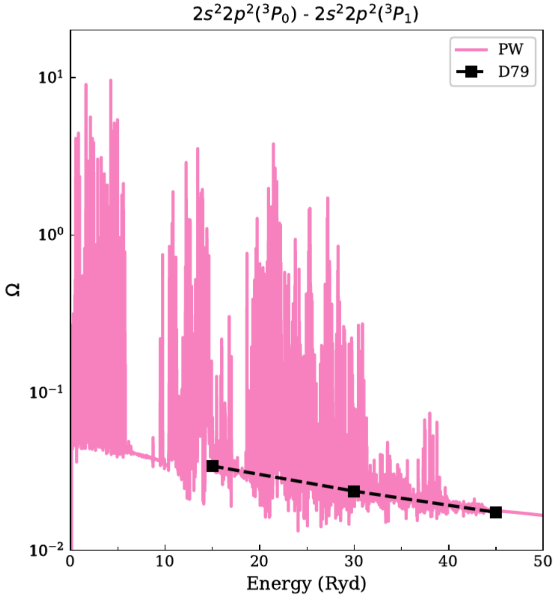
Magnetically-confined nuclear fusion and atomic data

Martin O'Mullane[1], N. R. Badnell[1], C. Balance[2], S. D. Loch[3], S. S. Henderson[4]

[1] University of Strathclyde, Glasgow
[2] Queen's University, Belfast
[3] Auburn University, Alabama
[4] UKAEA, Oxfordshire

Outline

- Magnetic confinement for fusion – conditions and implications for atomic and molecular physics.
- Are all ions equal?
- Uncertainty quantification of theoretical atomic data.
- Influence of model assumptions on the atomic data used in the analysis of fusion plasmas.
- Are we there yet – is atomic physics a roadblock to fusion engineering?



Ar^{12+}: Mao et al, A&A 634, A7 (2020)

Vacuum cell assembly at ITER (www.iter.org)

Fusion – the basics

Fusion Reactions

$D + T \rightarrow {}^4He(3.5MeV) + n(14.1MeV)$

$D + D \rightarrow {}^3He(0.82MeV) + n(2.45MeV)$

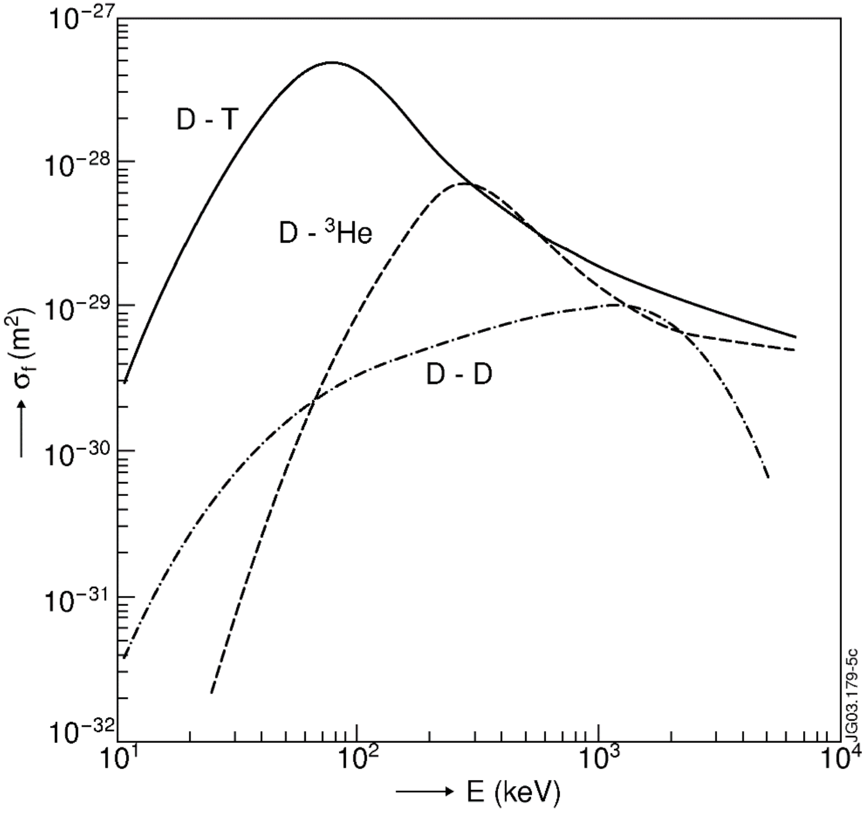
$D + D \rightarrow T(1.01MeV) + H(3.02MeV)$

Fusion Triple Product

$$n_i \tau_E T_i \geq 5x10^{21} m^{-3}.s.keV$$

Tritium Breeding

${}^6Li + n \rightarrow T + {}^4He\ (4.86MeV)$



Fusion – the basics

Fusion Reactions

D + T → ^{4}He(3.5MeV) + n(14.1MeV)

D + D → ^{3}He(0.82MeV) + n(2.45MeV)

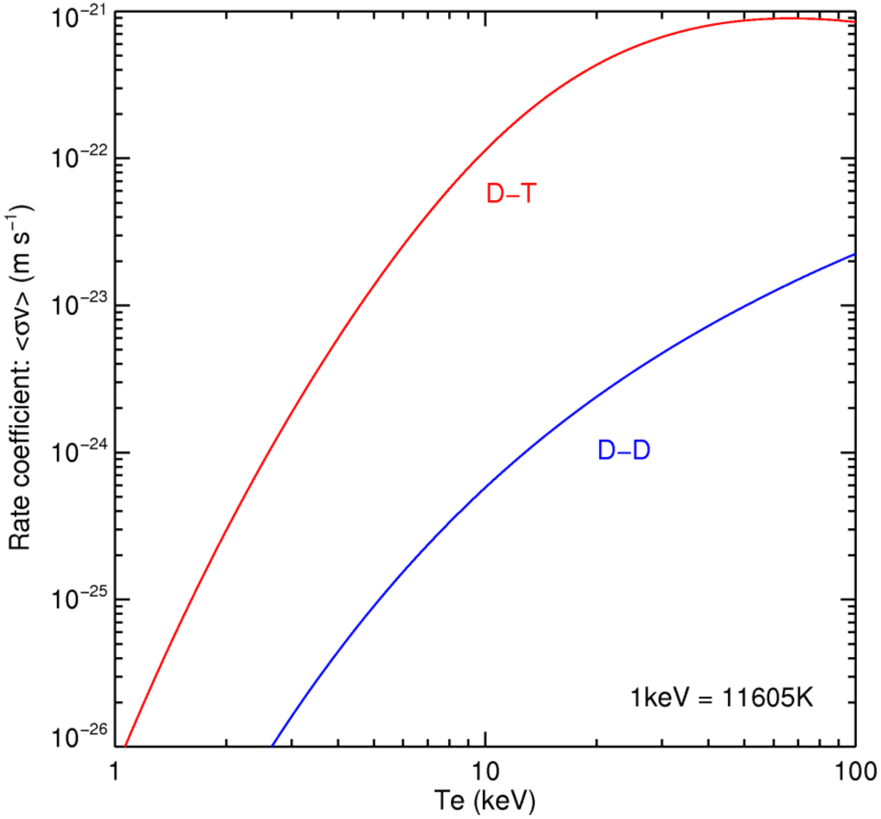
D + D → T(1.01MeV) + H(3.02MeV)

Fusion Triple Product

$$n_i \tau_E T_i \geq 5\text{x}10^{21} m^{-3}.s.keV$$

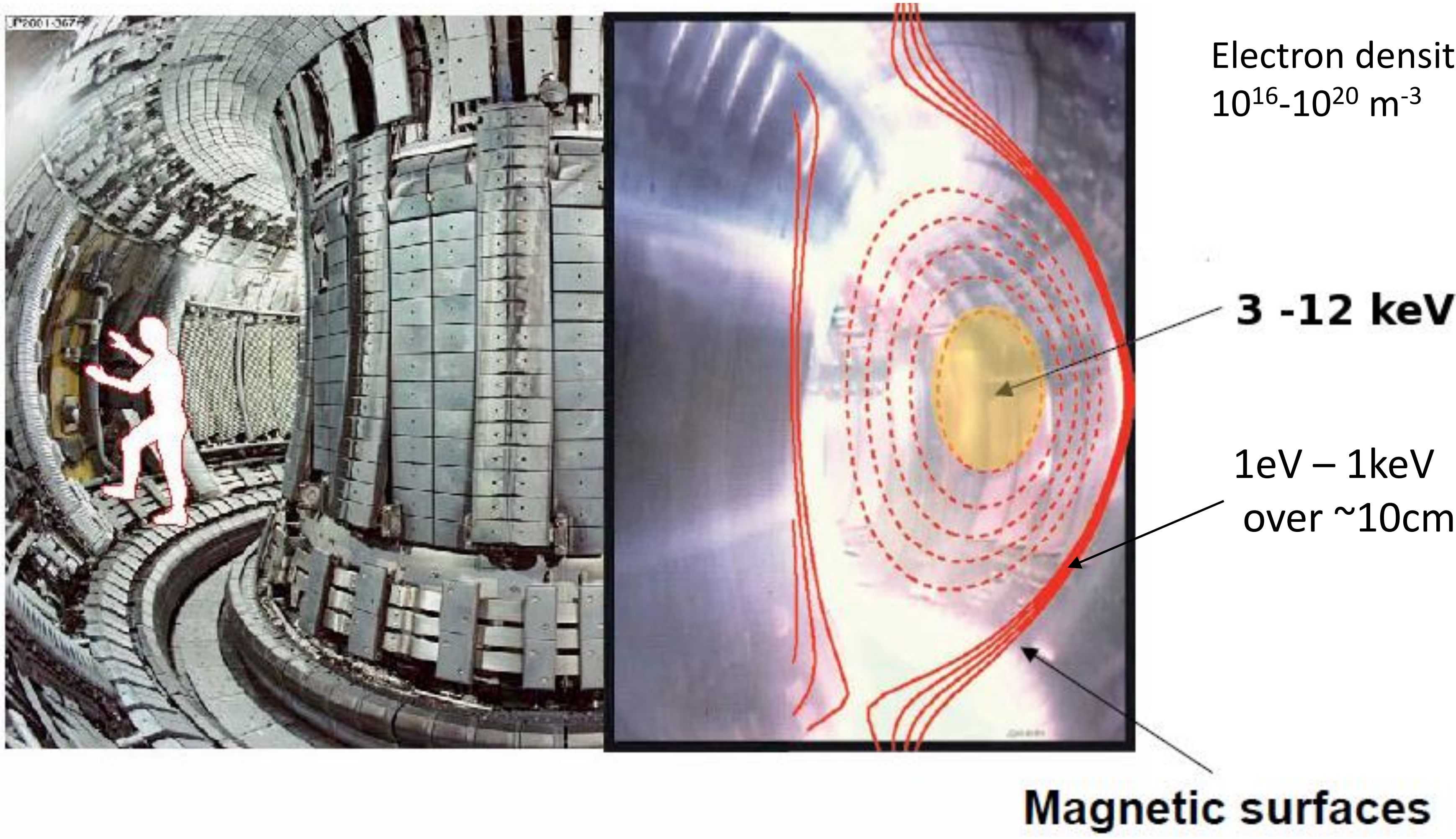
Tritium Breeding

^{6}Li + n → T + ^{4}He (4.86MeV)



Controlled Fusion plasma in a tokamak

JET: Radius 3.1m, vessel 3.96m x 2.4m, $80m^3$ plasma, up to 4MA and 4T.



