Modelling radiation from high-Z elements in tokamak plasmas
and similarities with X-ray sources

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and ADAS contributors

Potted history and outline

ADAS is an atomic data collection and set of modelling tools originating from the needs of magnetic confined fusion. It began at JET, the joint European tokamak experiment, and is now used in most MCF facilities. It continues to be developed at JET and is managed by University of Strathclyde.

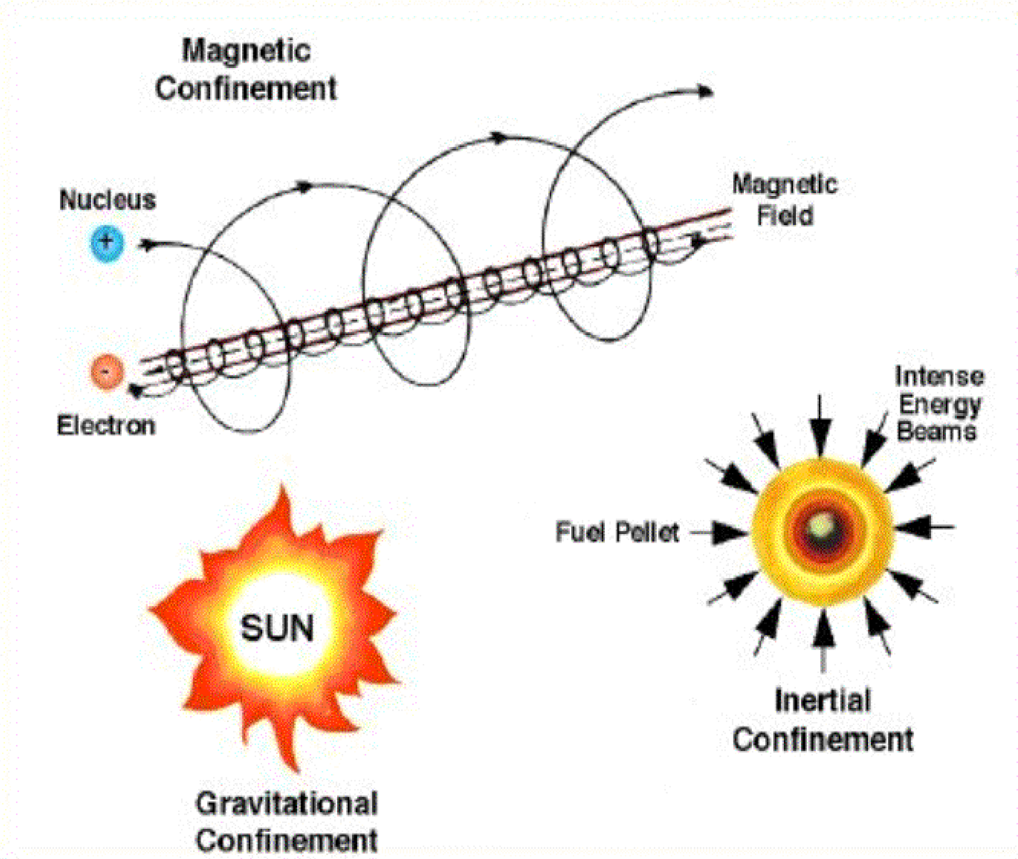
Effective coefficients, characterizing finite density conditions, are required for modelling and diagnostic interpretation. Collections of fundamental, individual process data, are needed to produce the derived, effective data.

OPEN-ADAS is the pathway for ADAS data and support software to be made publicly available and is an agreed and shared project between ADAS and IAEA.

- 60sec primer on tokamak plasmas.
- Use of spectroscopy in fusion experiments.
- ADAS population model.
- Calculation, optimization and validation of atomic data.
- Similarities with X-ray and VUV source plasmas.

Controlled Fusion

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

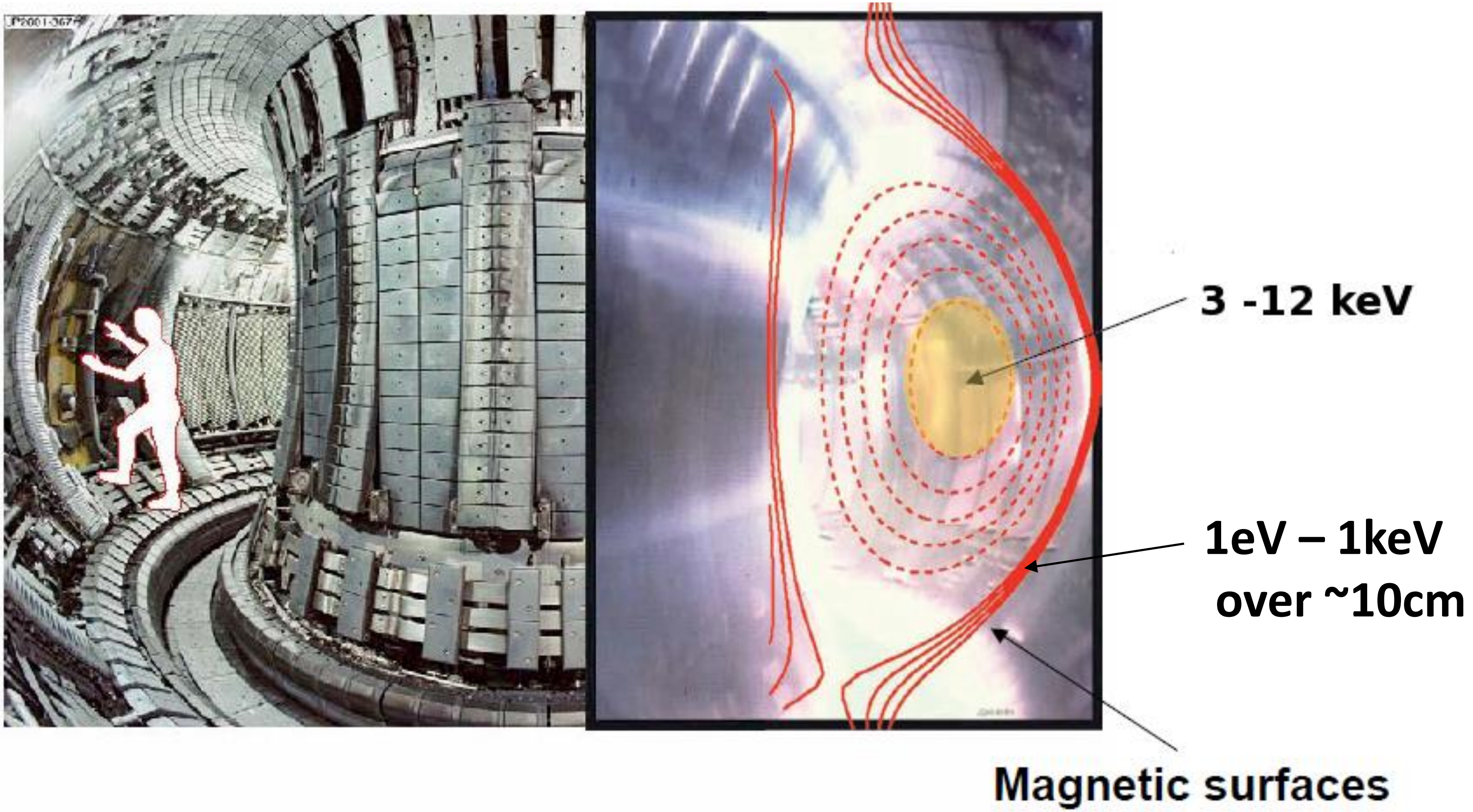


Two approaches:

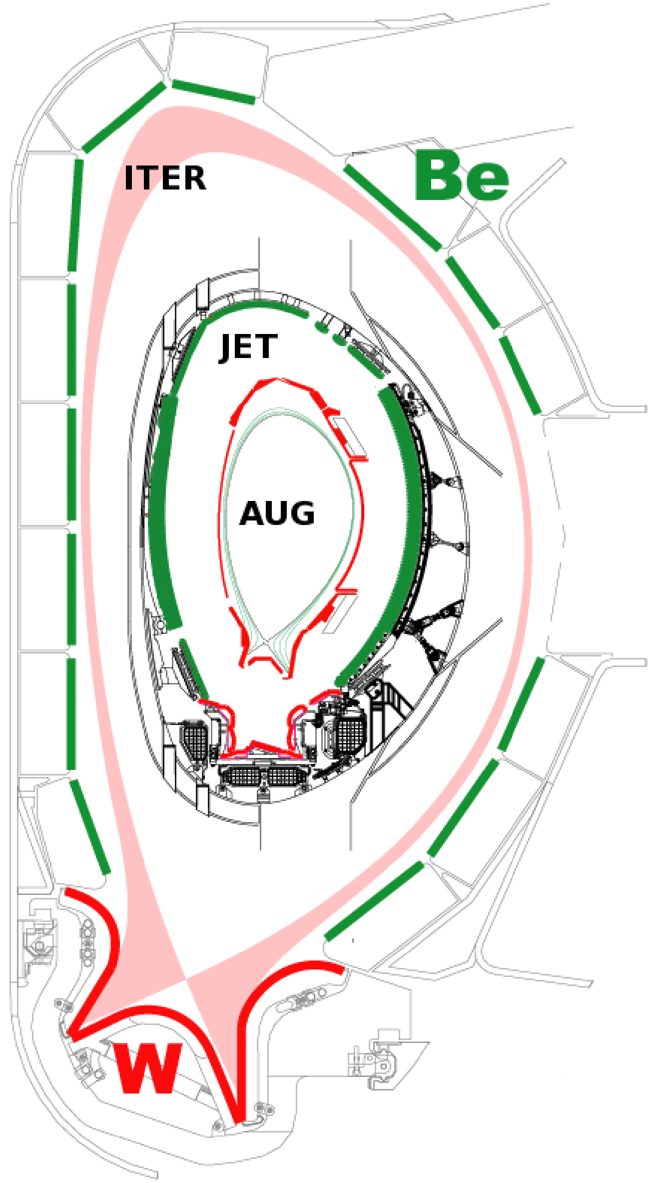
- Magnetic confinement – large volume, long duration plasmas.
- Inertial confinement – small volume and short duration.

