: determine the effect on ionization and power balance.

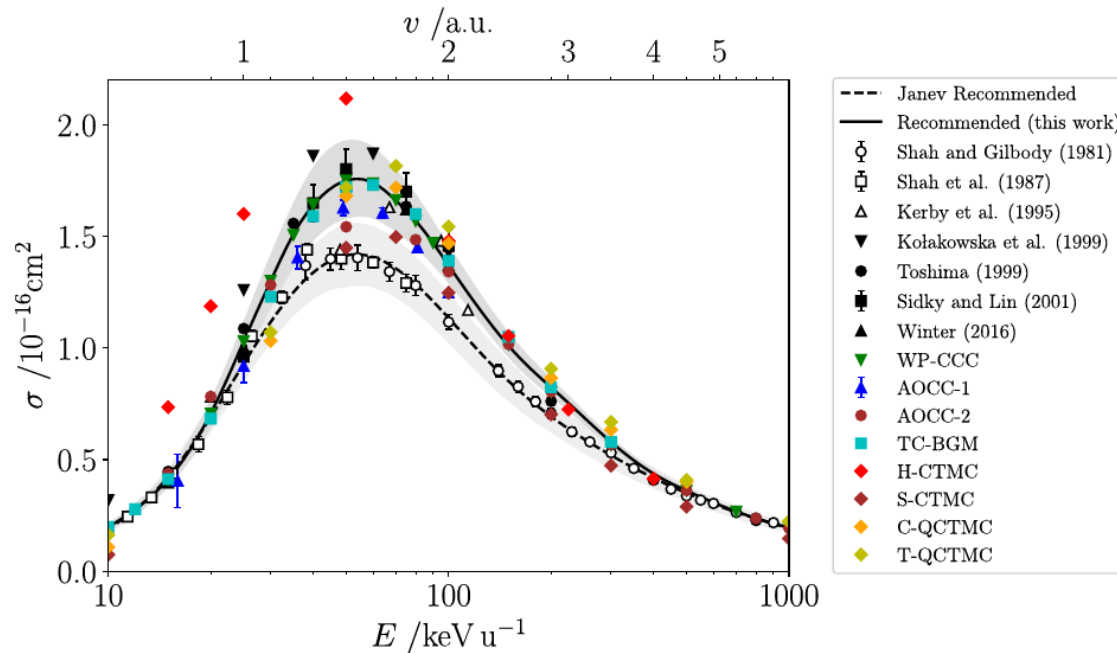# Hydrogen – when do we disbelieve experiment?

p + H⁰ ionization

Figure 4. Experimental and calculated cross sections for proton-impact ionization of ground-state hydrogen. Solid and open black symbols are as for figure 1; dashed line with uncertainty interval band: recommended cross sections obtained from the fit function of Janev and Smith [6]. New calculations are: the WP-CCC results from [27] (this paper reported both 1-center and 2-center results; here, 2-center results are shown), the AOCC-1 results from [26], the TC-BGM results from [25], the S-CTMC, T-QCTMC, and C-QCTMC results from [84], the AOCC-2 and H-CTMC results are present calculations.

- CRP on atomic data for neutral beams (Hill et al, 2023).
- Convergence of sophisticated methods indicate that experimental cross section measurements from the 1980s may not be correct.
- How do we incorporate such conclusions into our modelling?
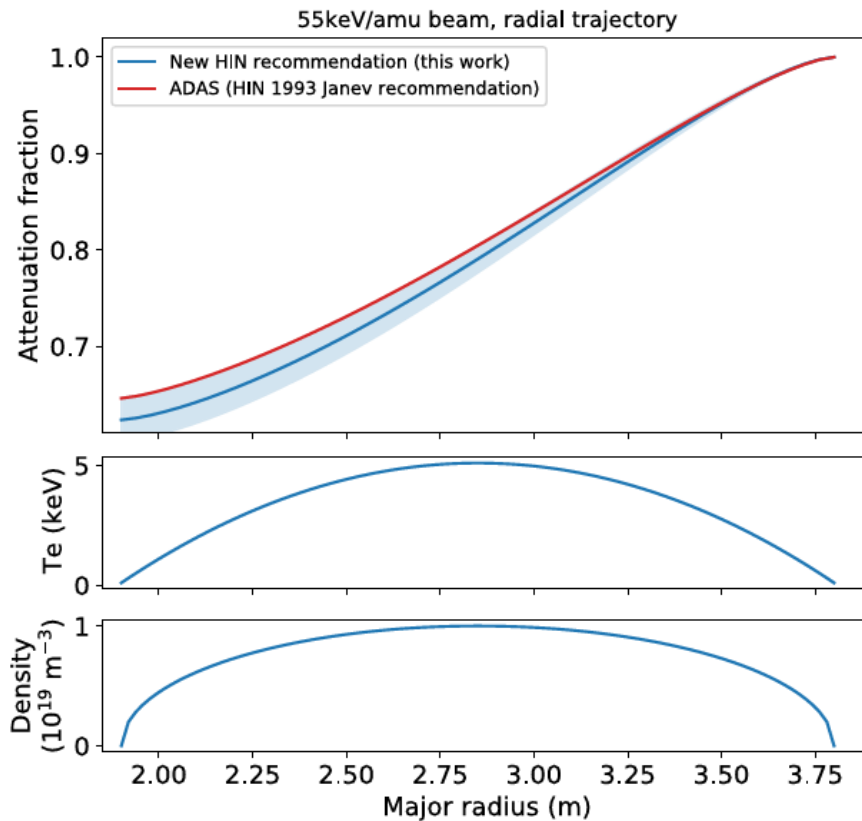
UQ – propagation of uncertainties

Figure 14. A simple, pencil-like, neutral beam launched into JET-like conditions shows the growing nature of attenuation and the difference between the same model when just the proton-neutral hydrogen ionization cross section is changed.

- Envelope of values can be used to propagate the uncertainty in fundamental data through to measurable quantities.
- Tokamaks measurements are rarely good enough to distinguish between competing atomic evaluations.
- But we should strive to add an 'atomic error' to all predictions from synthetic diagnostics.

