Fundamental atomic data for tungsten and hydrogen and the effect of the finite density edge plasma

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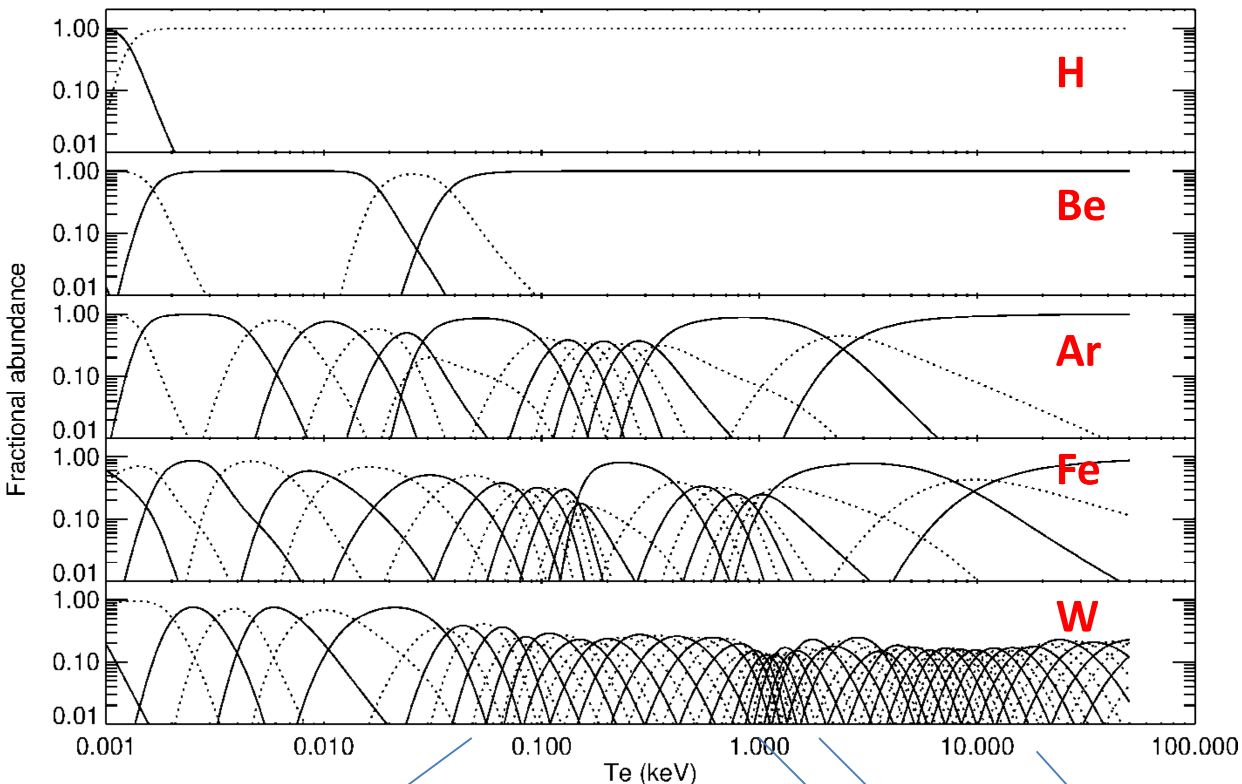
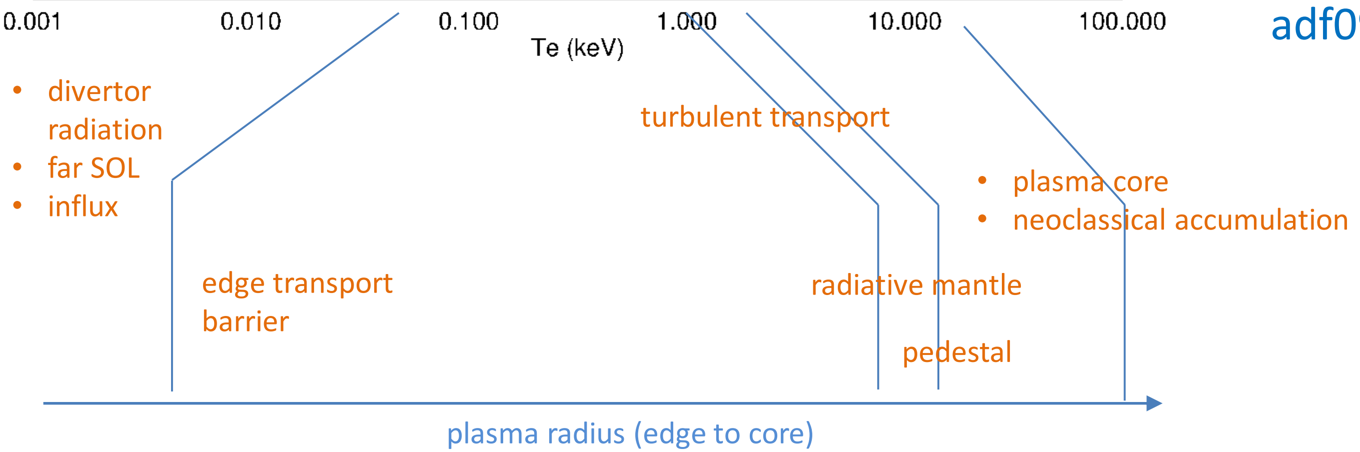
and ADAS contributors

