Transformation of fundamental atomic data for use in interpreting diagnostics and plasma modelling

Martin O'Mullane

Hugh Summers, Nigel Badnell, Simon Preval, Stuart Henderson, Matthew Bluteau, Ephrem Delabie, Alessandra Giunta and many ADAS contributors

Outline

- Lithium – example of how fundamental data relates to the ‘atomic data’ used in magnetic confined fusion modelling
- ADAS – atomic models and database to store both fundamental and effective atomic data.
- Tungsten.
- Perspectives from marshalling and data provision.

Fundamental vs. derived data – ionization of Li^0

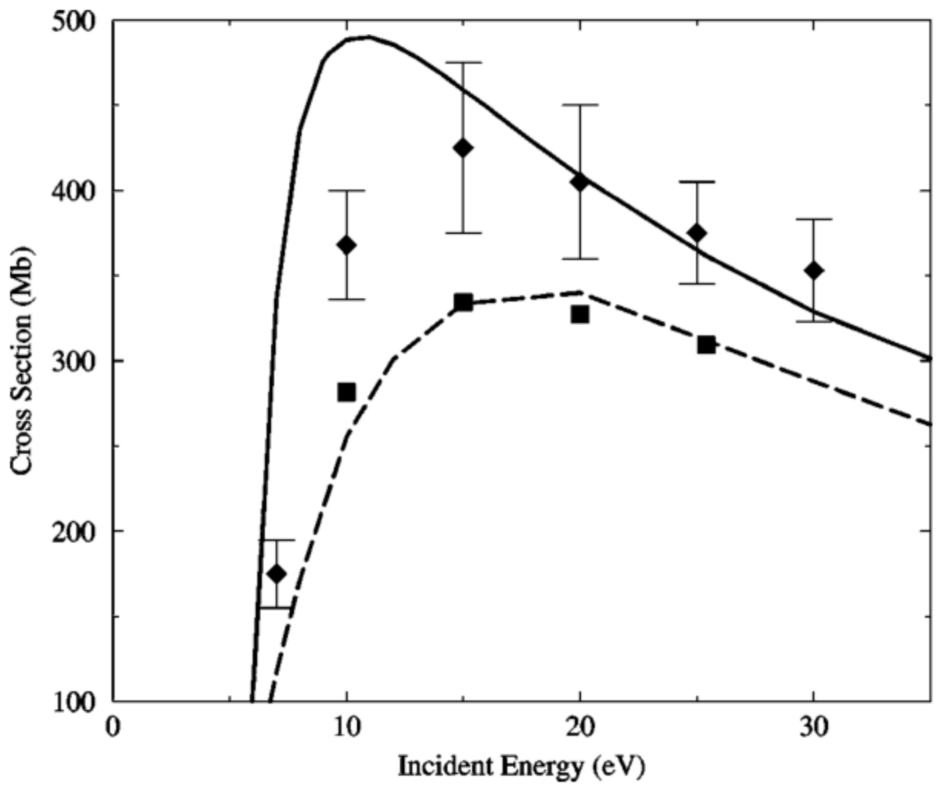
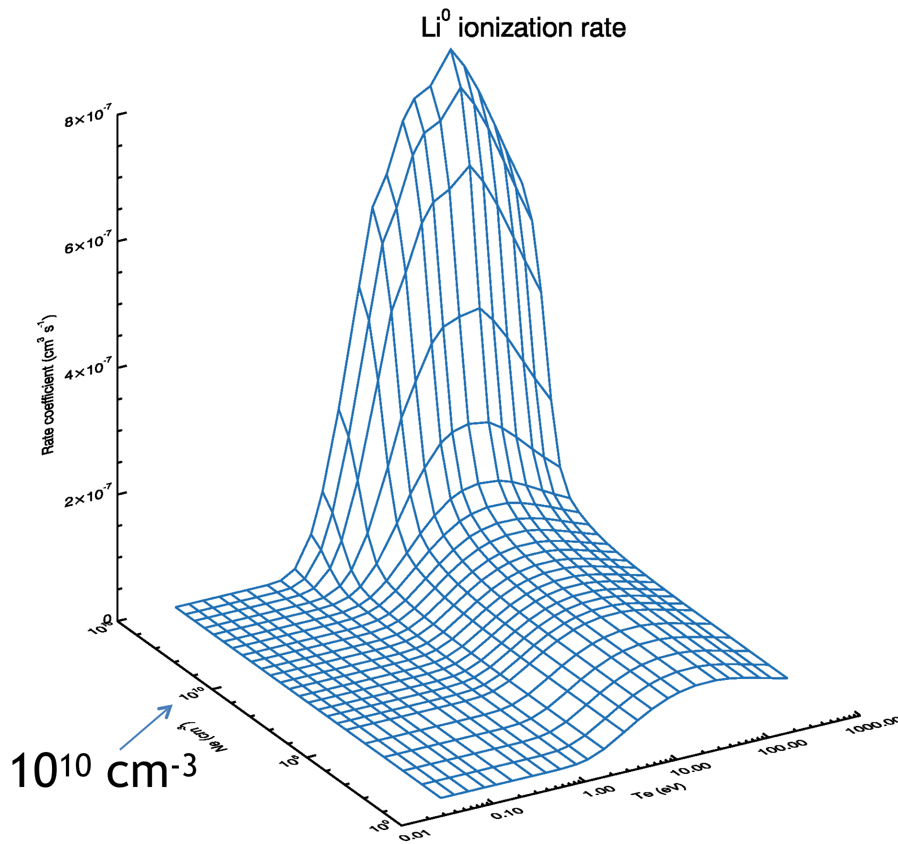


FIG. 2. Total electron-impact ionization cross section for electron scattering from lithium. Solid squares: time-dependent close-coupling method, solid line: distorted-wave method, dashed line: convergent close-coupling method [2], solid diamonds with error bars: experiment [10]. (1.0 Mb = 1.0×10^{-18} cm^2.)

J Colgan et al, Phys Rev A. **63**, 062709 (2001)



ADAS effective rate for Li^0 + e ionization.

A derived coefficient dependent on the local electron temperature and density.

The collisional-radiative model is a good description of a finite density plasma

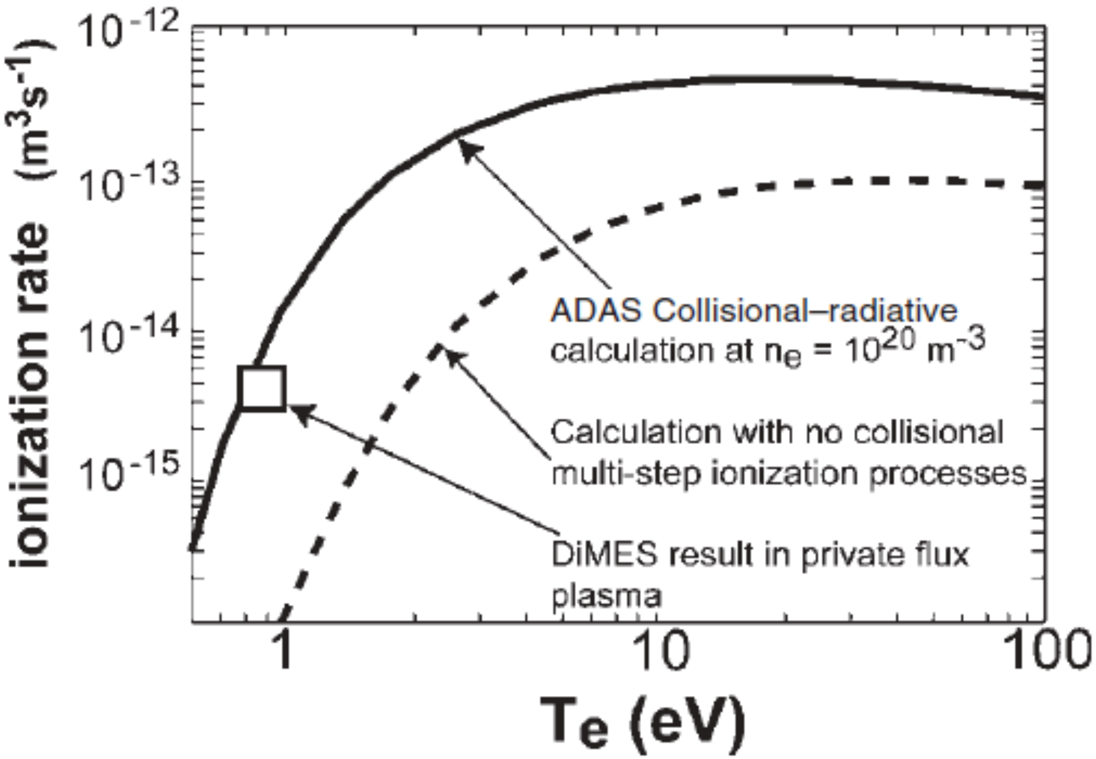
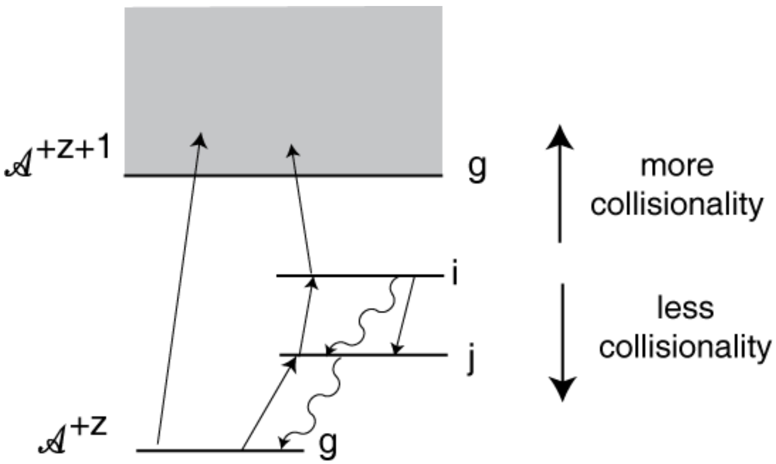


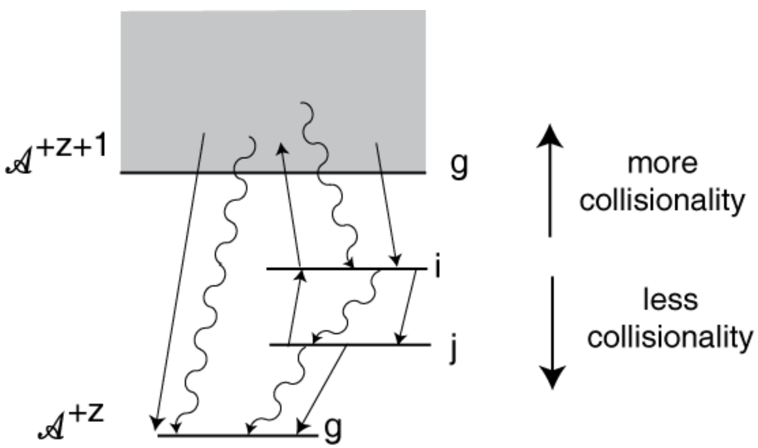
Figure 8. Ionization rate of sputtered lithium atoms as a function of electron temperature under PF plasma bombardment in H-mode plasma. Figure shows how the ADAS collisional–radiative model must be used to explain experimental data from Li–DiMES in PF plasma.