Controlled Fusion – MCF

JET at Culham, near Oxford, UK. Radius 3.1m, vessel 3.96m x 2.4m, 80m^3 plasma, up to 4MA and 4T.

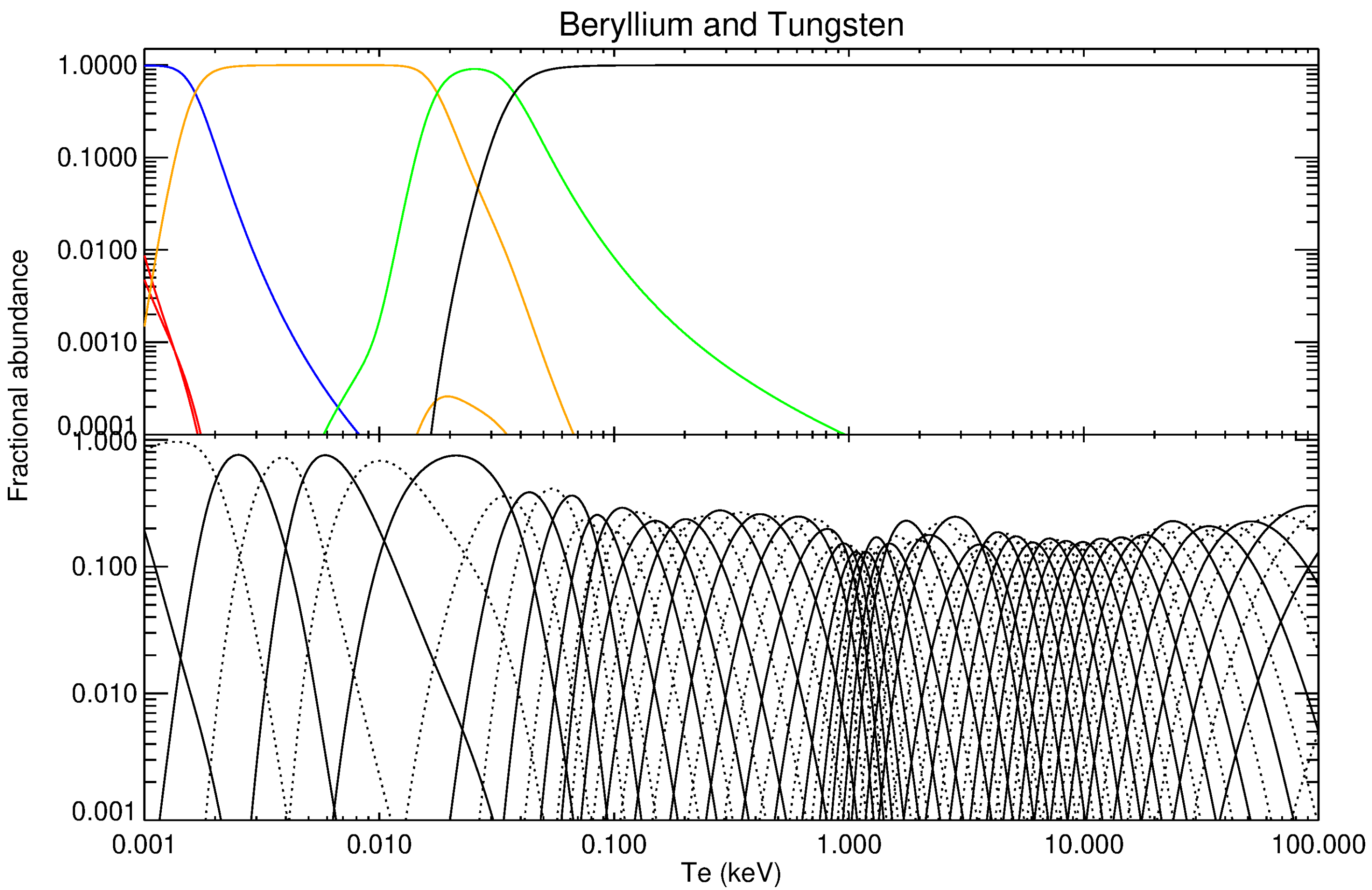


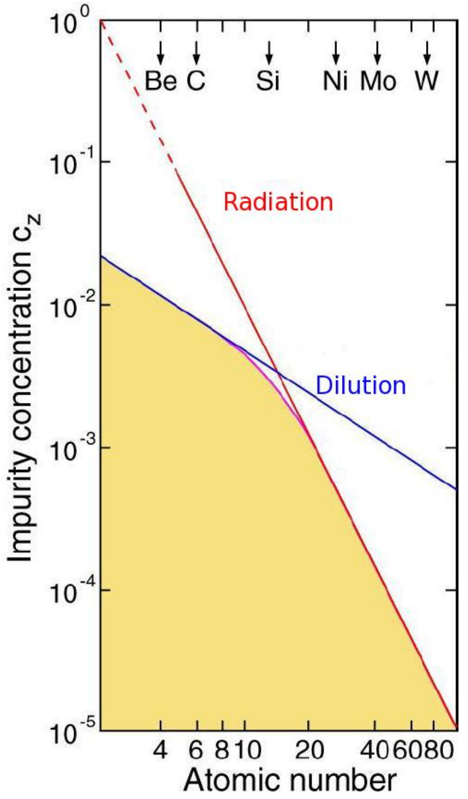
ITER – the next-step international experiment



- Collaboration between China, EU, India, Japan, Korea, Russia and USA.
- 830m^3 with radius of 6.2m
- Goal is 500MW of fusion power and Q>10.
- Tungsten is an integral plasma facing material.

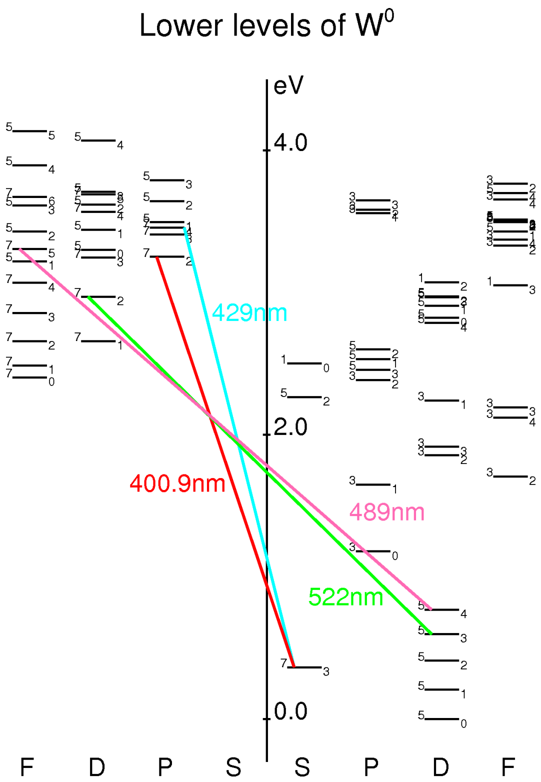
Tungsten – a challenge for atomic data

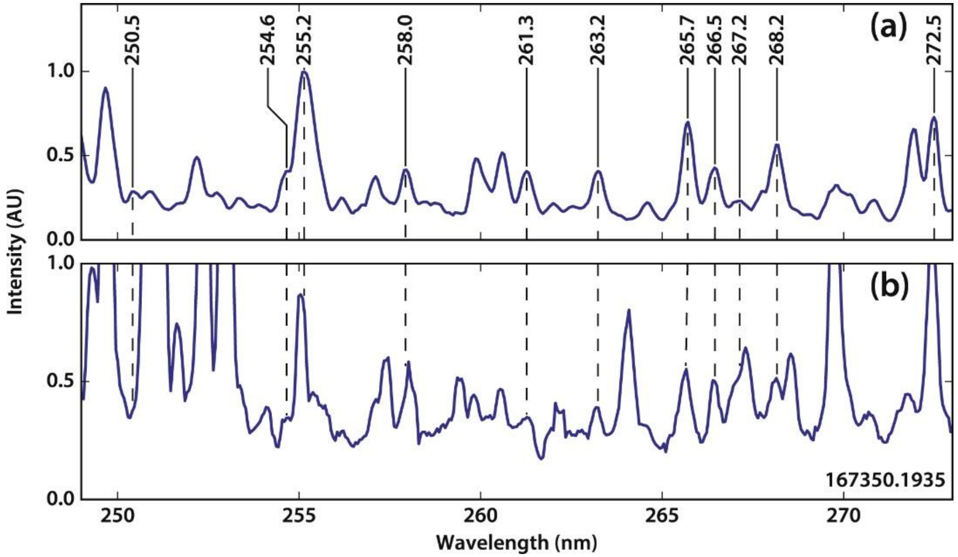




- Fusion – a mixture of simple elements (H, Be, He) and very complex tungsten.
- Ni-like tungsten, W46+ with $3d^{10}$ ground state has IP~4keV.
- Divertor and SOL emission from stages with n=5 and open 4d and 4f shells.

Tungsten spectroscopy – influx

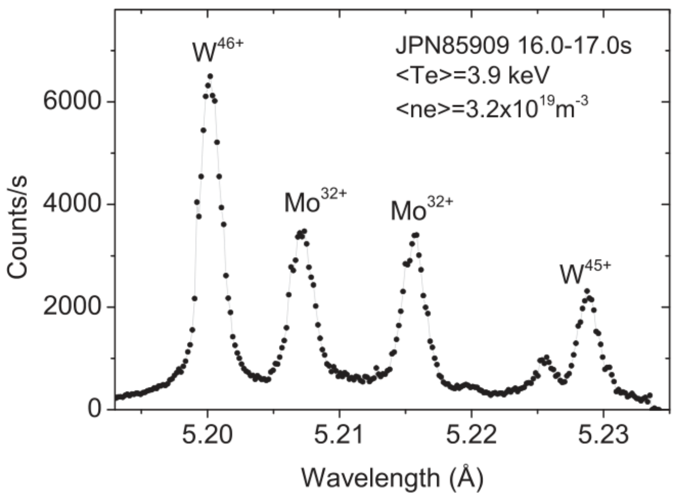




C Johnson et al, PPCF, **61**, 095006 (2019)
CTH and DIII-D VUV spectra of W^0.