Electron density 10^{16}-10^{20} m^{-3}

3 -12 keV

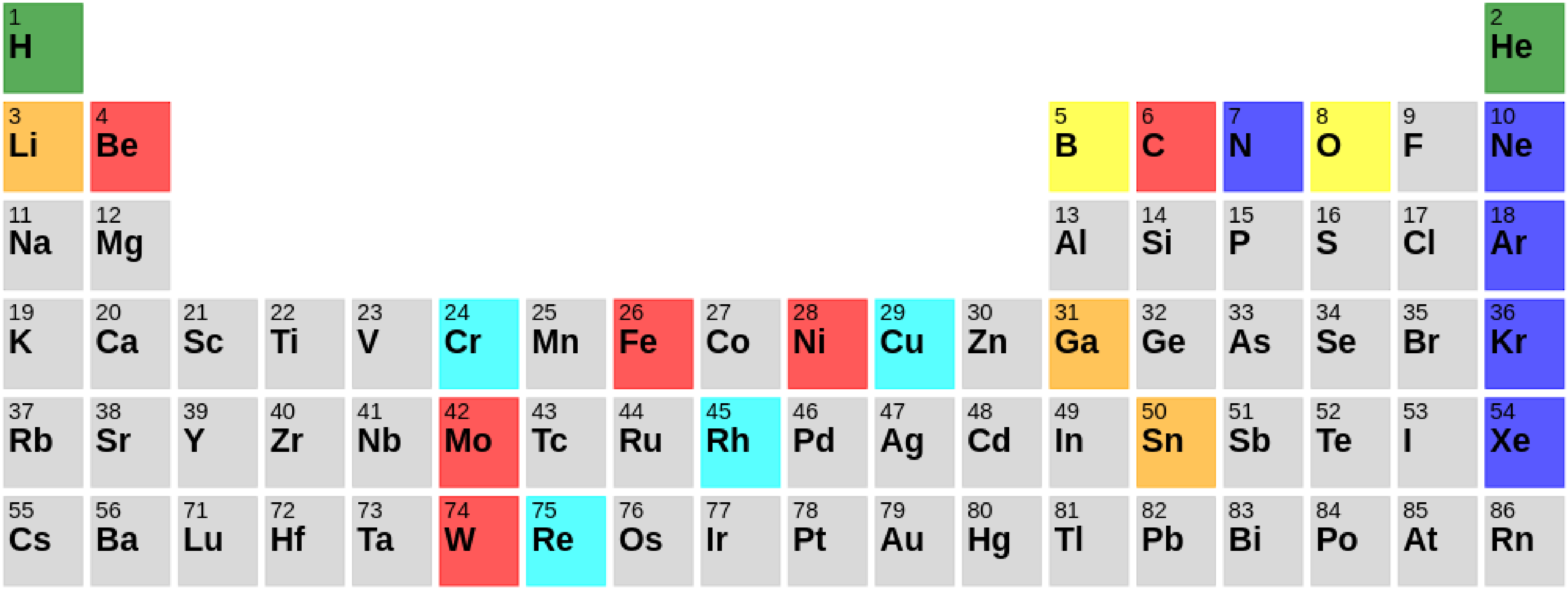
1eV – 1keV over ~10cm

Magnetic surfaces

ITER: radius 6.2m, $830m^3$ volume, up to 15MA, 5.3T, central Te~25keV

Palette of elements in MCF

Chosen for engineering, availability, practicality and to minimize activation
Need atomic data for low, mid and high Z elements



1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn

Fuel – isotopes of hydrogen and He by-product of D + T → ^{4}He(3.5MeV) + n(14.1MeV)

Plasma facing components – anything in direct contact with the plasma

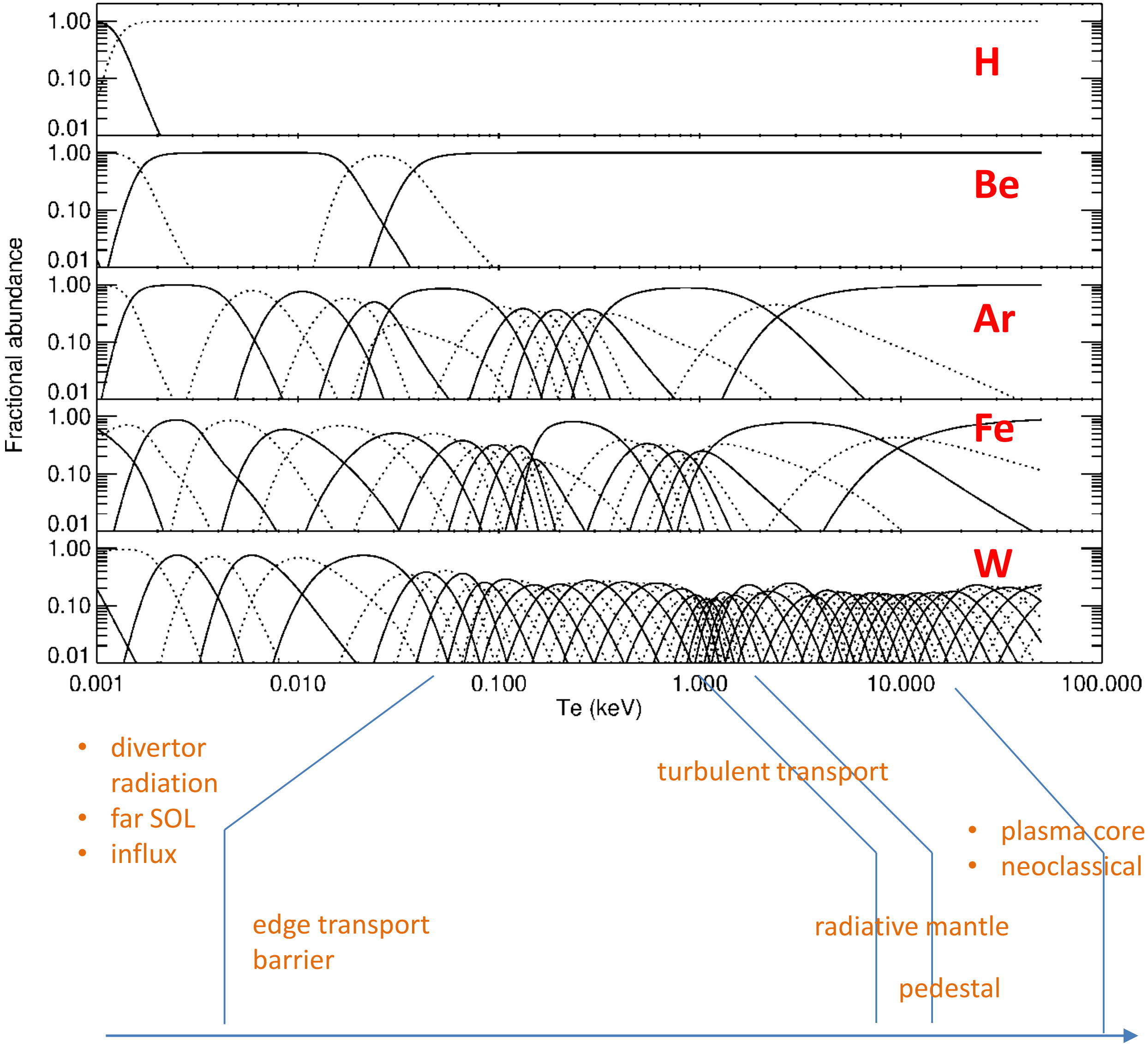
Radiated power actuators – to dissipate power, prevent disruptions and for diagnostics

Oxygen and getter mitigation

Liquid metal surfaces – an alternative PFC concept

Components of in-vessel structures – alloys and diagnostic mirrors etc.

A fusion perspective: complete data for each element of interest



- divertor radiation
- far SOL
- influx

turbulent transport

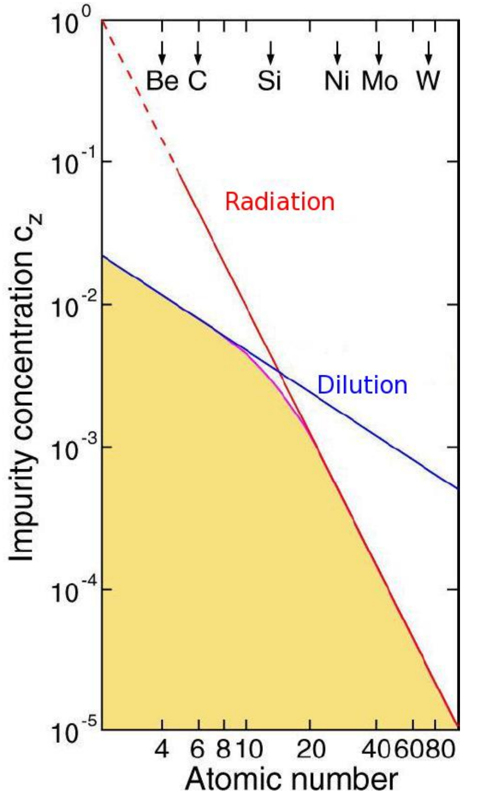
- plasma core
- neoclassical accumulation

edge transport barrier

radiative mantle

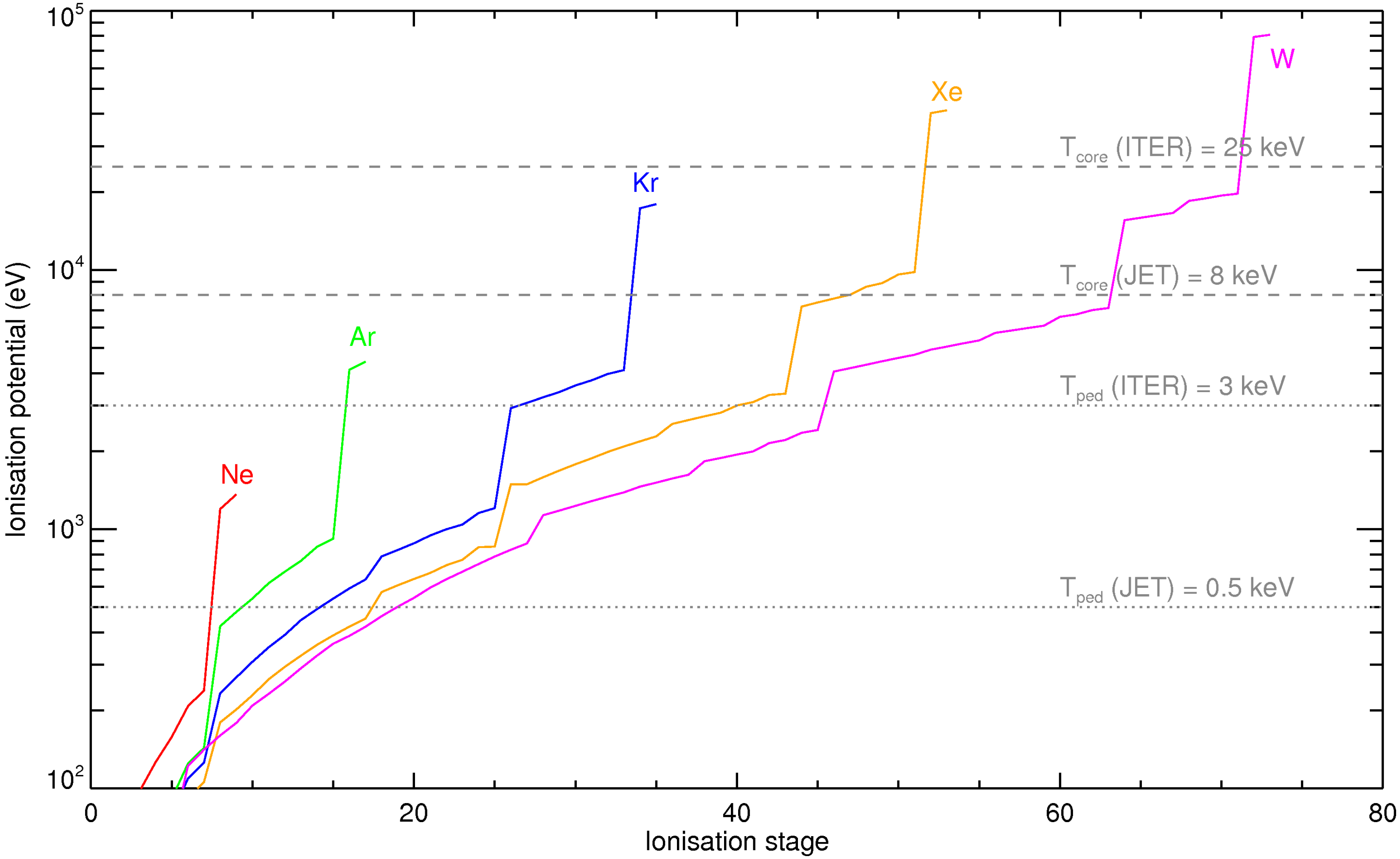
pedestal

plasma radius (edge to core)



Operational limits

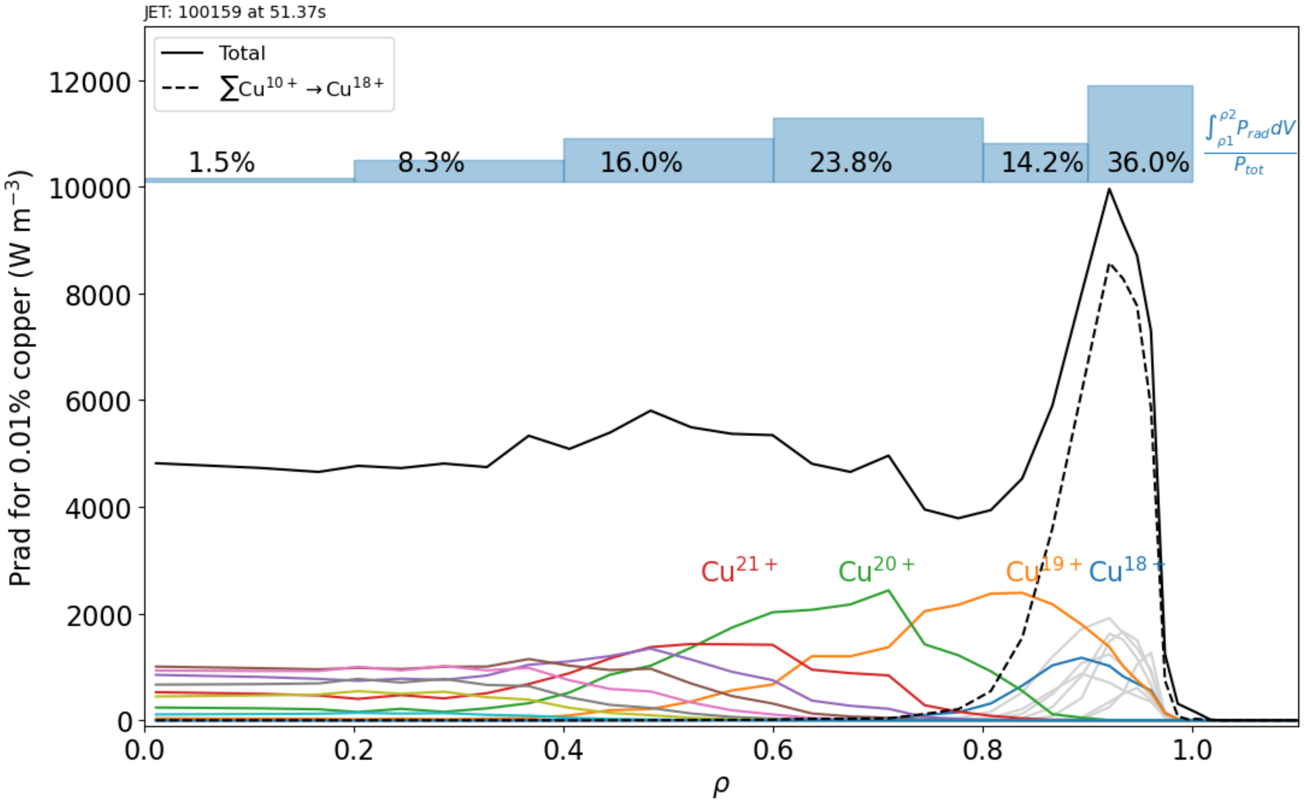
Contribution of ionization stages depend on local conditions



- With increasing Z
  - more and more ion stages exist in a small spatial region.
  - individual emission shells become narrower and less distinctive.
  - more electrons generally complicates the atomic structure spreading emission across many transitions – the notorious 4f electrons.

