Recent updates to the ADAS atomic database and new developments in ADAS data production and atomic models

Martin O'Mullane, Stuart Henderson, Nigel Badnell,
Hugh Summers, Matthew Bluteau
and many ADAS contributors

Outline

ADAS is a set of computer codes and a reaction database oriented to the needs of magnetic confined fusion and astrophysics research.

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.

- New data in ADAS
  - Radiated power with optimized choice of configurations.
  - Iso-nuclear sets of excitation data
  - Iso-nuclear dielectronic and radiative recombination data for tungsten
  - New adf15 data (photon emissivities)
- New codes in ADAS
  - Lifting our baseline quality
  - Extend population models – non-Maxwellian, mono-energetic
- Proposed data for ADAS and OPEN-ADAS
  - Ion impact in a new *adf06* specification

New data – since 2015 DCN meeting

- ~3000 new datasets.
- Mostly tungsten data – adf04 (excitation), adf09 (DR) and adf48 (RR)
- New Al-like iso-electronic adf09 (Sh. A. Abdel-Naby et al, Astron. & Astrophys., A40, p537 (2012). This may be the last of the fully level-resolved adf09 data. Tungsten is archived in a more compact fashion.
- Update of iron adf04 files, Fe2+, Fe8+, Fe12+
- Balmer and Paschen series Hydrogen adf15 (PEC) files.
- New adf15 files for Ca19+, Ni27+, O2+
- New Lithium CX data (adf01, adf12) to support liquid metal first wall studies.

- Molecular data for H2 added to ADAS in support of (mothballed) diatomic population model. OPEN-ADAS availability not currently under consideration since the data is a mix of numerical and fits.

OPEN-ADAS: http://open.adas.ac.uk

OPEN-ADAS
Atomic Data and Analysis Structure

Freeform | Wavelength | Ion

About OPEN-ADAS

OPEN-ADAS is a system to search and disseminate key data from the Atomic Data and Analysis Structure (ADAS).

ADAS is a computer program managed by the University of Strathclyde and made up of a consortium of over twenty members.

The OPEN-ADAS system enables non-members, with an interest in fusion and astrophysics, to download and use ADAS data.

More about OPEN-ADAS

03 July 2017– More Tungsten Project DR data available
Dielectronic and radiative recombination from the K-like to Kr-like iso-electronic sequences of tungsten are now available. Read more

Freeform search

Search | ▸ Freeform search examples

Freeform search | Search by wavelength | Search by ion

The OPEN-ADAS data classes

The data contained within ADAS is strictly organised and precisely formatted. There are over fifty distinct types of data file. The scope of OPEN-ADAS is targetted on and limited to the release and organisation of general user relevant data from the ADAS databases and the provision of code, subroutines and procedures to enable such users of OPEN-ADAS to read the released data. These data classes are given below.

FUNDAMENTAL CLASSES

ADF 01 — Charge exchange cross sections
nl-resolved charge exchange cross-sections over a range of n-shells for a donor neutral atom and ionised impurity receiver

ADF 04 — Resolved specific ion data collections
Coefficient data for a given ion which includes spontaneous emission coefficients and electron impact collisional rates and other optional processes.

ADF 07 — Electron impact ionisation coefficients
Collections of Maxwell averaged electron impact ionisation rate coefficients for both direct ionisation and excitation/autoionisation.

ADF 08 — Radiative recombination coefficients
Maxwell-averaged radiative recombination coefficients i.e. spontaneous free-bound transitions of Maxwellian electrons excluding dielectronic recombination.

ADF 09 — Resolved dielectronic recombination coefficients
Collections of state-selective dielectronic recombination coefficients of Maxwellian free electrons resolved by initial and final metastable and captured n-shell.

ADF 38 — Photoexcitation-autoionisation rate coefficients
Fundamental data for inner shell excitation followed by autoionisation

ADF 39 — Photoionisation cross-sections
Fundamental data for direct (including and especially inner shell) photoionisation.

ADF 48 — Radiative recombination rate coefficients
Partial final-state resolved radiative recombination rate coefficients from both ground and metastable levels.

DERIVED CLASSES

ADF 11 — Iso-nuclear master files
Effective (collisional–radiative) coefficients which are required to establish the ionisation state of a dynamic or steady-state plasma.

ADF 12 — Charge exchange effective emission coefficients
Collections of effective emission coefficients for spectrum lines emitted by ions of elements following charge transfer from neutral beam donor atoms.

ADF 13 — Ionisation per photon coefficients
Data collections useful in analysis of a spectrum line from an ionisation stage of an element, which is inflowing into a plasma from a surface.

ADF 15 — Photon emissivity coefficients
Fully density dependent and metstable resolveed effective emissitivy coeffeicients from a collisional–radiative model.

ADF 21 — Effective beam stopping/excitation coefficients
They are effective ionisation coefficients, including charge transfer losses, which leave the beam atoms ionised.

ADF 22 — Effective beam emission/population coefficients
Coefficients for the emission from a beam when it enters an ionised plasma including impurities. Results are fully density dependent output from a collisional–radiative model.

- Fundamental data
- Derived data for modelling and diagnostics

Tungsten DR Project

Aim is to generate nl-resolved (and total) DR rates for all ionisation stages of tungsten using AUTOSTRUCTURE

PHYSICAL REVIEW A **93**, 042703 (2016)

Partial and total dielectronic recombination rate coefficients for W^{73+} to W^{56+}

S. P. Preval,* N. R. Badnell, and M. G. O'Mullane
Department of Physics, University of Strathclyde, Glasgow G4 0NG, United Kingdom
(Received 20 December 2015; published 7 April 2016)

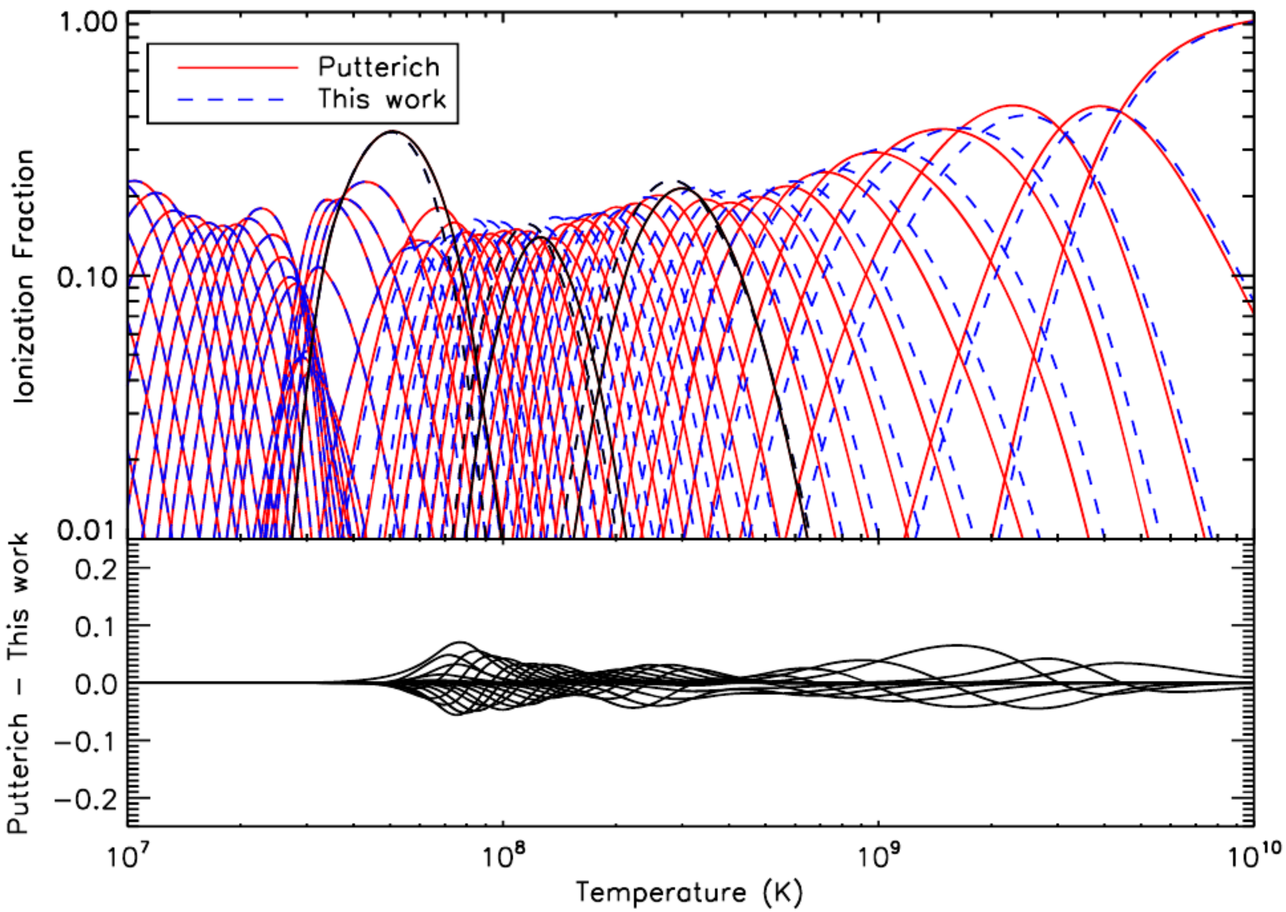
IOP Publishing Journal of Physics B: Atomic, Molecular and Optical Physics
J. Phys. B: At. Mol. Opt. Phys. **50** (2017) 105201 (17pp) https://doi.org/10.1088/1361-6455/aa6a3c

Partial and total dielectronic recombination rate coefficients for W^{55+} to W^{38+}

S P Preval, N R Badnell and M G O'Mullane

Department of Physics, University of Strathclyde, Glasgow G4 0NG, United Kingdom

Tungsten DR Project



- The next row is complete and being readied for submission.
- Data for Xe and Sn has been produced and will also be archived in ADAS and OPEN-ADAS

Optimizing the radiated power

- At the 23rd DCN we outlined a method to develop rule-based methods to optimize the total radiated power.
- Complementary to the one-method, self-consistent, approach.