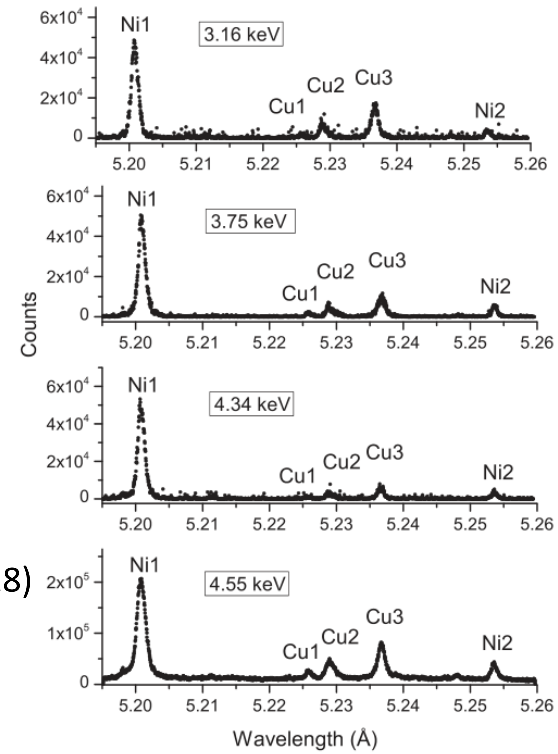
- W0 is a measure of influx of tungsten: Γ = S/XB * I
- Requires ionization (S), excitation (X) and structure atomic data.
- Dominant lines are in VUV but practical measurements are in visible.
- Lower levels are metastable – all with significant population.
- Active area of interest, in particular for ionization data.

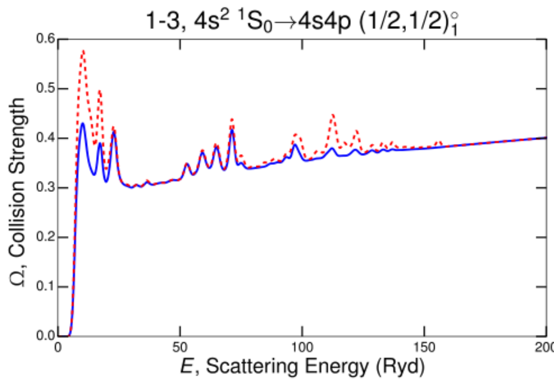
Tungsten spectroscopy – core

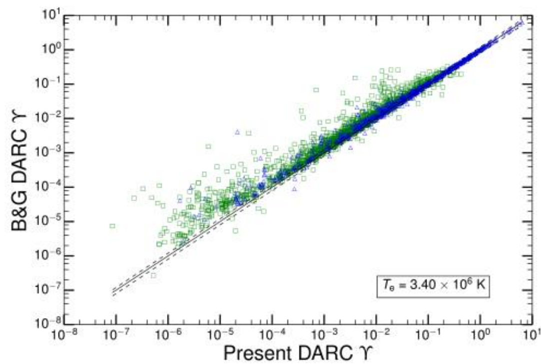


J Rzadkiewicz et al, Phys Rev A97, 052501 (2018)

JET X-ray spectra supported by EBIT measurements





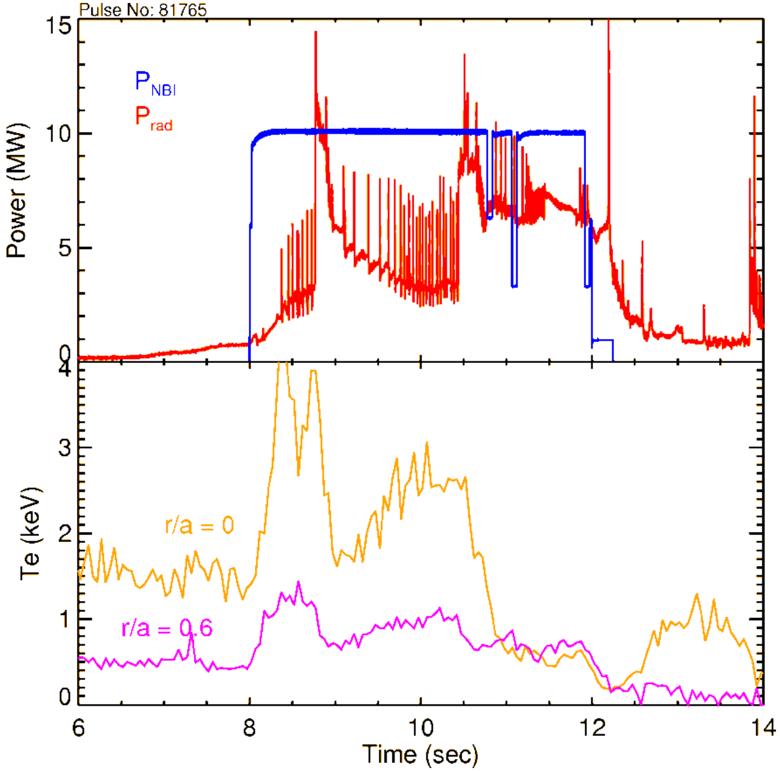


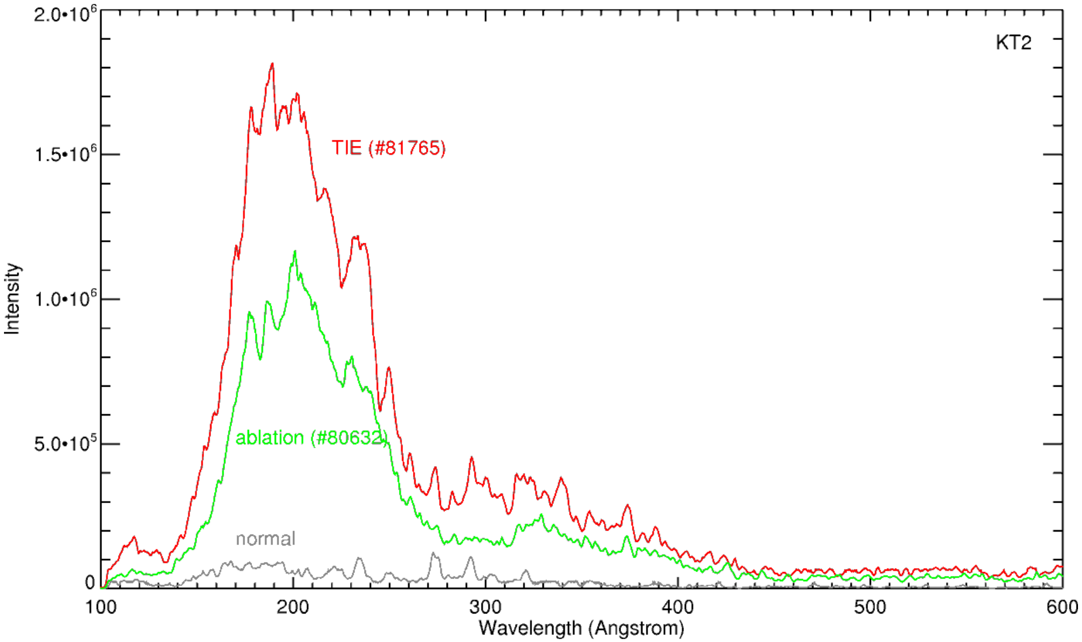
M Bluteau et al, J Phys B, **48**, 195701 (2015)

- Isolated lines from relatively simple ion stages – around Ni-like for JET and Ne-like for ITER.
- Relativistic R-matrix excitation calculations – independent results so comparisons are possible.
- Used for ion temperature and concentration diagnostics of core plasma.

Tungsten spectroscopy – edge and pedestal region

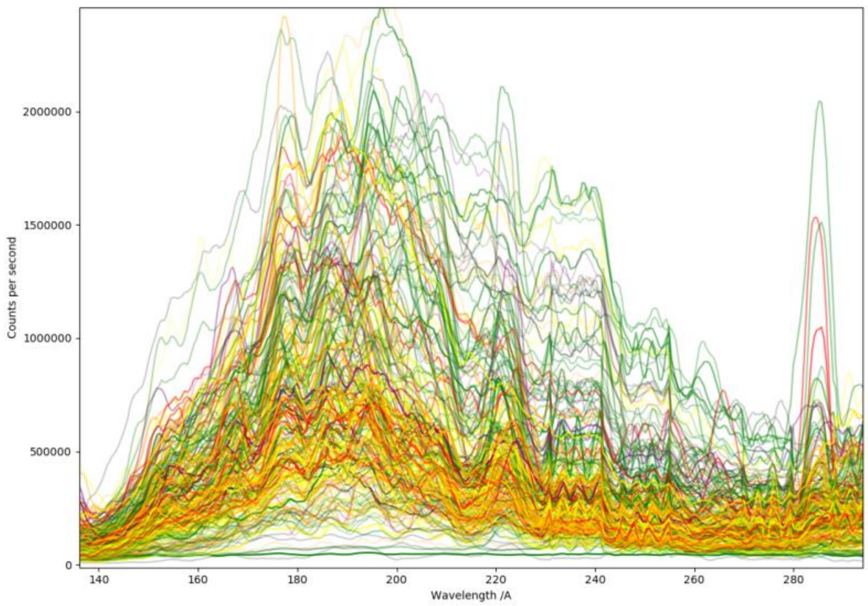
Transient impurity events are random events due to particles (dust/flakes) entering the plasma.