Metrics to assess importance of individual ions – gross behaviours

Consider copper in a JET L-mode plasma – Te ~ 1.5keV in core falling to 30eV at the last closed flux surface.



- Radiated power and the distribution of ionization stages are important for fusion.
- Atomic data for ionization, recombination (RR, DR and CX) and power are required.
- The selection of configurations, summing the line emission, topping-up for omitted configurations and continuum/recombination are choices.

Themes for atomic data in fusion – the ADAS viewpoint

completeness

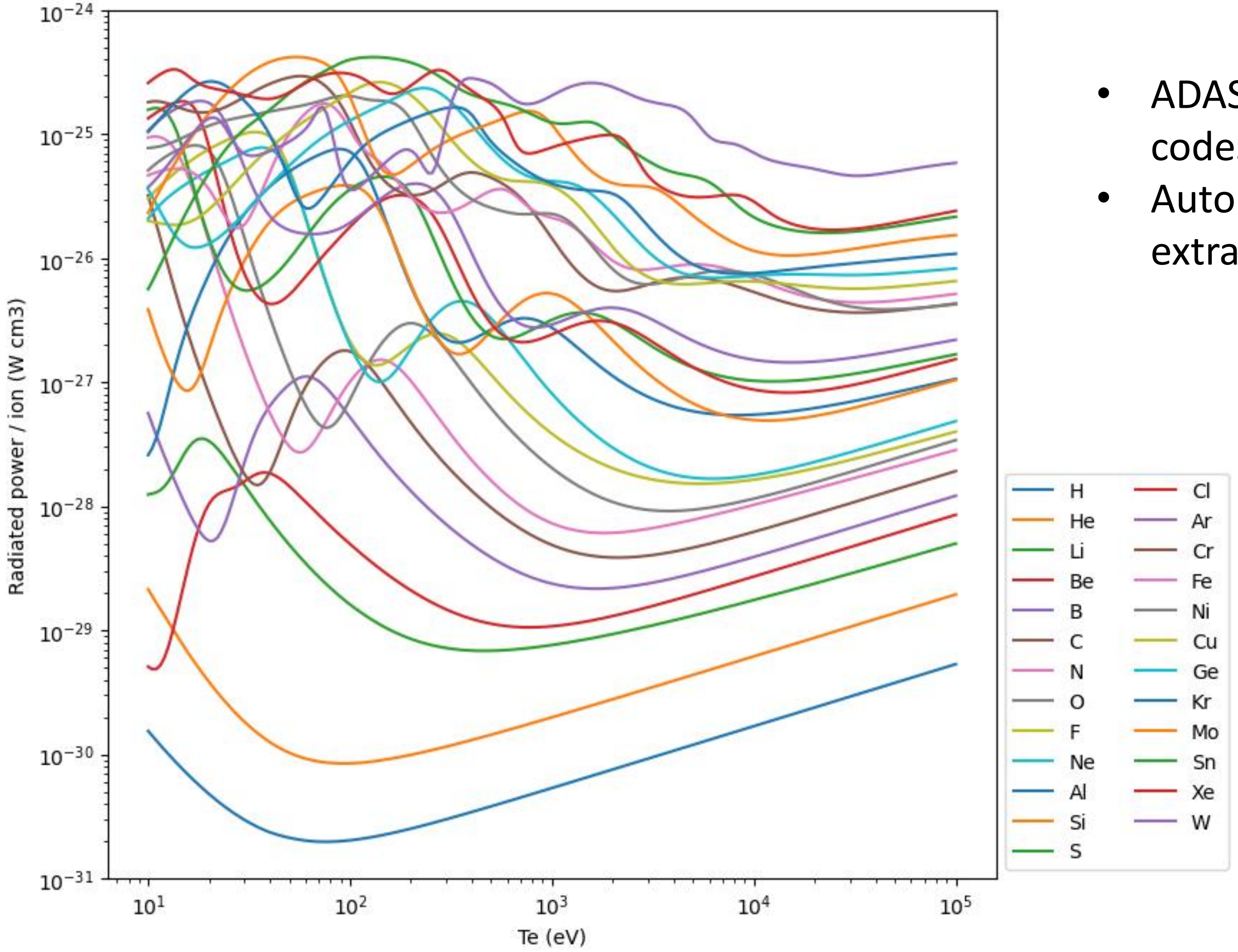
precision

provenance

availability

Completeness for an element and an estimation of the precision of the data are the most important aspects for fusion – the others are guiding principles.

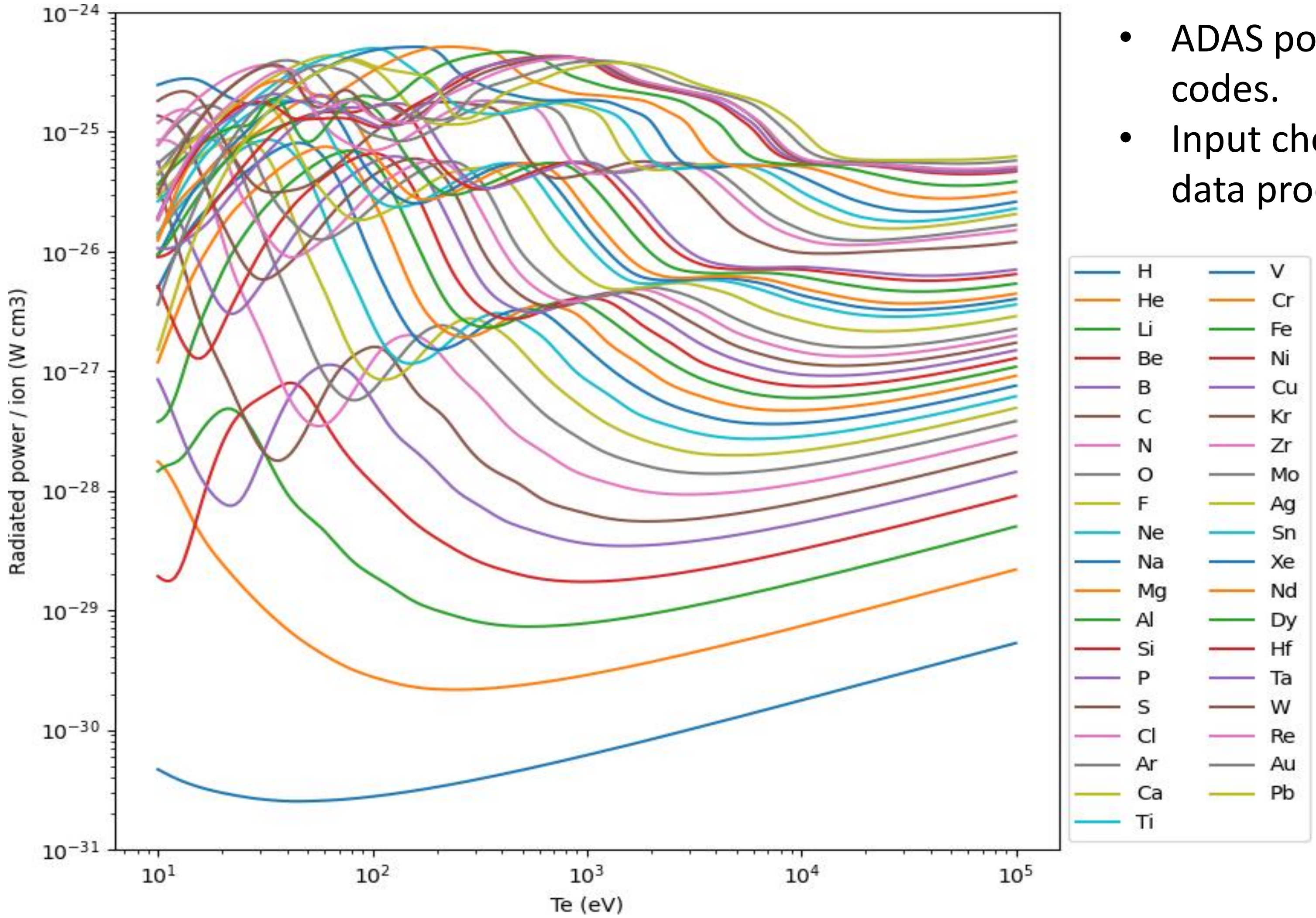
Baseline cooling curves for fusion



- ADAS semi-empirical codes.
- Automated parameter extraction.

ADAS407/ADAS408 codes operating on adf04 sets of data

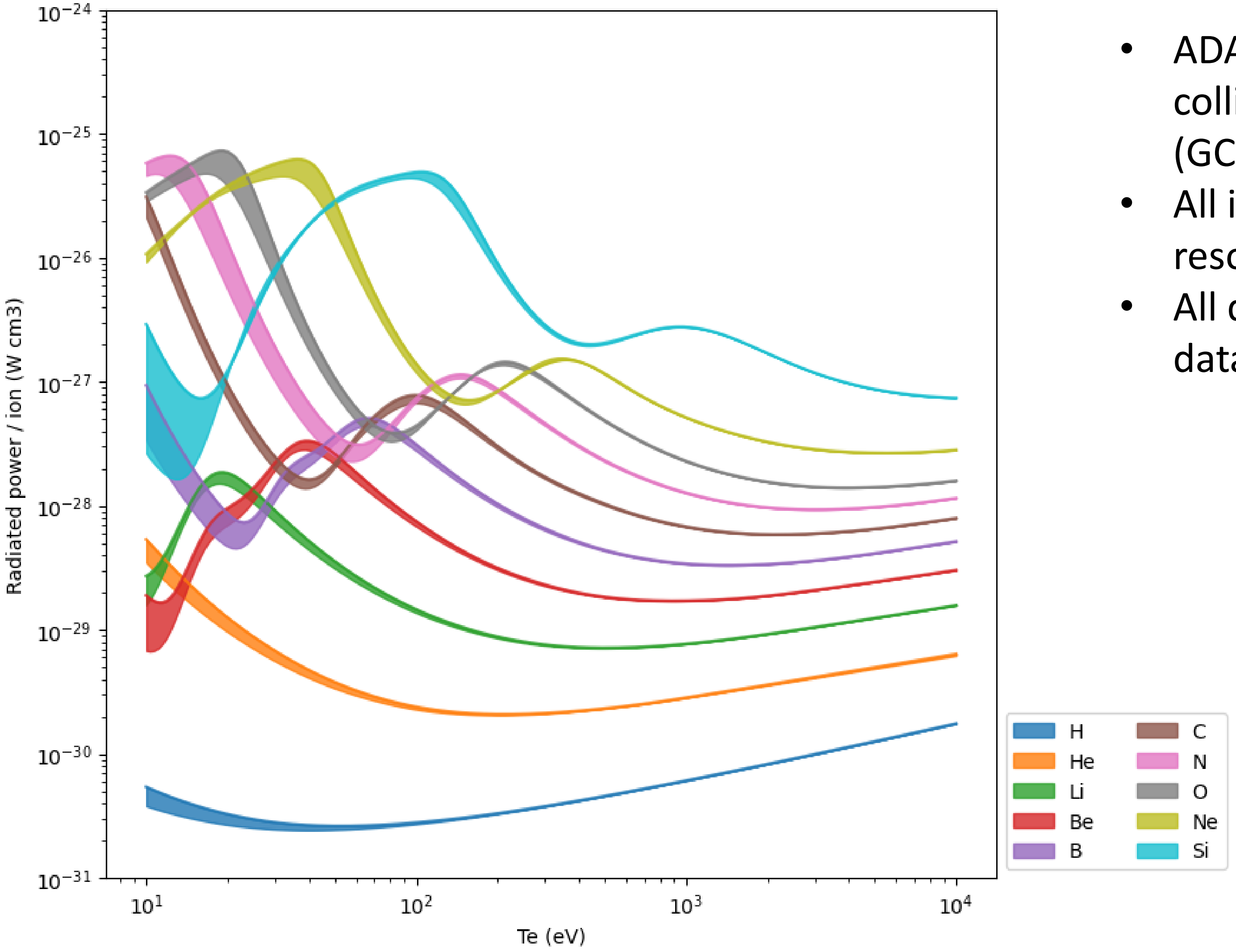
Another consistent set of cooling curve data



- ADAS population codes.
- Input choices from the data producer.