Effect on the concentration

Apply CHEAP to Ne10+ concentration measurement with: bms-sd bms bms+sd
and separate out the new 'atomic error'
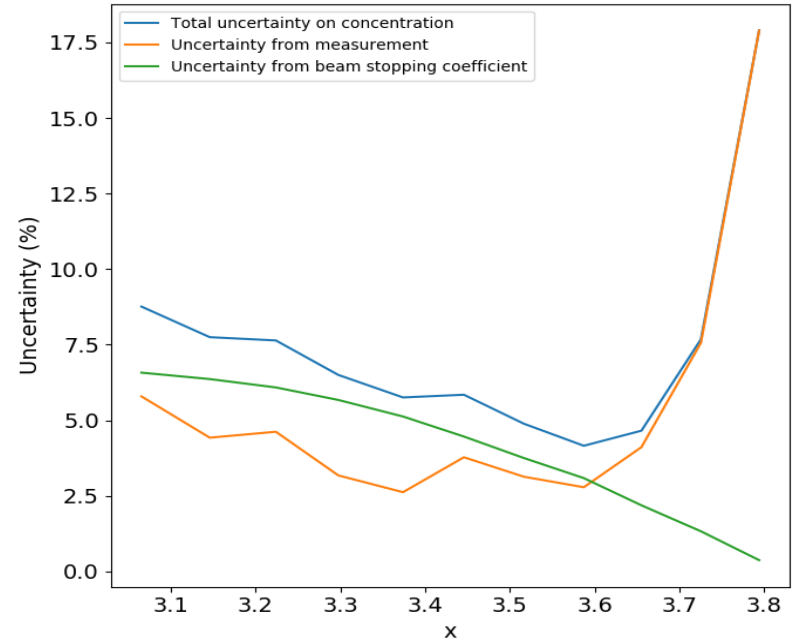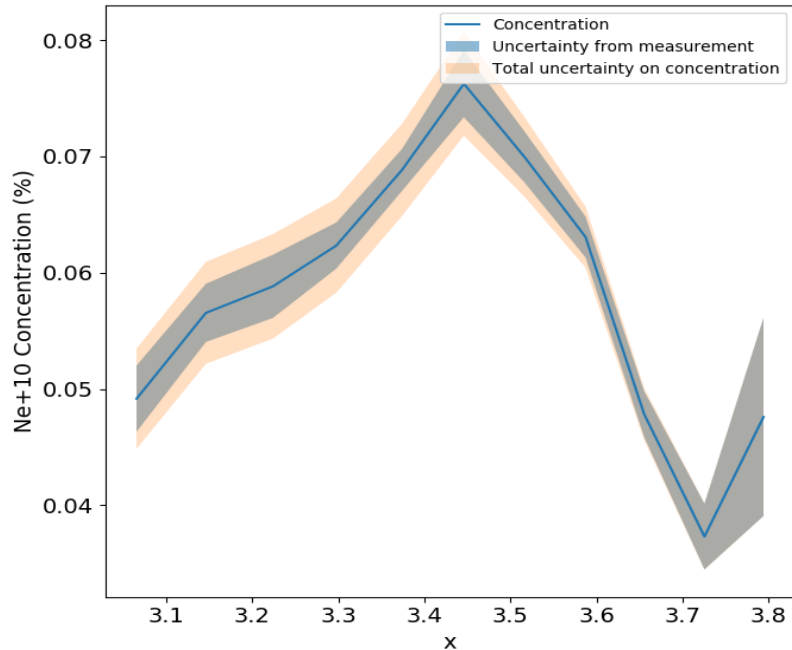
- Uncertainties on the diagnosed parameter due to atomic inputs are of same order as measurement errors.
- Important to properly determine this uncertainty and to reduce it as much as possible.

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Extending adf11 data format – adding energy-resolution

Two types of ADAS power coefficients – line (PLT) and continuum (PRB)

- current adf11 power data are not energy resolved
- line power (PLT) is the sum of all the transitions in the adf04 dataset
- GCR improves the PLT value by projecting the influence of upper levels onto the adf04 set – these are Rydberg bundle-n levels.
- power arising from omitted configurations is absent – but this is a good model for light elements
- for higher Z (higher than Mo, 42) including all configurations that contribute a noticeable fraction (~1% or more) to PLT results in extremely large adf04 files.
- 2 related problems – choosing the set of configurations and bringing the PLT closer to 'true' value – were addressed by using configuration-averaged adf04 files.
- PLT is topped-up with CA transitions and an algorithmic approach is used to select the set of configurations.

- continuum (PRB) is less dominant than line power until all electrons are ionized and bremsstrahlung takes over.
- GCR PRB follows the cascade of electrons in an n=999 calculation.
- empirical/baseline PRB is empirical for DR. RR and bremsstrahlung are based on Gaunt factors for both GCR and empirical methods.

Line (PLT) vs continuum (PRB) contribution in equilibrium
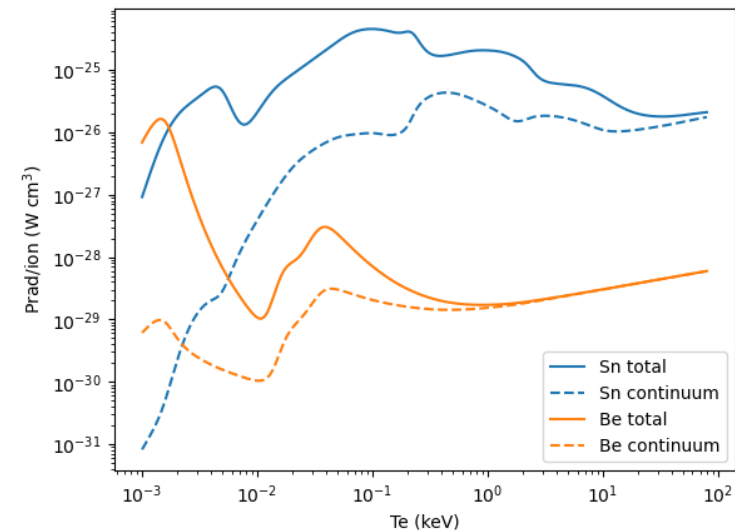
Optimisation and assessment of theoretical impurity line power coefficients relevant to ITER and DEMO

paper on choosing configurations

S S Henderson[1], M Bluteau[1], A Foster[2], A Giunta[3], M G O'Mullane[1], T Pütterich[4] and H P Summers[1]

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PLT power coefficients – location of radiation

PLT

- the energy of the lines are known so any binning scheme can be used
- CA top-up adds a little complexity – where to put the CA transitions
- W^{26+} shows a top-up correction of x1.5 at Te of peak abundance.