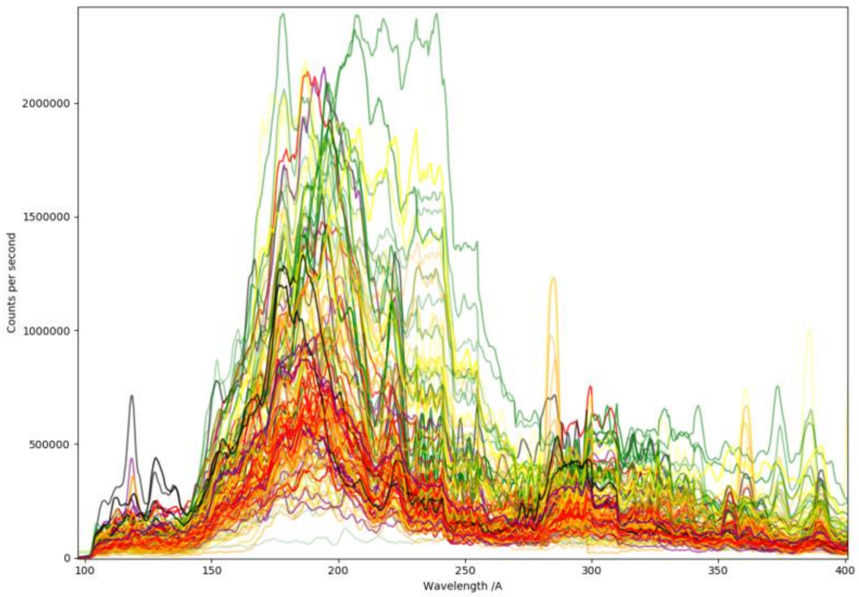




- Primarily in XUV and VUV regions.
- Carry significant power (~MW) and can cool and even disrupt the plasma.
- Emission is from complex ion stages – W^{6+} – W^{40+}.

Tungsten spectroscopy – edge and pedestal region

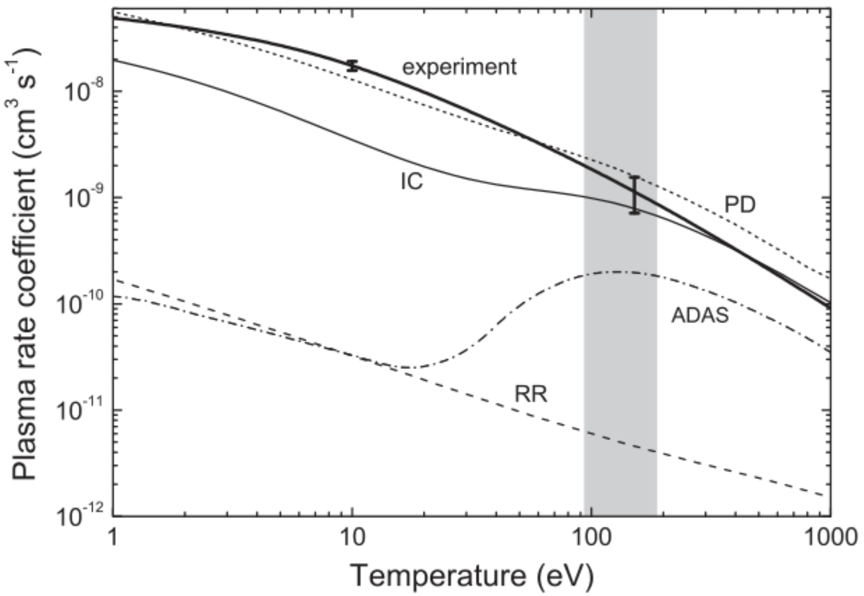




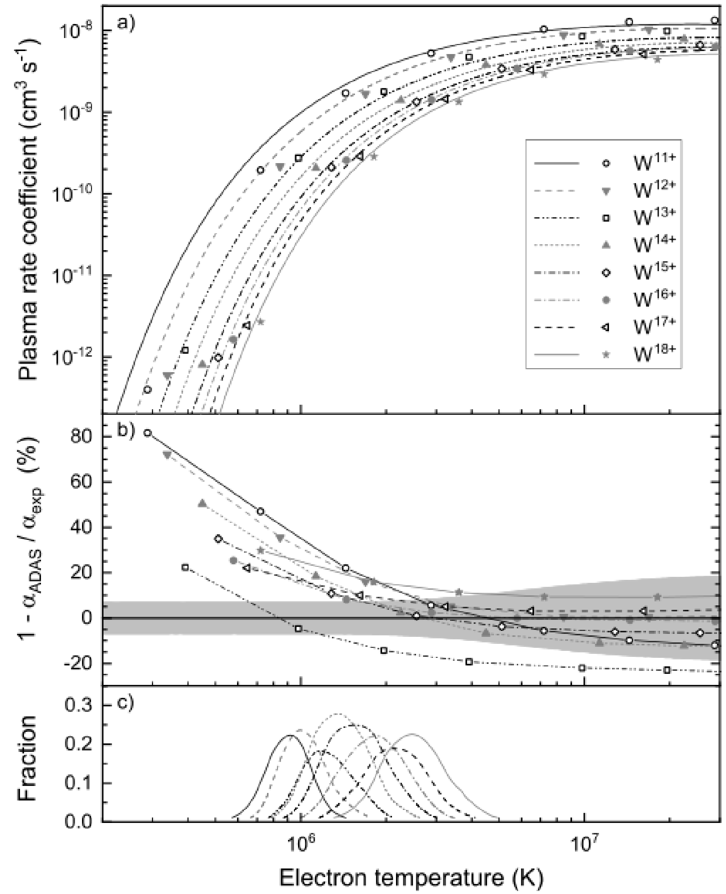
- Emission pattern varies with conditions.
- Edge-like and core-like can be classified.
- No satisfactory quantitate model yet.
- Spectrometer instrument function is broad and dispersion is not flat.
- Edge and pedestal region are characterized by large gradients in temperature and density and cross-field plasma transport is significant.
- It is essential to be able to model the ionization balance.

Tungsten ionization balance – problems with atomic data

Measurements of DR and ionization cross sections indicated that the models in use needed to be improved.



K Spruk et al, Phys Rev A 90, 032715 (2014)

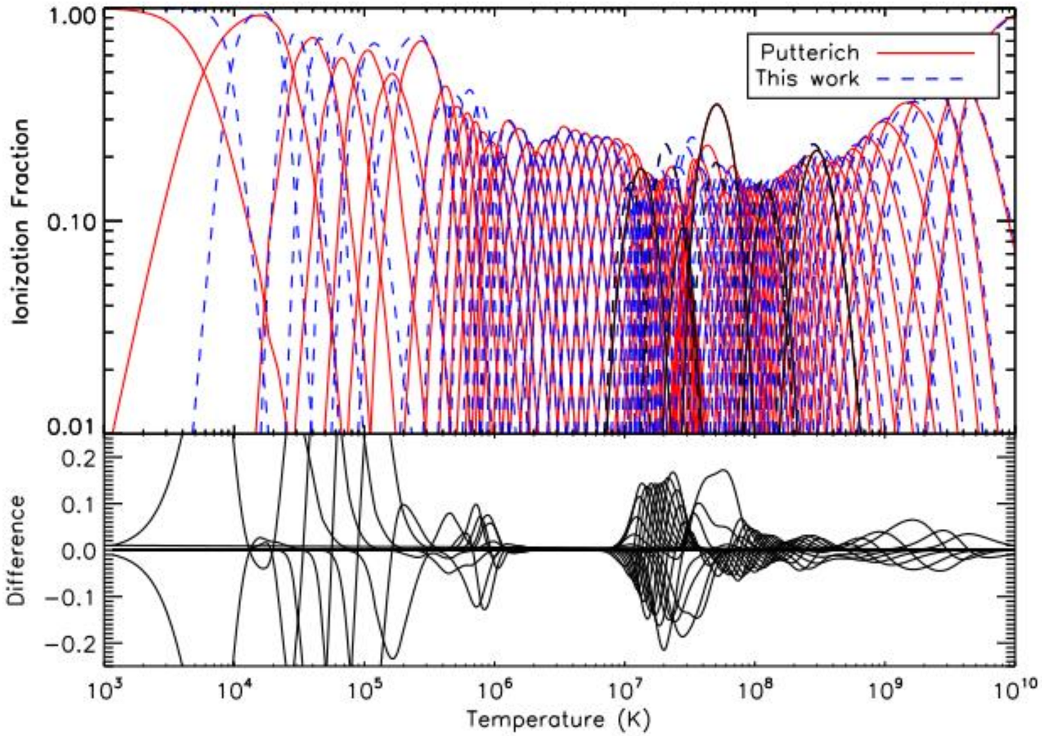


D Schury et al, arXiv 1910.08482 (2019)

- Dielectronic recombination rates were severely underestimated for ions with open 4f shells.
- Ionization is also showing a (smaller) discrepancy between models and measurements.

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** and is ongoing…….