T Pütterich et al, Nuclear Fusion, **59** (2019) 056013

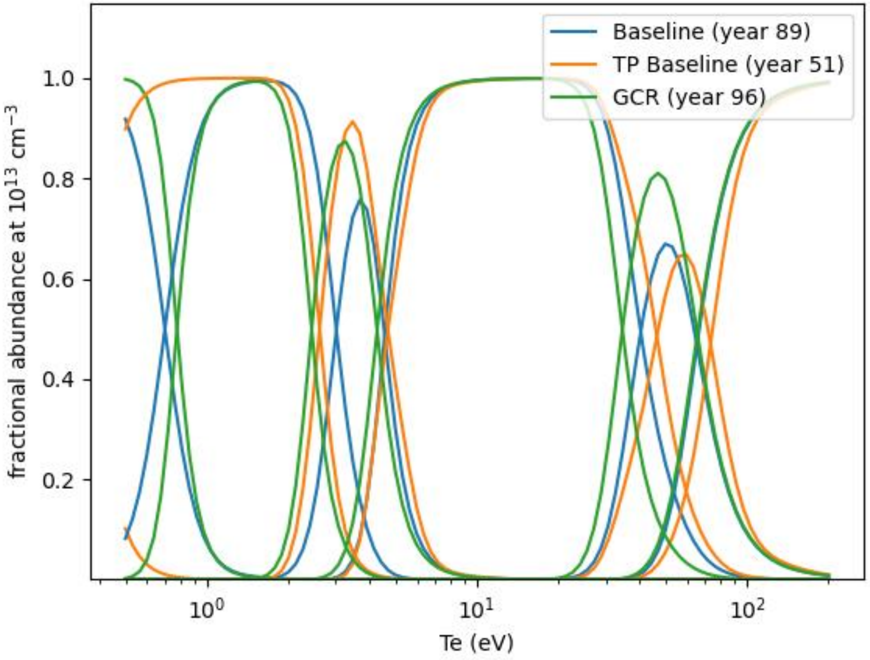
Metastable resolved, density-dependent cooling data

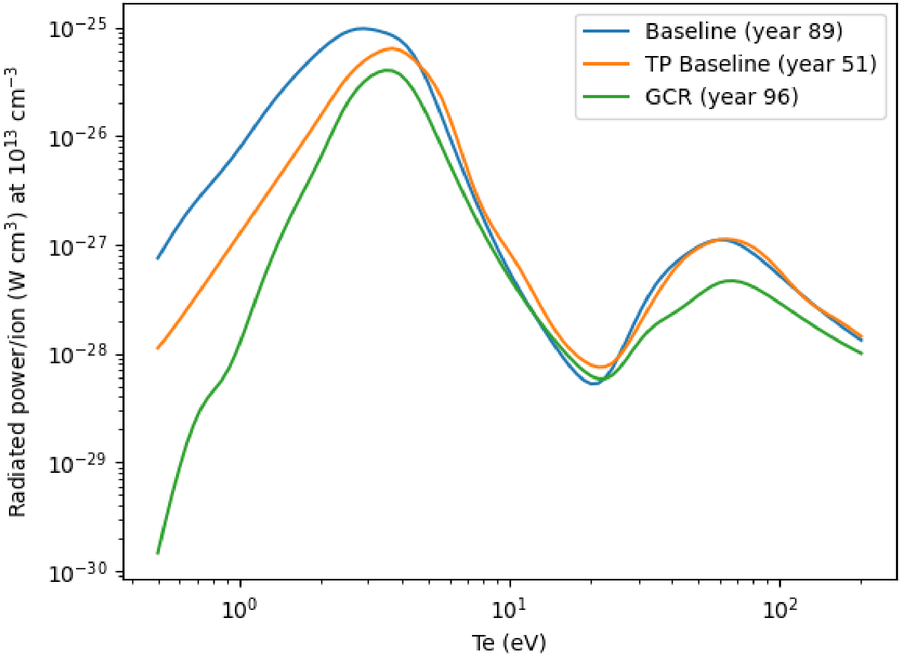


- ADAS generalized collisional-radiative (GCR) model.
- All input data term resolved.
- All data assessed by data producer.

H P Summers et al, PPCF, 48 (2006), 263

Variation in cooling data





- Baseline data is adequate.
- Improvements in CR model are significant.
- Subsequent improvements will be incremental – hopefully!

Sources of data for cooling curves

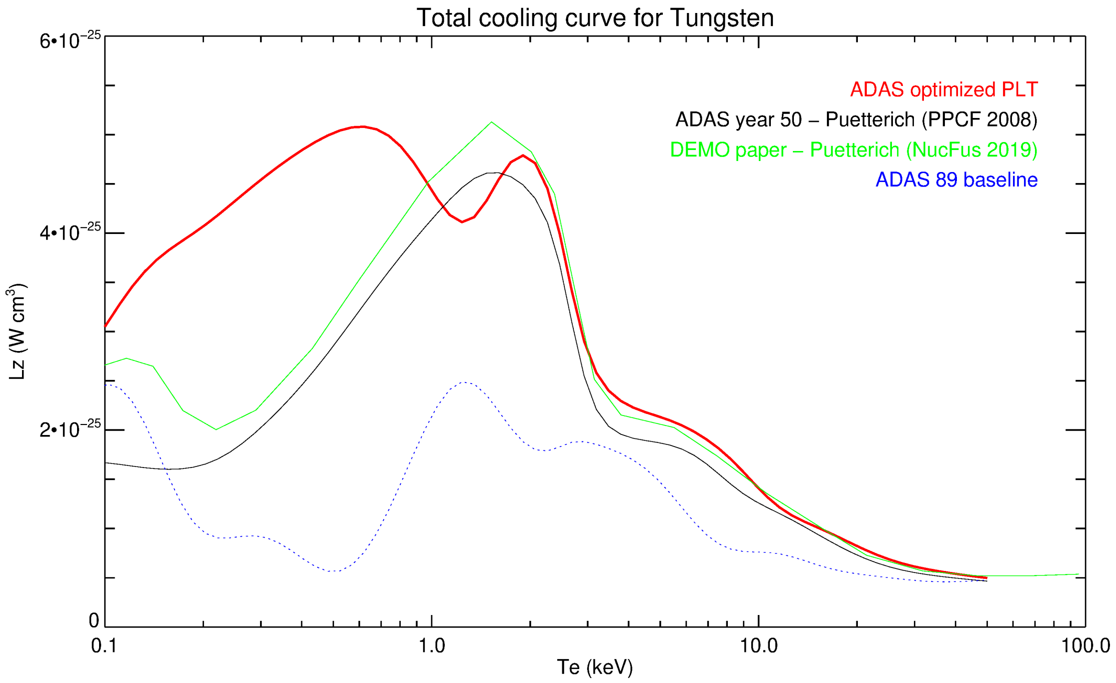
- Excitation
  - extensive R-matrix calculations from APAP network.
  - some data from literature
  - top-up with Cowan (plane wave Born) and AUTOSTRUCTURE (distorted wave)
  - adjust energies to NIST
  - review A-values

not to same level as CHIANTI

- Dielectronic recombination
  - extensive set of level and term resolved DR data from AUTOSTRUCTURE – N R Badnell collection.
- Radiative recombination
  - Burgess-Summers Gaunt factor approach with quantum defect corrections.
  - moving to AUTOSTRUCTURE data with levels sets that are consistent with DR.
- Ionization
  - Split recommended data, eg collections of Bell or Dere.
  - CADW, sometimes with improved Auger factors.
  - moving to R-matrix but slow progress
- Charge exchange
  - whatever we can get!

Radiated power from tungsten – different choices

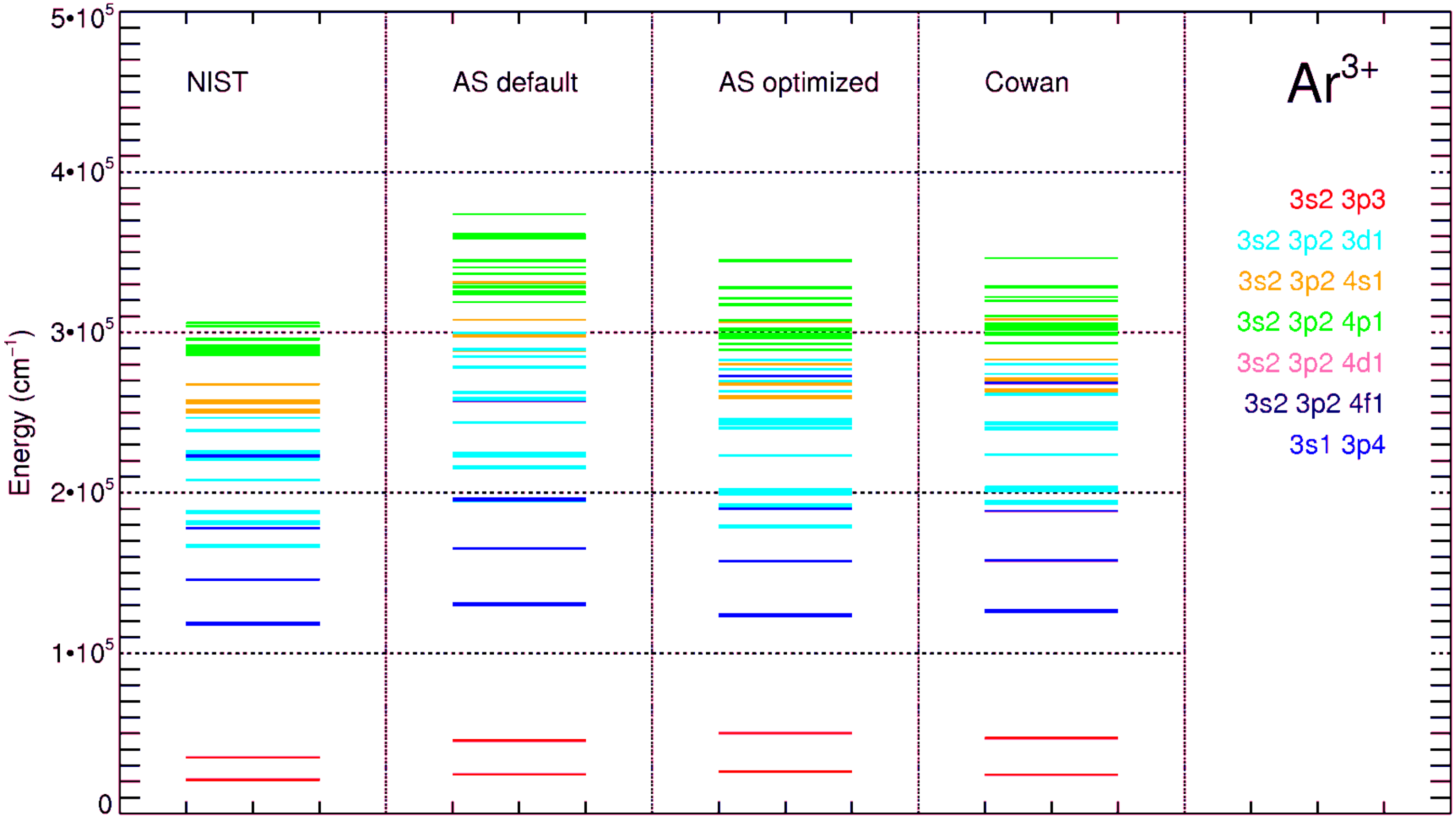
Cooling curve from different sources



- Different ionization balances and choice of contributions in each stage.
- Convergence at higher Te for charge states with simpler atomic structure.
- Emission from $4f^{(n-2)}$ from W^{20+} - W^{27+} is more efficient than expected and results in the difference below 1keV.
- ADAS optimized PLT is an algorithmic approach with optimizing power are the success metric.
- Baseline data (similar to average ion model) is adequate – important for fusion!