$$\mathcal{PLT}^{tot} = \mathcal{PLT}^{ic(cs)} \frac{\mathcal{PLT}^{ca(cl)}}{\mathcal{PLT}^{ca(cs)}}$$
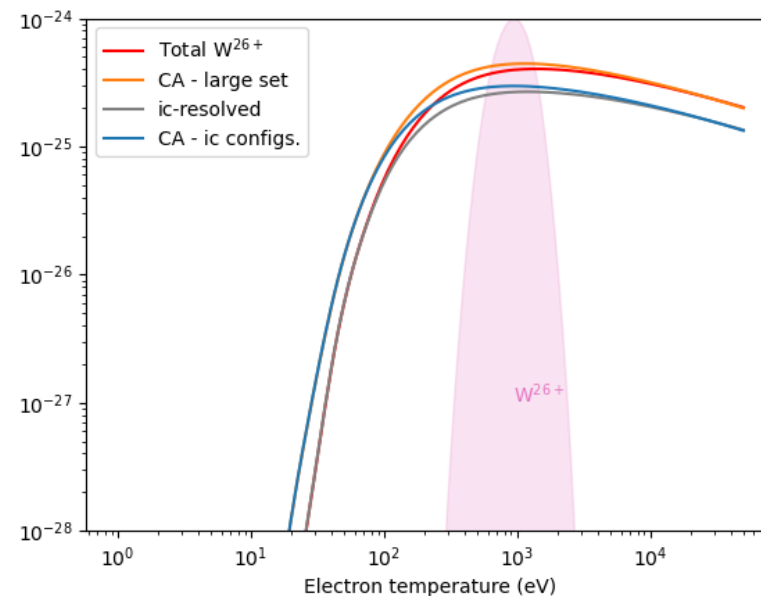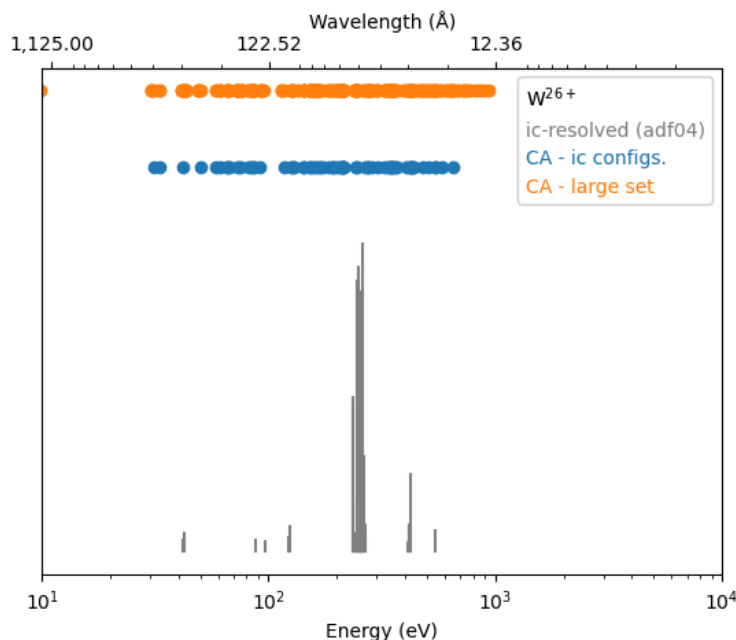
- Strong lines of W^{26+} from adf04 file. Ground is $4d^{10}\,4f^2$.
- energies of CA transitions – the set corresponding to intermediate-coupling resolution lines in the adf04 file – PLT $^{ca(cs)}$
- larger set of configurations – PLT $^{ca(cl)}$

- low Te dominated by low level (ic) spectroscopic levels
- high Te significant radiation from 'missing' configurations
- how does this compare to spectroscopy measured at LHD?

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Energy resolved PLT power coefficients
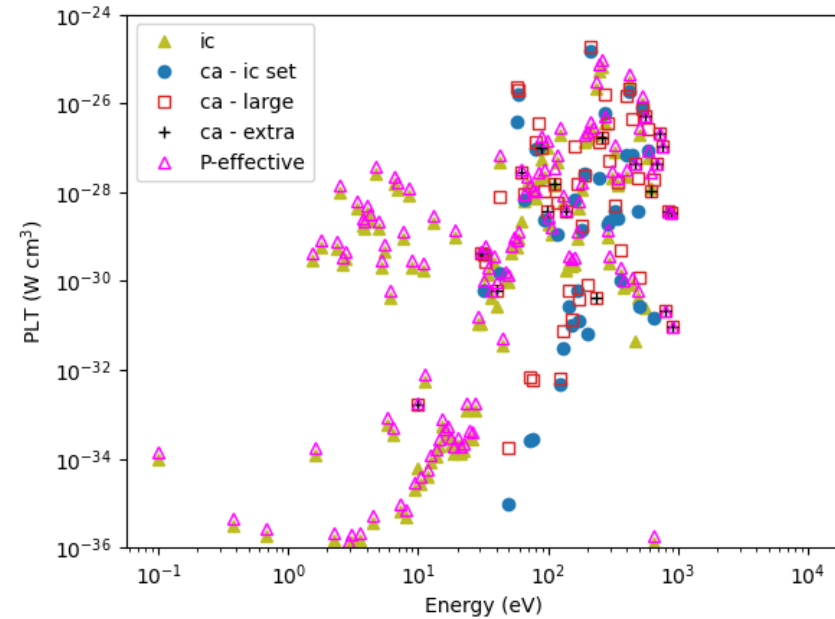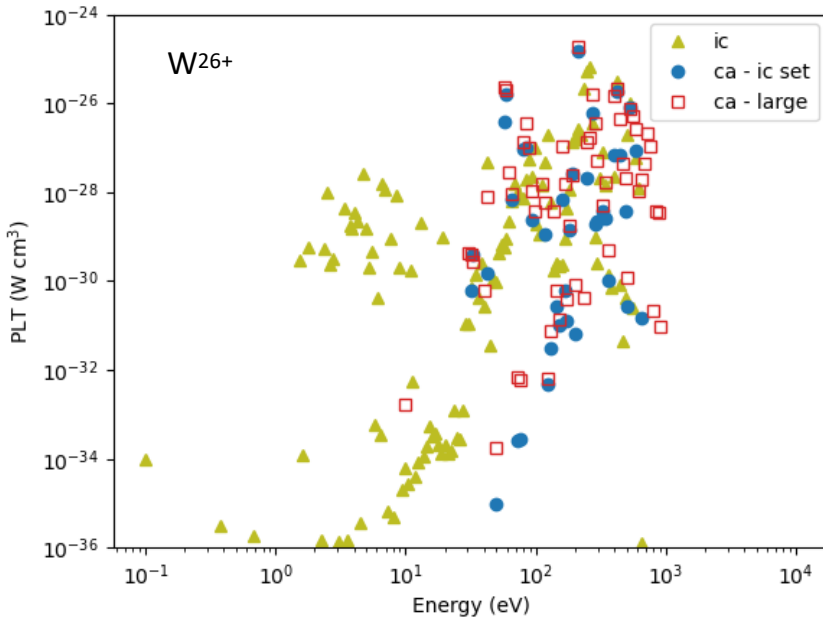
$$\mathcal{PLT}_{\text{eff}}(E) = \mathcal{PLT}^{ic(cs)}\frac{\mathcal{PLT}^{ca(cl \in cs)}}{\mathcal{PLT}^{ca(cs)}} + \mathcal{PLT}^{ca(cl \notin cs)}$$

When summed over energy (E) there is < 0.5% difference with the un-resolved effective PLT coefficient.