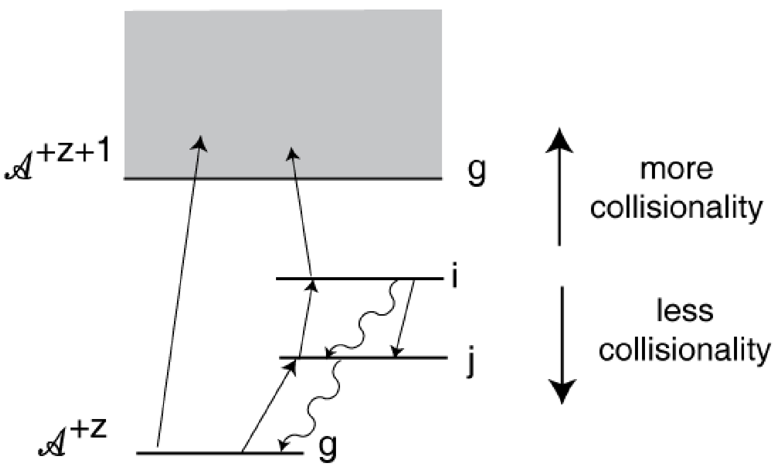


- $4f^n$ still an issue
- But now constrained from both sides
- It's the pedestal region for JET (100-1000eV)

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

Finite density environment

collisonal-radiative picture for ionisation and recombination

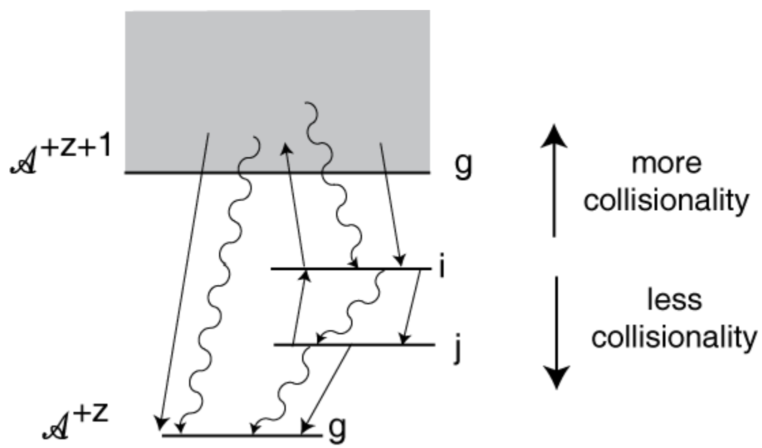


Reactions:

At higher densities, collisional excitation and de-excitation between excited levels compete with spontaneous emission.

$$\mathcal{A}^{+z}(i) + e \rightleftharpoons \mathcal{A}^{+z}(j) + e$$

Indirect pathways lead to line emission and ionisation may occur in a stepwise manner.



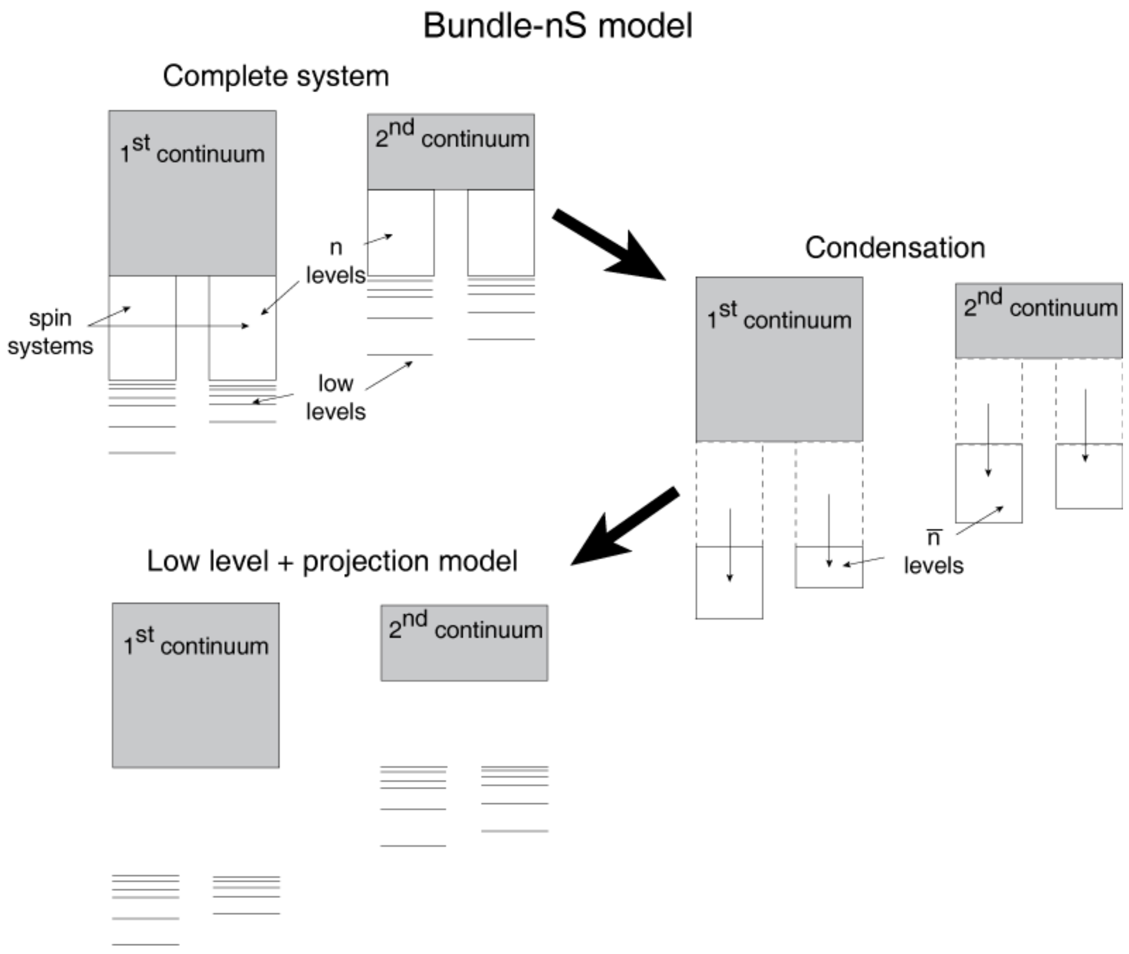
Three-body recombination must be added to the reactions which pairs with collisional ionisation from excited states

$$\mathcal{A}^{+z}(i) + e \rightleftharpoons \mathcal{A}^{+z+1}(g) + e + e$$

Not all recombinations lead to growth of the ground population of the recombined ion.

Finite density environment

generalized collisonal-radiative approach – projection of high-n levels

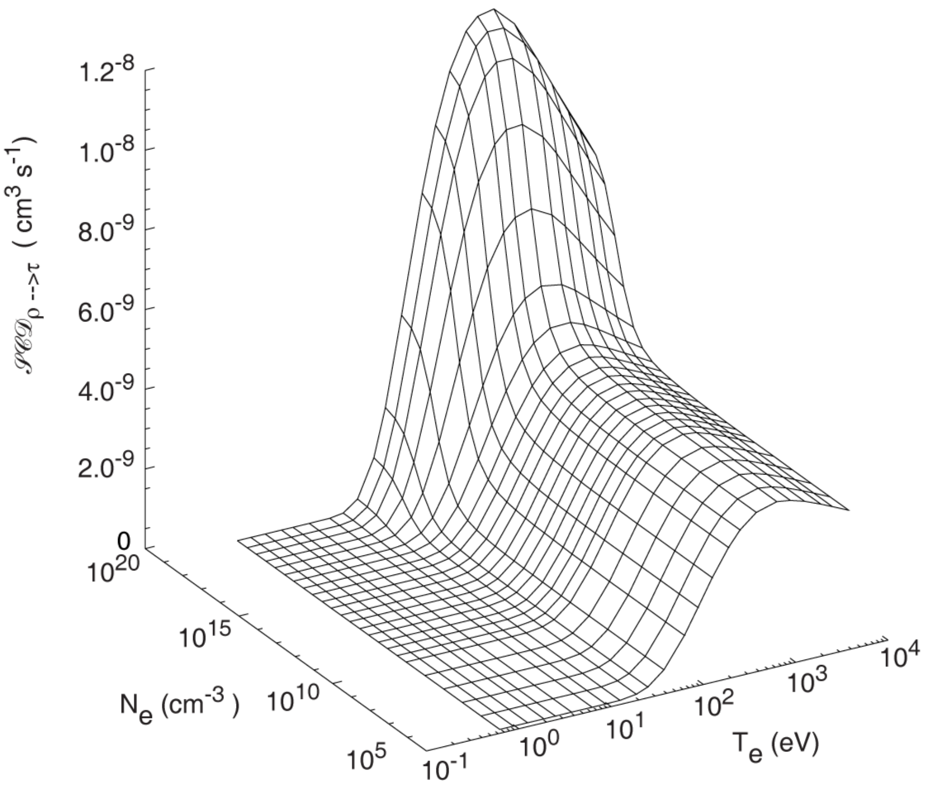


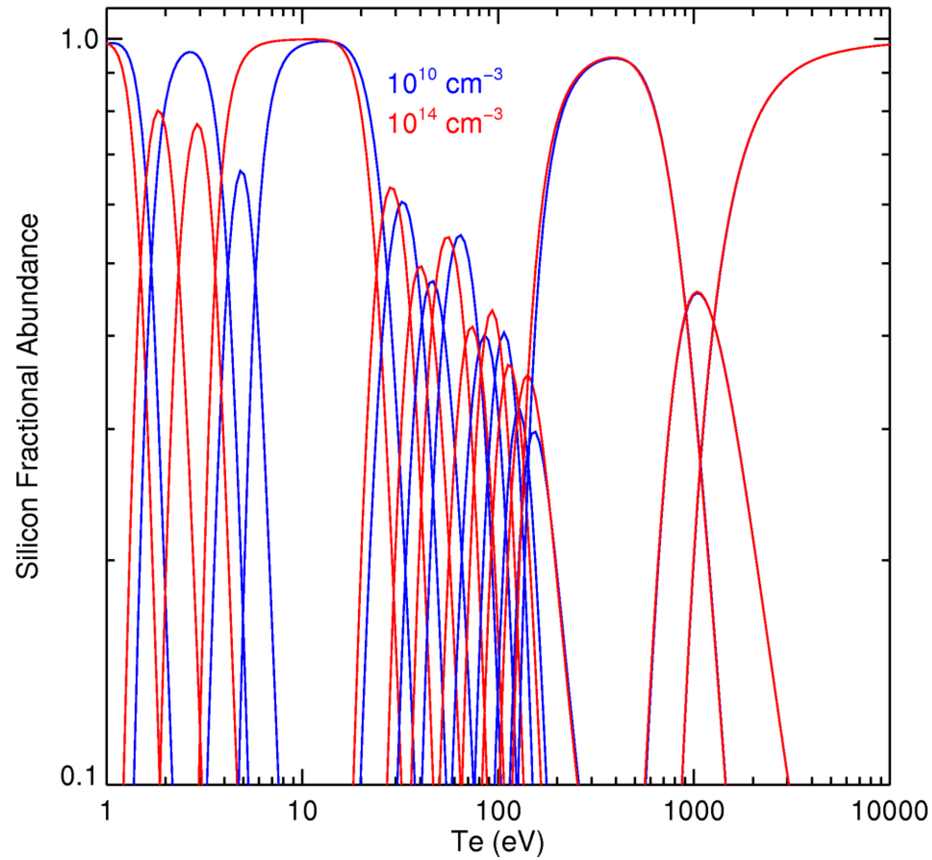
- For light/medium weight elements there is a truncation problem since the true atom with its infinite number of Rydberg states.
- Dielectronic recombination populates high lying states.
- Setup a bundle-n collisional-radiative matrix for the whole system. Use the inverse sub-matrix propagator for the ry n-shells to project onto the ry_{ls} n-shells.
- Eliminate the direct couplings and expand statistically over the ry_{ls} nS-shell substructure and add to the more exact collisional-radiative matrix for ry.