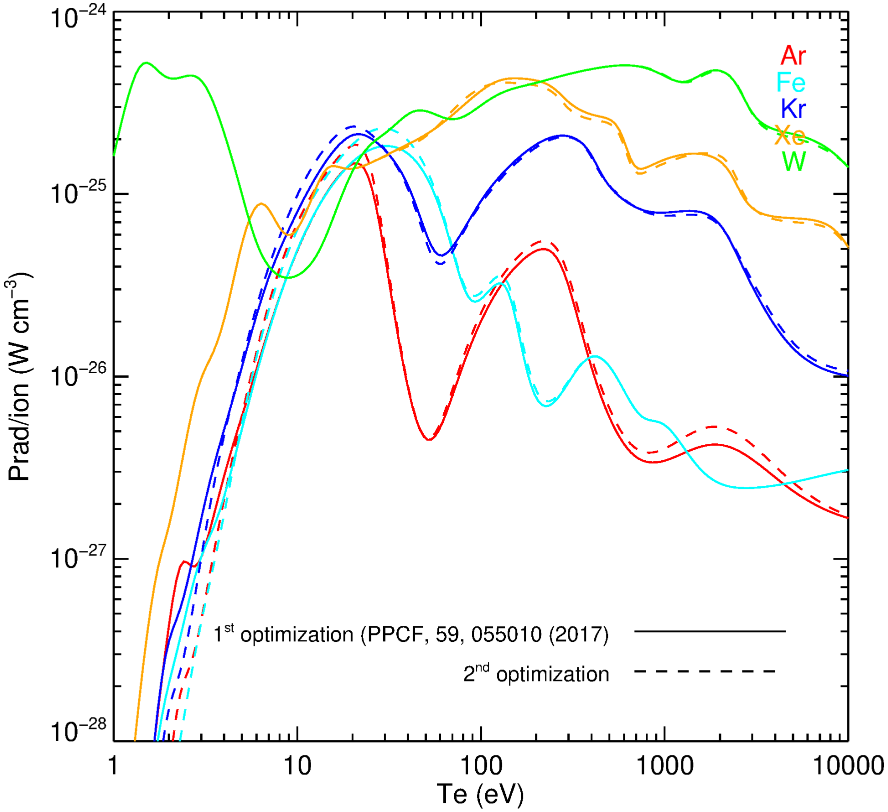
Further enhancement over configuration choice optimization

- AUTOSTRUCTURE uses a Thomas-Fermi potential but individual orbitals can be scaled to improve results.
- Usually thwarted by a lack of observed (in reality NIST) data.
- Cowan with its default setting, or GRASP, can be used as a target structure for AS.

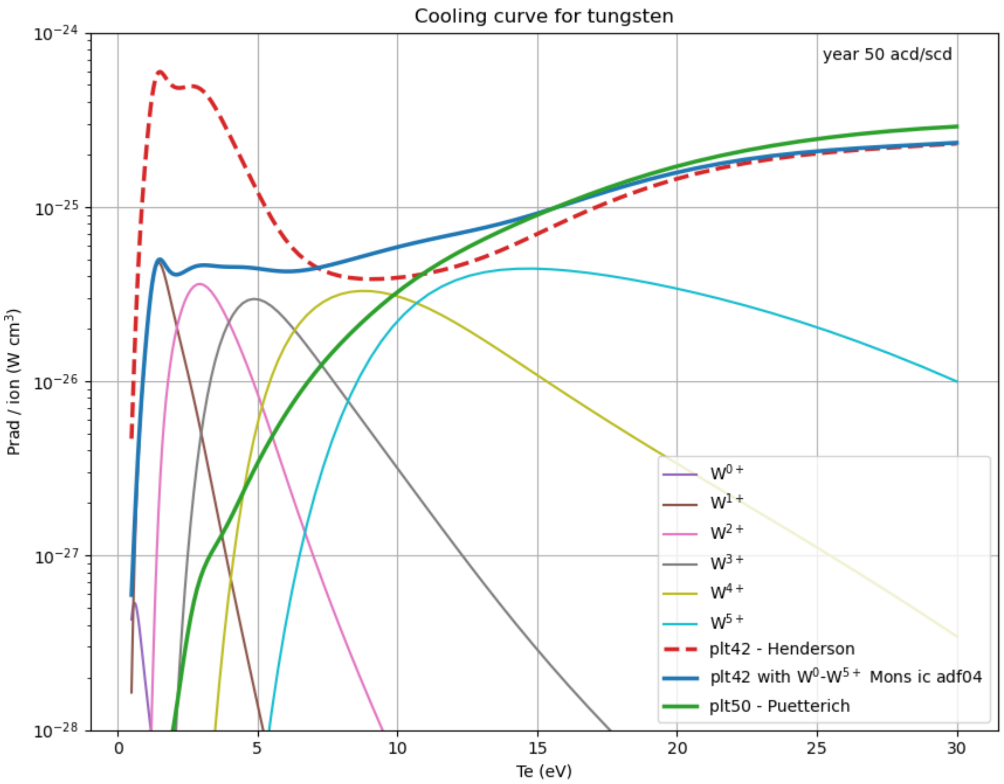


Further enhancement over 2017 optimization

- There is a modest change which indicates that configuration choice is the more important optimization.
- The more complex ionization stages were not considered.
- Spectroscopy and total power are different metrics.



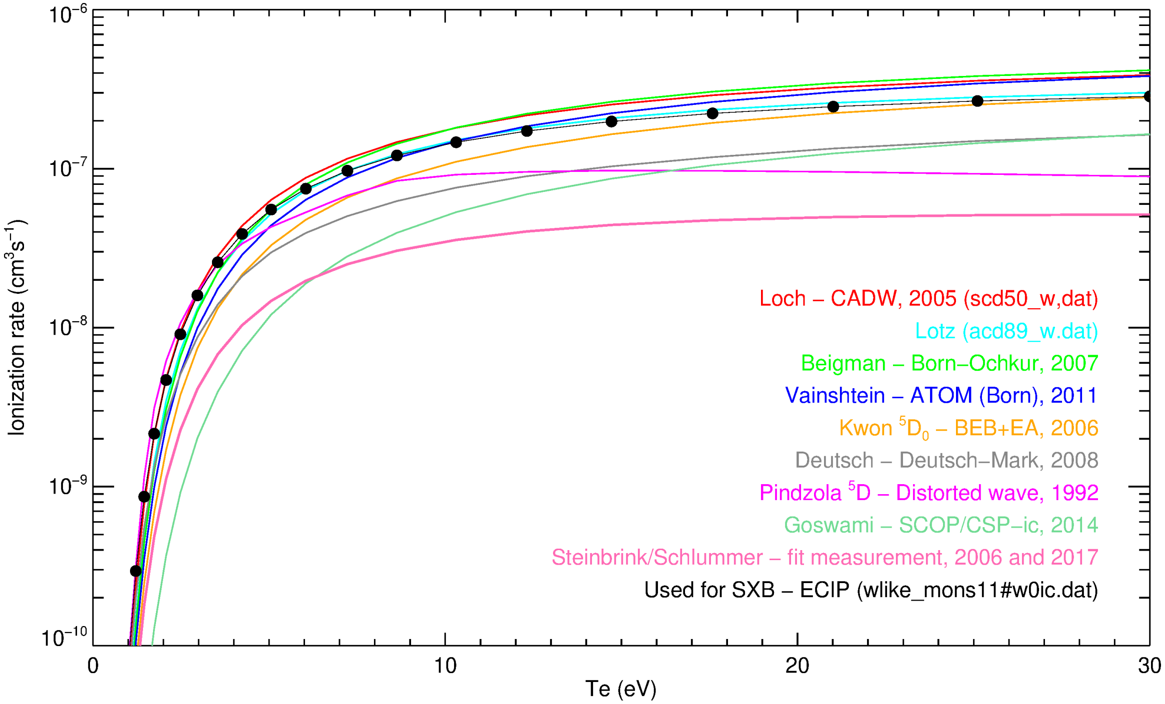
Radiated power from tungsten – different choices at low Te



- 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+} almost ready.
- W^{3+} from C P Ballance et al, J Phys B, 46, 055202 (2013)
- Note configuration-average top-up not applied here but may be needed.

A very open question – ionization of neutral tungsten

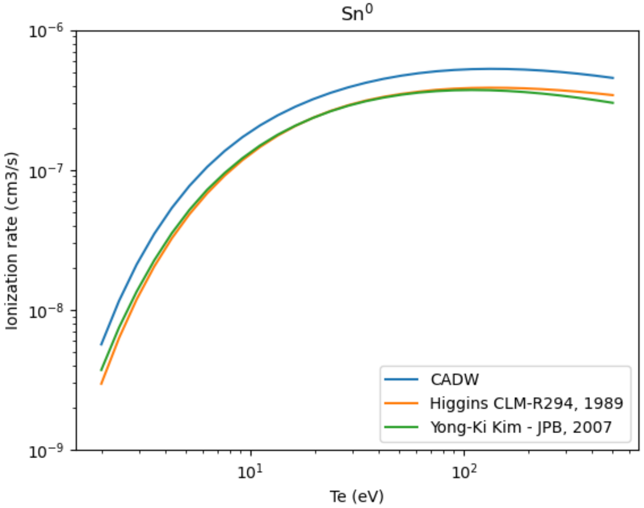
Total rate from ground configuration

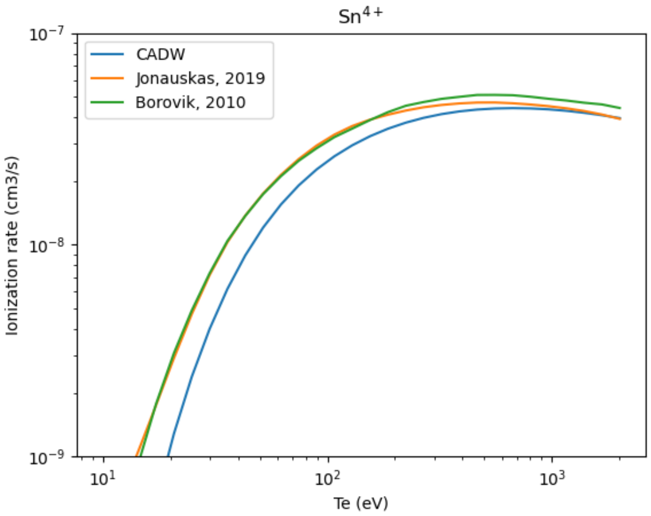


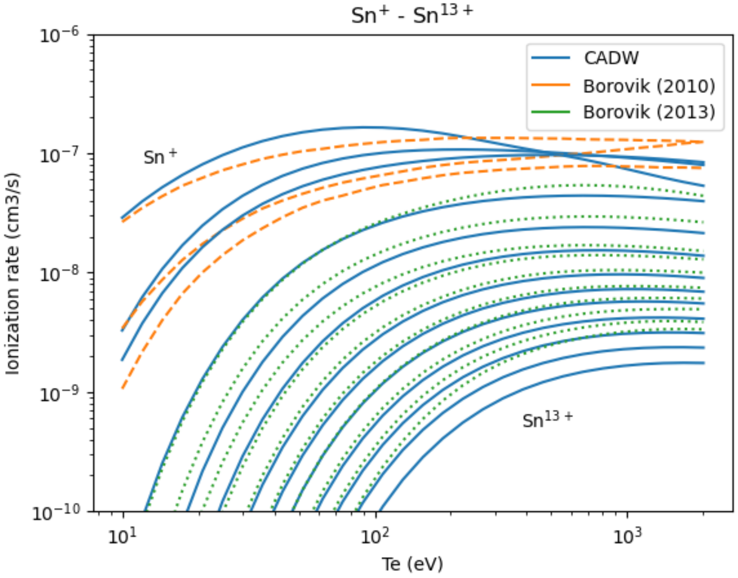
- ADAS uses ECIP (exchange classical impact parameter) for ionization out of excited levels – empirical formula developed by comparing measured ionization cross sections of light elements. But it is robust and is non-divergent.
- This pathway may be larger than the rate from ground.
- No convergence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

Completeness – Sn ionization

Current ‘best’ ionization data for tin – how to archive and recommend this?

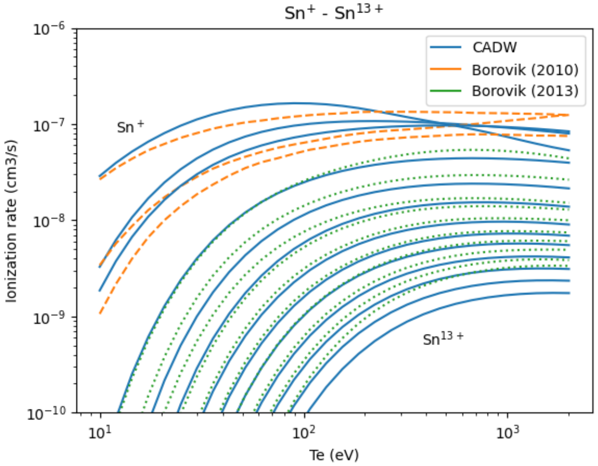




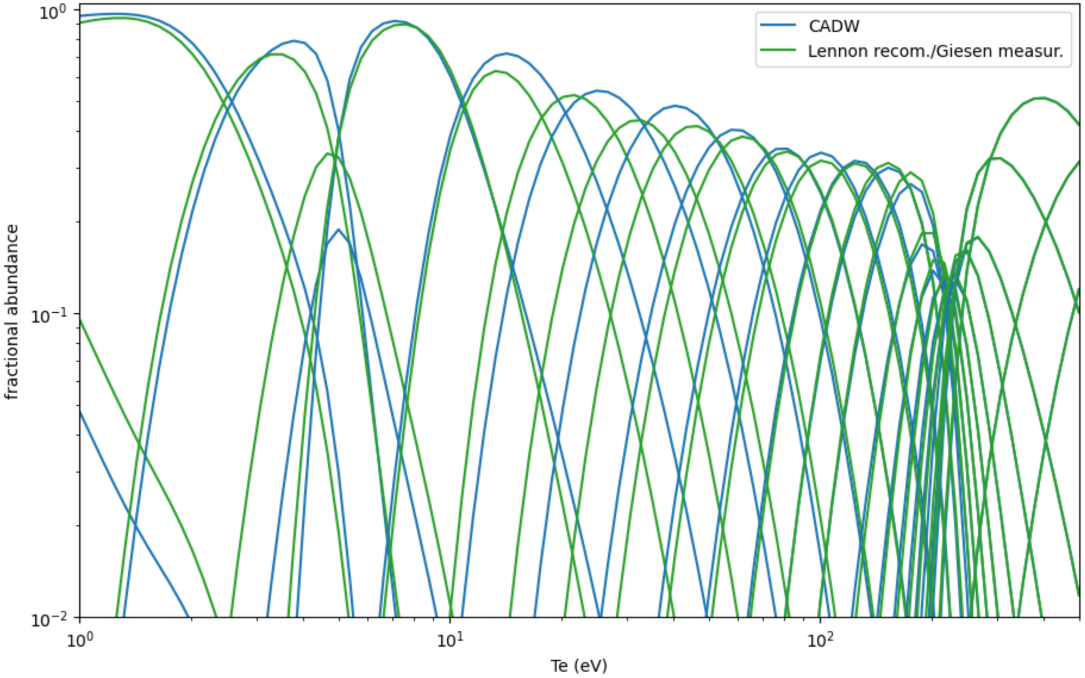


- Some good data/measurements for some ions.
- More than one calculation for others.
- The CADW baseline is reasonable but may need optimization.
- No fully assessed/validated data for all ions which leave a gap.
- But waiting until they are filled is also ‘wrong’.