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Radiated power from tungsten – different choices at low Te

Cooling curve for tungsten

year 50 acd/scd
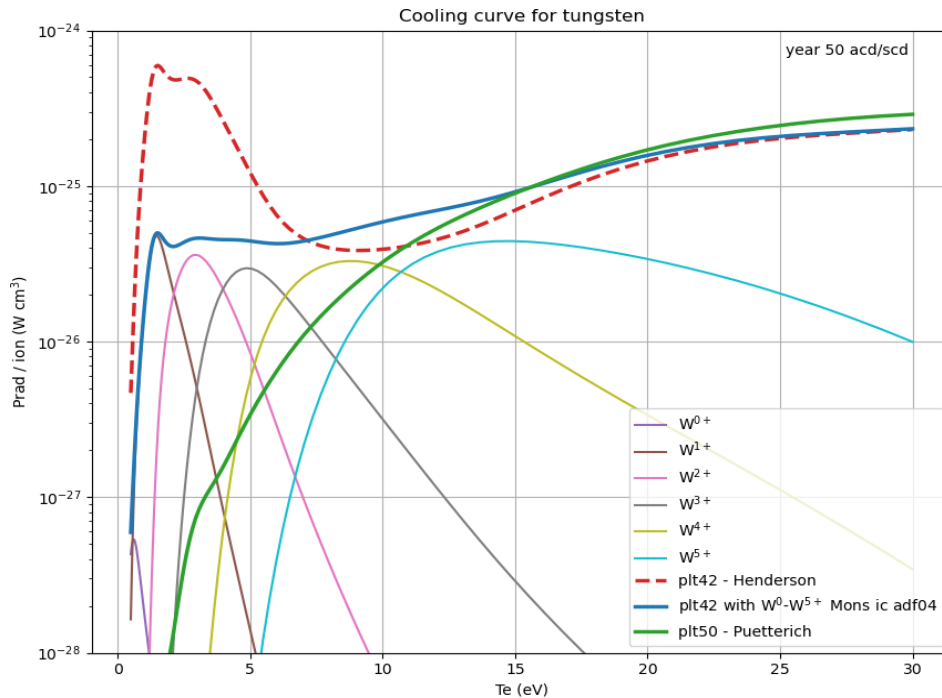
Cowan data with U Mons polarisation corrections
- wlike_mons11#w0ic.dat
- talike_mons11#w1ic.dat
- hflike_mons11#w2ic.dat
- lulike_mons11#w3ic.dat
- yblike_mons11#w4ic.dat
- tmlike_mons11#w5ic.dat

Comparison with R-matrix collision data is next step.
- W^0 from R T Smyth et al, Phys Rev A, 97, 052705 (2018)
- W^+ from N Dunleavy et al, J Phys B, 55, 175002 (2022)
- W^{2+} from M McCann – in preparation
- W^{3+} from C P Ballance et al, J Phys B, 46, 055202 (2013)

Is configuration-average top-up essential?

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W+ R-matrix data and validation

J. Phys. B: At. Mol. Opt. Phys. 55 (2022) 175002   N L Dunleavy et al
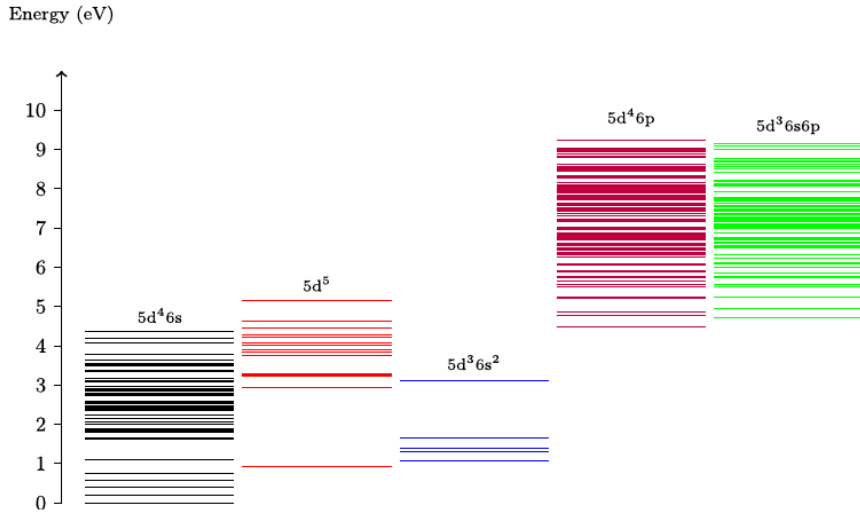
Figure 1. Energy level spectrum of W II organised by electronic configuration (for the first 5 configurations which contribute to the lowest-lying levels). Each horizontal line designates a specific fine structure level (taken from the NIST database).
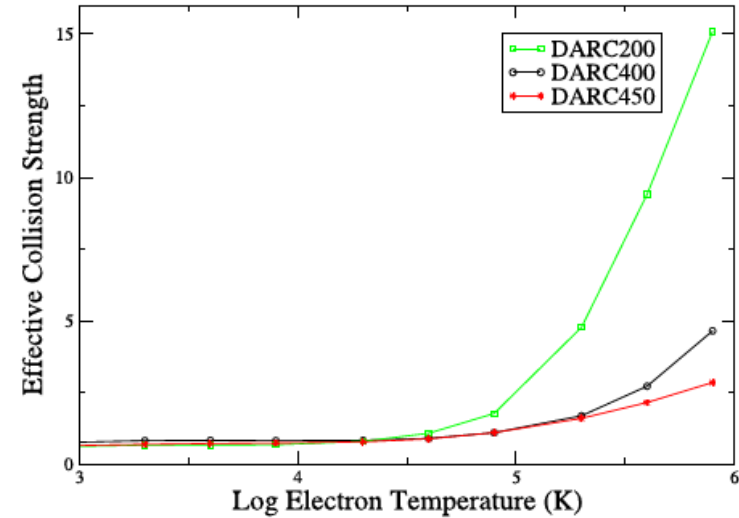
- Complex set of lower levels.
- It may be impossible to ignore metastables.
- Correctness of the excitation collision strengths is determined via convergence of models with increasing number of levels.