Coefficients are functions of T_e *and* N_e

The **SCD** coefficient increase to a new limit at high density as excitations lead to ionisation

$O^{+3}(2s^2\ 2p\ ^2P) \rightarrow O^{+4}(2s^2\ ^1S)$





With Silicon the effect is greater effect at edge than in core

Optimizing the calculation of atomic data

- ADAS makes extensive use of Cowan structure code for baseline data provision.
- AUTOSTRUCTURE is a better collision model (DW vs PWB) but it is non-trivial to produce a good structure.
- Sophisticated R-matrix (Breit-Pauli/ICFT and DARC) are applied to diagnostically significant ions.
- Calculation along iso-electronic sequences is preferred in the atomic domain but iso-nuclear data is needed to interpret plasma measurements.

- The Tungsten DR project showed the value of treating even very complex ions in a systematic fashion.
- We would like a rule-based algorithmic method to optimize the structure calculations.
- And consequently the excitation data for spectroscopy and power.

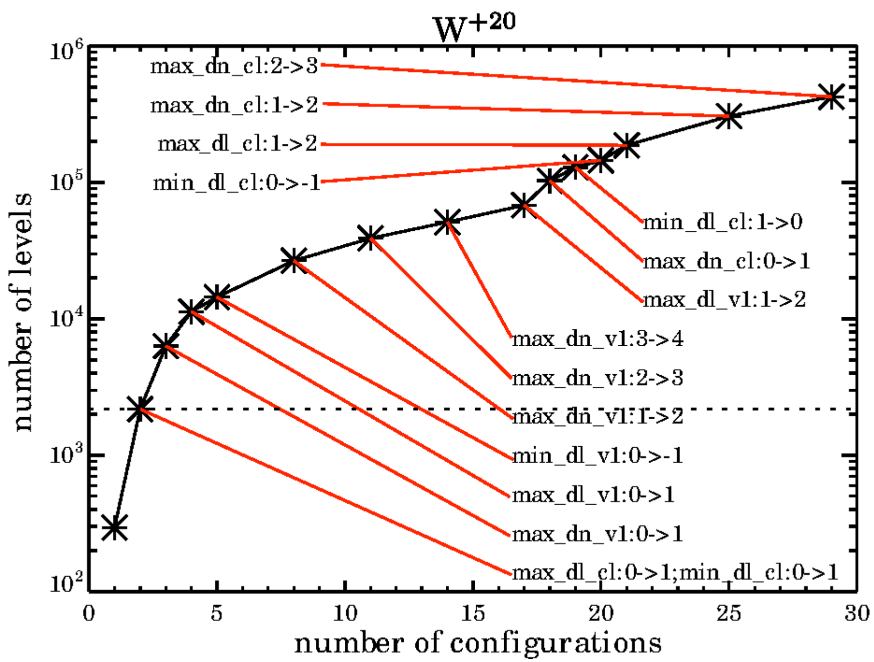
Optimizing the calculation of atomic data

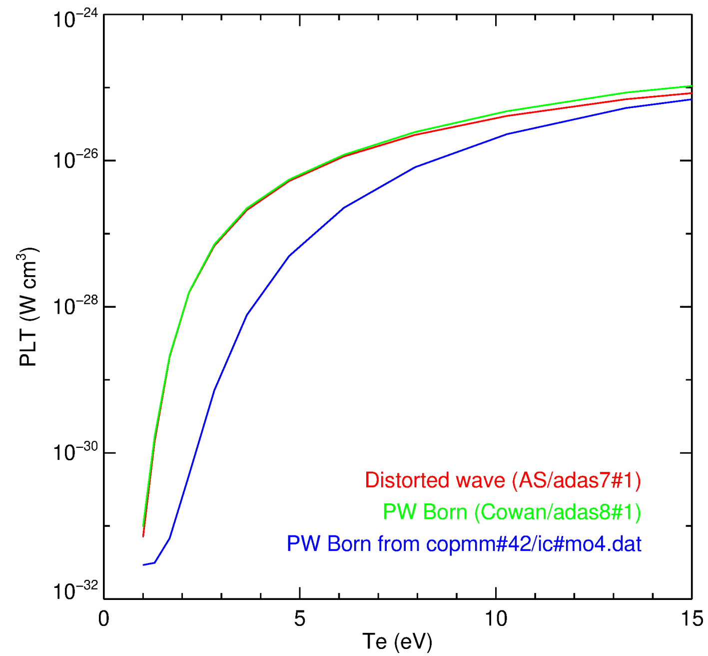
- Choice of correction configurations is most important.
- Use total radiated power as the metric to optimize.
- Other criteria could be considered – eg a spectral interval.

IOP Publishing Plasma Physics and Controlled Fusion
Plasma Phys. Control. Fusion **59** (2017) 055010 (8pp) https://doi.org/10.1088/1361-6587/aa6273

Optimisation and assessment of theoretical impurity line power coefficients relevant to ITER and DEMO

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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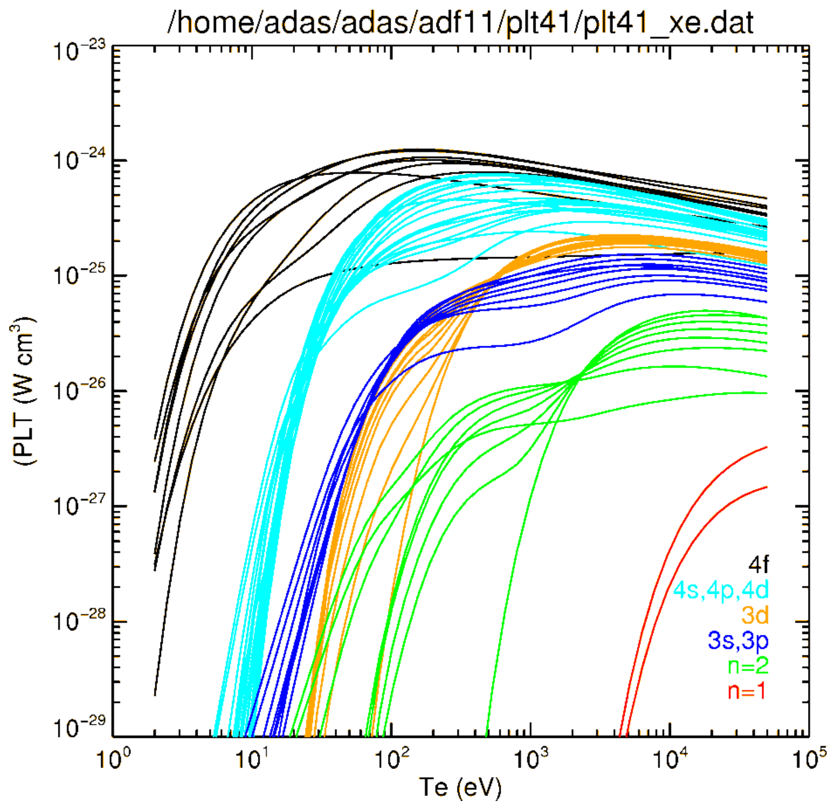
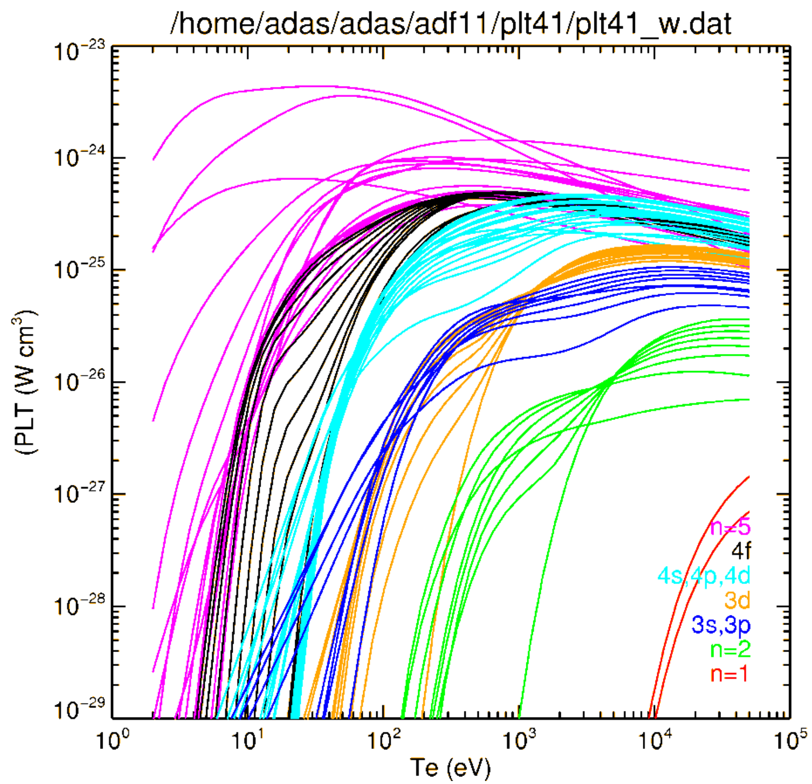
Optimizing the radiated power

- Data from Cowan code with AS supplementation for spin-changing and higher multipole transition probabilities