Completeness – Sn ionization



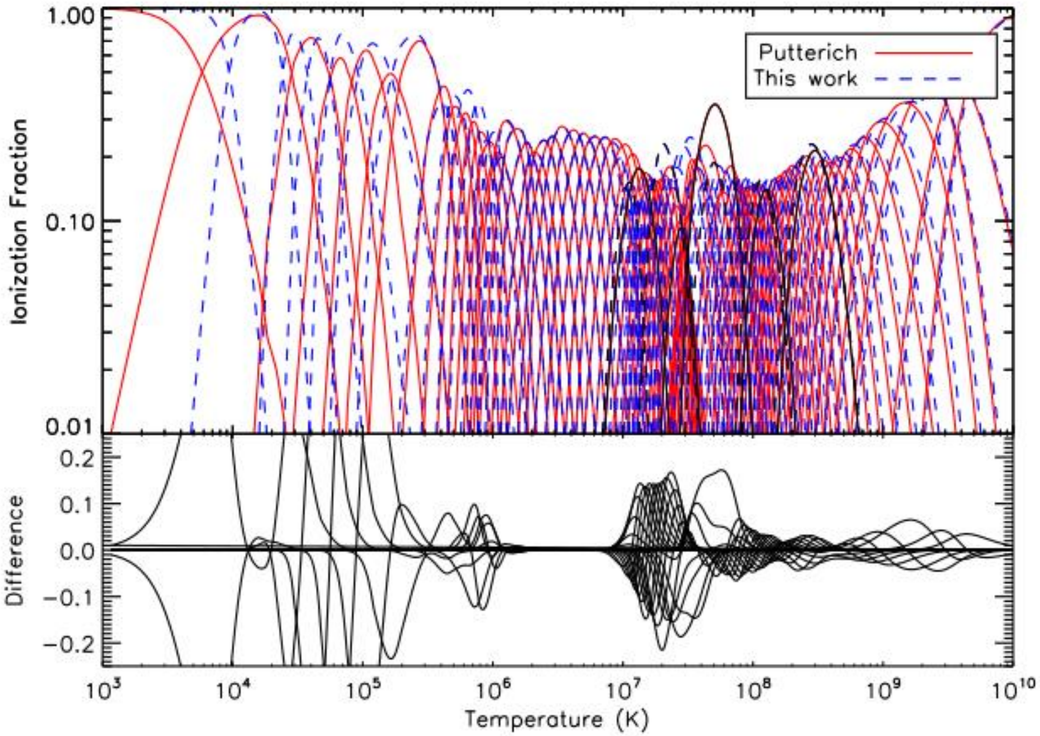
- Do not have the luxury of waiting.
- UQ assignation here will be more opinionated out of necessity.
- The ionization balance is affected.



Tungsten DR Project

- Dielectronic recombination rates for tungsten were the most poorly calculated input to the ionization balance.
- T Puetterich scaled the ADPAK average ion rates to match AUG measurements
- Limited to 2keV < T_e < 10keV (W^{20+} – W^{55+} or Xe-like to K-like) PPCF, v50, 085016 **2008**
- DR rates for ions with open $4f^n$ shell ions are x3 higher than expected

  Schippers et al, Phys Rev A 83, 012711, **2011** & Badnell et al, Phys Rev A 85, 052716 **2012**
- ADAS DR Projected started in **2016** – if we can do W other elements should be simpler!

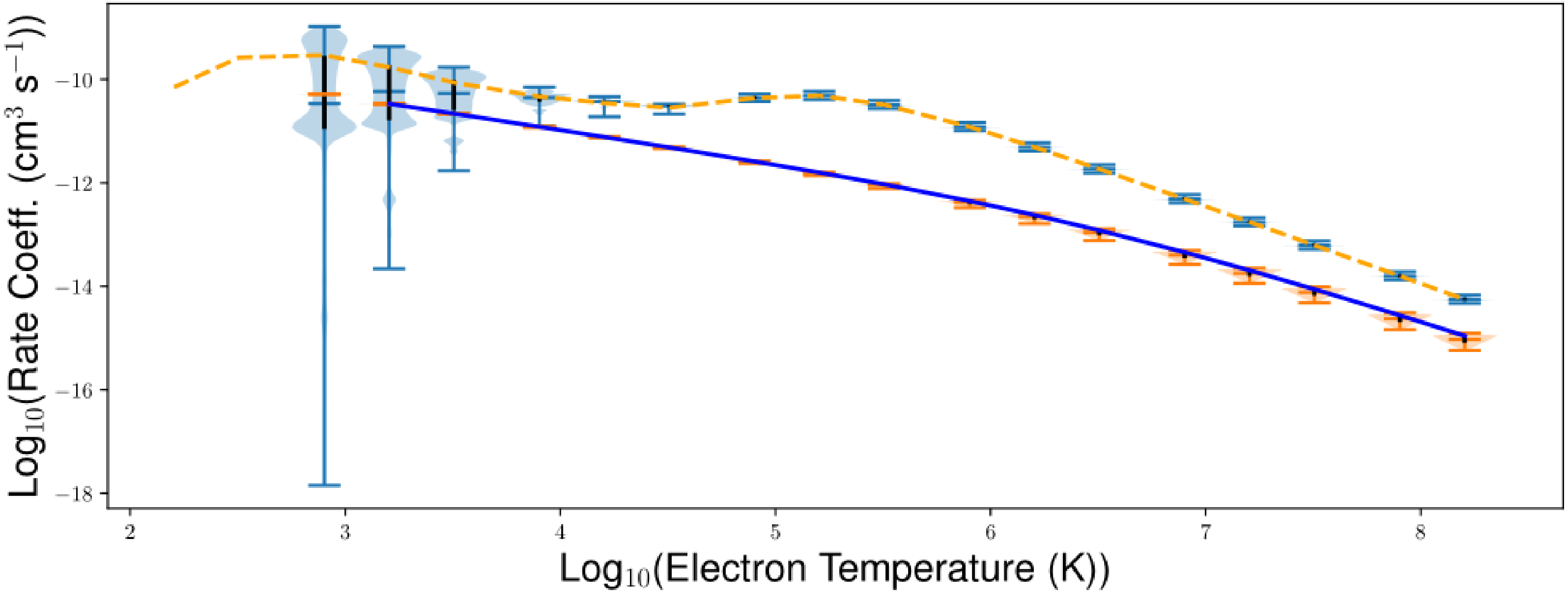


- $4f^n$ still an issue
- But now constrained from both sides
- It's the pedestal region for JET (100-1000eV)

- Preval et al,
- 73 – 56: PRA 93, 042703 (2016)
- 55 – 38: JPB 50, 105201 (2017)
- 37 – 28: JPB 51, 015004 (2018)
- 27 – 14: not complete
- 13 – 1: JPB52, 025201 (2109)

UQ on DR and effects on abundances

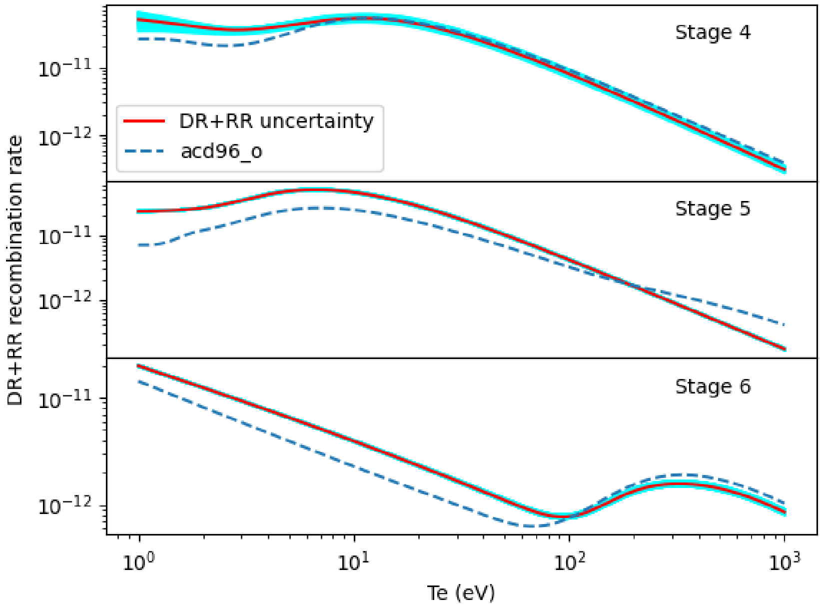
- Project to instrument *ab initio* codes to produce an error bar.
- Use AUTOSTRUCTURE for DR on oxygen and take variation of resonance position as the metric.
- Results in a distribution of possibilities which can be sampled to propagate the effects.

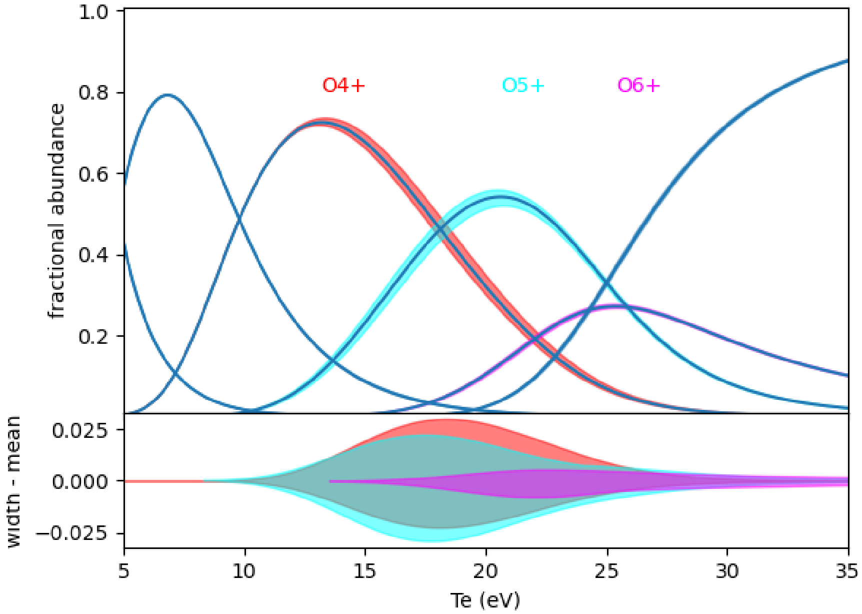


- Low Te behaviour may be worrisome for photo-ionized plasmas.
- Look like much less spread at collisional (ie fusion) conditions.

UQ on DR and effects on abundances

- Sample the uncertainty distributions for a few ionization stages.