IOP Publishing   Plasma Physics and Controlled Fusion

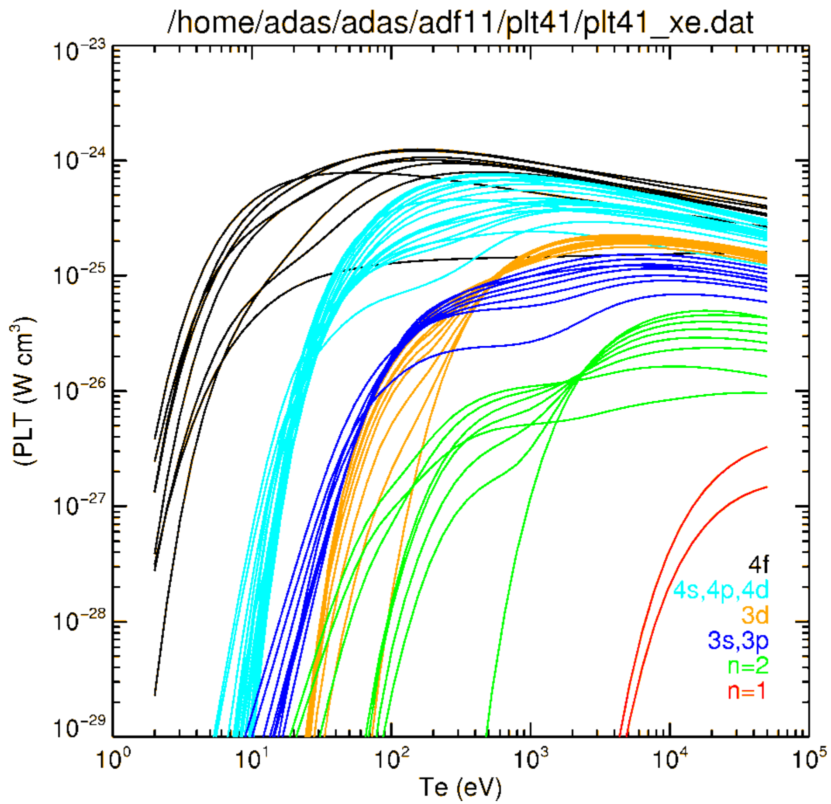
Plasma Phys. Control. Fusion **59** (2017) 055010 (8pp)   https://doi.org/10.1088/1361-6587/aa6273

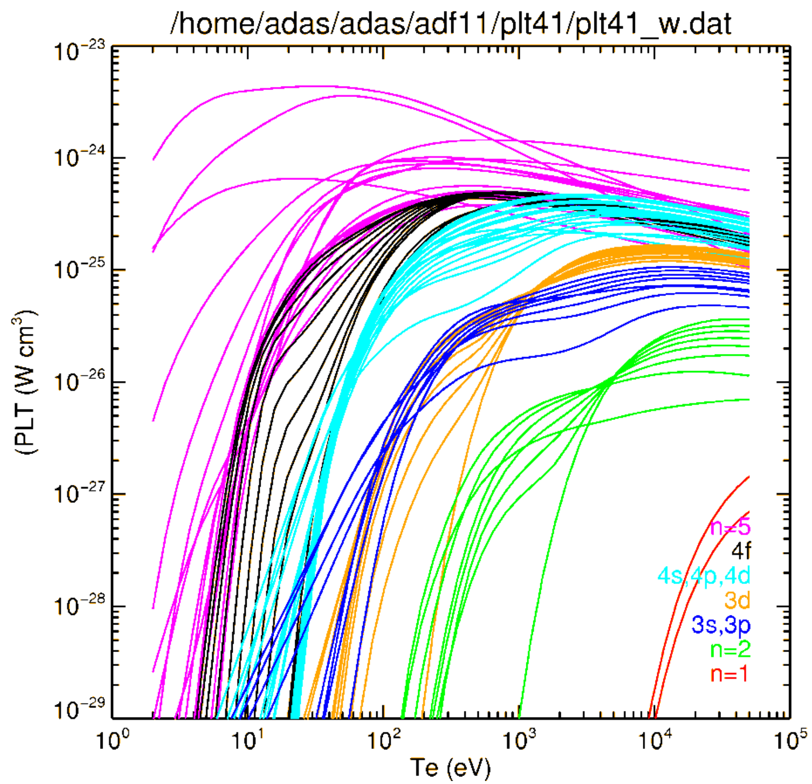
Optimisation and assessment of theoretical impurity line power coefficients relevant to ITER and DEMO

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]

Optimizing the radiated power

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

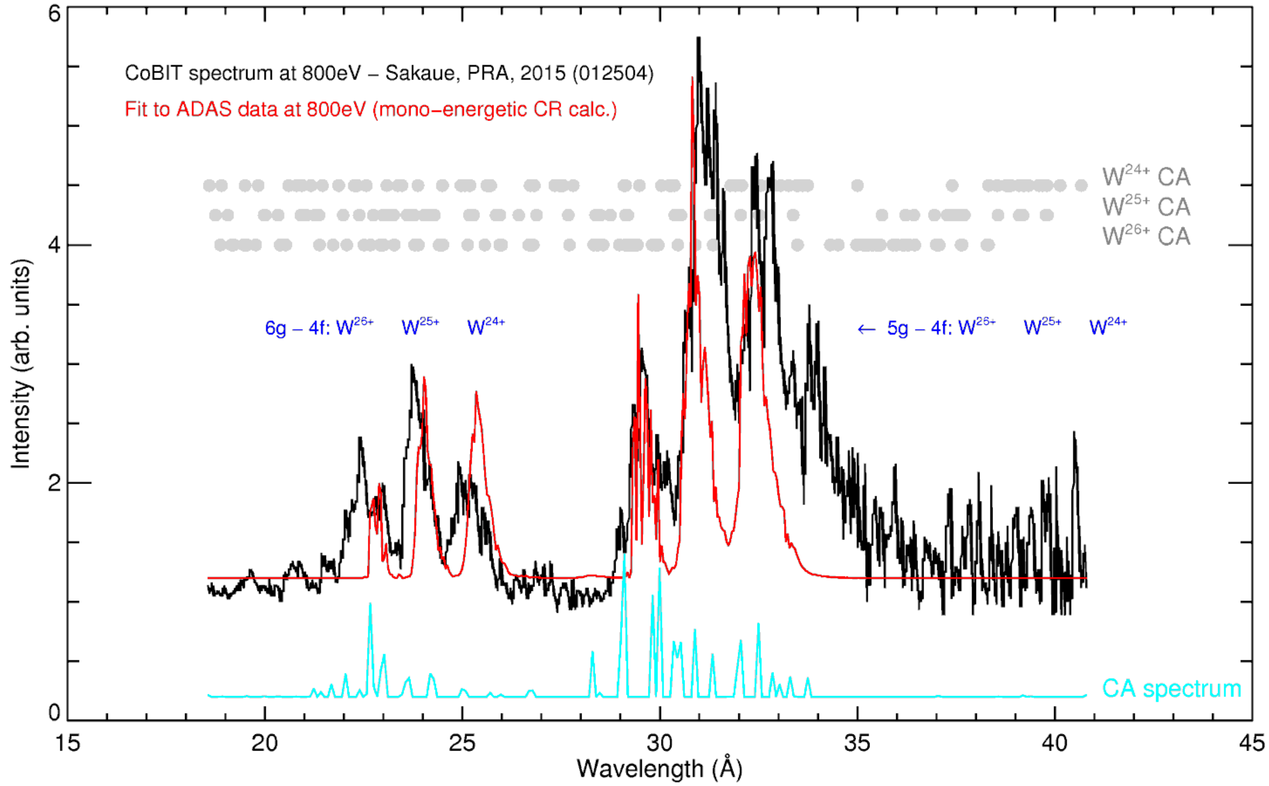




It's one (important) part of the story – but we need DR and neutral (I-IV) before we can endorse a complete solution suitable for modelling tungsten