J P Allain *et al*, Nuclear Fusion, **44** (2004) p655

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.

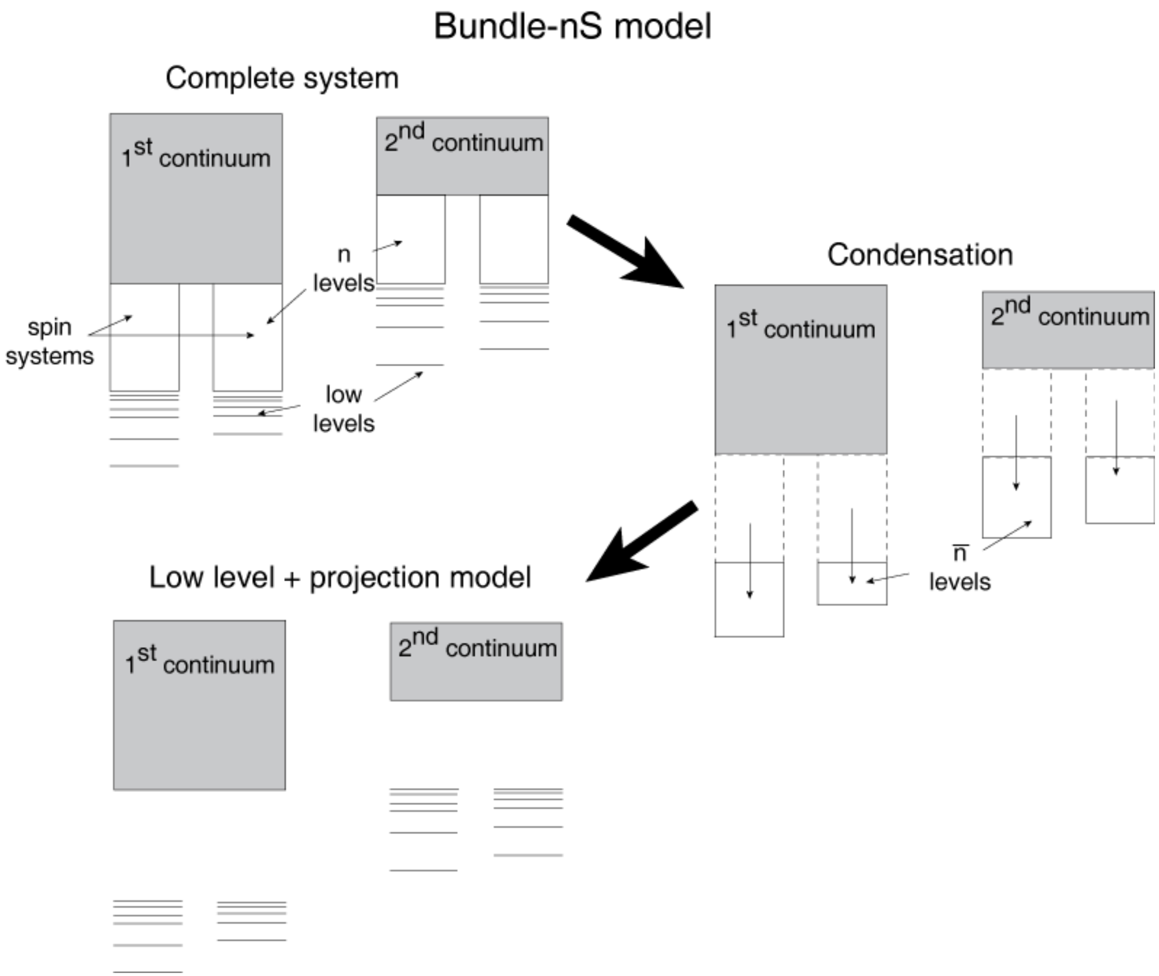
Three-body recombination must be added to the reactions which pairs with collisional ionisation from excited states

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

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.

Timescales for transport and atomic processes

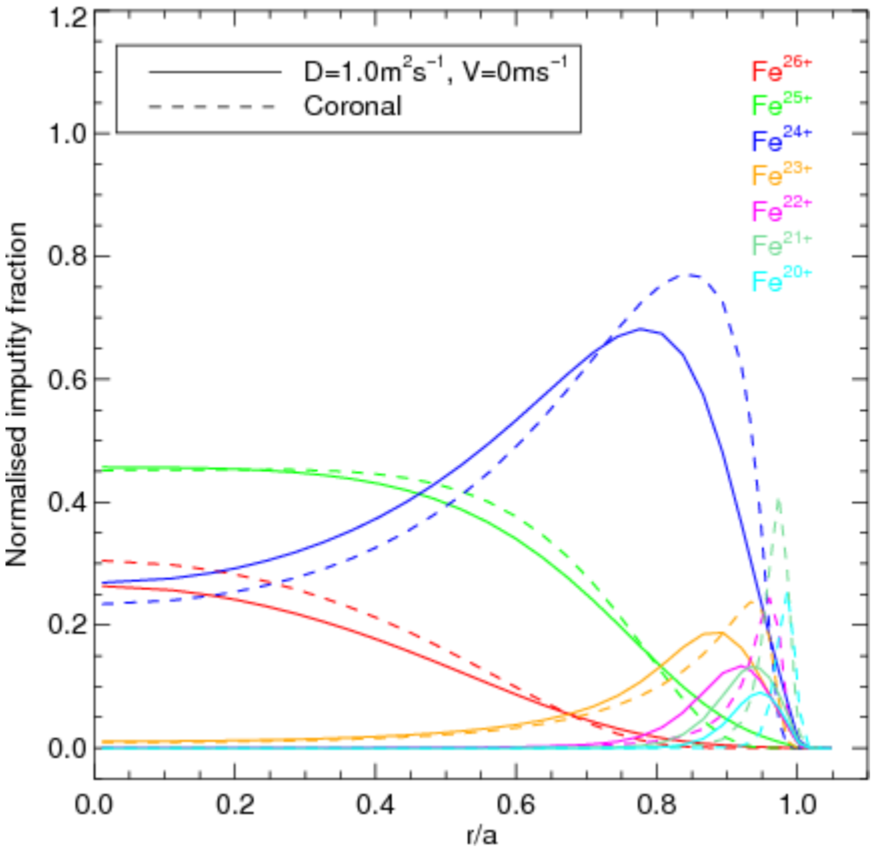
Emission	$n_e X \approx 10^{20}\ \mathrm{m^{-3}} \times 10^{-12}\ \mathrm{m^3/s} \approx 10^8/\mathrm{sec}$
Ionisation	$n_e S \approx 10^{20}\ \mathrm{m^{-3}} \times 10^{-14}\ \mathrm{m^3/s} \approx 10^6/\mathrm{sec}$
Diffusion	$D/(0.1\ a)^2 \approx 1\ \mathrm{m^2/sec}\ /\ 0.01\mathrm{m^2} \approx 100/\mathrm{sec}$
Convection	$v/(0.1\ a) \approx 1\ \mathrm{m/sec}\ /\ 0.1\mathrm{m} \approx 10/\mathrm{sec}$
Recombination	$n_e \alpha \approx 10^{20}\ \mathrm{cm^{-3}} \times 10^{-20}\ \mathrm{m^3/s} \approx 1/\mathrm{sec}$

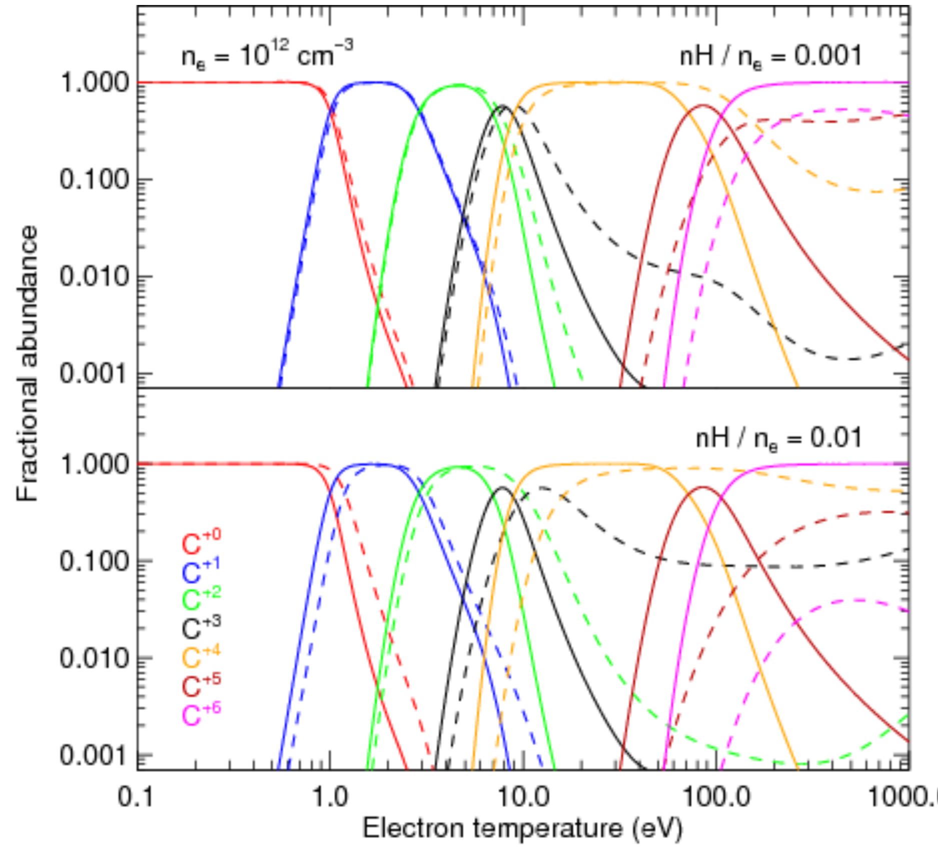
- Emission is a local process
- Timescale for transport is slower than ionisation but faster than recombination, therefore density profile of individual ionisation stage is determined non-locally