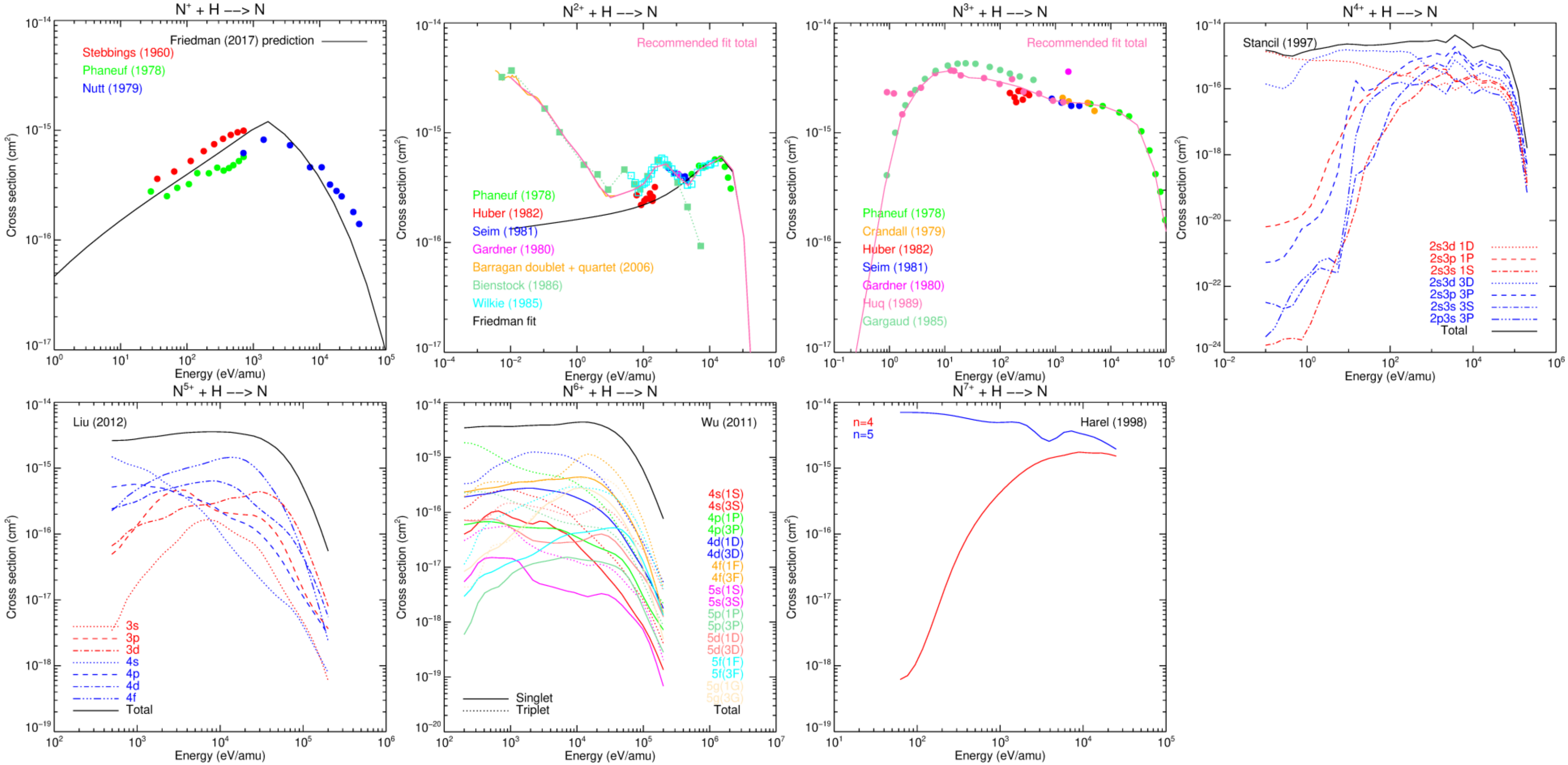




- Noticeable effect over a number of stages.
- Ionization uncertainty may have a comparable influence.
- All stages must be considered before comparing atomic error to other sources of uncertainty.

Thermal charge exchange

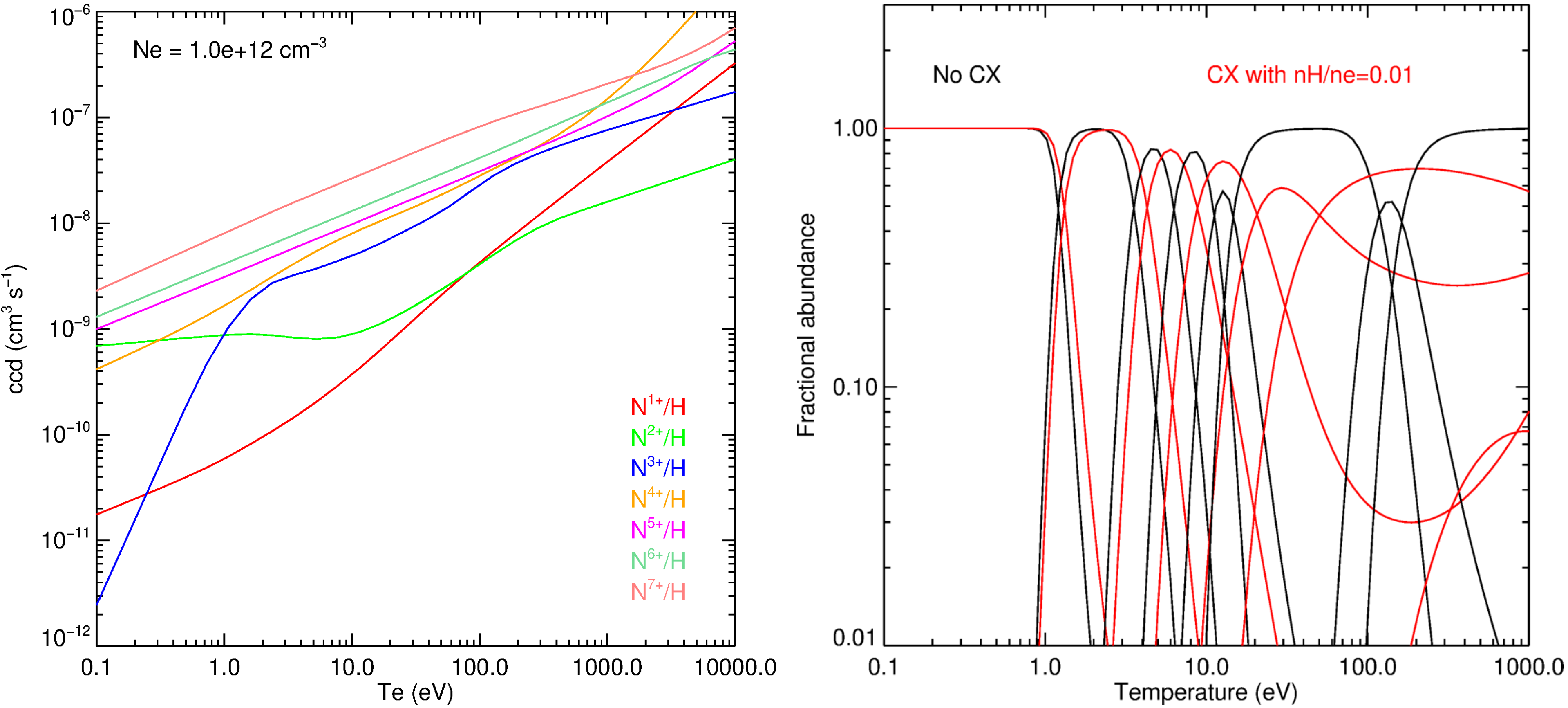
- ADAS adds CX as a process in GCR (adas208). H-line in adf04 file.
- No comprehensive method for low and high energy regimes.



State-selective CX cross sections for nitrogen ions

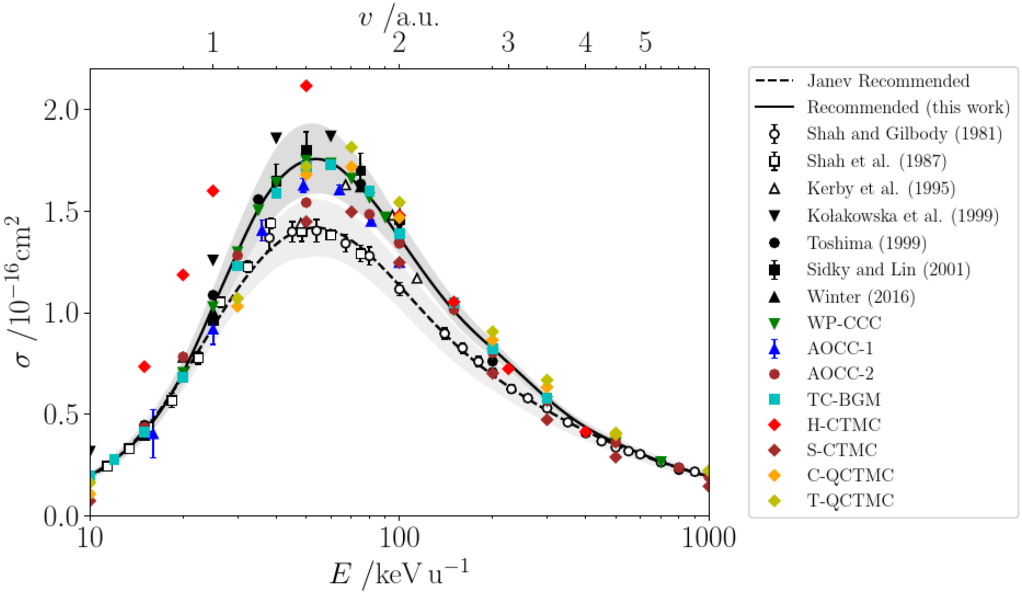
Thermal charge exchange

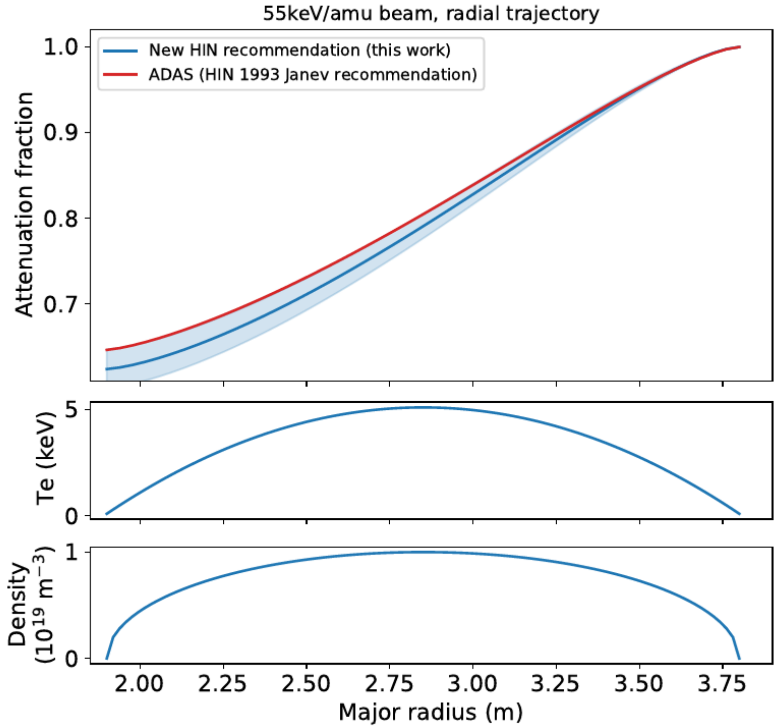
- ADAS adds CX as a process in GCR (adas208). H-line in adf04 file.



GCR CX rates (adf11/ccd96/) and effect on equilibrium balance

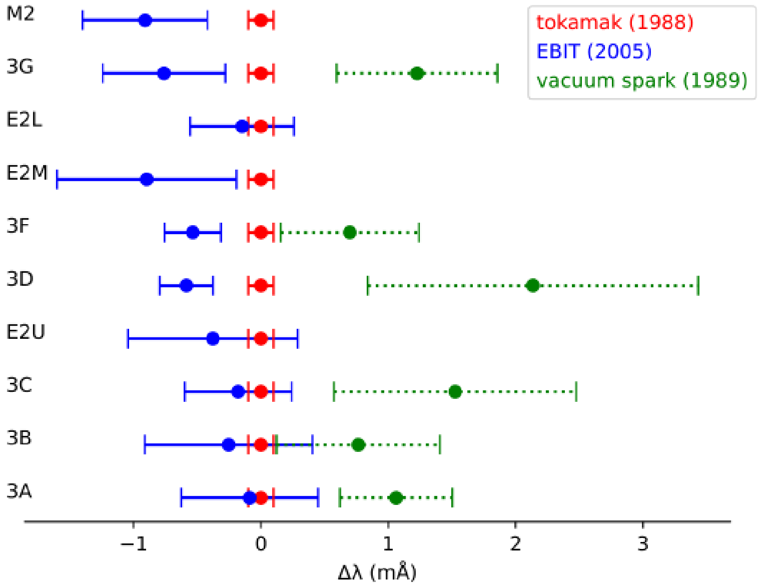
Not always electrons – ion impact and beam stopping

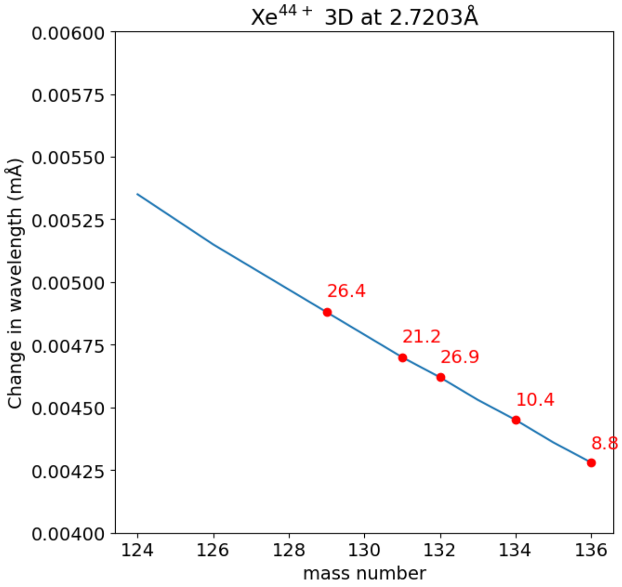




- The cross section for proton impact ionization of hydrogen atoms was scrutinized at a recent IAEA co-ordinated research project.
- The consequences of uncertainty in the cross section are significant for beam attenuation predictions.
- What is the protocol for favouring new calculations over old experimental data?