Optimizing the radiated power

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

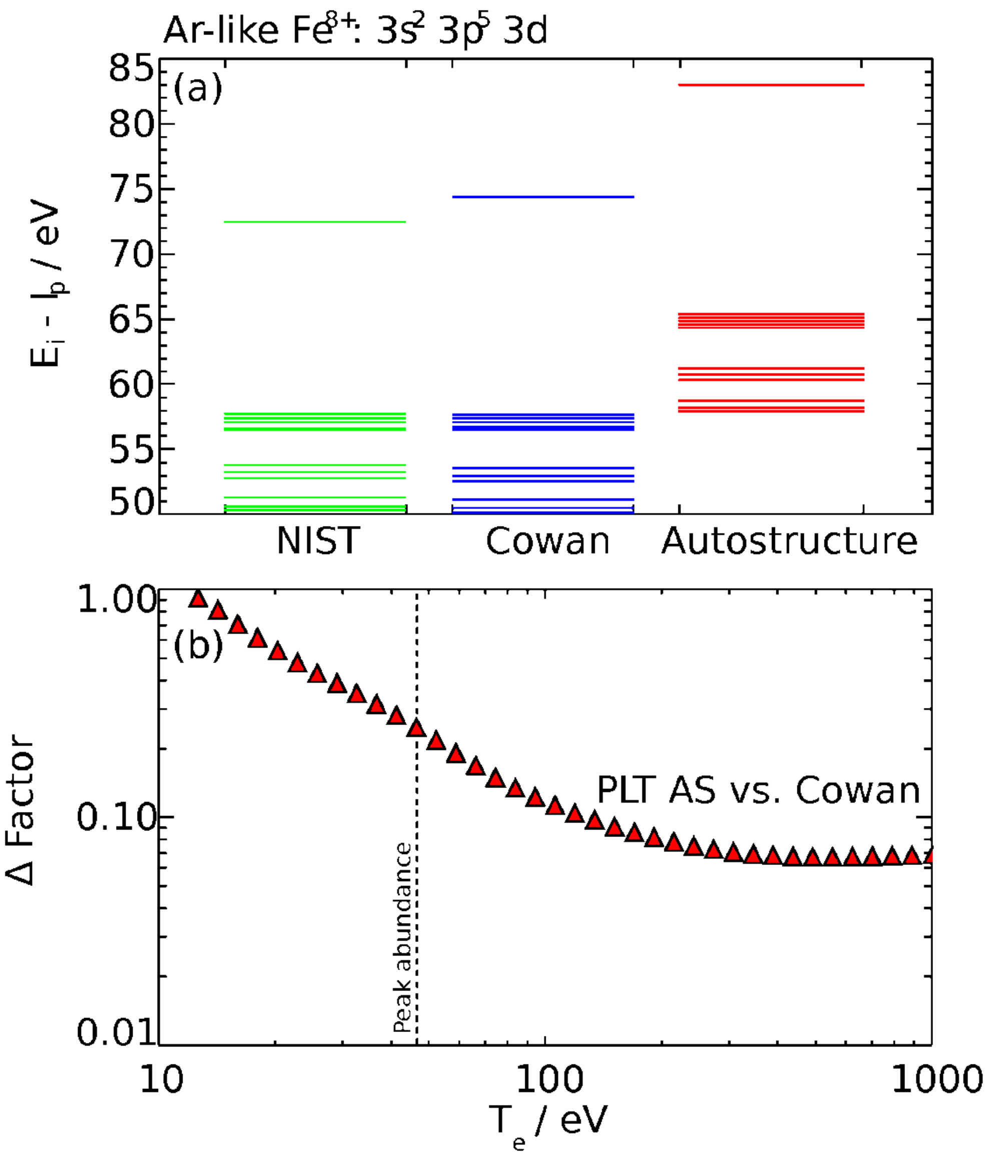


- Mono-energetic ADAS population model, producing a spectral feature, fitted to an EBIT spectrum with ADAS feature-fitting LSQ code.
- Goal is to apply (shifted) features to tungsten emission from tokamaks.

Optimizing atomic structure

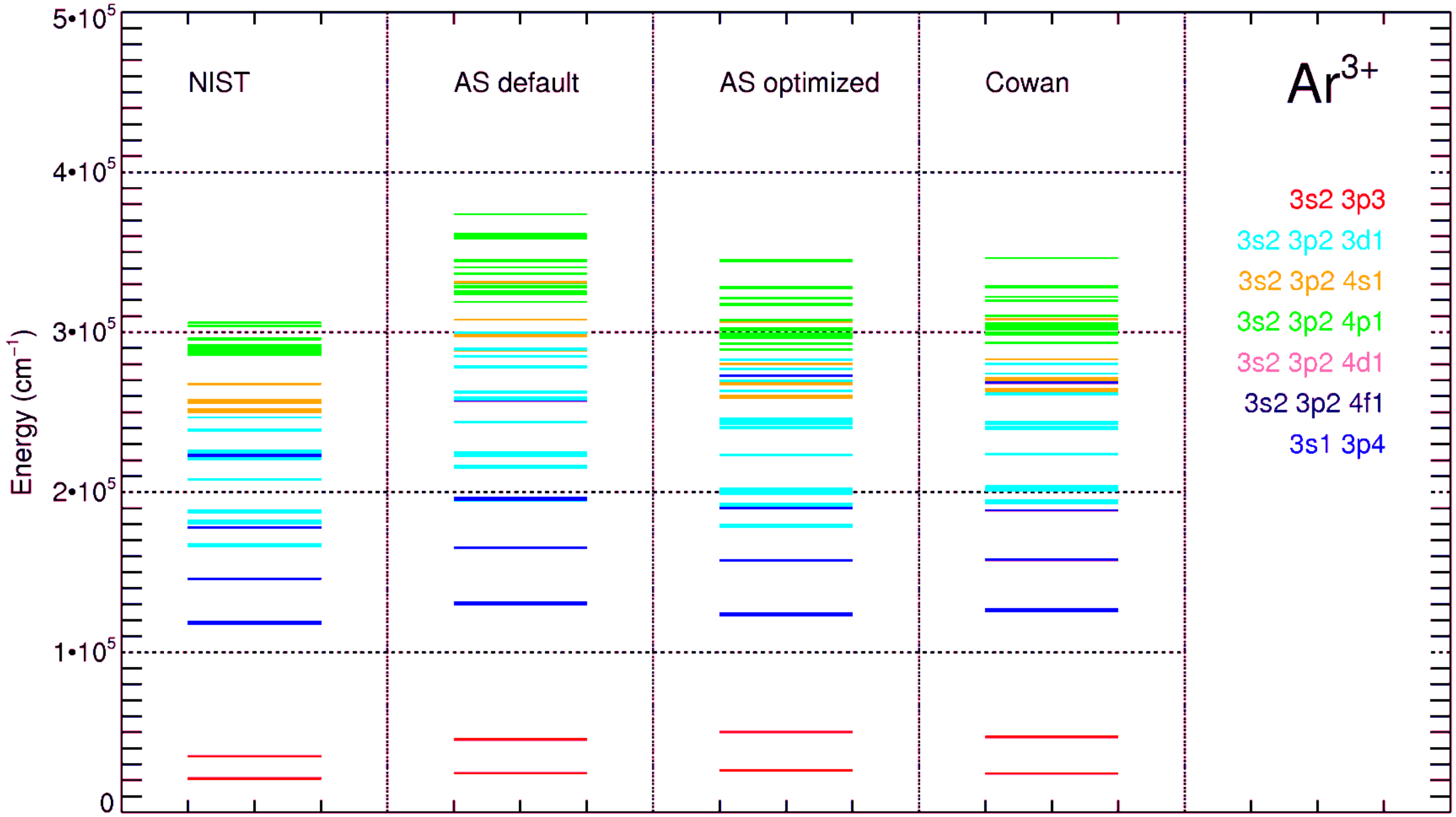
- Wish to move to AUTOSTRUCTURE distorted-wave as a new baseline quality.
- Also can drive R-matrix.
- Good atomic structure is essential for high quality derived data.
- And is the basis for uncertainty estimation.

- Default results could be better.