ADAS perspective: wish for complete data for all elements

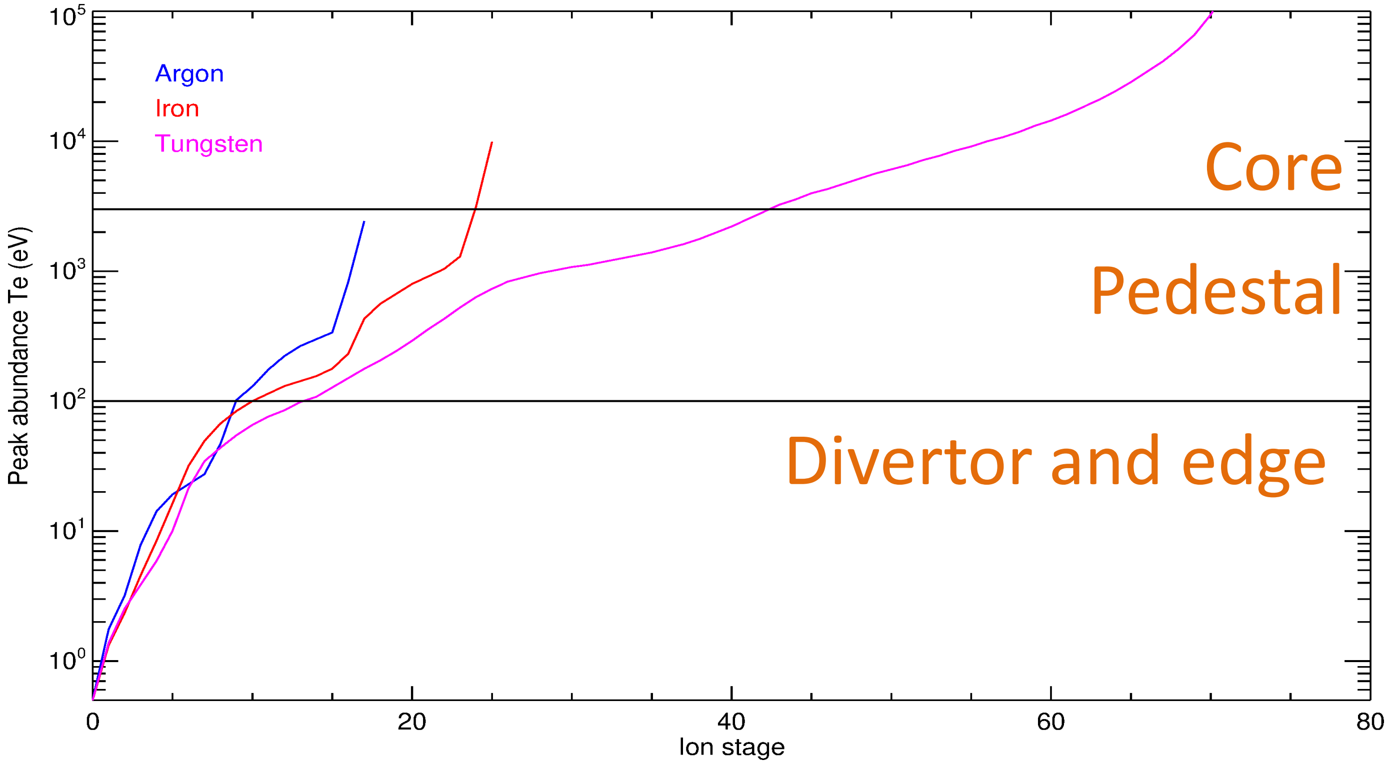


Equilibrium balance

- rate coefficients for ionisation balance (adf11)
- influx S/XB measure (adf15)
- Radiated power (adf11)
- Spectroscopy (adf15)
- All fundamental atomic data calculated by ADAS group and close collaborators (adf04, adf09, adf48, adf23)



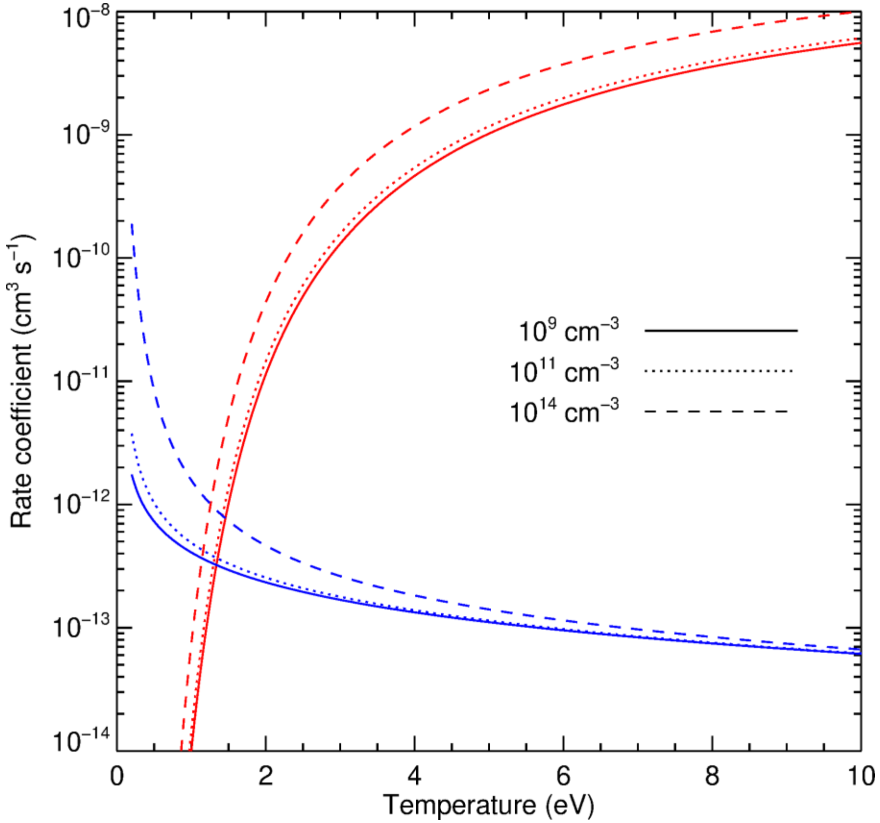
What is an edge ion?

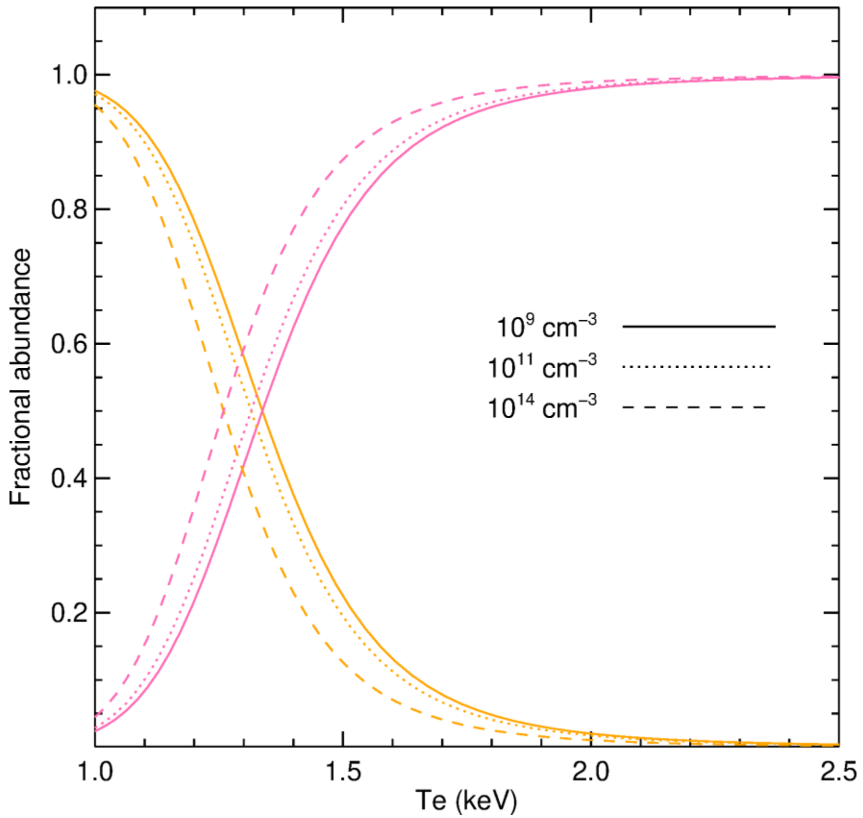


- With increasing Z
  - more and more ion stages exist in a small spatial region
  - individual emission shells become narrow which limits the contribution function of a line
  - more electrons generally complicates the atomic structure spreading emission across many transitions