Spatial Distribution of Ions

Equilibrium (coronal) ionisation balance is not a safe assumption for tokamak plasm

X-ray ← visible

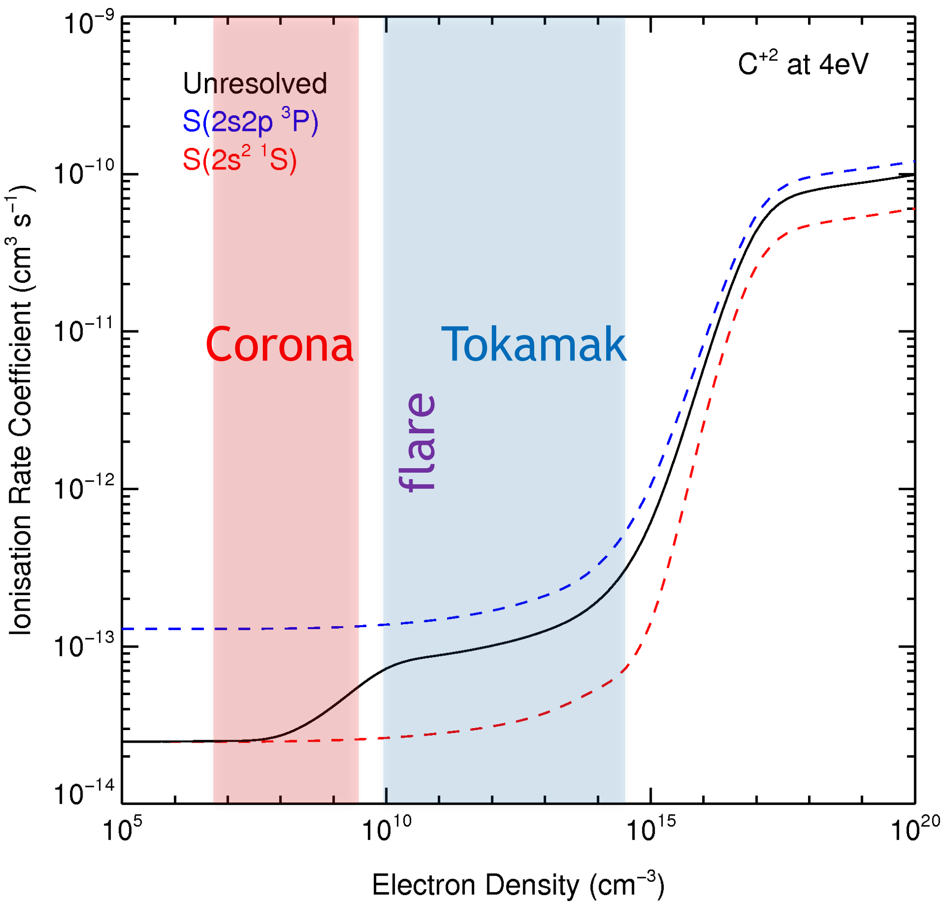


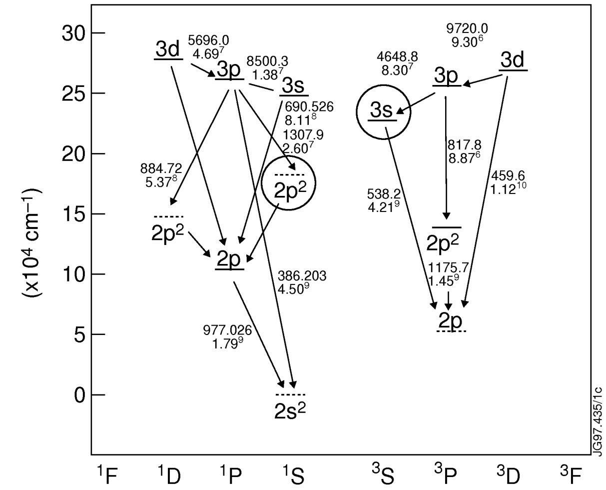


Charge exchange with neutral hydrogen can also be a significant contributor to overall recombination

Finite density and metastables

- A finite electron density plasma results in ‘effective’ source coefficients.





Finite density and metastables

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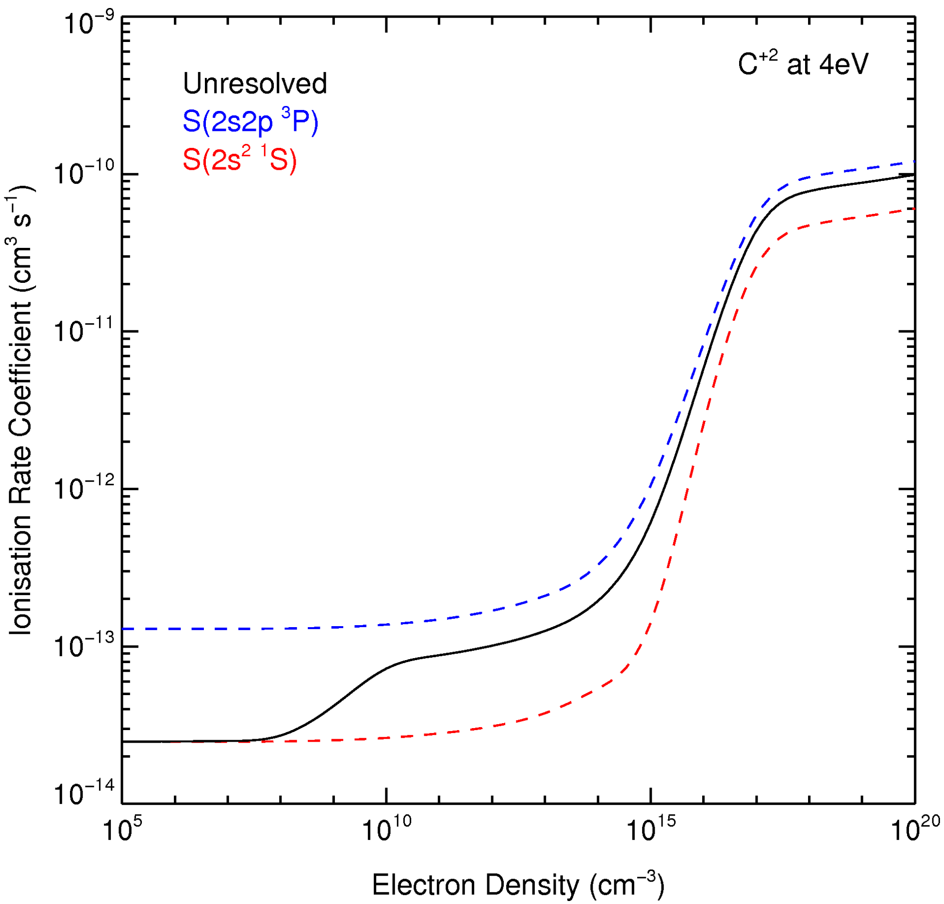
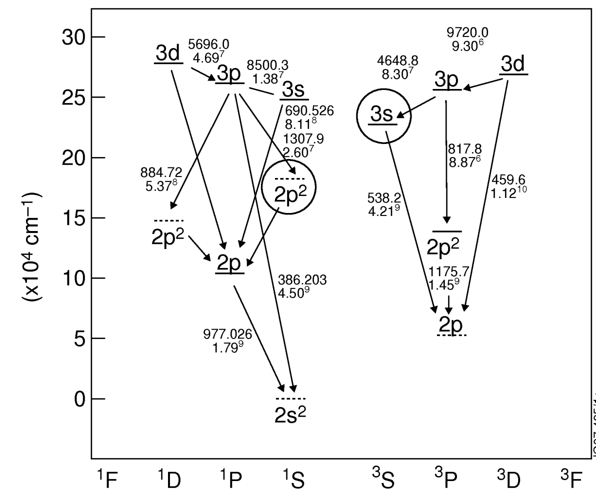