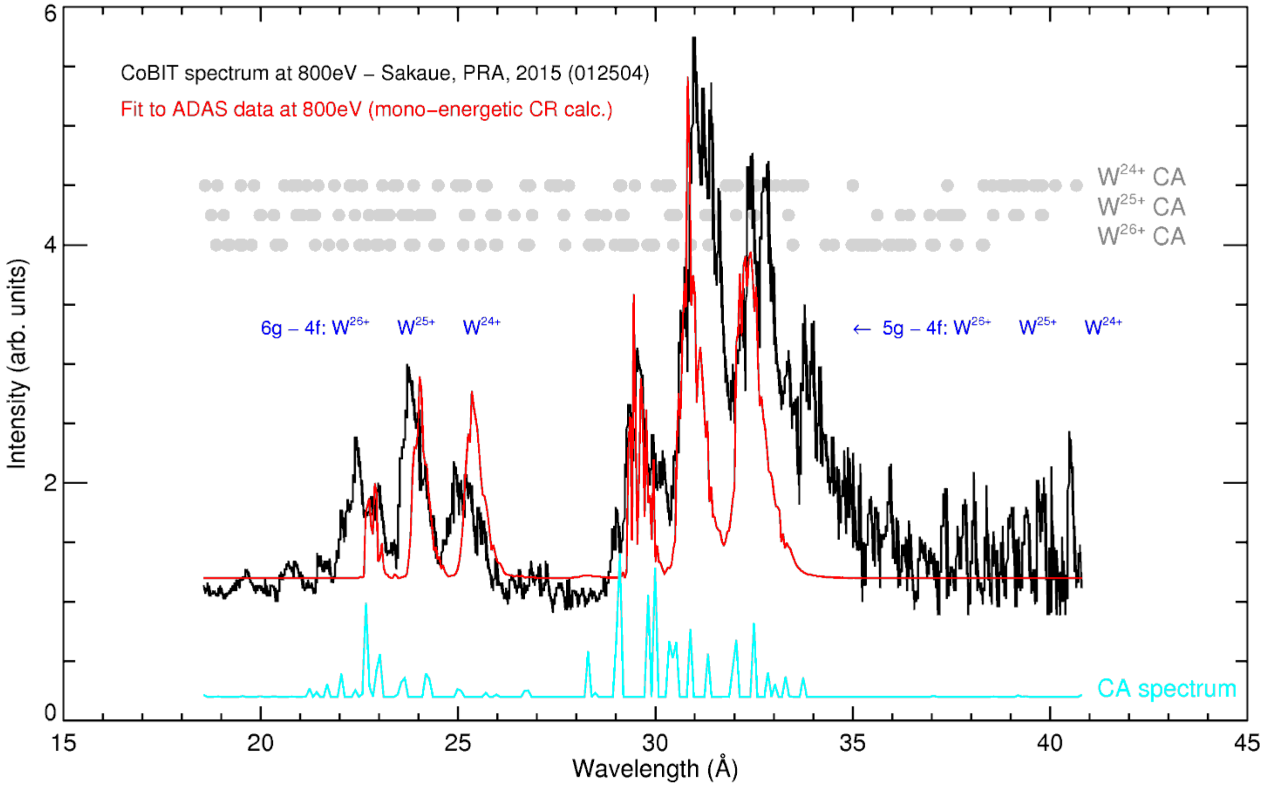




Top-up from configuration-average calculation is required to supplement the radiation from the low-lying, spectroscopic, levels.

Optimizing the radiated power – validation of atomic data

- One outcome is a set of adf04 excitation data in collision strength and effective collision strength forms.
- These can be applied to spectral problems

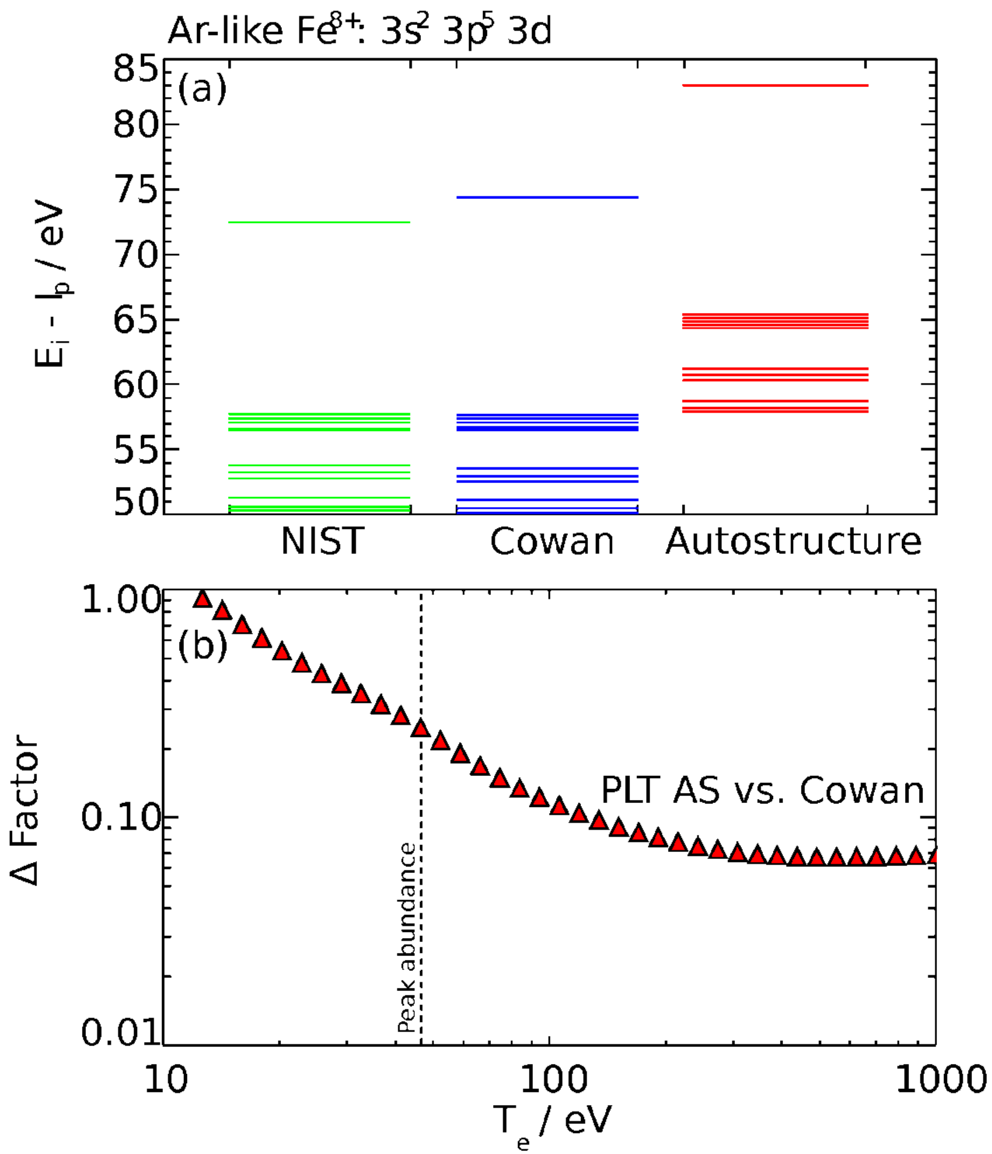


- Mono-energetic ADAS population model, producing a spectral feature, fitted to an EBIT spectrum with ADAS feature-fitting LSQ code.
- Goal is to apply (shifted) features to tungsten emission from tokamaks.

Optimizing atomic structure

- Wish to move to AUTOSTRUCTURE distorted-wave as a new baseline quality.
- Also can drive R-matrix.
- Good atomic structure is essential for high quality derived data.
- And is the basis for uncertainty estimation.

- Default results could be better.