Fundamental rates alone are not sufficient

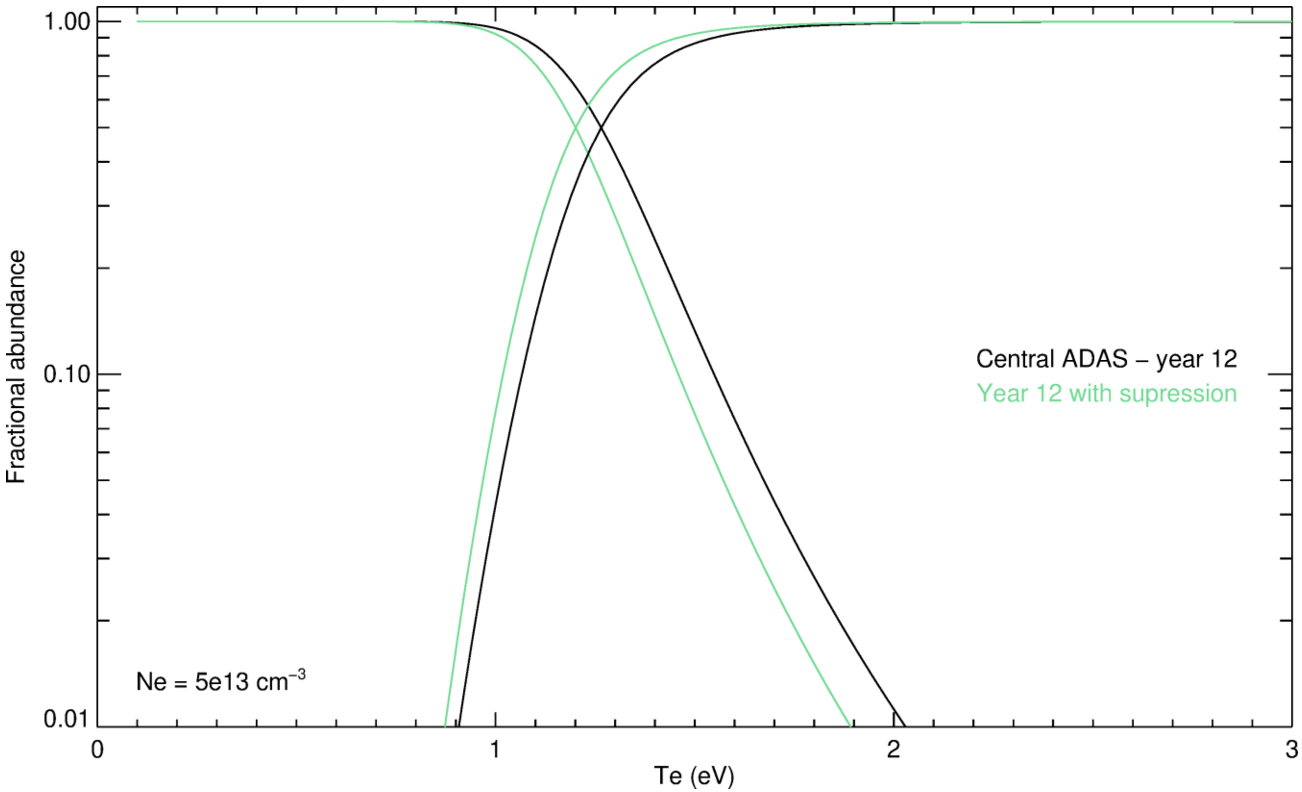
ADAS generalized collisional-radiative model





- Simple equilibrium balance – no thermal CX or molecular processes.
- Variation with density is possibly greater than any uncertainty in atomic data – particularly for hydrogen.

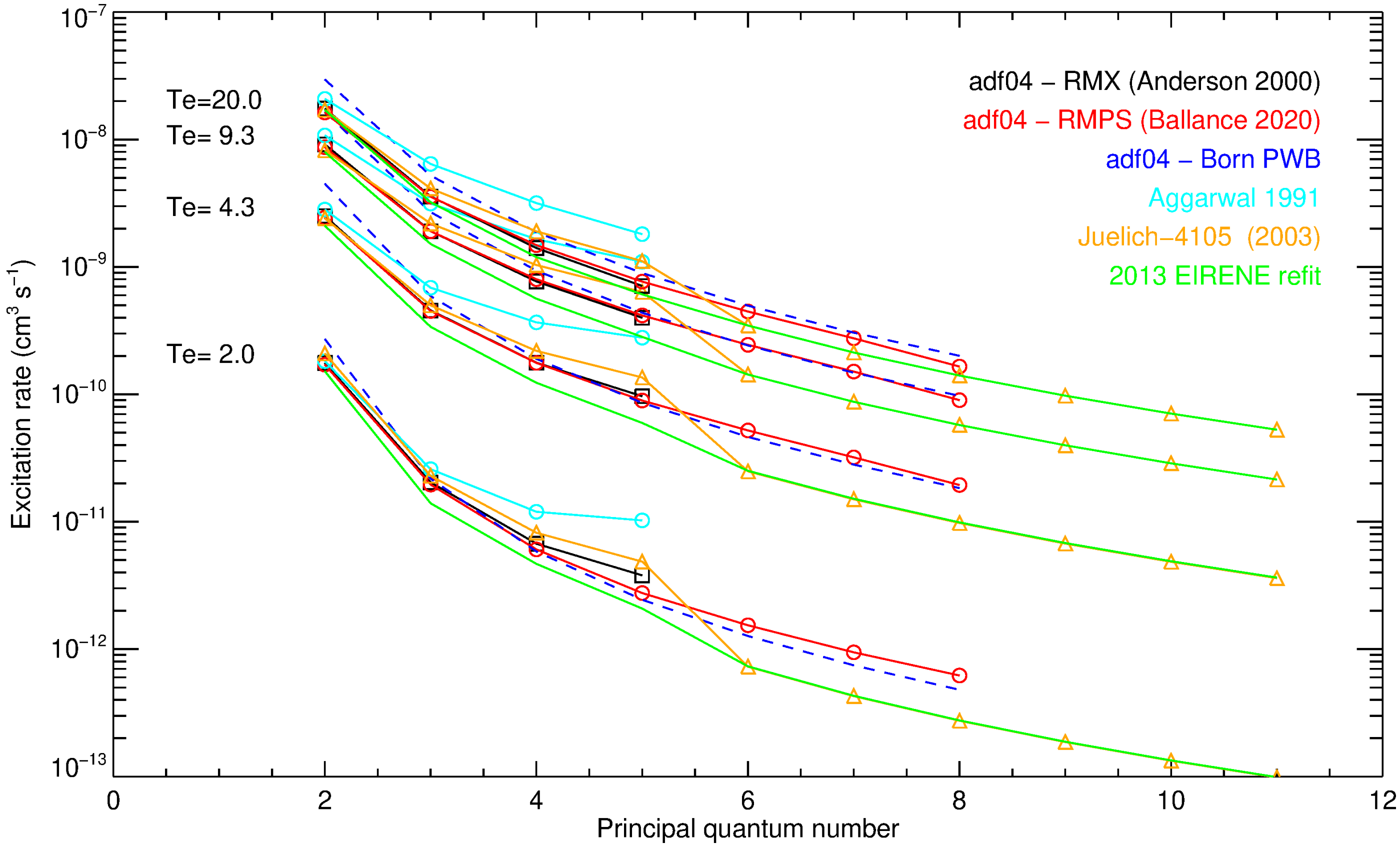
Opacity effects



- ADAS generalized collisional-radiative model
- Transition probabilities of Lyman-α reduced to 10% and Lyman-β to 55%.
- Not as extreme as astrophysical Case A.
- Consistent ionization and recombination rates calculated.