Metastables are followed in time

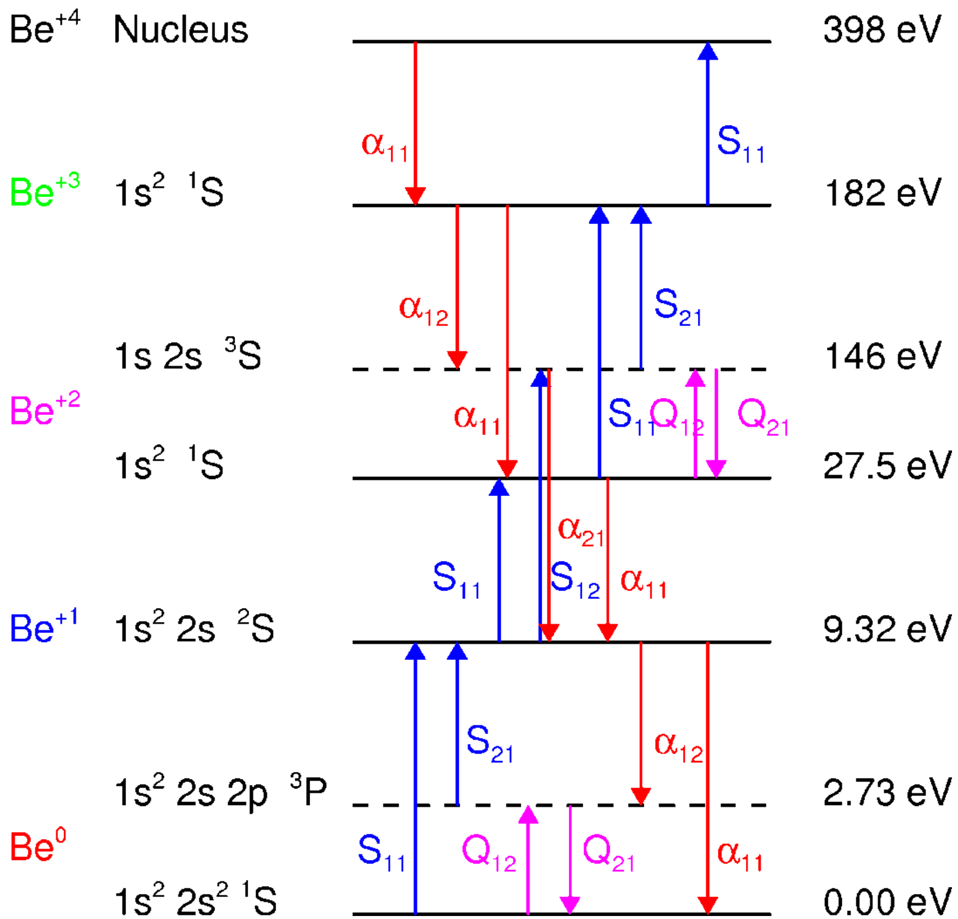
$$\frac{d}{dt}N_\rho^z \neq 0 \quad 1 \leq \rho \leq m$$

Ordinary levels are in quasi-stati
equilibrium with their metastabl

$$\frac{d}{dt}N_i^z = 0 \quad i > m.$$

GCR coefficients

$$\frac{dN_{\rho}^{+z}}{dt} = -(N_e S_{CD,\sigma\rightarrow\nu} N_{\sigma}^{+z} + N_e \alpha_{CD,\nu'\rightarrow\rho} N_{\nu'}^{+z+1} + N_e Q_{CD,\sigma\rightarrow\rho} N_{\sigma}^{+z}) + \ldots$$



What we need to model emission from fusion plasmas

If we wish to interpret/predict the emission from plasmas:

- Require atomic and molecular data
- Not necessarily of highest quality – completeness is as important
- Fundamental data mediated via models to be useful for modelling and
  diagnostic use.
- The derived/effective data must be a parameterization of atomic features with macroscopic plasma quantities (Te, Ti, Ne, B, I etc.).
- Large amounts of data involved.

Necessary tasks:

- Gather/calculate fundamental data.
- Develop appropriate (collisional-radiative) models.
- Store data in a well defined way.
- Assess the quality of the data.

Most data within ADAS is *ab initio*

Rely on the atomic codes being benchmarked against experiment when possible

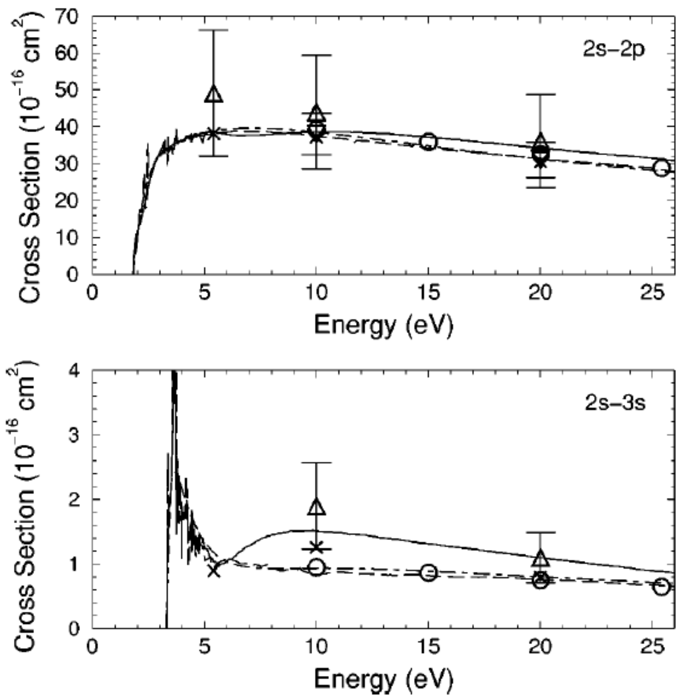


FIG. 2. Total electron-impact excitation cross sections for the $2s \rightarrow 2p$ and $2s \rightarrow 3s$ transitions in Li. Solid curves, present 14-state *R*-matrix calculation; dashed curves, present 55-state RMPS calculation; open circles, present TDCC calculation; dot-dashed curves, from fits to the CCC calculations given by Schweinzer *et al.* [10]; crosses, CCO calculation of Bray *et al.* [9]; upward triangles, experimental measurements of Williams *et al.* [11]; downward triangles, experimental results of Vušković *et al.* [12].

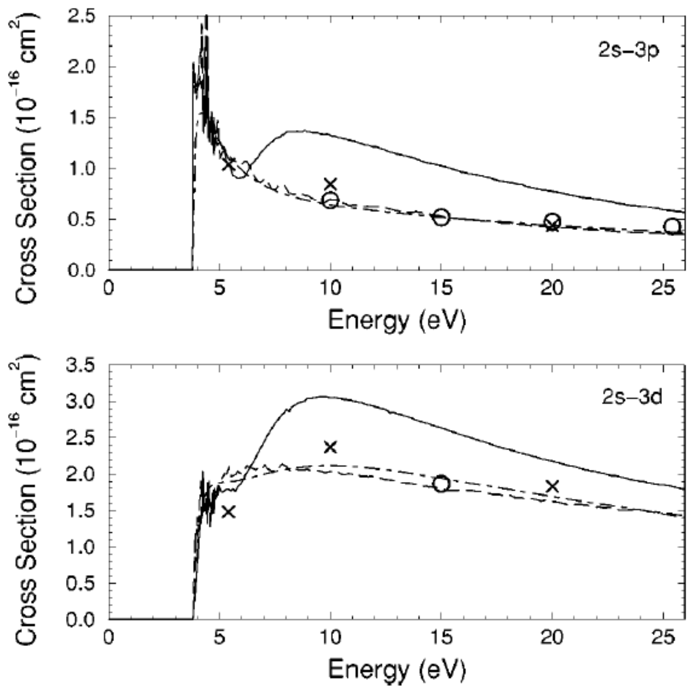
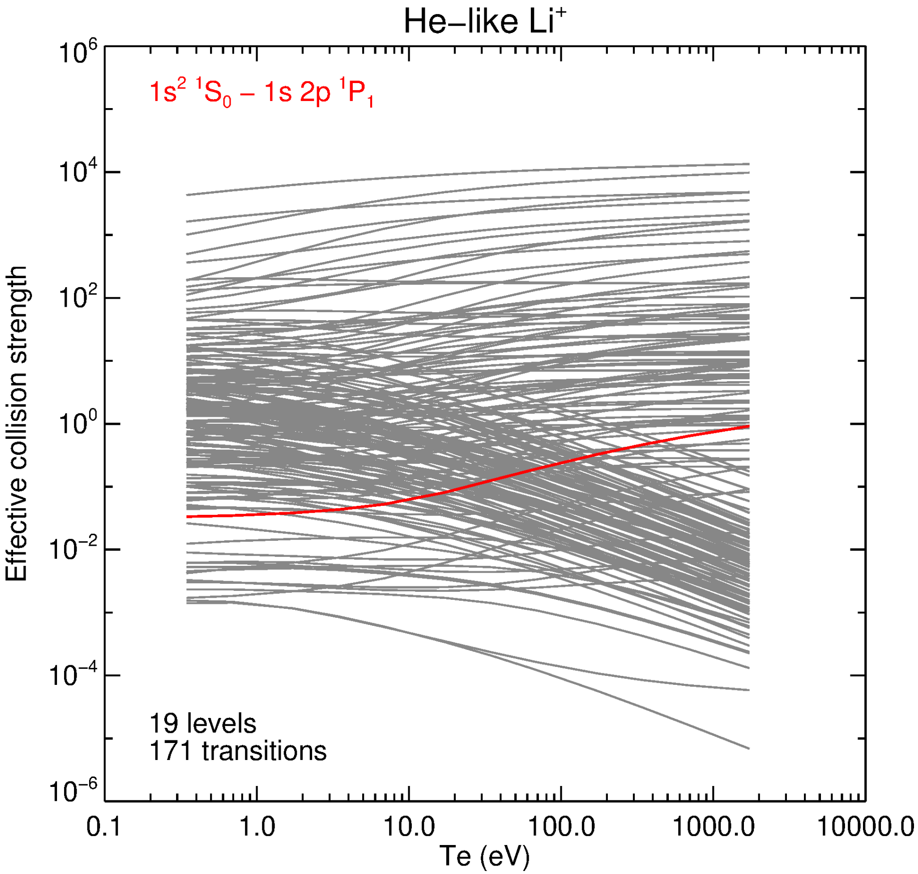
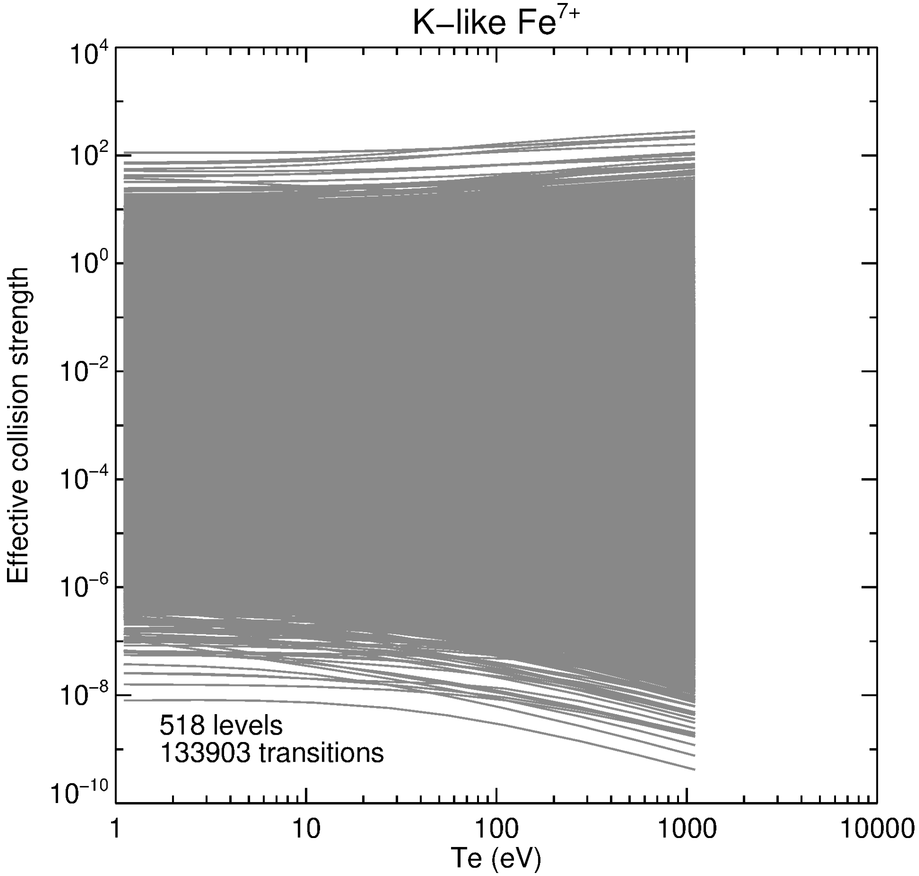