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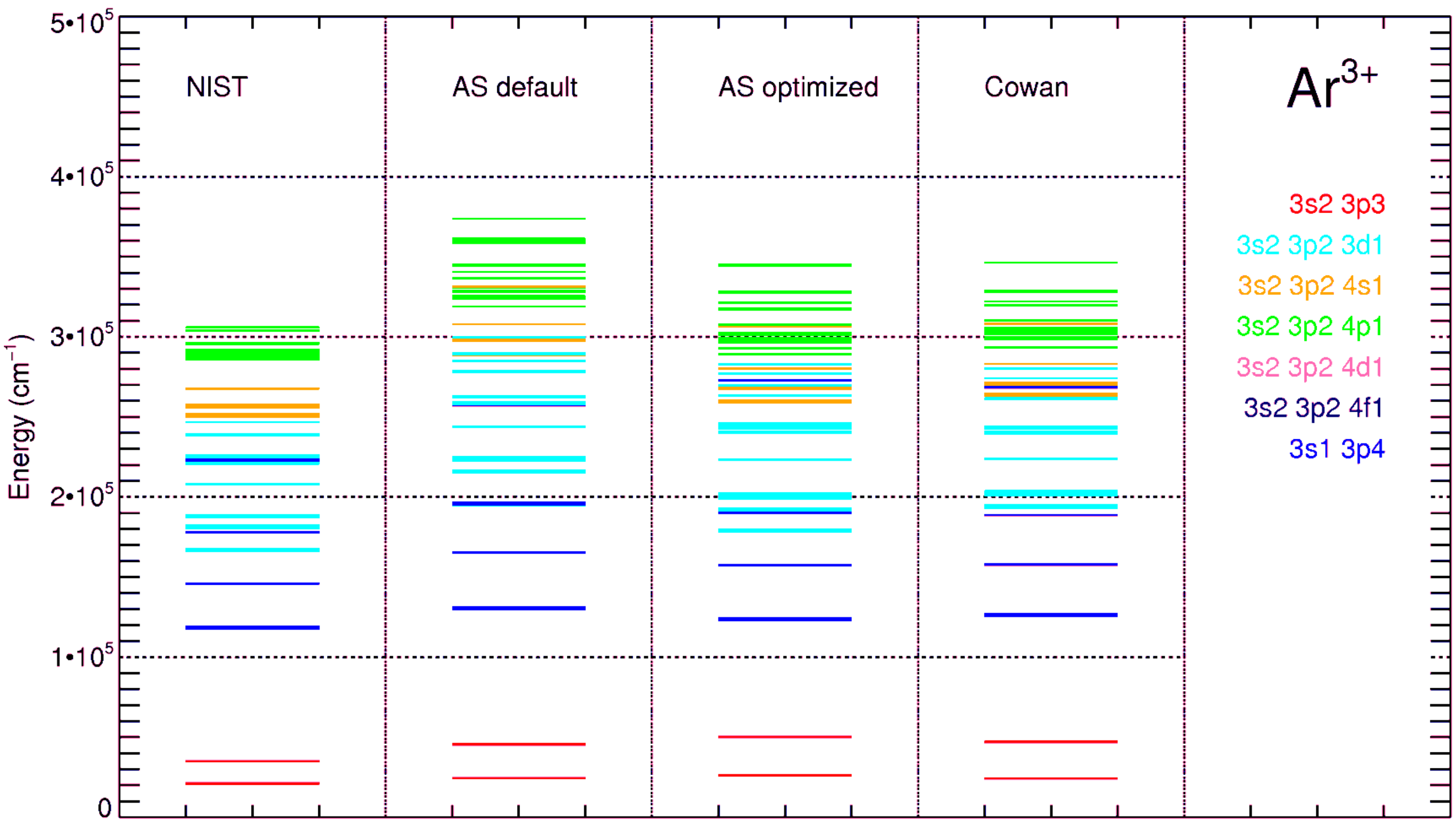
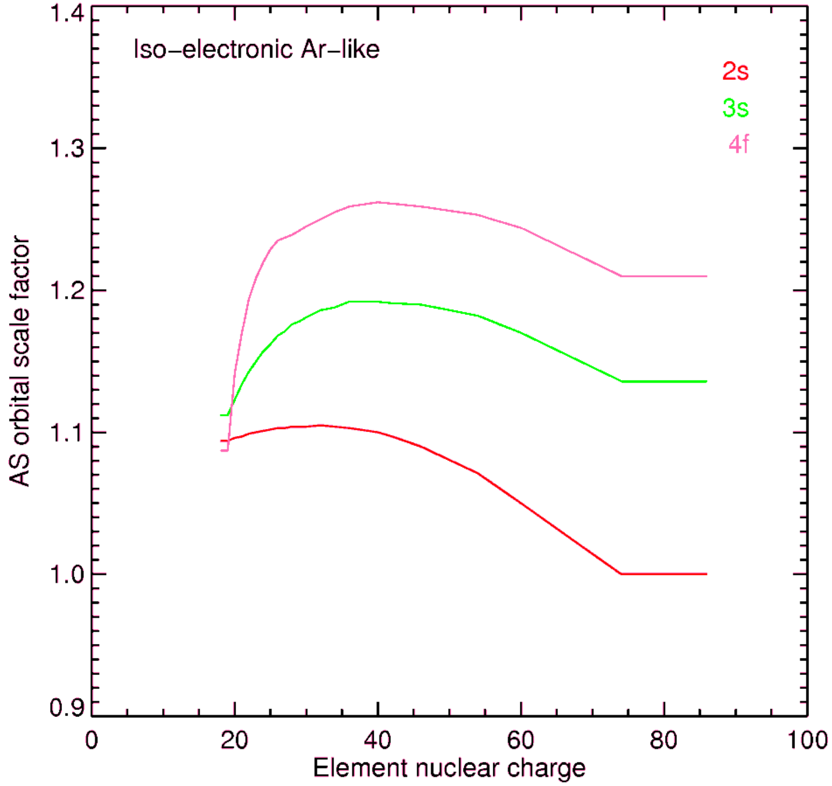
Optimizing structure across iso-electronic and iso-nuclear sequences

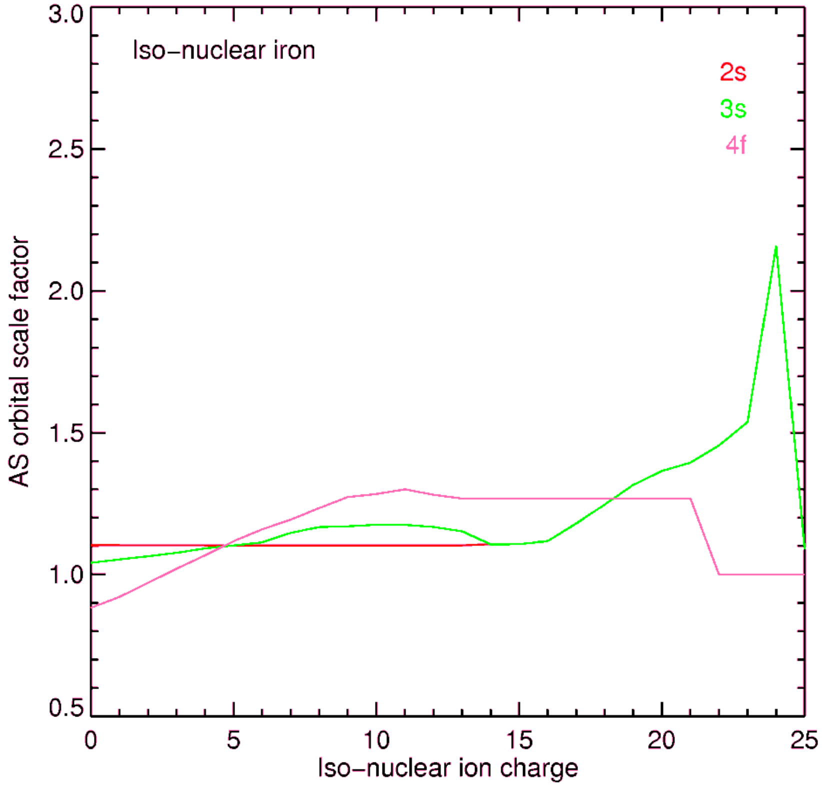
- AUTOSTRUCTURE uses a Thomas-Fermi potential.
- Individual orbitals can be scaled to improve results.
- But what is improvement?



Optimizing structure across iso-electronic and iso-nuclear sequences

- Start with configurations identified in power optimization.
- Include equivalent electron complex.
- Use AS minimization selectively locking orbitals as we move along sequences
- Construct a smooth surface of scaling parameters.

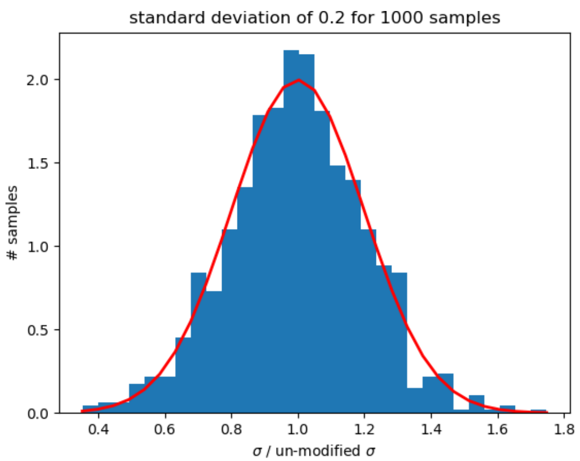


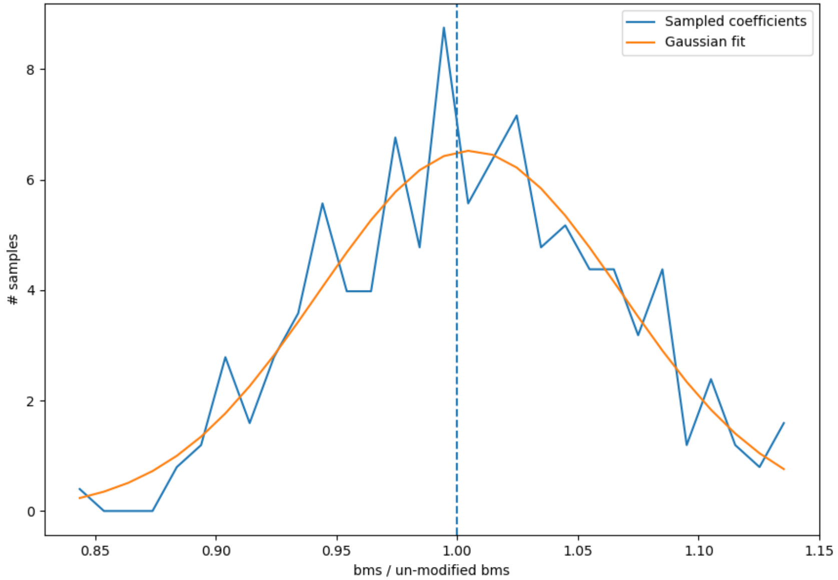


Validation via propagation of uncertainty – beam example

An instrumented ADAS beam model (adas316) is a bundle-n collisional-radiative calculation:

- CR model driven by atomic cross sections; excitation, de-excitation and ionization
- Plasma ion and electron populations are the drivers.
- Beam stopping and emission are parameterized by beam energy and Te, Tion, Ne and Nion.
- Assume a normal distribution for each atomic process and see if we recover sufficiently normal bms and bme coefficients.





- Apply sd=0.2 for ion impact ionization
- sd=0.1 for e-impact ionization
- 250 samples for each

Result: bms/un-modified bms mean is 1.0055 with sd=0.0619

Can a similar approach be applied to spectral features?

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Concluding remarks

- Advancing the atomic data required for fusion is still important
- High Z species – calculation of data and development of models underway

- The way atomic data will be used is changing
- Embedded into complex analysis chains, some with machine protection implications (and responsibilities).
- Provenance of atomic data is important
- Validation and assessment must take greater prominence.

- Need to maintain flow of the highest quality data into ADAS
    - Not all data in ADAS is perfect – ideally when faults are found outside the ADAS team an improved dataset would be provided.
- Models must also advance.