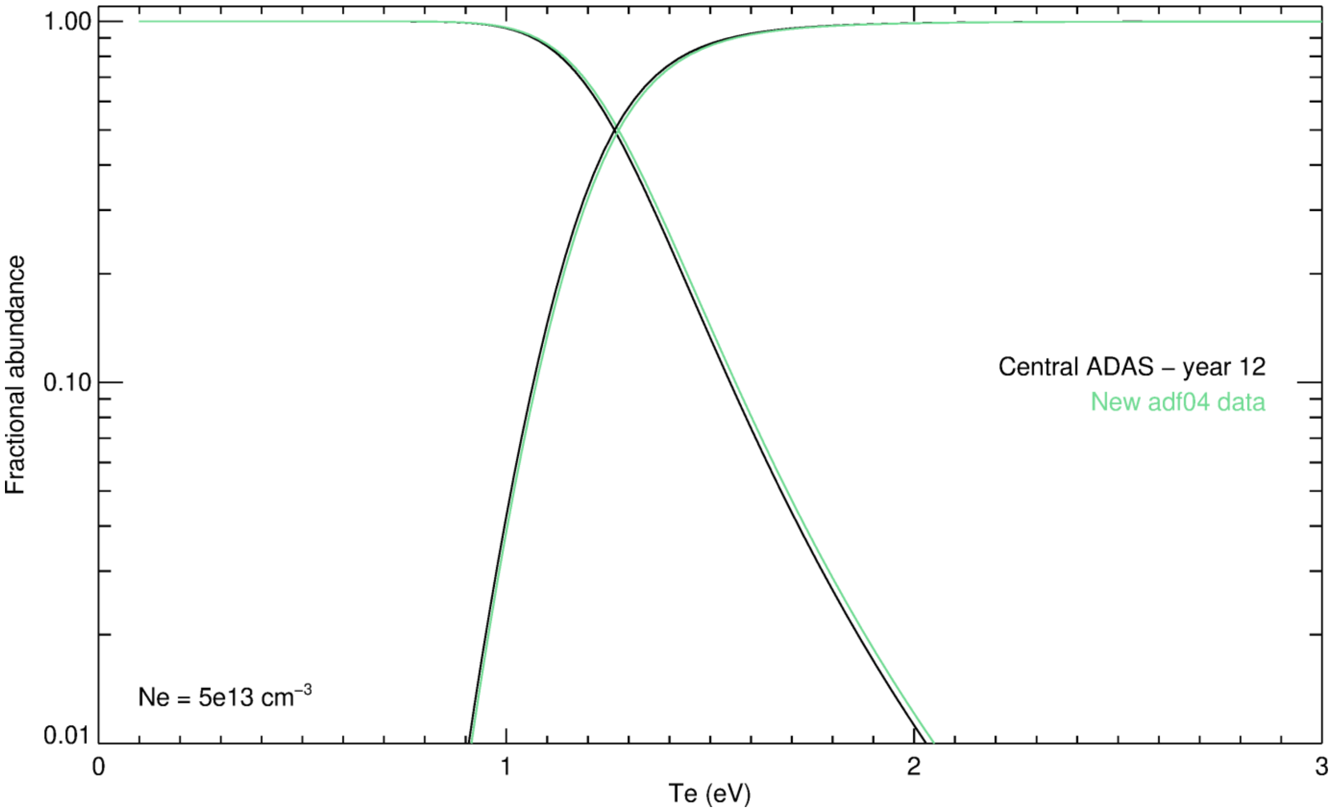
- The change is of same order as density variation.
- Demands high precision of the underlying atomic data.
- And correctness of the CR model.

New neutral hydrogen excitation data



- 1958 – first measurement of 2p→ground (Fite and Brackmann).
- 1963 – close coupling calculation (Burke).
- 2020 – R-matrix up to n=8.
- hydrogen may never be 'done'.

New excitation data – n=1-5 only

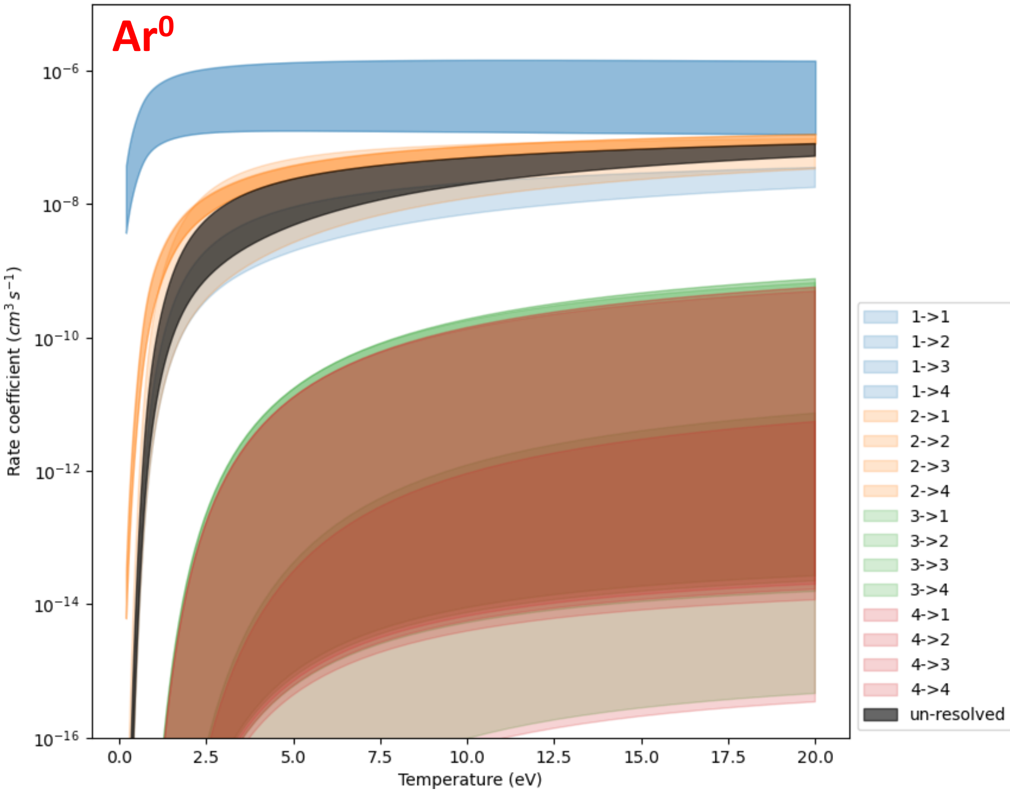


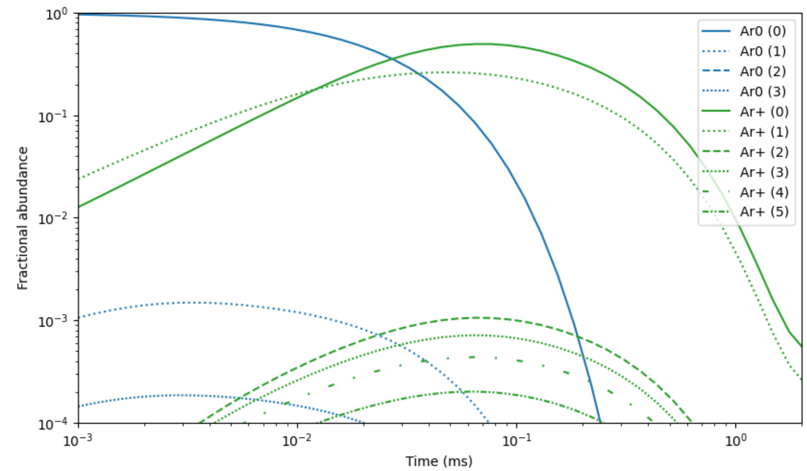
- ADAS generalized collisional-radiative model
- Have **not** used higher-n to modify high n-n' transitions so the effect may be greater.

- The change is more modest but this does not show the effect on the spectroscopy of the Lyman and Balmer series.
- Confirms the need for high precision of the underlying atomic data.
- And correctness of the CR model.