W⁺ R-matrix data and validation
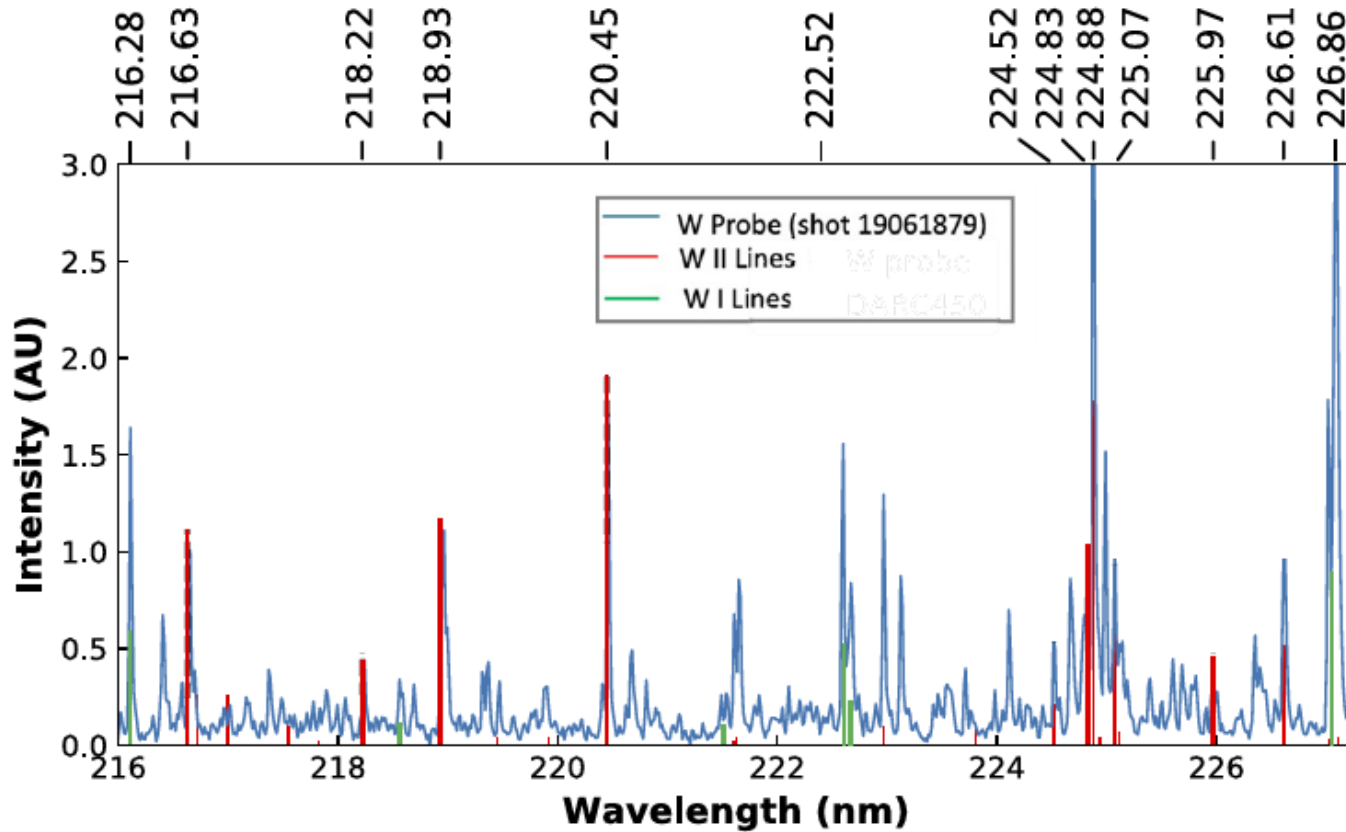
- Experimental comparisons to CTH spectra.
- Disc of tungsten on a reciprocating probe.

Extending traditional analysis

- Machine learning approaches can be applied to spectral measurements.
- Test application to using many W⁰ lines simultaneously rather than identifying the prefect pair of lines.
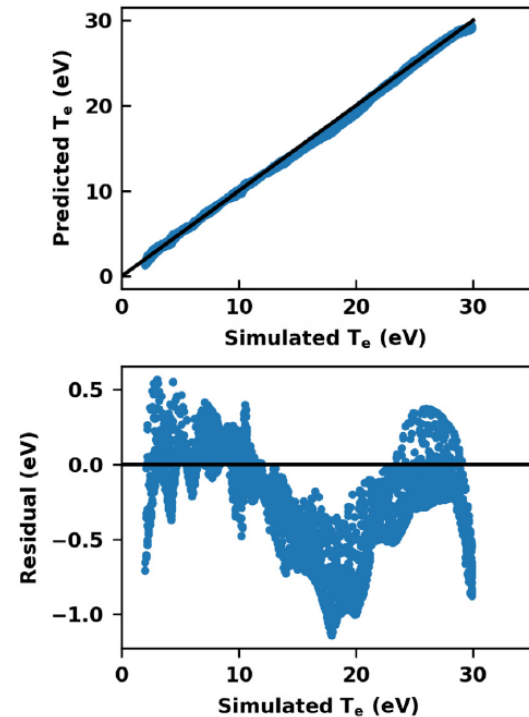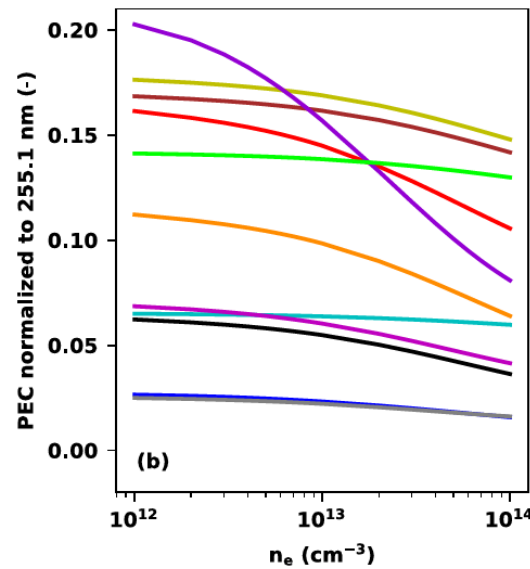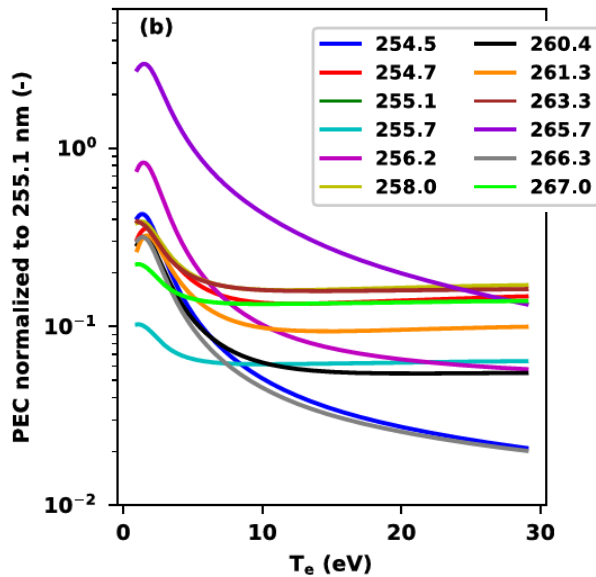
- Training set of normalized photon emissivity coefficients.
- Successful test of NN-model results against Te from Langmuir probes.

C Johnson et al, Nuc. Mater. Energy, 34 (2023) 101304

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Non-tokamak laboratory experiments are essential