FIG. 3. Total electron-impact excitation cross sections for the $2s \rightarrow 3p$ and $2s \rightarrow 3d$ transitions in Li. Solid curves, present 14-state *R*-matrix calculation; dashed curves, present 55-state RMPS calculation; open circles, present TDCC calculation; dot-dashed curves, from fits to the CCC calculations given by Schweinzer *et al.* [10]; crosses, CCO calculation of Bray *et al.* [9].

Li^0 excitation cross sections

Excitation data for population modelling

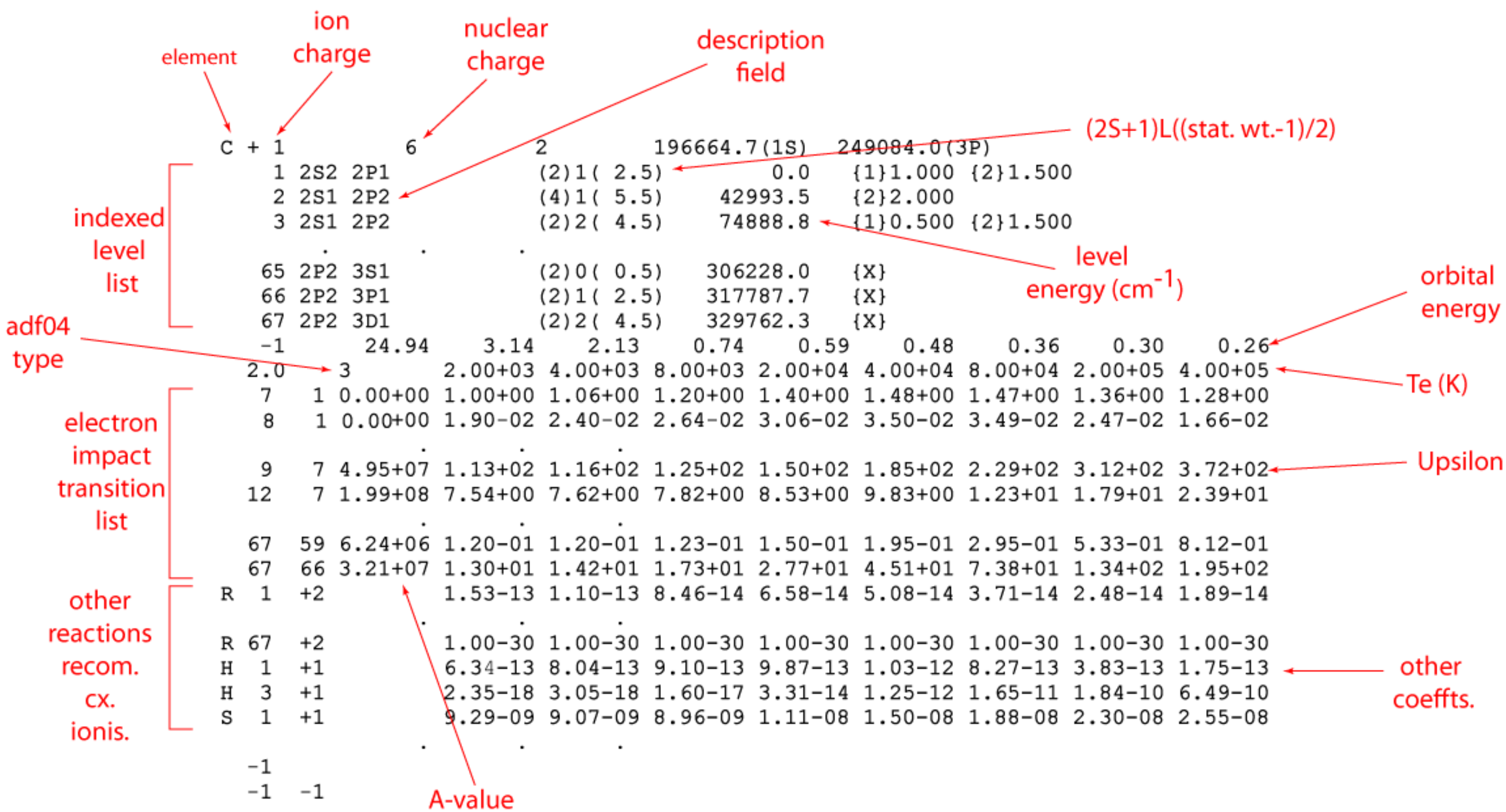




Scrutiny of individual transitions becomes difficult when the complexity of the ion structure increases.

ADAS data formats (*adf*)

All ADAS data is stored in a well defined, tightly specified, format – eg. *adf04* f



A free-format comment section at the end details the source and responsible per

Modelling lithium results in 64 datasets

Driver for adas8#1 adf04
adf34/lithium/li0.dat
adf34/lithium/li1.dat
adf34/lithium/li2.dat

Baseline adf04 to give baseline fill-in and A-values
adf04/copmm#3/ls#li0.dat
adf04/copmm#3/ls#li1.dat
adf04/copmm#3/ls#li2.dat

R-matrix data from Connor Ballance and Don Griffin
adf04/lilike/lilike_cpb02#li0.dat
adf04/helike/helike_cpb02#li1.dat
adf04/hlike/hlike_cpb02#li2.dat

Metastable and excited state resolved ionisation data from S Loch
adf07/szd02#li/szd02#li_li0.dat
adf07/szd02#li/szd02#li_li1.dat
adf07/szd02#li/szd02#li_li2.dat

State resolved radiative recombination from Nigel Badnell
adf48/nrb05#he/nrb05#he_li1ls.dat
adf48/nrb05#h/nrb05#h_li2ls.dat
adf48/nrb05##/nrb05##_li3ls.dat

State resolved dielectronic recombination from N Badnell and M Bautista
adf09/nrb00#h/nrb00#h_li2ls12.dat
adf09/nrbmb00#he/mb00#he_li1ls12.dat
adf09/nrbmb00#he/mb00#he_li1ls23.dat

Fully specified adf04 file for processing
adf04/adas#3/cpb02_ls#li0.dat
adf04/adas#3/cpb02_ls#li1.dat
adf04/adas#3/cpb02_n#li2.dat

Mapping high-n to low levels
adf18/a17_p208/exp96#li/exp96#li_li0ls.dat
adf18/a17_p208/exp96#he/exp96#he_li1ls.dat
adf18/a17_p208/exp96#h/exp96#h_li2n.dat

Projection matrices
adf17/cbnm96#li/cbnm96#li_li0ls.dat
adf17/cbnm96#he/cbnm96#he_li1ls.dat
adf17/cbnm96#h/cbnm96#h_li2ls.dat

iso-electronic GCR data
adf10/acd96/pj#acd96_li11.dat
adf10/acd96/pj#acd96_li21.dat
adf10/scd96/pj#scd96_li11.dat
adf10/scd96/pj#scd96_li21.dat
adf10/xcd96/pj#xcd96_li12.dat
adf10/xcd96/pj#xcd96_li21.dat
adf10/plt96/pj#plt96_li##.dat
adf10/prb96/pj#prb96_li10.dat
adf10/prb96/pj#prb96_li20.dat

iso-nuclear source and power - resolved
adf11/acd96r/acd96r_li.dat
adf11/scd96r/scd96r_li.dat
adf11/qcd96r/qcd96r_li.dat
adf11/xcd96r/xcd96r_li.dat
adf11/plt96r/plt96r_li.dat
adf11/prb96r/prb96r_li.dat

iso-nuclear source and power - unresolved
adf11/acd96/acd96_li.dat
adf11/scd96/scd96_li.dat
adf11/ecd96/ecd96_li.dat
adf11/ycd96/ycd96_li.dat
adf11/zcd96/zcd96_li.dat
adf11/plt96/plt96_li.dat
adf11/prb96/prb96_li.dat

Ionisations per photon
adf13/sxb96#li/sxb96#li_pjr#li0.dat
adf13/sxb96#li/sxb96#li_pju#li0.dat
adf13/sxb96#li/sxb96#li_pjr#li1.dat
adf13/sxb96#li/sxb96#li_pju#li1.dat
adf13/sxb96#li/sxb96#li_pjr#li2.dat
adf13/sxb96#li/sxb96#li_pju#li2.dat

Photon emissivity coefficients
adf15/pec96#li/pec96#li_pjr#li0.dat
adf15/pec96#li/pec96#li_pju#li0.dat
adf15/pec96#li/pec96#li_pjr#li1.dat
adf15/pec96#li/pec96#li_pju#li1.dat
adf15/pec96#li/pec96#li_pjr#li2.dat
adf15/pec96#li/pec96#li_pju#li2.dat

In OPEN-ADAS

Lithium – only 3 electrons

ELSEVIER

Available online at www.sciencedirect.com

ScienceDirect

Atomic Data and Nuclear Data Tables 92 (2006) 813–851

Atomic Data AND Nuclear Data Tables

www.elsevier.com/locate/adt

Generalised collisional-radiative model for light elements. A: Data for the Li isonuclear sequence

S.D. Loch [a,*], J. Colgan [a], M.C. Witthoeft [a], M.S. Pindzola [a], C.P. Ballance [b], D.M. Mitnik [b], D.C. Griffin [b], M.G. O'Mullane [c], N.R. Badnell [c], H.P. Summers [c]

[a] *Department of Physics, Auburn University, Auburn, AL 36849, USA*
[b] *Department of Physics, Rollins College, Winter Park, FL 32789, USA*
[c] *Department of Physics, University of Strathclyde, Glasgow G40NG, UK*

- 64 adf datasets
- 43 in OPEN-ADAS: fundamental data (excitation, DR, RR and ionisation)
  derived data (source, power, S/XB and PEC coefficients)

What is ADAS?