Density variation and metastable evolution

eg, intermediate-coupled (resolved in J) argon



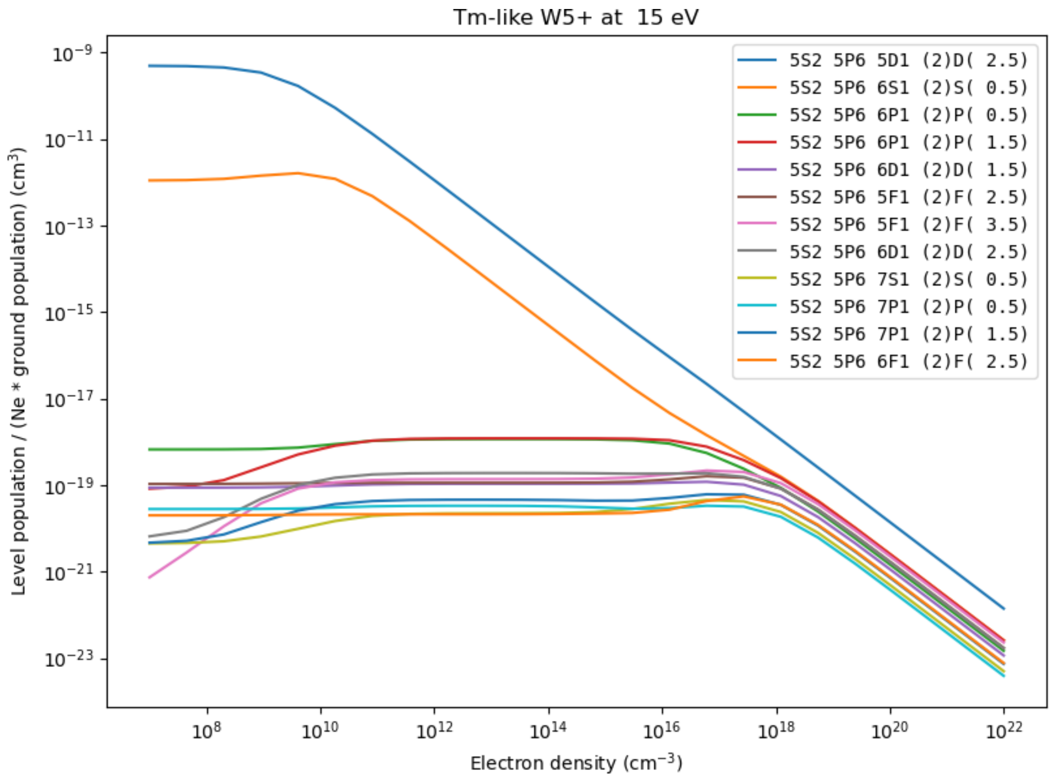


- Ar^0 into a 7.5eV/10^{14} cm^{-3} plasma.
- Ar3+ is the dominant stage in these conditions.

```
Ar0 1  3s2 3P6     (1)0(0.0)       0.0
    2  3s2 3P5 4S1 (3)1(2.0)   93143.8
    3  3s2 3P5 4S1 (3)1(1.0)   93750.6
    4  3s2 3P5 4S1 (3)1(0.0)   94553.7
Ar+ 1  3s2 3p1     (2)1(1.5)       0.0
    2  3s2 3p1     (2)1(0.5)    1431.6
    3  3s1 3p1     (2)0(0.5) 108721.5
    4  3s2 3p1     (4)2(3.5) 132327.4
    5  3s2 3p1     (4)2(2.5) 132481.2
    6  3s2 3p1     (4)2(1.5) 132630.7
    7  3s2 3p1     (4)2(0.5) 132737.7
```

- Ne = $10^9 - 10^{14}$ cm^{-3}.
- Higher lying metastables are sensitive to density.

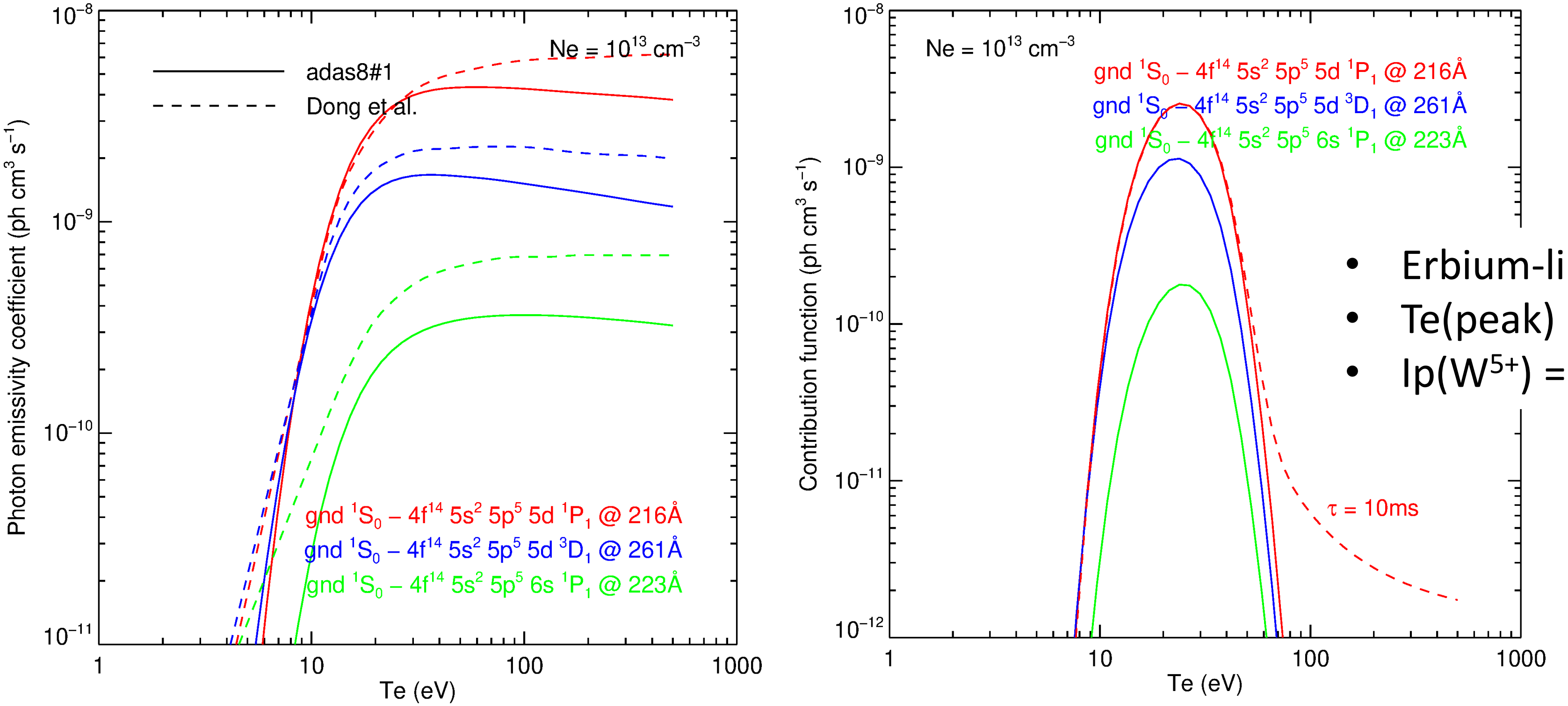
Tungsten – density effects and metastables



- Thulium-like W^{5+}.
- Te(peak) = ~10eV
- Ip(W^{5+}) = 64.7eV.

- Cowan plane wave Born (adas8#1) modified following Mons approach of Quinet et al, J Phys B43 (2010)
- Ground state: `3d10 4s2 4p6 4d10 4f14 5s2 5p6 5d1`.
- Note that 6s is metastable and is lower lying than 5f configuration – a 'problem' common to the lowly-ionized tungsten ions.