Measured X-ray emission from highly charged Xe with Ti^{20+} and Ti^{21+} calibration spectrum
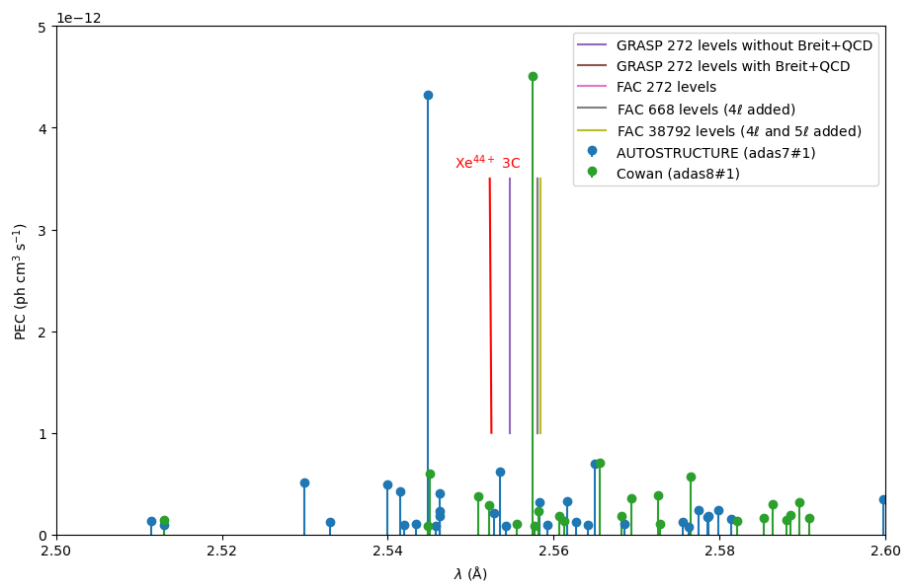
- ADAS data for intensity estimations (AUTOSTRUCTURE and Cowan) agree well for emission but not in wavelength.
- Convergence between GRASP and FAC atomic structure codes has been reported (see doi:10.1016/j.adt.2009.11.002)
- The line adjacent to 3C should be well separated which was confirmed by a recent measurement at EBIT-I at LLNL.
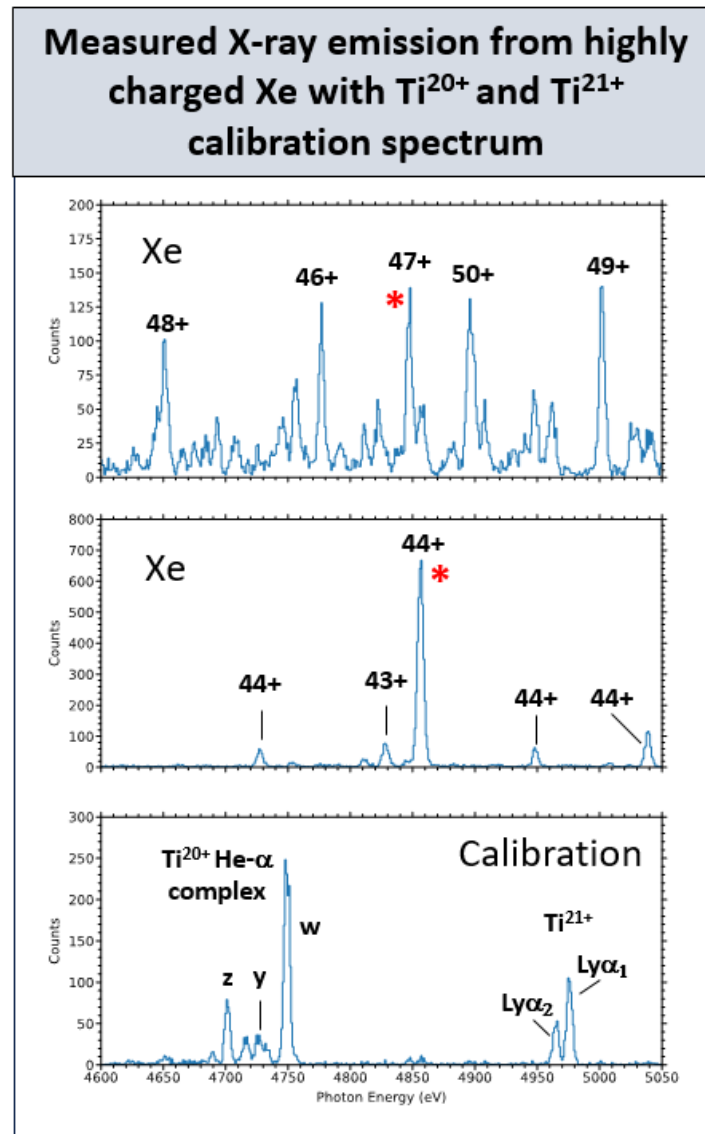
G. V. Brown, N. Hell, A. Fairchild, M. Eckart

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Total rate from ground configuration
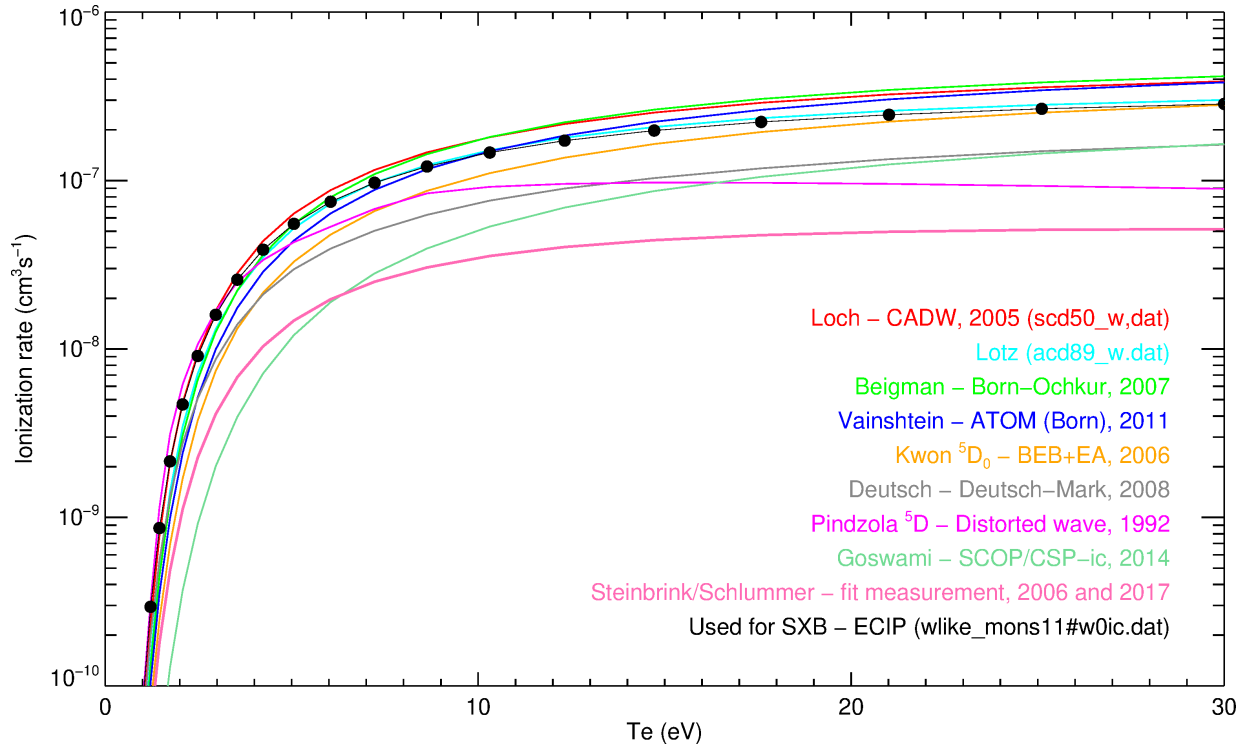
- ADAS uses ECIP (exchange classical impact parameter) for ionization out of excited levels – empirical formula developed by comparing measured ionization cross sections of light elements. But it is robust and is non-divergent.
- This pathway may be larger than the rate from ground.
- No convergence to a consensus yet and the spread is too wide to use for an uncertainty analysis.
- An outstanding challenge for ab initio calculations and experiment.