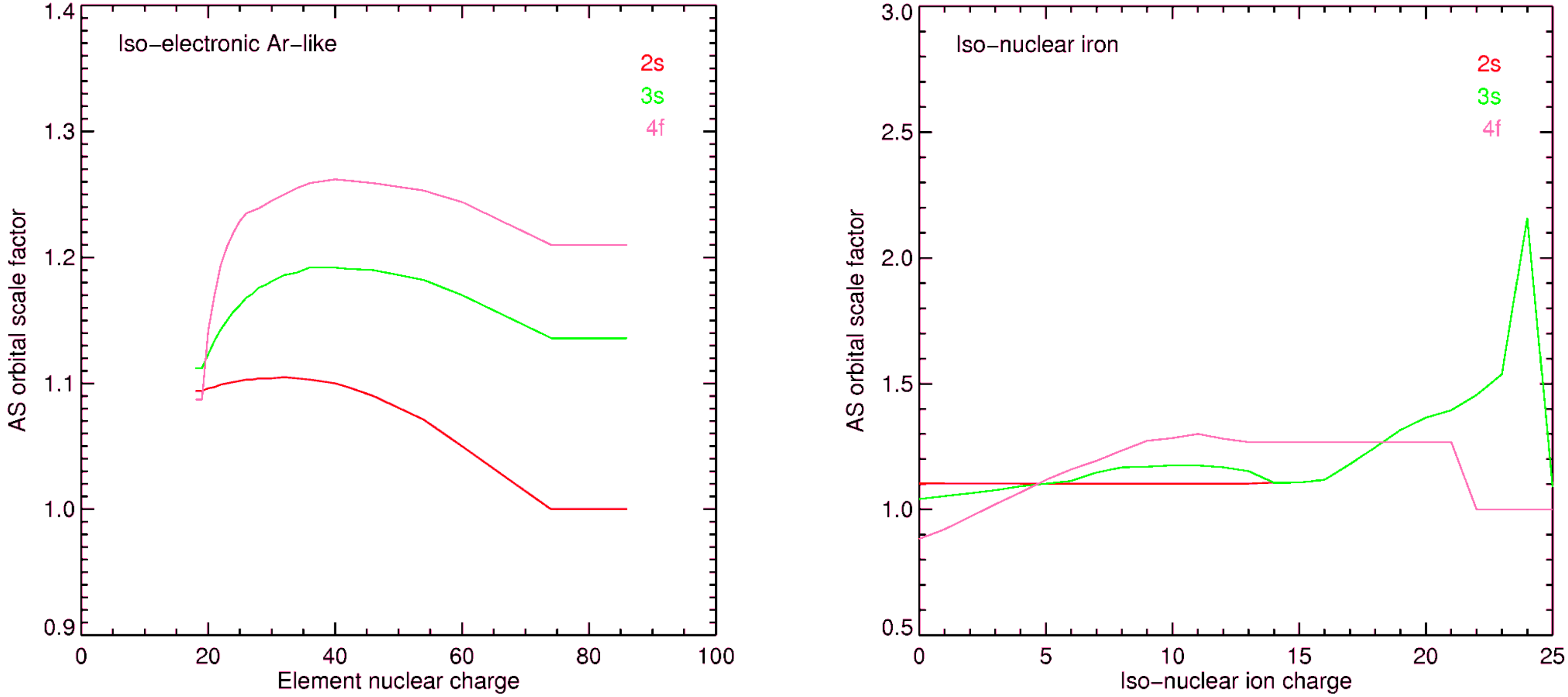
Optimizing structure across iso-electronic and iso-nuclear sequences

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



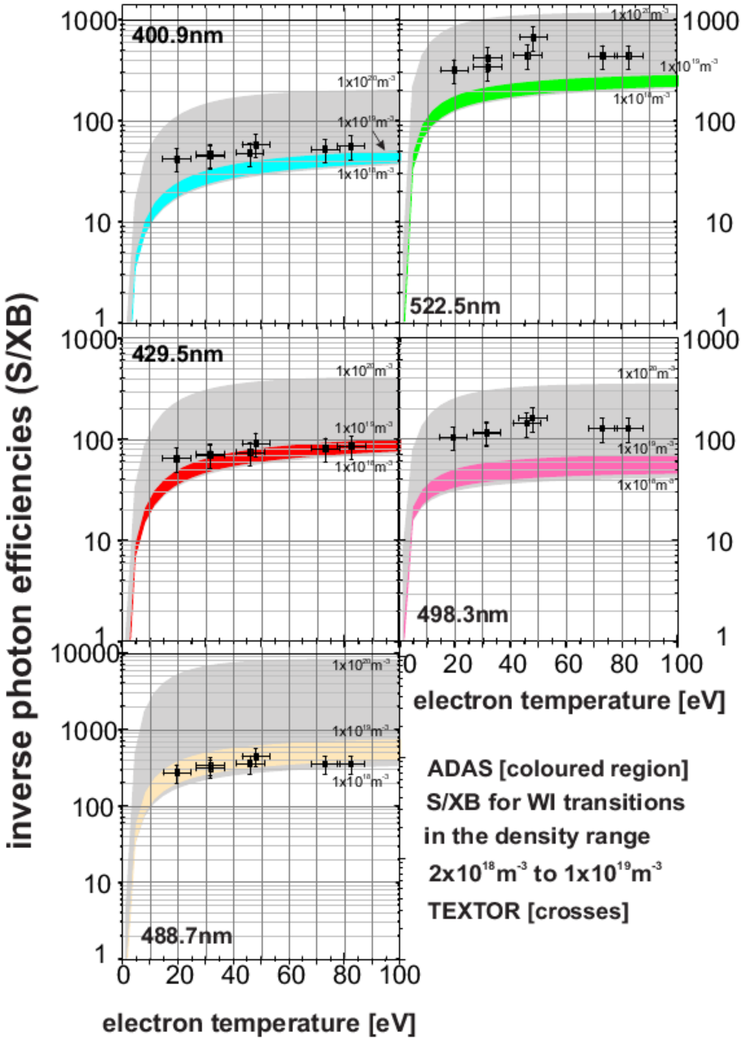
Optimizing structure across iso-electronic and iso-nuclear sequences

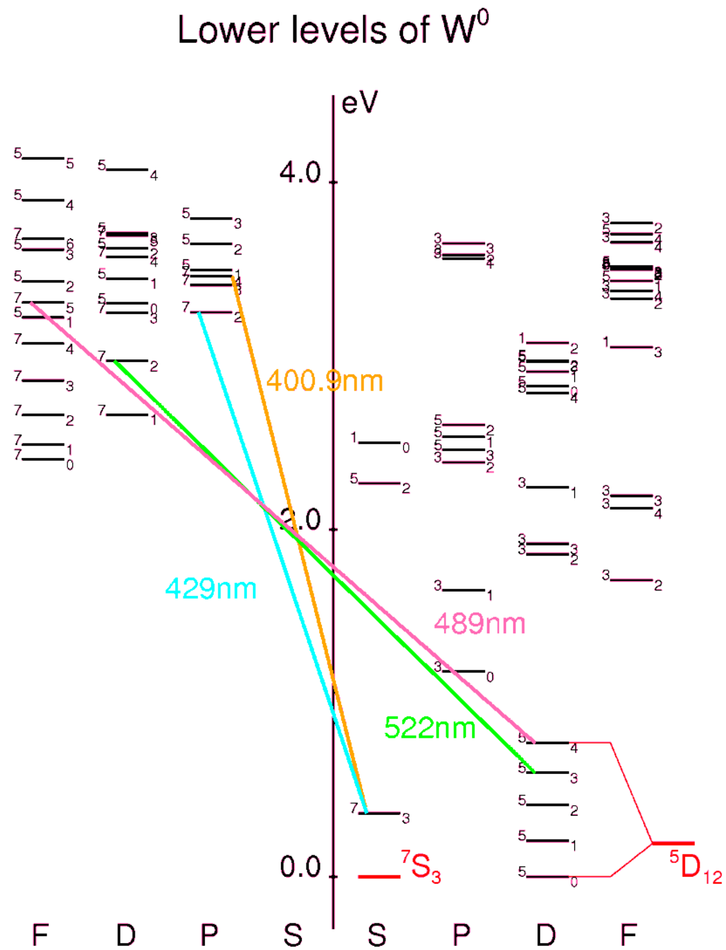
- Start with configurations identified in power optimization.
- Include equivalent electron complex.
- Use AS minimization selectively locking orbitals as we move along sequences
- Construct a smooth surface of scaling parameters.



Ionizations per photon

- Influx studies of tungsten (and Cr and Mo) for first wall.