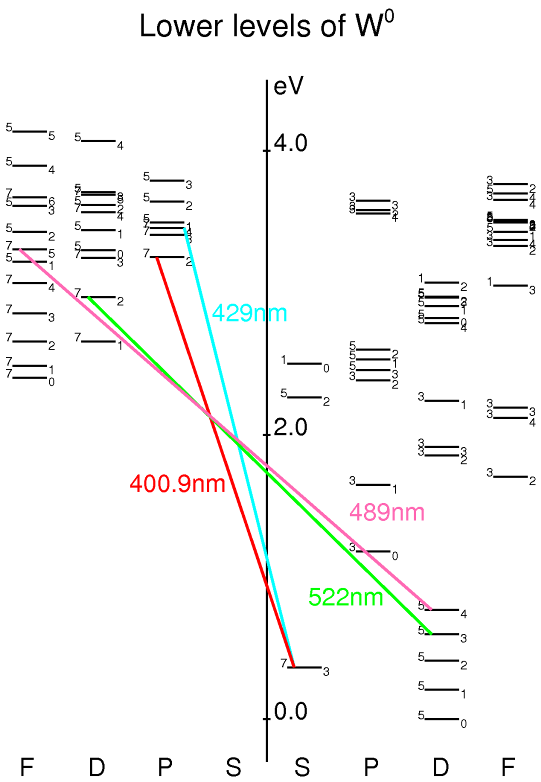
Tungsten – excitation data for the lowly ionized ions

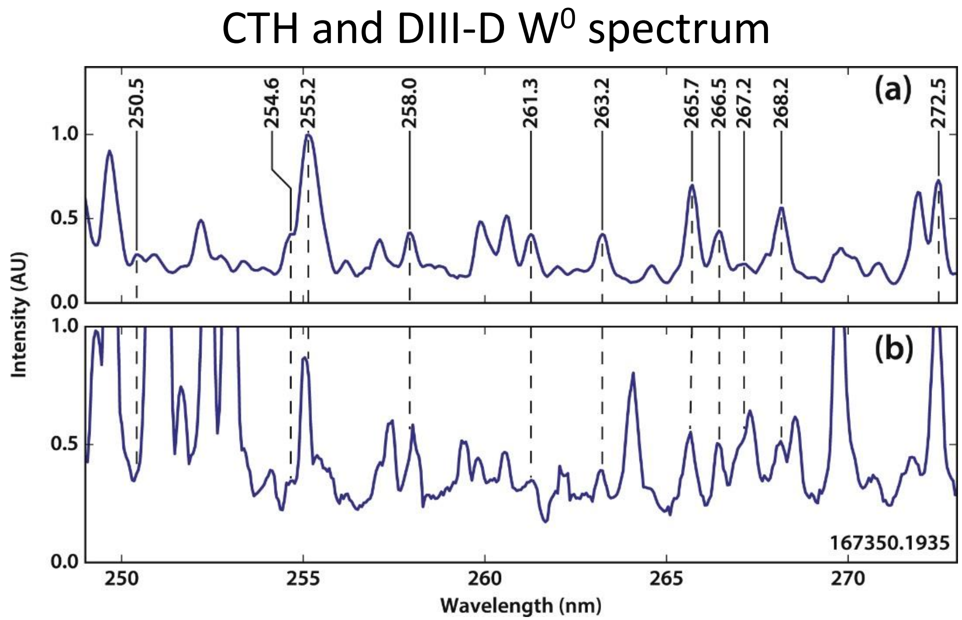


- Erbium-like W^{6+}.
- Te(peak) = ~21eV
- Ip(W^{5+}) = 122eV.

- Ground state: `3d10 4s2 4p6 4d10 4f14 5s2 5p6`.
- The lowering of 6s is not an issue here and the 1st excited configuration is from the promotion of 4f: `4d10 4f13 5s2 5p6 5d1`
- Photon emissivity coefficients based on Cowan excitation data are compatible with HULLAC calculations (Dong et al, Nuc. Fusion, 59 (2019))
- Ewa Pawelec/Kerry Lawson has observed these lines at JET.
- Contribution function folds abundance and PEC to localize emission layer temperature.
- Lines are not sensitive to a simple confinement time mimic for transport.

Neutral tungsten



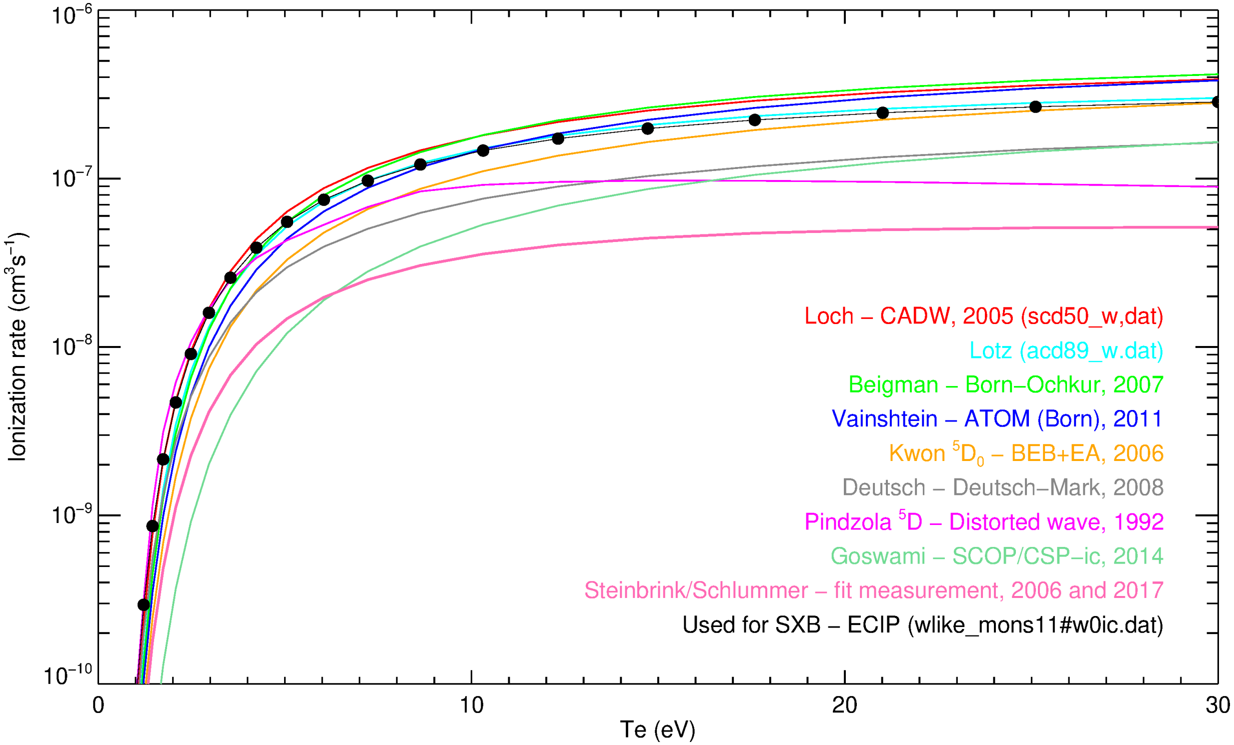


C A Johnson (PPCF 61, 2019)

- W^0 can be a measure of influx of tungsten: Γ = S/XB * I
- Requires ionization (S), excitation (X) and structure atomic data.
- Dominant lines are in VUV which are connected to ground.
- But practical measurements are in visible but are driven by metastables.
- Lower levels are metastable – all with significant population.
- Active area of interest, in particular for ionization data.

Neutral tungsten ionization

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.