- ADAS, as a database delivers:
  - extensive fundamental and derived data tuned for plasma modelling and spectroscopic analysis,
  - provides ‘baseline’ level data for any element and ion stage.
  - atomic data source for many modelling codes and systems,
  - makes a significant quantity of data publically available via OPEN-ADAS http://open.adas.ac.uk (with IAEA).

- ADAS, as a computer system, is designed to:
  - provide a set of interactive codes which are easy to use,
  - provide subroutine libraries for inclusion in other codes,
  - allow direct access to diagnostically relevant data.

- ADAS, as a collaborative organisation:
  - provides guidance (training courses, visits etc.) on running codes,
  - gives recommendation on the best data to use,
  - assists in analysis and development of analysis tools and models.

It is structured as a self-funded consortium between most major fusion laboratories and universities. Its historical roots are in JET and is now managed by Strathclyde University but governed by a steering committee of the participating members.

ADAS data and computational overview

There are 55 different ADAS data formats

Some key ADFs and MDFs for general application

ADF01 : charge exchange cross sections
ADF04 : specific ion data
ADF11 : coll.-rad. ionis., recom. and related coefficients.
ADF13 : ionisation per photon ratios
ADF15 : emissivity coefficients
ADF40 : envelope feature photon emiss. coefficients
ADF21 : beam stopping coefficients
ADF39 : photoionization cross sections

MDF00: fundamental diatomic molecular constants
MDF01: rovibronic models
MDF02: fundamental cross-section data
MDF04: specific molecule data

Interactive user interface

ADAS series (9 series with 85 programs)

The application interface

ADAS Fortran subroutine (~1900) , IDL procedure (~1700) and python (~30) routine libraries

Data extraction procedures and subroutines by format: xxdata_<nn> , read_adf<nn>, xxdatm_<nn> , read_mdf<nn> .

Offline-ADAS for large scale production

6 large scale production packages: adas7#1, adas7#3, adas8#1, adas8#2, adas8#3, adas8#4 .

Documentation – examples, manual and course material.

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

Freeform search

Search | Freeform search examples

Freeform search | Search by wavelength | Search by ion

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

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.

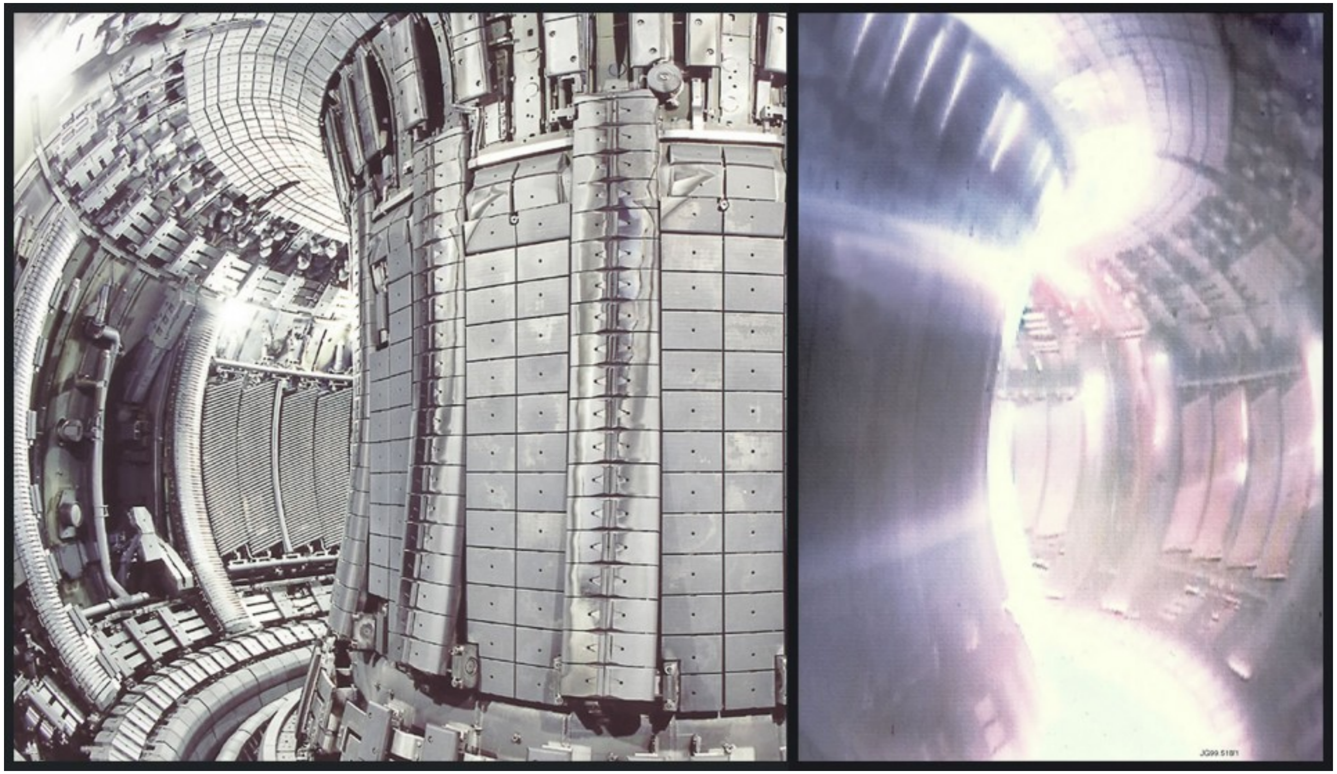
DERIVED CLASSES

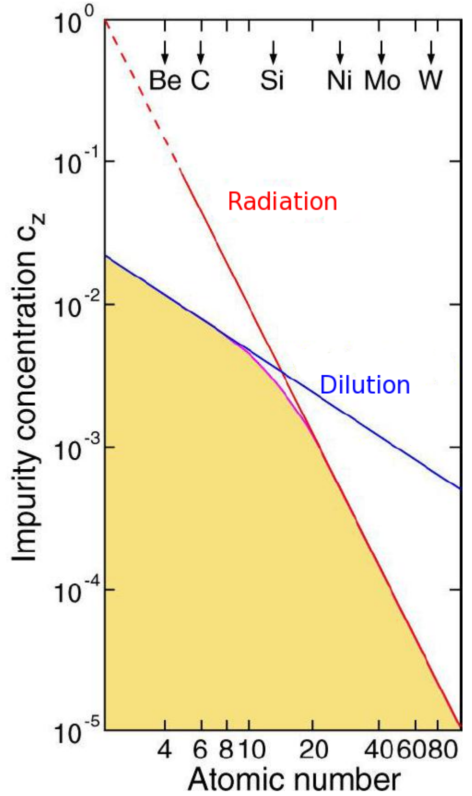
- ADF 11 — Iso-nuclear master files: Effective (collisional–radiative) coefficients which are required to establish the ionisation state of a dynamic or steady-state plasma.
- ADF 12 — Charge exchange effective emission coefficients: Collections of effective emission coefficients for spectrum lines emitted 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 coeffeicents 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

Who thought that tungsten was a good idea?

- Interpret emission from fuel (H, D, T and He) and impurities (Be, Ne, Ni, W).





Although emission from impurities gives information, their presence is not always benign.