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Ionizations per photon

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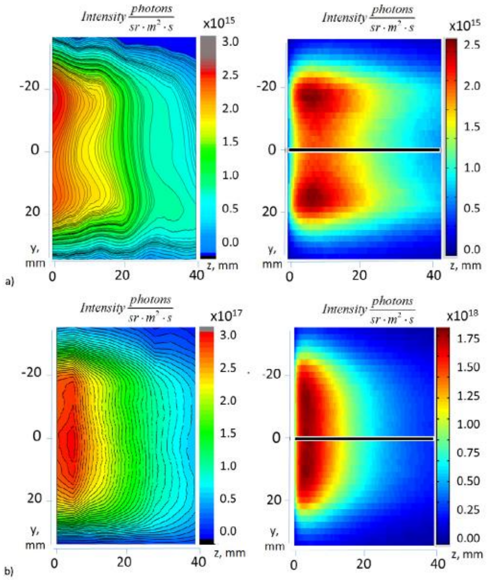


Fig. 9. 2D emission intensity patterns (λ = 4009 A) obtained in the Ar experiment with the spectrometer (left) and calculated with ERO (right). Black line – direction of axial intensity profiles extraction. a) "Low" discharge power case, U_b = 150 V, experiment 3 (see Table 1); b) "High" discharge power case, U_b = 150 V, experiment 2 (see Table 1).

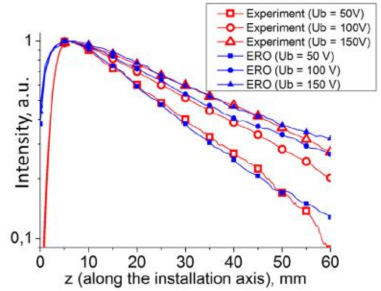
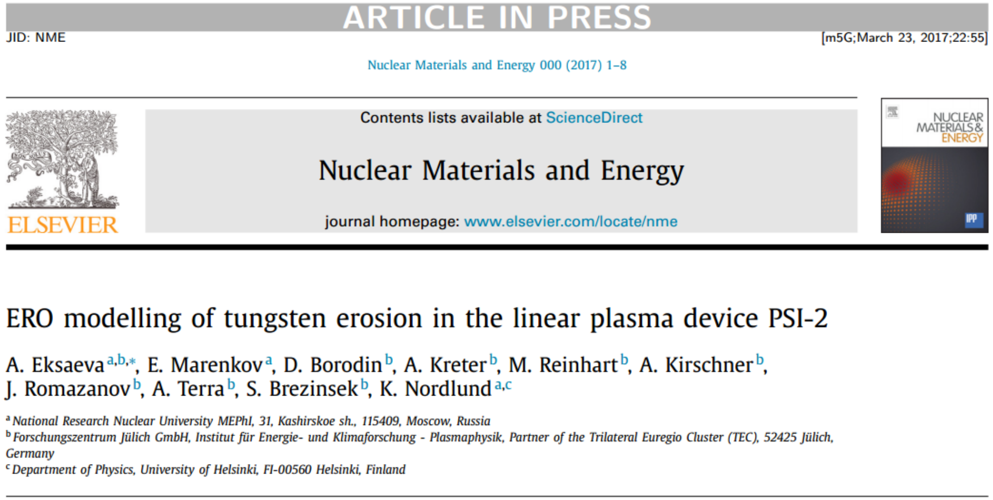


Fig. 10. Axial WI (λ = 400.9 nm) intensity profiles (normalized) – Ar experiment and ERO simulations. "Low" discharge power, U_b = 50–150 V, experiment 1 (see Table 1).



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Nuclear Materials and Energy 000 (2017) 1–8

Contents lists available at ScienceDirect

Nuclear Materials and Energy

journal homepage: www.elsevier.com/locate/nme

ERO modelling of tungsten erosion in the linear plasma device PSI-2

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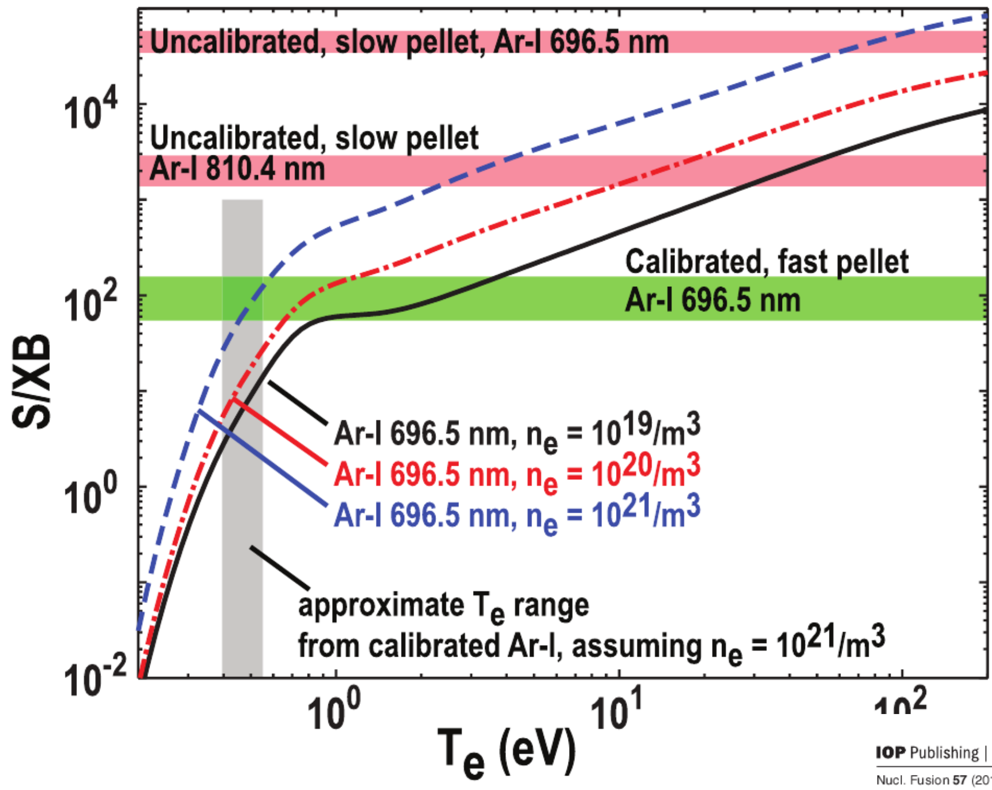
[c] Department of Physics, University of Helsinki, FI-00560 Helsinki, Finland

Ionizations per photon

- Argon for disruption and runaway electron mitigation.



IOP Publishing | International Atomic Energy Agency

Nuclear Fusion

Nucl. Fusion **57** (2017) 016008 (10pp)