Xenon X-ray lines – accuracy needed for rotation measurement



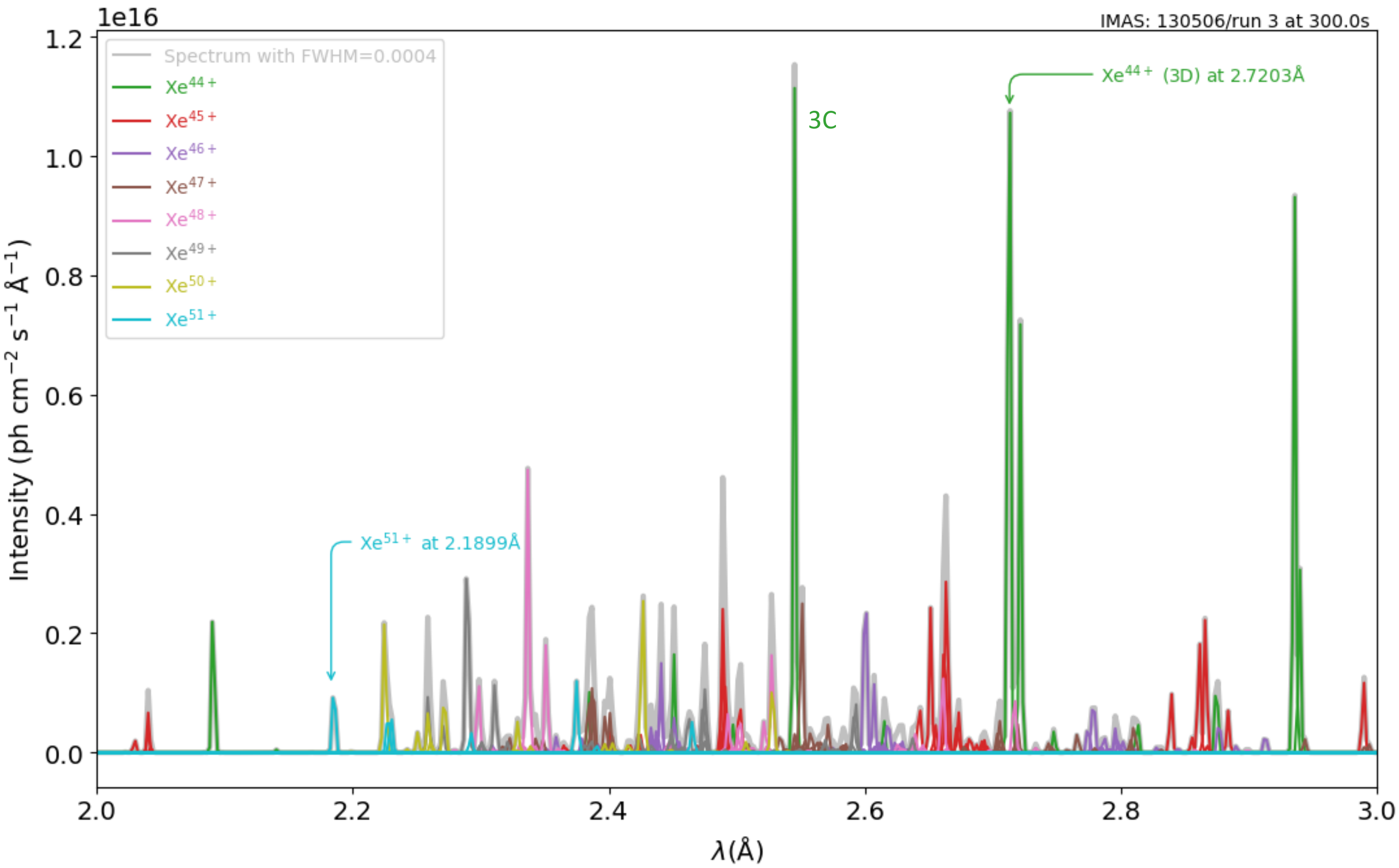


- Xe^{44+} X-ray lines normalized to tokamak (PLT) measured spectra
- Wavelength variation shows the precision of the measurements (but may reflect the different environments).
- The ultimate calibration depends on QCD calculation of He-like titanium used as a reference.
- All are well within the bandpass of the proposed Tion diagnostic.

- There are a number of stable isotopes of Xe^{44+}, with the most abundant highlighted.
- The mass effect shift in wavelength is modest.
- Gas suppliers can provide ~99% pure isotope so specification will eliminate this variation from the measurement.

Modelled X-ray spectrum of Xe^{44+} – Xe^{51+}

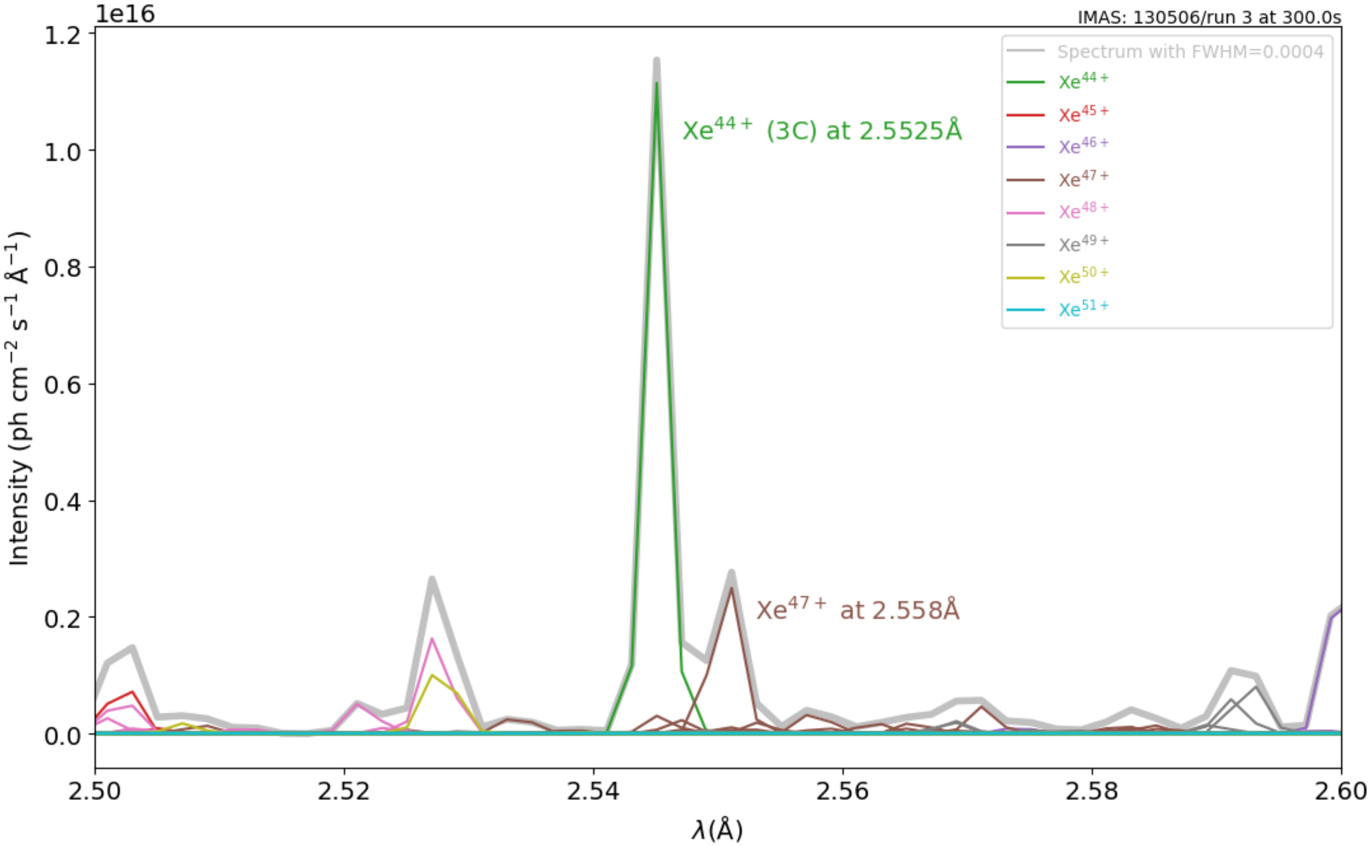
Each stage between Xe^{44+} and Xe^{51+} also radiates in the same X-ray spectrum.



- The original choice of the Xe^{51+} line and the strong Xe^{44+}(3D) line is because of their relative isolation and well-characterized (ie measured) wavelengths.
- The 3C line is almost as strong and is adjacent to a line from Xe^{47+} which may be used to give extra spatial information.

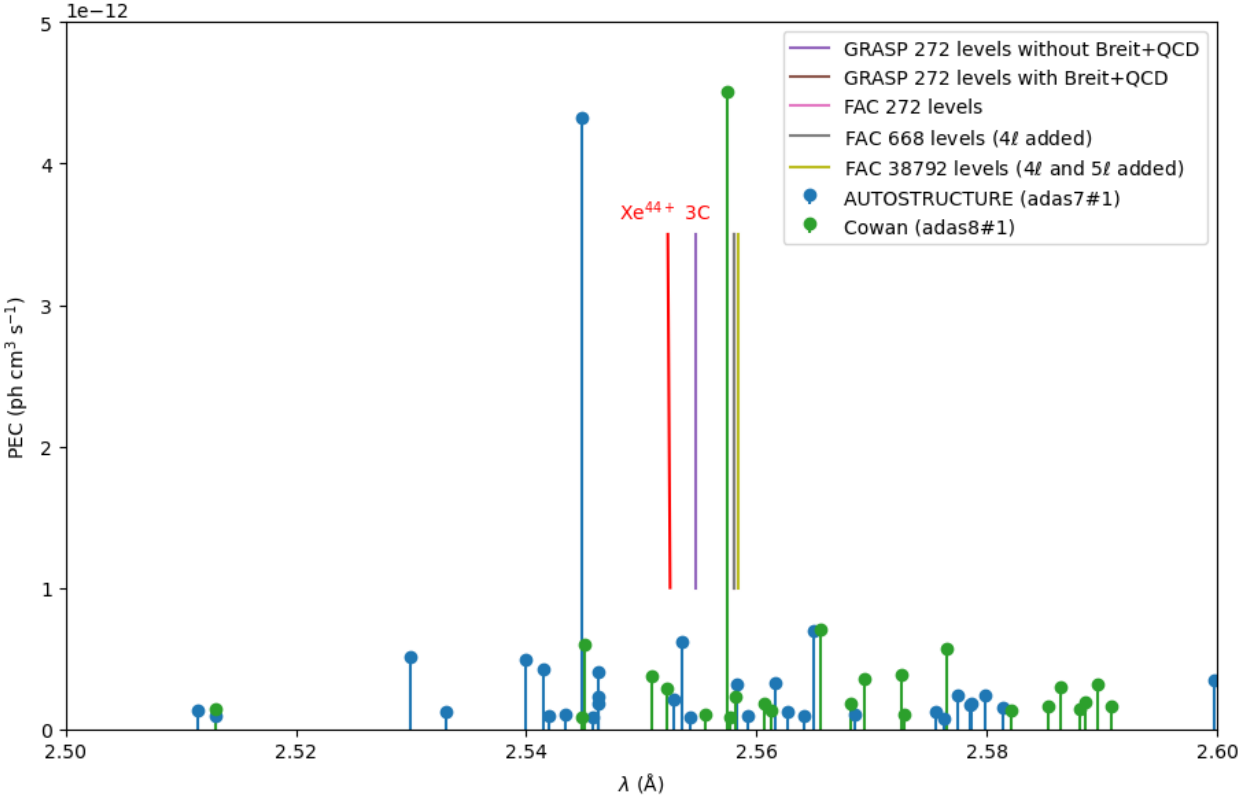
X-ray spectrum of Xe^{44+} and Xe^{47+}

Each stage between Xe^{44+} and Xe^{51+} also radiates in the same X-ray spectrum.



- The Xe^{44+}3C line is almost as strong as the 3D line and is adjacent to a line from the Xe^{47+} stage (ground – $2s^2\ 2p^2(^1S)3d\ ^4D_{5/2}$).
- Both lines lie within the very narrow bandpass of the instrument but do they overlap which would complicate the Tion measurement.

X-ray wavelengths of N-like Xe^{47+} have not been measured



- There are no measurements of any Xe^{47+} lines.
- 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 but confirmation of this via an EBIT experiment at LLNL is underway.

Concluding remarks

- Atomic physics is deeply embedded in magnetic confined fusion.
- Often it is hidden in codes and may never be updated – this attitude is changing.
- Some atomic data (and models) have safety implications – eg predicting the attenuation of the beam.
- The accuracy of the atomic data is not quantified to the expectations for engineering use.

- Low and high temperature plasma environments are important for different reason – data for all ion stages is usually needed.
- Spectroscopy encodes a lot of information and may be under-exploited.
- Some applications need very high precision data (wavelengths, intensities, ratios) but others would benefit from a robust estimate of its uncertainty.
- Laboratory plasmas have luxury of independent measurements of temperature and density.

- Our goal is to add a realistic and well formulated 'atomic error' to fusion analysis and modelling codes.