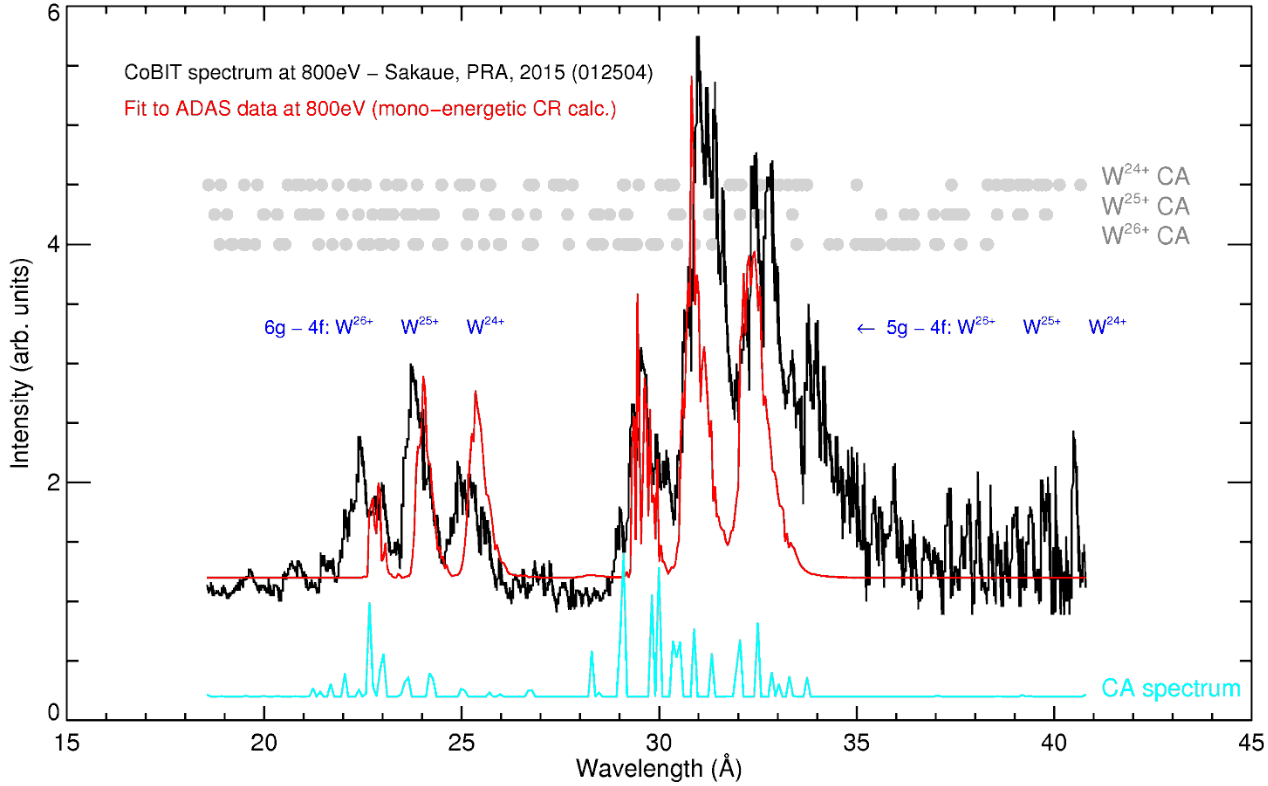
W+ to W13+

0	7.86403220d+00	1s2	2s2	2p6	3s2	3p6	3d10	4s2	4p6	4d10	4f14	5s2	5p6	5d4	5f0	5g0	6s2	(5)2(	0.0)
1	1.63659135d+01	1s2	2s2	2p6	3s2	3p6	3d10	4s2	4p6	4d10	4f14	5s2	5p6	5d4	5f0	5g0	6s1	(6)2(	0.5)
2	2.60242821d+01	1s2	2s2	2p6	3s2	3p6	3d10	4s2	4p6	4d10	4f14	5s2	5p6	5d4				(5)2(	0.0)
3	3.82119283d+01	1s2	2s2	2p6	3s2	3p6	3d10	4s2	4p6	4d10	4f14	5s2	5p6	5d3				(4)3(	1.5)
4	5.15898227d+01	1s2	2s2	2p6	3s2	3p6	3d10	4s2	4p6	4d10	4f14	5s2	5p6	5d2				(3)3(	2.0)
5	6.47656229d+01	1s2	2s2	2p6	3s2	3p6	3d10	4s2	4p6	4d10	4f14	5s2	5p6	5d1				(2)2(	1.5)
6	1.22012844d+02	1s2	2s2	2p6	3s2	3p6	3d10	4s2	4p6	4d10	4f14	5s2	5p6					(1)0(	0.0)
7	1.41217996d+02	1s2	2s2	2p6	3s2	3p6	3d10	4s2	4p6	4d10	4f13	5s2	5p6					(2)3(	3.5)
8	1.60187577d+02	1s2	2s2	2p6	3s2	3p6	3d10	4s2	4p6	4d10	4f14	5s2	5p4					(3)1(	2.0)
9	1.79033175d+02	1s2	2s2	2p6	3s2	3p6	3d10	4s2	4p6	4d10	4f14	5s2	5p3					(2)1(	1.5)
10	2.08913365d+02	1s2	2s2	2p6	3s2	3p6	3d10	4s2	4p6	4d10	4f14	5s2	5p2					(3)1(	0.0)
11	2.31602473d+02	1s2	2s2	2p6	3s2	3p6	3d10	4s2	4p6	4d10	4f13	5s2	5p2					(4)3(	3.5)
12	2.58259074d+02	1s2	2s2	2p6	3s2	3p6	3d10	4s2	4p6	4d10	4f14	5s2						(1)0(	0.0)
13	2.90742933d+02	1s2	2s2	2p6	3s2	3p6	3d10	4s2	4p6	4d10	4f13	5s2						(2)3(	3.5)

- Complex lower stages due to 6s and 6p – complicates atomic structure.
- Multiple metastables complicates the spectral model.
- Mons-style excitation data for W^0 – W^{6+}
- R-matrix for W^0 – R Smyth et al, Phys Rev A97 (2018)
- R-matrix for W^+ – coming (see Connor Ballance's talk)
- R-matrix for W^{3+} - C Balance et al, J Phys B46 (2013)
- More in the pipeline? DW may be sufficiently good at this point.
- CADW for ionization and AUTOSTRUCTURE for DR/RR recombination data but these must be verified by models and experiment.

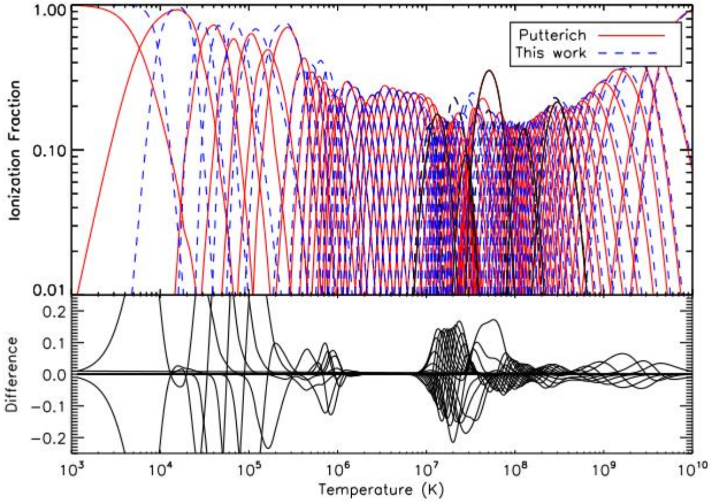
Tungsten up to pedestal

- One outcome of the power optimization work is a set of adf04 excitation data in collision strength (cross sections) and effective collision strength (rates) forms.
- These can be applied to spectral problems



- Mono-energetic ADAS population model, producing a spectral feature, fitted to an EBIT spectrum with ADAS feature-fitting LSQ code.
- Goal is to apply (shifted) features to tungsten emission from tokamaks.