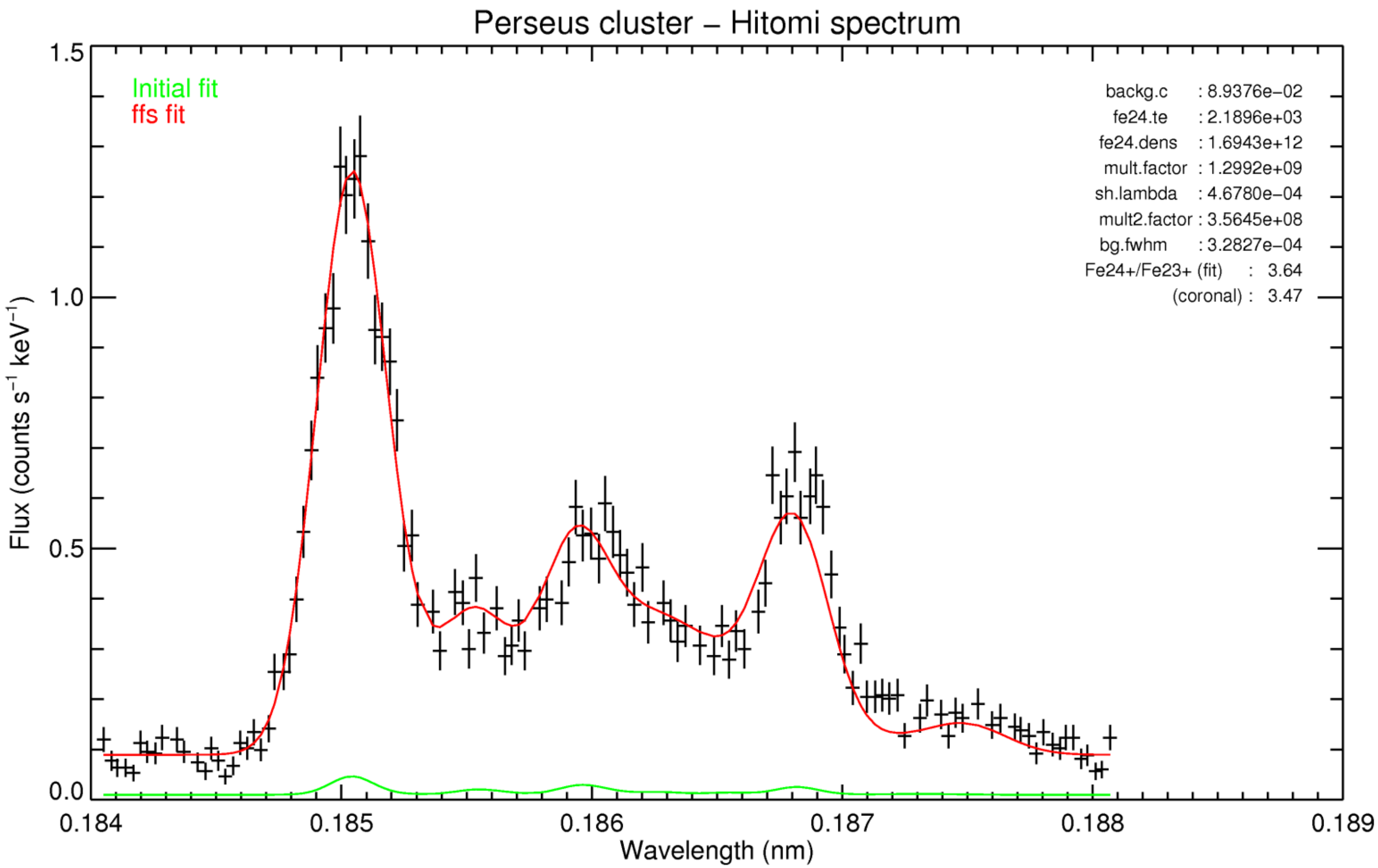
doi:10.1088/0029-5515/57/1/016008

Use of Ar pellet ablation rate to estimate initial runaway electron seed population in DIII-D rapid shutdown experiments

E.M. Hollmann[1], N. Commaux[2], R.A. Moyer[1], P.B. Parks[3], M.E. Austin[4], I. Bykov[1], C. Cooper[3], N.W. Eidietis[3], M. O'Mullane[5], C. Paz-Soldan[3], D.L. Rudakov[1] and D. Shiraki[2]

Other ADAS models

- He-like satellite spectrum
- R-matrix He-like structure, AS for satellite lines
- ADAS population model and feature fitting routine.



Other ADAS models

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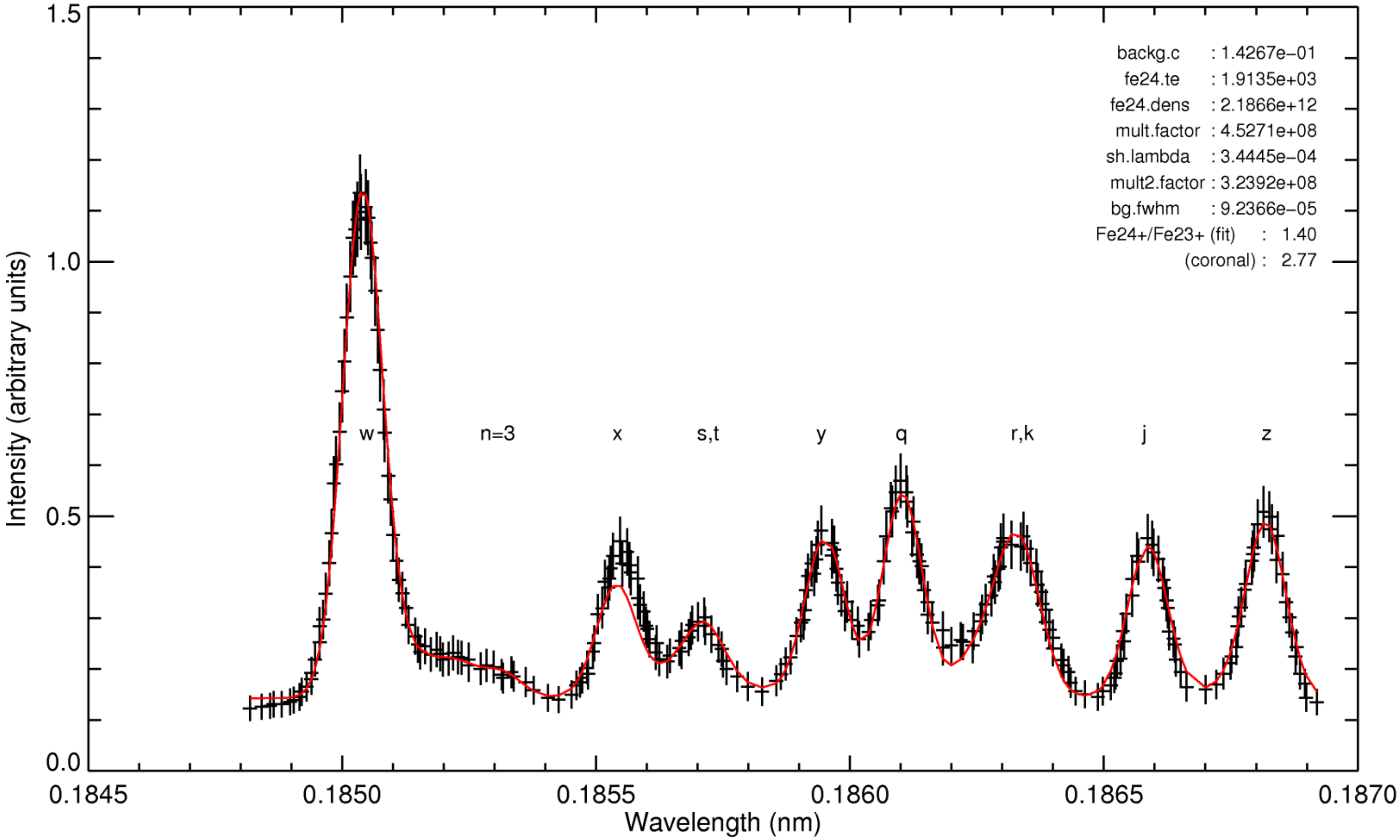
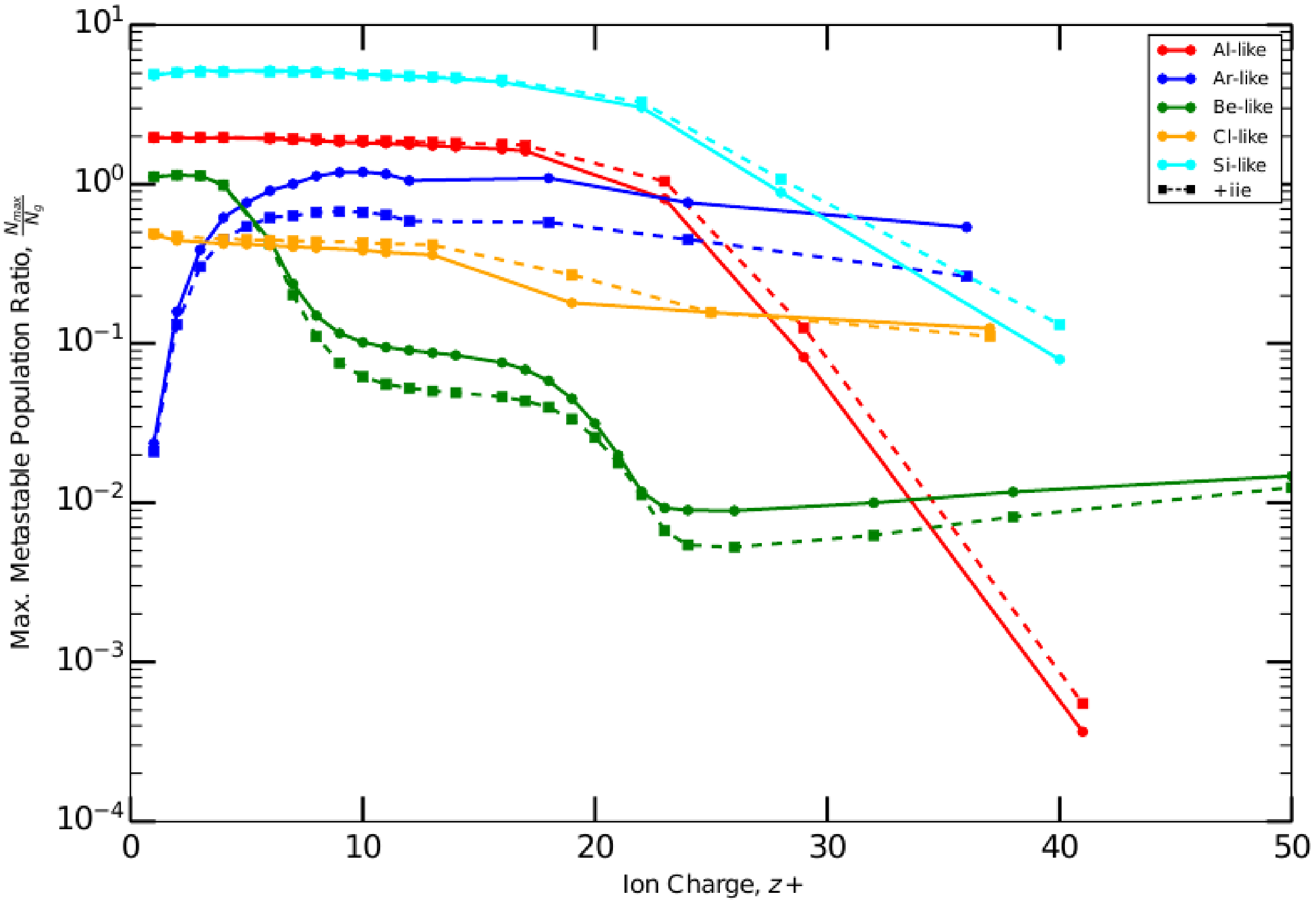