Many high resolution spectra of different W ions

SIR spectrum - WEST#55506

2.00-9.50 sec (exp. 204-704)

W^{45+} W^{42+} W^{44+} W^{43+}

Counts/s
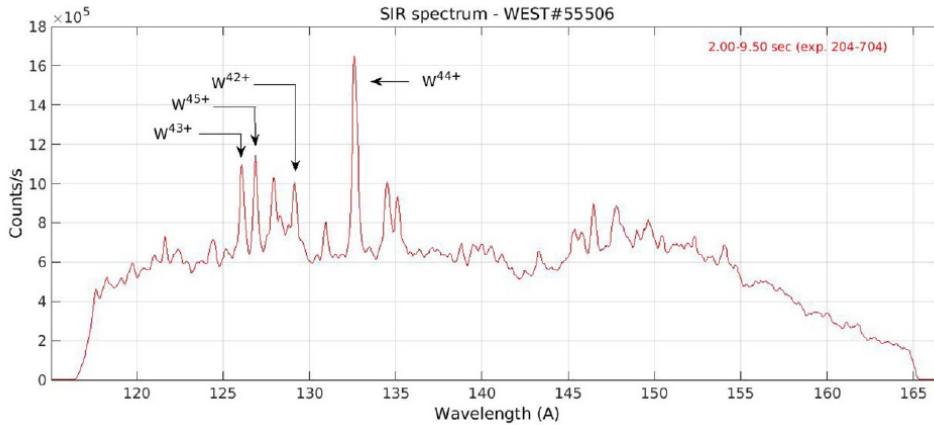
Wavelength (A)

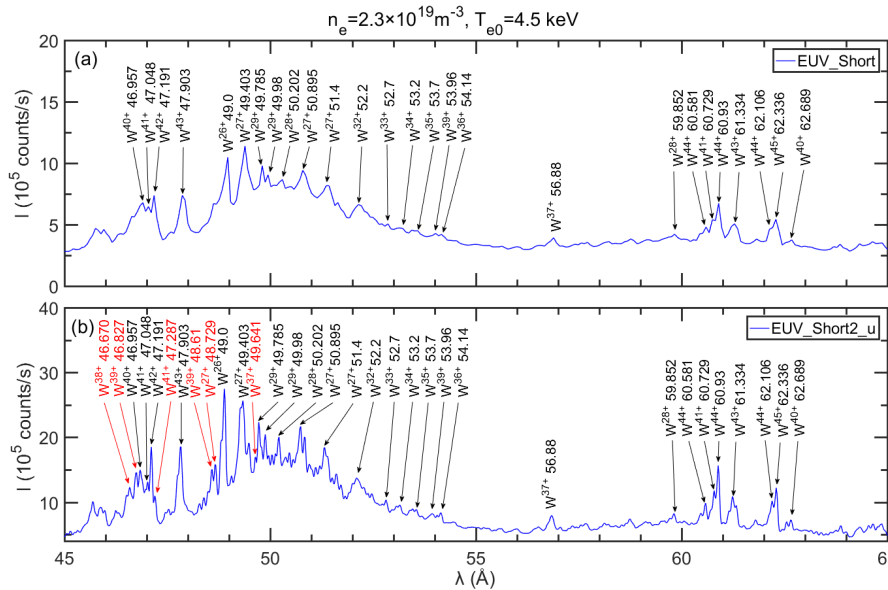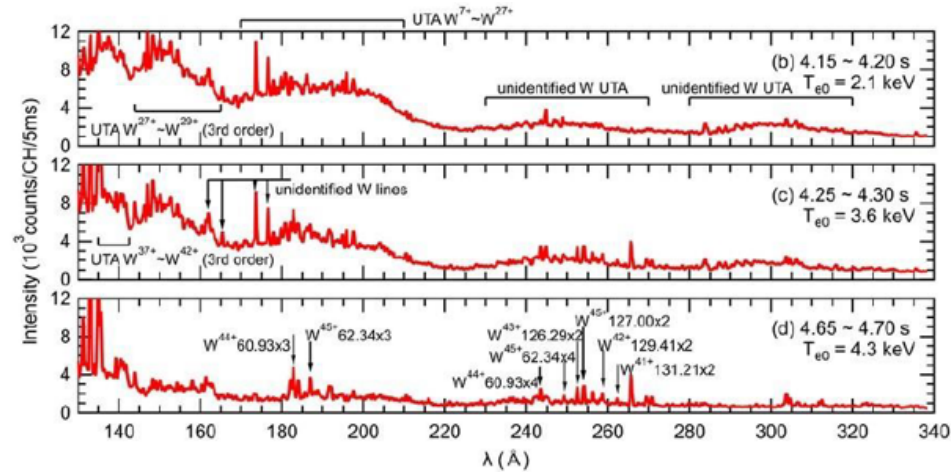| Present measured wavelength (Å)	Emitting ion	Lower level	Upper level	Previous measured wavelength (Å)
121.6	W^{44+}	$4s^2\,^1S_0$	$4s4p\,^1P_1$	60.931×2
124.4	W^{45+}	$4s\,^2S_{1/2}$	$4p\,^2P_{3/2}$	62.335×2
• 126.1	W^{43+}	$4s^2 4p\,^2P_{1/2}$	$4s^2 4p\,^2P_{3/2}$	126.29
				126.39
• 126.8	W^{45+}	$4s\,^2S_{1/2}$	$4p\,^2P_{1/2}$	127.12
				127.20
127.9	W^{43+}	$4s^2 4p\,^2P_{1/2}$	$4s4p^2\,^4P_{1/2}$	128.17
				128.24
• 129.2	W^{42+}	$4s^2 4p^2\,^3P_0$	$4s^2 4p^2\,^1D_2$	129.41
				129.45
131.0	W^{41+}	$4s^2 4p^3\,^2D_{3/2}$	$4s^2 4p^3\,^2D_{5/2}$	131.24
				131.21
• 132.6	W^{44+}	$4s^2\,^1S_0$	$4s\,4p\,^3P_1$	132.88
	(blended)			132.87

R. Guirlet, PPCF, 24 (2022) 101304

WEST   EAST   LHD

$n_e=2.3\times10^{19}m^{-3}$, $T_{e0}=4.5$ keV

(a) EUV_Short

(b) EUV_Short2_u

Y.X. Cheng *Rev. Sci. Instrum.* 93 (2022)123501

(b) 4.15 ~ 4.20 s $T_{e0}=2.1$ keV — UTA W^{7+}~W^{27+}, unidentified W UTA

(c) 4.25 ~ 4.30 s $T_{e0}=3.6$ keV — UTA W^{27+}~W^{39+} (3rd order), UTA W^{37+}~W^{42+} (3rd order), unidentified W lines

(d) 4.65 ~ 4.70 s $T_{e0}=4.3$ keV — W^{44+}60.93×3, W^{45+}62.34×3, W^{43+}126.29×2, W^{45+}127.00×2, W^{45+}62.34×4, W^{42+}129.41×2, W^{44+}60.93×4, W^{41+}131.21×2

T. Oishi et al, 25th International Conference on Line Shapes

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Atomic data for tungsten ions – adf04 files

- $W^0 - W^{3+}$ R-matrix (RMPS).
- W^{44+}, W^{45+}, W^{46+} R-matrix (ICFT).
- These are effective collision strengths (Maxwellian EEDF) but cross sections (interval averaged to maintain resonance nature) can be produced.