W^{18+} dielectronic recombination

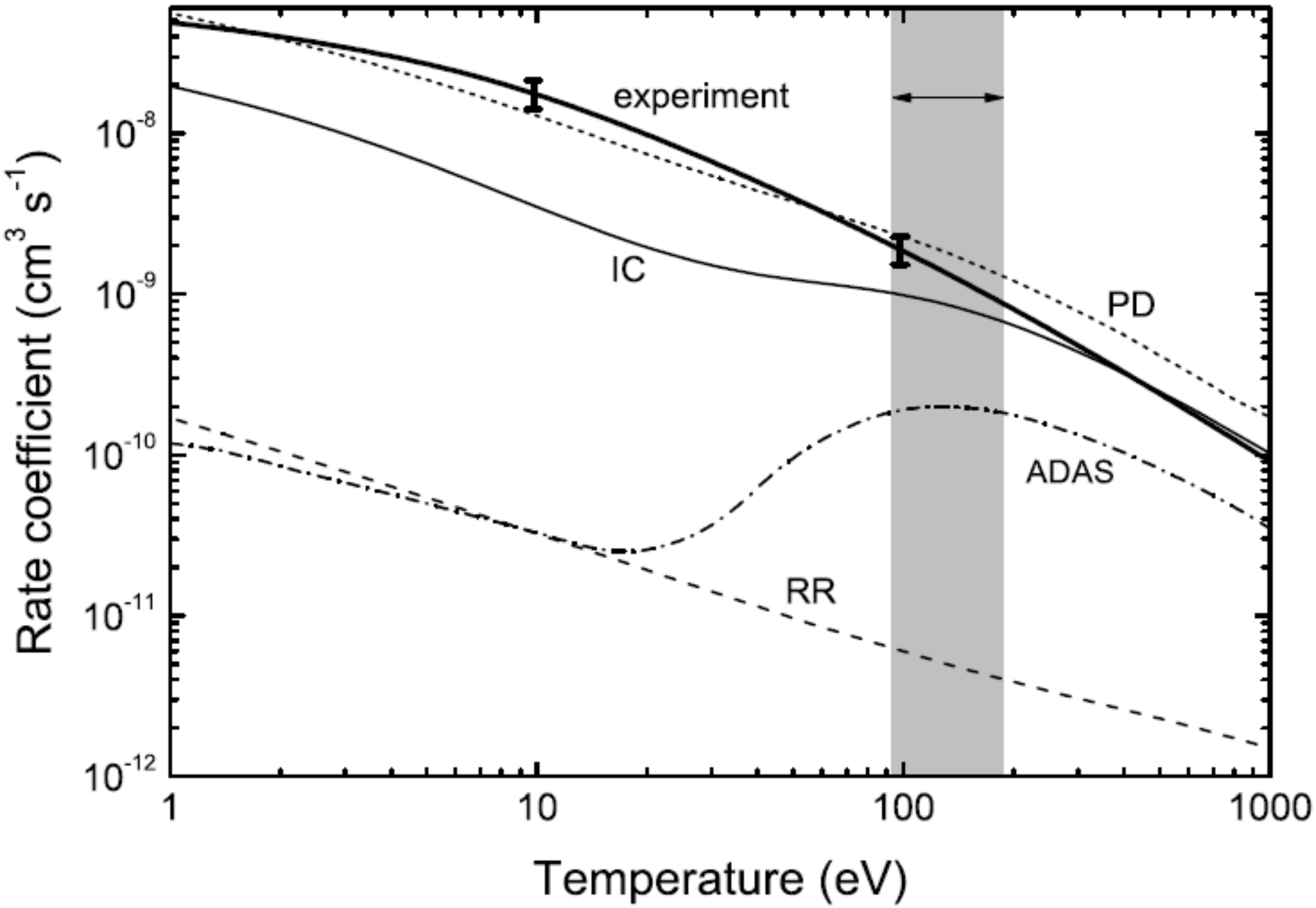
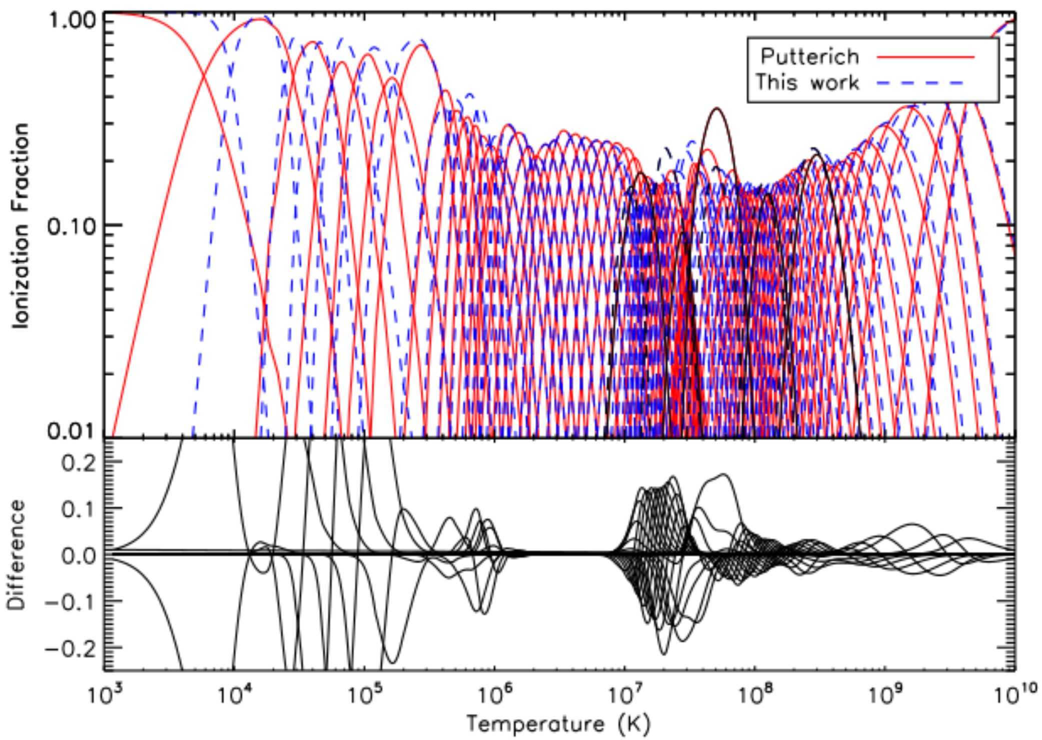


Fig 4. Plasma recombination rate coefficients for W^{18+} (Spruck et al. Phys.Rev.A **90**, 032715,2014) Thick solid curve: experimentally derived rate coefficient; thin solid curve: IC theory; short-dashed curve (PD) partitioned and damped calculation; Dot-dashed curve: ADAS plasma recombination rate coefficient (Foster 2008).

Tungsten DR and ionization balance

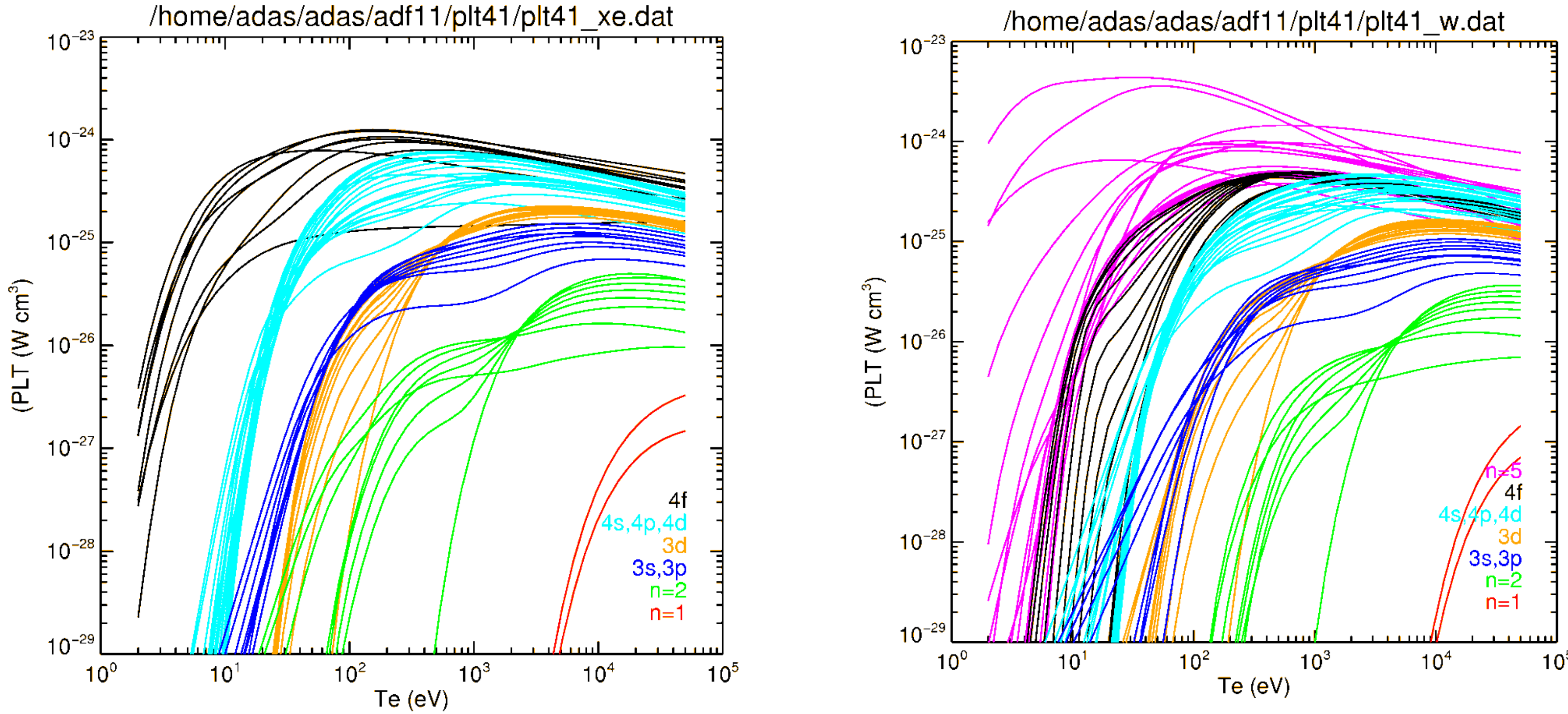
- Dielectronic recombination rates for tungsten were the most poorly calculated input to the ionization balance.
- T Pütterich scaled the ADPAK average ion rates to match AUG measurements.
- Limited to 2keV < T_e < 10keV (W^{20+} – W^{55+} or Xe-like to K-like) PPCF, v50, 085016 **2008**
- DR rates for 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,



oing.
- $4f^n$ 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

Optimizing the radiated power

- A rule-based algorithm to choose the configurations needed based on the metric of optimizing the total radiated power.
- Data from Cowan with AUTOSTRUCTURE supplementation for spin-changing and higher multipole transition probabilities