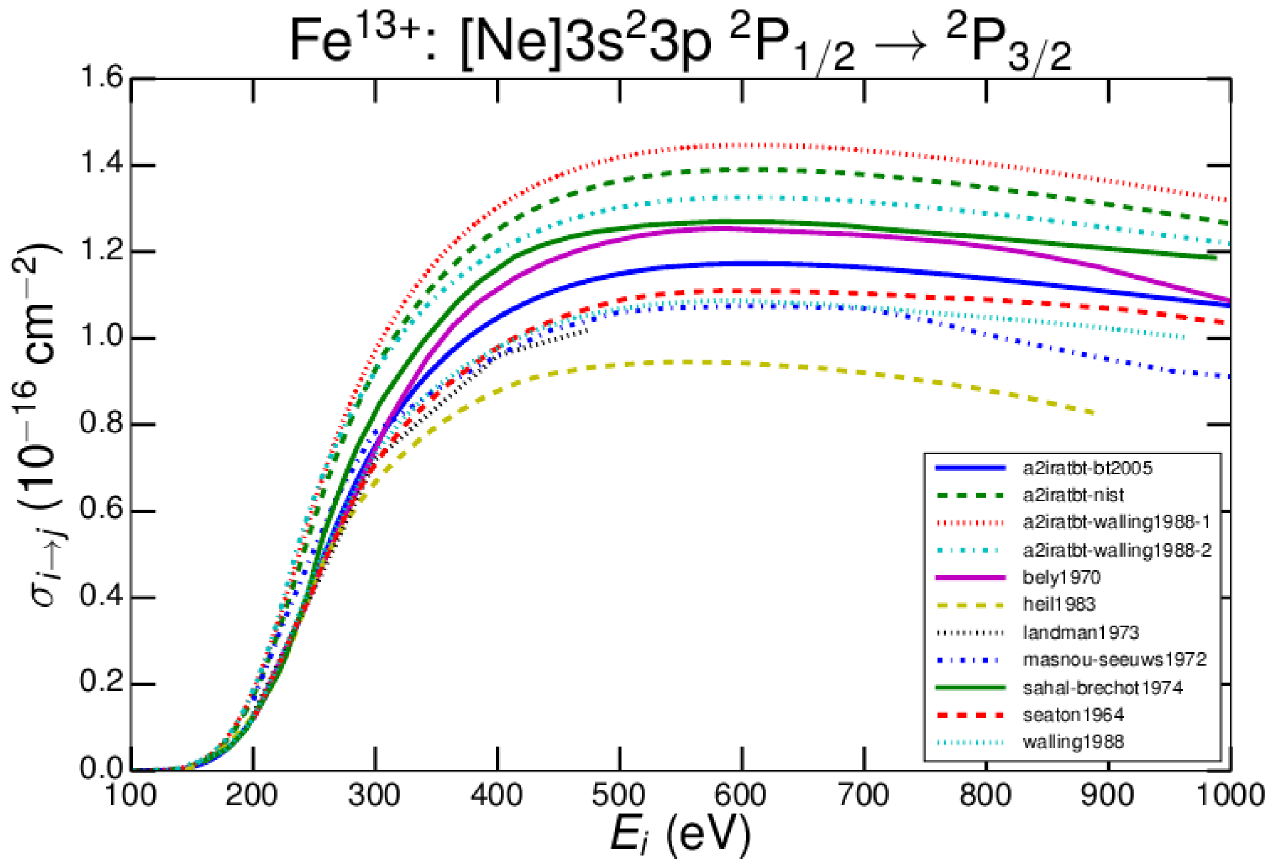
New ion impact data

- Needed for intermediate coupling ionization balance.
- Mixed collidors required for tokamak plasmas.
- New ADAS data format designed to store data.



New ion impact data

- Relatively simple impact parameter method chosen for baseline production and providing an extensive set of data.
- More sophisticated techniques can be used but including the ion impact process is the primary concern.



New ion impact data

- New ADAS code and body of data for proton, He+, Li2+…Ne9+ collidors

```
LI+ 0         3         1     43489.0(1S)   516797.0(3S)
    1 1S2 2S1             (2)0( 0.5)          0.0000    {1}1.000    {2}1.500
    2 1S2 2P1             (2)1( 2.5)      14903.9000    {1}1.000
    3 1S2 3S1             (2)0( 0.5)      27206.1000    {1}1.000
    4 1S2 3P1             (2)1( 2.5)      30925.4000    {1}1.000
    5 1S2 3D1             (2)2( 4.5)      31283.1000    {1}1.000
    6 1S2 4S1             (2)0( 0.5)      35012.1000    {1}1.000
    7 1S2 4P1             (2)1( 2.5)      36469.6000    {1}1.000
    8 1S2 4D1             (2)2( 4.5)      36623.4000    {1}1.000
    9 1S2 4F1             (2)3( 6.5)      36630.2000    {1}1.000
   -1
  1.0     1        1.00+00 1.11+00 1.23+00 1.37+00 1.52+00 1.69+00 1.87+00 2.08+00 2.31+00 2.57+00 2.85+00 3.16+00 3.51+00 3.90+00 4.33+00
/mt  =    6.9410 /zp =    1.00 /mp =    1.0073 /   1^H  impact /
   2    1 0.00+00 6.64+00 8.04+00 9.64+00 1.15+01 1.35+01 1.58+01 1.84+01 2.13+01 2.45+01 2.81+01 3.20+01 3.63+01 4.10+01 4.62+01 5.18+01
   3    1 0.00+00 7.03-01 7.53-01 7.78-01 7.74-01 7.38-01 6.71-01 5.77-01 4.65-01 3.49-01 2.42-01 1.61-01 1.21-01 1.34-01 2.09-01 3.50-01
   4    1 0.00+00 6.61-01 7.27-01 8.12-01 9.31-01 1.10+00 1.32+00 1.59+00 1.90+00 2.23+00 2.55+00 2.83+00 3.07+00 3.26+00 3.39+00 3.48+00
   5    1 0.00+00 3.55-01 4.04-01 5.00-01 6.51-01 8.59-01 1.13+00 1.46+00 1.87+00 2.34+00 2.88+00 3.49+00 4.15+00 4.84+00 5.54+00 6.24+00
                                                                              .....
                                                                              .....
                                                                              .....
   9    5 0.00+00 5.51+00 6.81+00 8.41+00 1.04+01 1.28+01 1.57+01 1.91+01 2.30+01 2.75+01 3.27+01 3.87+01 4.59+01 5.47+01 6.58+01 8.01+01
   7    6 0.00+00 2.82+02 3.11+02 3.43+02 3.79+02 4.17+02 4.60+02 5.08+02 5.60+02 6.17+02 6.80+02 7.50+02 8.27+02 9.12+02 1.01+03 1.11+03
   8    6 0.00+00 1.14+02 1.21+02 1.29+02 1.37+02 1.46+02 1.56+02 1.65+02 1.76+02 1.87+02 1.99+02 2.12+02 2.25+02 2.40+02 2.55+02 2.71+02
   9    6 0.00+00 1.29+02 1.37+02 1.47+02 1.57+02 1.68+02 1.80+02 1.92+02 2.05+02 2.19+02 2.35+02 2.51+02 2.68+02 2.87+02 3.06+02 3.28+02
   8    7 0.00+00 3.24+03 3.36+03 3.48+03 3.60+03 3.73+03 3.86+03 4.00+03 4.14+03 4.28+03 4.43+03 4.59+03 4.75+03 4.92+03 5.10+03 5.28+03
   9    7 0.00+00 1.77+03 1.79+03 1.80+03 1.81+03 1.83+03 1.84+03 1.86+03 1.87+03 1.89+03 1.90+03 1.92+03 1.93+03 1.95+03 1.96+03 1.98+03
   9    8 0.00+00 1.89+04 1.92+04 1.95+04 1.98+04 2.01+04 2.04+04 2.08+04 2.11+04 2.14+04 2.18+04 2.21+04 2.25+04 2.28+04 2.32+04 2.36+04
S  1   +1          3.35+01 3.56+01 3.72+01 3.84+01 3.92+01 3.97+01 4.00+01 4.02+01 4.03+01 4.03+01 4.04+01 4.05+01 4.06+01 4.07+01 4.09+01
S  2   +1          1.17+02 1.25+02 1.32+02 1.39+02 1.46+02 1.52+02 1.58+02 1.64+02 1.70+02 1.75+02 1.80+02 1.85+02 1.90+02 1.94+02 1.98+02
S  3   +1          1.09+02 1.13+02 1.17+02 1.20+02 1.22+02 1.24+02 1.24+02 1.24+02 1.23+02 1.22+02 1.21+02 1.20+02 1.19+02 1.19+02 1.20+02
S  4   +1          2.13+02 2.31+02 2.49+02 2.67+02 2.85+02 3.03+02 3.21+02 3.39+02 3.56+02 3.72+02 3.88+02 4.03+02 4.18+02 4.31+02 4.44+02
S  5   +1          3.39+02 3.70+02 4.02+02 4.35+02 4.69+02 5.03+02 5.37+02 5.71+02 6.04+02 6.37+02 6.68+02 6.99+02 7.28+02 7.56+02 7.83+02
S  6   +1          1.70+02 1.79+02 1.86+02 1.94+02 2.01+02 2.08+02 2.14+02 2.20+02 2.26+02 2.31+02 2.36+02 2.40+02 2.44+02 2.48+02 2.52+02
S  7   +1          3.86+02 4.15+02 4.46+02 4.77+02 5.08+02 5.39+02 5.70+02 5.99+02 6.28+02 6.55+02 6.82+02 7.07+02 7.31+02 7.53+02 7.74+02
S  8   +1          6.12+02 6.64+02 7.21+02 7.81+02 8.41+02 9.02+02 9.64+02 1.02+03 1.08+03 1.14+03 1.20+03 1.26+03 1.31+03 1.36+03 1.41+03
S  9   +1          8.38+02 9.10+02 9.88+02 1.07+03 1.15+03 1.24+03 1.32+03 1.40+03 1.49+03 1.57+03 1.64+03 1.72+03 1.79+03 1.86+03 1.93+03
  -1
  -1   -1
```