- All stages: distorted wave (AUTOSTRUCTURE) – rates and cross sections.

- Desirable to have HULLAC and FAC data.
- There are a number of papers on different ions in the academic literature but not easily available.
- For ADAS (☺) but also collisionDB.

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Spectral measurements from EBITs

- Individual spectra from various tungsten ions have been measured over the years.
- Could act as a fiducial measurement to validate the *ab initio* atomic calculations of low lying (spectroscopic) transitions.
- Do we need more complete coverage to improve our validation effort.
- Easily available database of EBIT spectra (IAEA perhaps?) would be helpful.

Ion stage	Wavelength range (Å)	Machine	Year	Reference
$W^{5+} - W^{7+}$	180–280	EBIT-I	2015	[59]
$W^{5+} - W^{8+}$	180–250	SH-HtscEBIT	2022	[60]
$W^{7+} - W^{8+}, W^{10+}$	4200–6400	SH-HtscEBIT	2015	[61, 61]
$W^{11+} - W^{15+}$	160–270	SH-HtscEBIT	2015	[62]
W^{26+}	2600–5020	SH-PermEBIT	2014	[63]
W^{28+}	3300–4000	SH-HtscEBIT	2014	[64]
$W^{21+} - W^{45+}$	45–70	Berlin	2001	[65]
$W^{24+} - W^{33+}$	15–35	CoBIT	2013	[66]
$W^{39+} - W^{47+}$	40–200	NIST	2007	[67]
$W^{40+} - W^{50+}$	5–6	LLNL	2004	[68]
W^{45+}, W^{46+}	5.19–5.26	Shanghai	2018	[69]
$W^{48+} - W^{61+}$	27–41	LLNL	2013	[70]
W^{64+}	0.9–1.77	Tokoyo	1996	[54]
$W^{65+} - W^{71+}$	6.5–7.7	SuperEBIT	2009	[71]

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Large variation

- The spectral features vary with conditions so an accurate atomic model is essential for understanding and untangling transport effects.
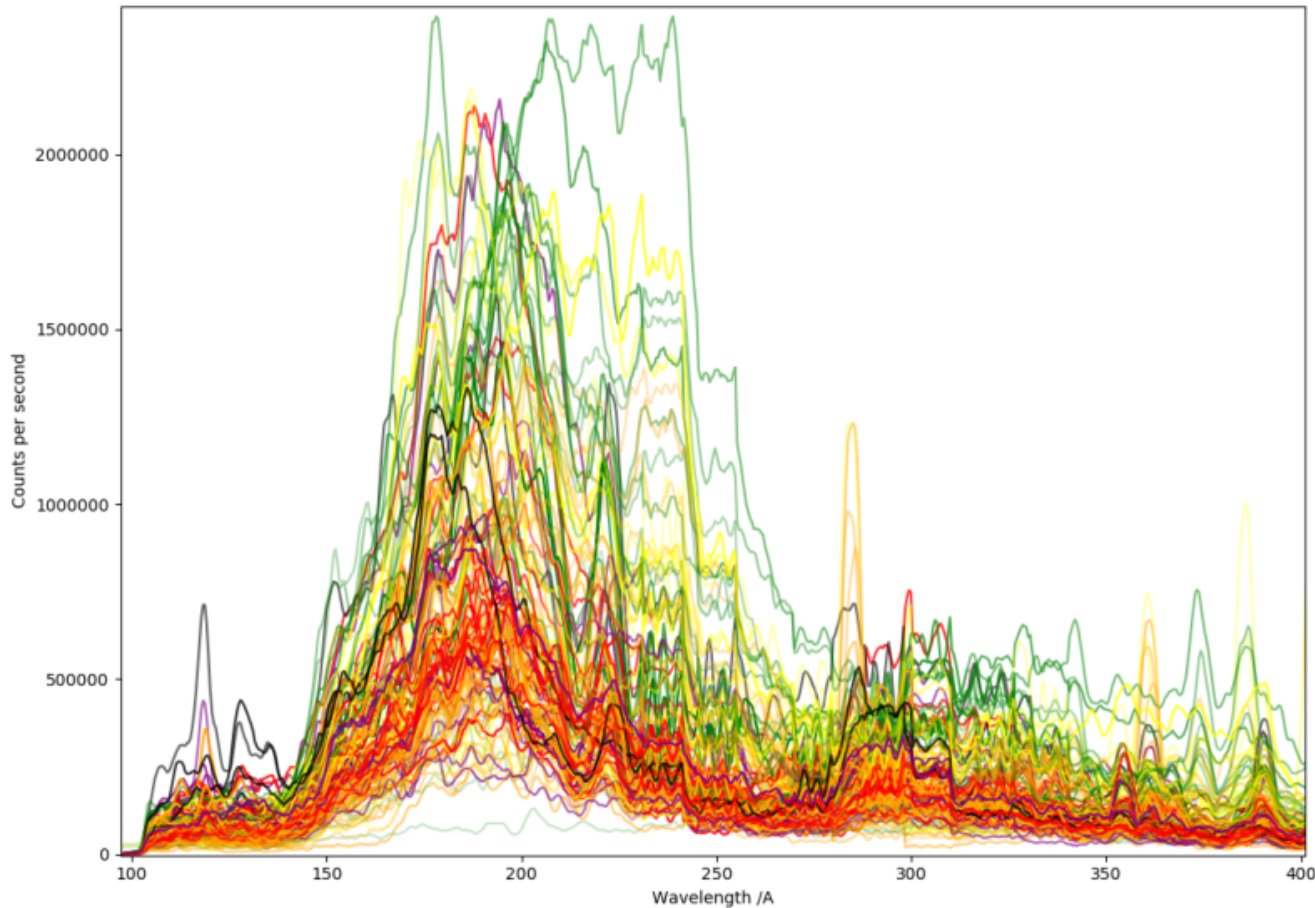
- JET VUV W feature, T Kloska
- No strong correlations of shape with various plasma parameters

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Conclusions and outlook

- A lot of progress has been made in measurements, analysis, calculations and models.
- To answer the tungsten question for tokamaks input from many other areas was, and is, needed – storage rings, EBITs, linear plasmas, table-top experiments, theoretical advances and high performance computing.
- Hydrogen is similar but with a longer history.
- Still some missing pieces – DR for a handful of stages, W^0 ionization, forbidden lines, spectral features.
- But tungsten emission can now be used as a quantitative diagnostic in fusion.
- Collisional-radiative effective data for modelling is more available.