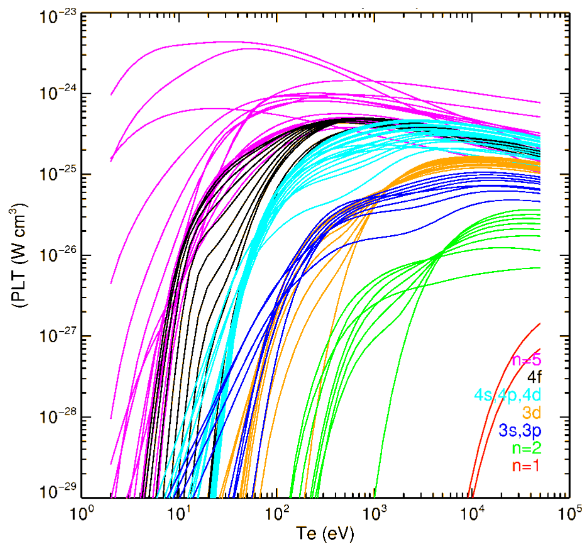
Tungsten in core

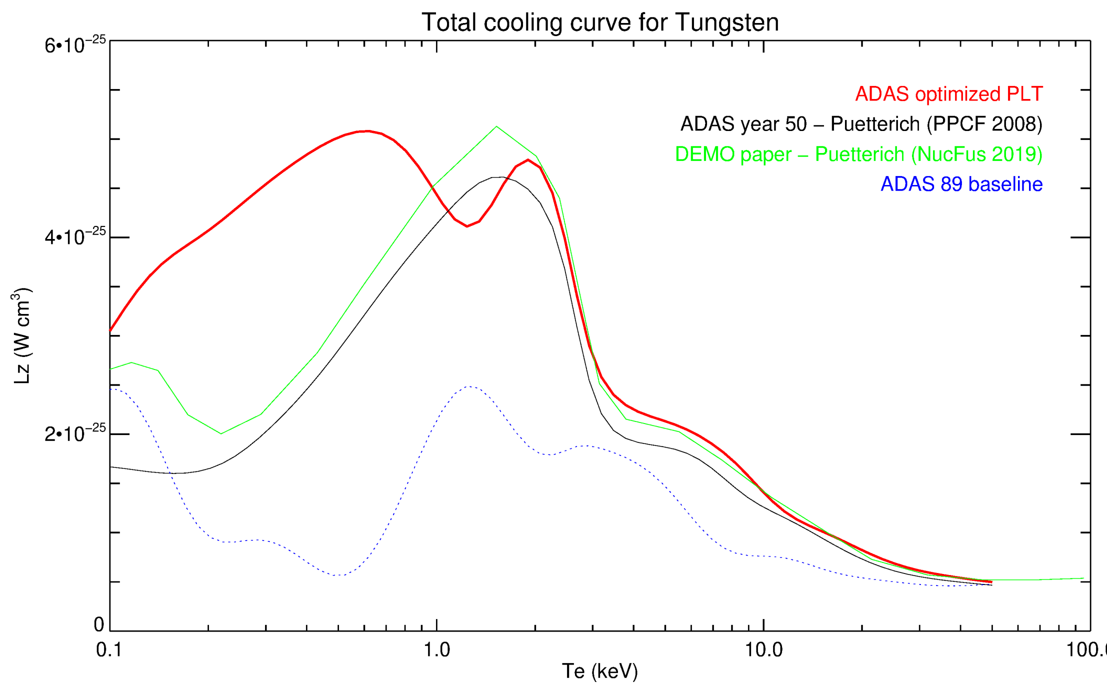


- $4f^n$ DR still an issue
- But now constrained from both sides
- But it's the pedestal region for JET (100-1000eV)

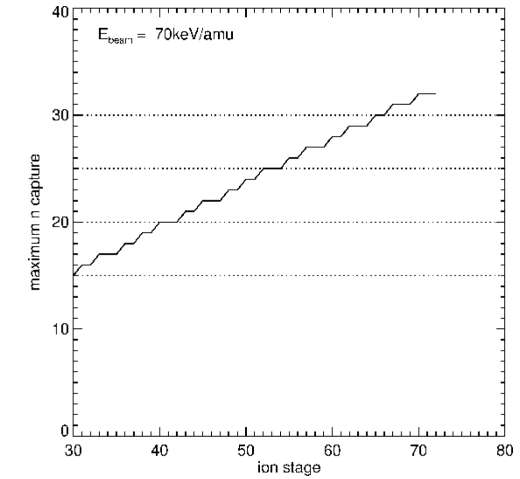
- Preval et al,
- 73 – 56: PRA 93, 042703 (2016)
- 55 – 38: JPB 50, 105201 (2017)
- 37 – 28: JPB 51, 015004 (2018)
- 27 – 14: calculations underway
- 13 – 1: JPB52, 025201 (2109)

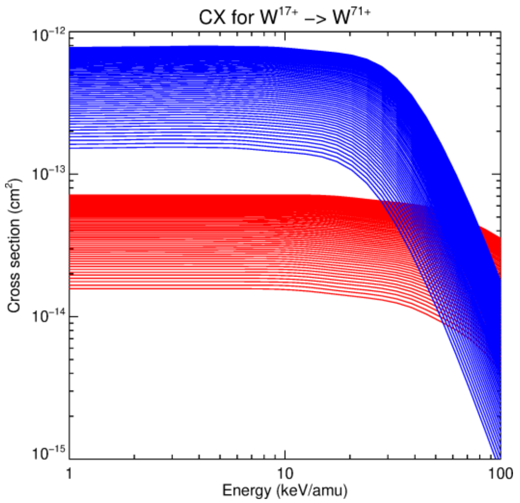
Optimised configuration choice for power calculations – year 42





Tungsten and charge exchange

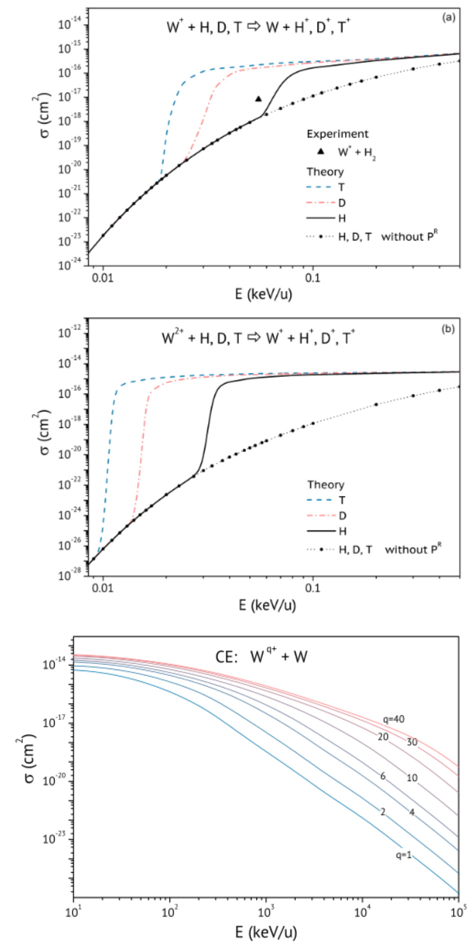




ADAS universal fit for CX cross sections

- with increasing Z the peak n for DR reduces (and may be supressed by density) but the peak n for CX moves upwards so CR models will be needed.
- Active CX for mid-Z, ~W^{26+}, are observed transiently at JET.
- Cross section data is not extensive.

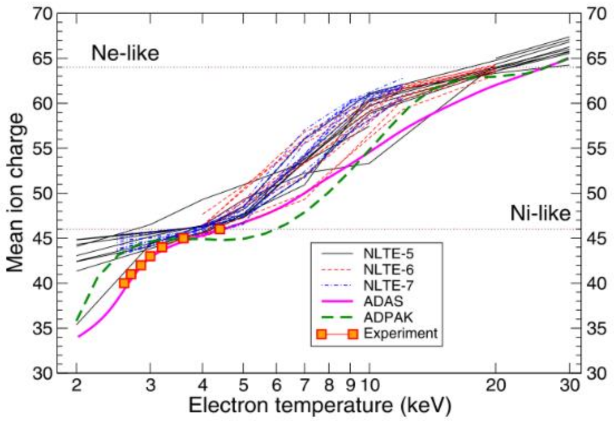
- Cross section data for W^{+} and W^{2+} exchanging with neutral H/D/T do exist.
- And for W^{0} as the donor.
- Not yet included in edge transport models?



I Yu Tolstikhina (J Phys B45, 2012)

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, 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.



Y Ralchenko (Plas Fus Res B8, 2013)

- Validation of atomic data for mid-Z shows convergence.
- Do we need something similar for data used to model and diagnose the edge plasma?