Data description and comparison activities

- Describing the data, its history and provenance, and recommendations is not a one-line activity.
- How to capture all the nuances? Example from a wiki at JET.

What ADAS year should I use?

The ADAS year for each species can be set in the SANCO extra namelist settings.

- For low Z (up to Neon), ADAS 96 is available and is the best quality data (most sophisticated method)
- For higher Z, ADAS 89 is available as a low quality baseline dataset for all species.
- For W, ADAS50 is an improved quality dataset based on the work of T. Puetterich (see below)
- For Ni, See below.

Tungsten ADAS50

On 04/10/16 14:08, Martin O'Mullane wrote:

The year '50' data for tungsten in central ADAS is that produced by Thomas Puetterich (PPCF 50 (2008), 085016) with adjustments to the recombination rates for W21+ -> W55+. At JET see,

```
/home/adas/adas/adf11/acd50/acd50_w.dat : recombination
/home/adas/adas/adf11/plt50/plt50_w.dat : ionisation
/home/adas/adas/adf11/prb50/prb50_w.dat : continuum power
/home/adas/adas/adf11/scd50/scd50_w.dat : line power
```

For SXR modelling with a transport code you need the PLT and PRB coefficients modified by the transmission of the diagnostic - a low energy cut-off due to the beryllium window and a high-energy decay due to the nature of the diode detector. The JET specific PLT and PRB files are stored at

```
/home/cxs/adas/adf11/plt88/plt88_w.jet_100.dat
/home/cxs/adas/adf11/plt88/plt88_w.jet_250.dat
/home/cxs/adas/adf11/plt88/plt88_w.jet_350.dat
```

and

```
/home/cxs/adas/adf11/prb88/prb88_w.jet_100.dat
/home/cxs/adas/adf11/prb88/prb88_w.jet_250.dat
/home/cxs/adas/adf11/prb88/prb88_w.jet_350.dat
```

for the three different Be window thickness in current and previous use (100 = 100microns). They are not in central ADAS since they are specific to JET's instruments and are not universal.

The acd and scd data for ionisation balance can be combined with the SXR filtered power coefficients. Note that these PLT and PRB make a different choice of contributing configurations than those in Thomas's year '50' PLT and PRB files. For self-consistency between total and SXR power the above directories also have plt88_w.dat and prb88_w.dat files.

The cooling curve can be constructed from acd/scd/plt/prb coefficients. Normally this curve is in equilibrium balance or infinite confinement. It is possible to mimic diffusive transport via a confinement time (add a Ne*tau loss term to the ionisation balance calculation) and, as Thomas said, transport in a tokamak is 'low' so such an approach allows one to bypass the transport calculation. We have supplied such cooling curves to Michael Kovari and Hanni Lux for use in the PROCESS code.

Turning to caveats. There is still much atomic physics work to be done.

(1) The biggest unknowns are the dielectronic recombination rates. Thomas's year 50 recombination data adjusted these to fit the Asdex Upgrade measurements. There is a lot of work underway to make better calculations but we need a full iso-nuclear set for transport studies. Simon Preval, a post-doc at Strathclyde is working on this. The first paper covered W73+ to W56+ (PRA, 93, 042703 (2016)). The second paper covering W55+ to W38+ was submitted last week so this data is nearly ready for inclusion in ADAS. There was also another review paper on DR comparisons submitted yesterday - the result of an IAEA TM which draws heavily on our new DR data. There are results from W5+, 6+, 18+, 19+, 20+, 27+, 28+, 29+, 35+, 37+ and other overlapping with our second W DR paper. We are authors on this IAEA paper.

Data description and comparison activities

- Astrophysics activity based on NLTE comparison workshops.
- Strong overlap with magnetic confined fusion
- Density effects are becoming important in astro modelling.

- Suite of data/model compilations agreed.
- Will be collated by Randall Smith and Adam Foster at CFA.

Data description and comparison activities

```
Z    4.0   4.1   4.2   4.3   4.4   4.5   4.6   4.7   4.8   4.9   5.0   5.1   5.2   5.3   5.4   5.5   5.6   5.7   5.8   5.9   6.0   6.1   6.2
#--------------------------------------------------------
# Hydrogen
#
  1      -23.36823975   -22.33324129   -21.73094828   -21.79996619   -22.07625817   -22.32447055   -22.53952849   -22.72977206   -22.89577346
#
# acd : /home/adas/adas/adf11/acd12/acd12_h.dat
# scd : /home/adas/adas/adf11/scd12/scd12_h.dat
# plt : /home/adas/adas/adf11/plt12/plt12_h.dat
# prb : /home/adas/adas/adf11/prb12/prb12_h.dat
#--------------------------------------------------------
# Helium
#
  2      -28.55229427   -26.30729954   -24.59703800   -23.17749469   -22.06352683   -21.56031451   -21.55114314   -21.53051656   -21.29775516
#
# acd : /home/adas/adas/adf11/acd96/acd96_he.dat
# scd : /home/adas/adas/adf11/scd96/scd96_he.dat
# plt : /home/adas/adas/adf11/plt96/plt96_he.dat
# prb : /home/adas/adas/adf11/prb96/prb96_he.dat
#--------------------------------------------------------
# Carbon
#
  6      -20.75174585   -20.54147638   -20.12161978   -19.74355082   -19.42187878   -19.12409571   -18.84074853   -18.57780899   -18.35624946
#
# acd : /home/adas/adas/adf11/acd96/acd96_c.dat
# scd : /home/adas/adas/adf11/scd96/scd96_c.dat
# plt : /home/adas/adas/adf11/plt96/plt96_c.dat
# prb : /home/adas/adas/adf11/prb96/prb96_c.dat
#--------------------------------------------------------
# Nitrogen
#
  7      -15.76024229   -16.48099188   -18.42080818   -19.59751996   -19.64685039   -19.46655051   -19.23416532   -18.99910205   -18.75371255
#
# acd : /home/adas/adas/adf11/acd96/acd96_n.dat
# scd : /home/adas/adas/adf11/scd96/scd96_n.dat
# plt : /home/adas/adas/adf11/plt96/plt96_n.dat
# prb : /home/adas/adas/adf11/prb96/prb96_n.dat
```

Concluding remarks

- A typical amount of data updates in ADAS and OPEN-ADAS.
- Continuing development of parameter-driven spectral features.
- Maintaining interaction with integrated tokamak modelling efforts – EUROfusion and ITER.

- Better atomic structure identified as principal need to improve the baseline ADAS data.
- Baseline should be of sufficient quality for high level modelling.
- Defined uncertainty evaluation should be part of this – but it is proving difficult to fund.
- Philosophy of moving cutting edge codes to routine production use.
- But maintain the focus of ADAS on modelling and diagnosing hot collisional plasmas.

- Modelling improvement focus will be on intermediate coupling resolved ionisation balance.
- Calculate and archive the ion collision data required for this task.
- Co-ordinate with plasma transport models to use these data.