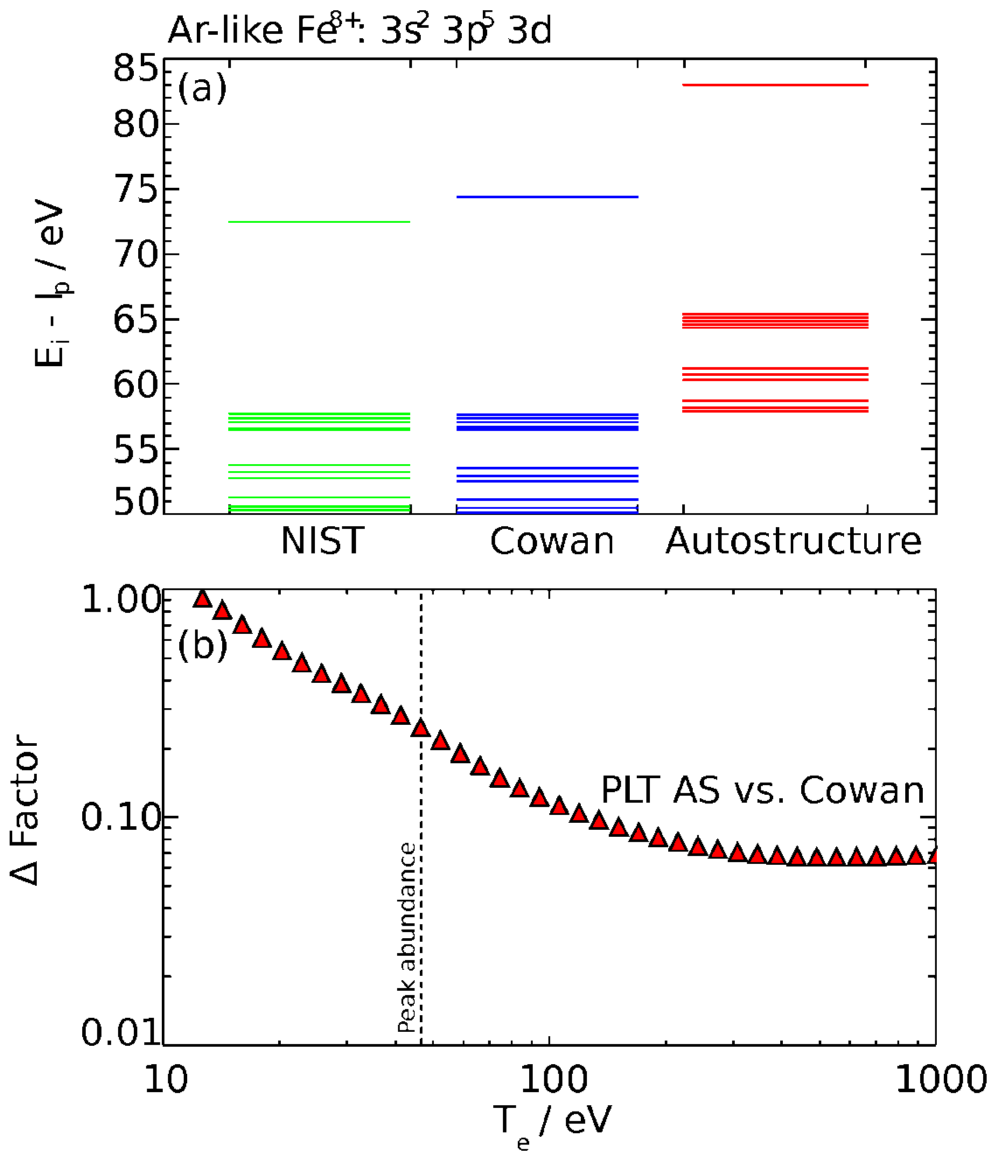
S Henderson et al, PPCF. **59**, 055010 (2017)

Optimizing atomic structure

- Wish to move to AUTOSTRUCTURE distorted-wave as a new baseline quality.
- Same driver files for R-matrix.

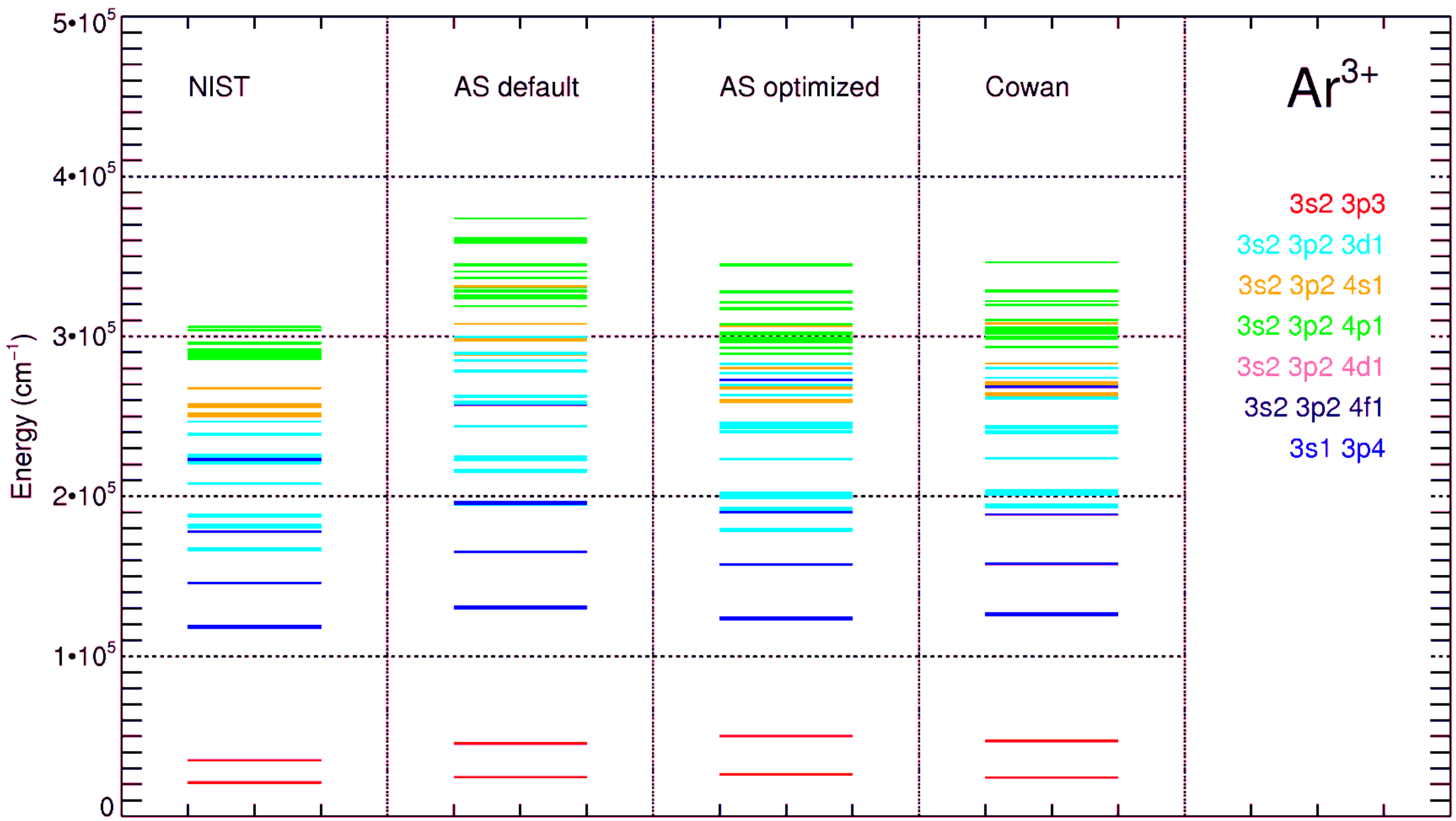
- Good atomic structure is essential for high quality derived data.
- And is the basis for uncertainty estimation.

- Default results could be better.
- Optimization converges quickly.
- But it needs a 'good' target.



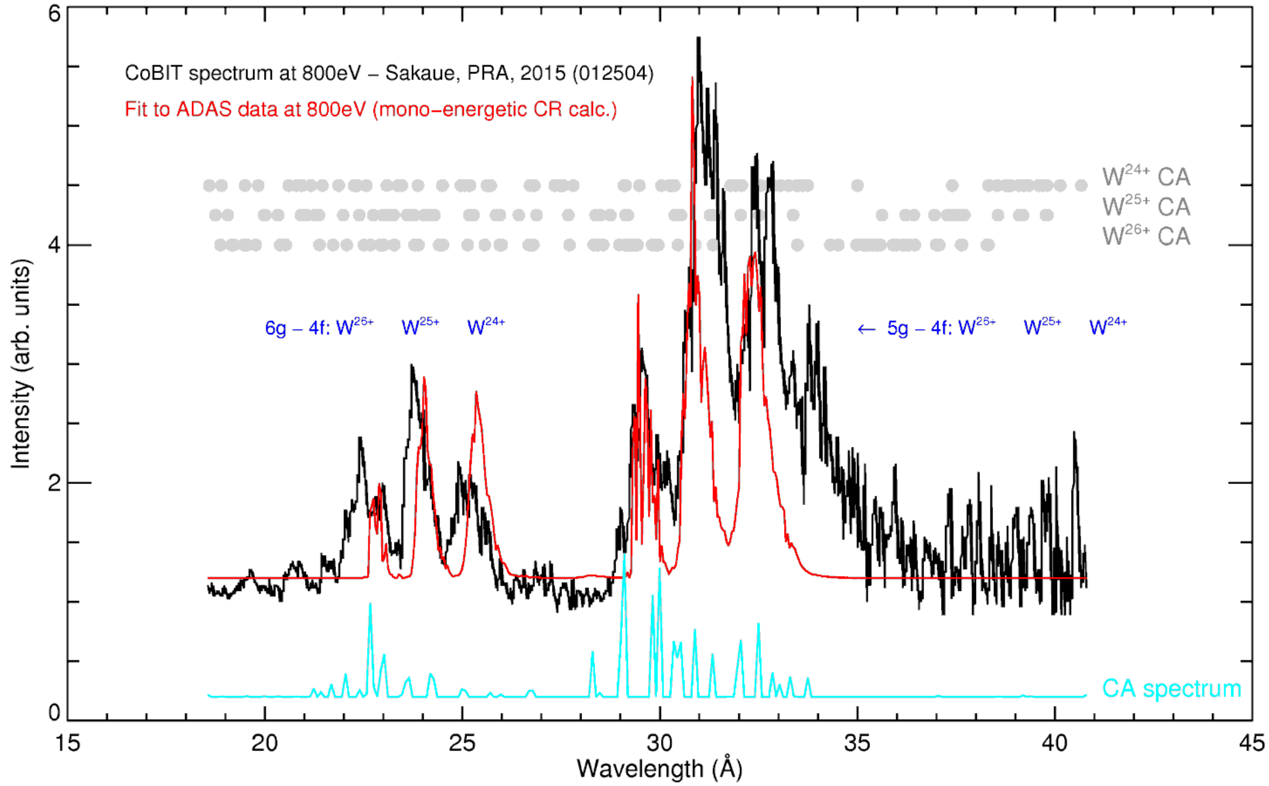
Optimizing structure across iso-electronic and iso-nuclear sequences

- AUTOSTRUCTURE uses a Thomas-Fermi potential and individual orbitals can be scaled to improve results along iso-electronic and iso-nuclear sequences.
- Unfortunately data from NIST becomes sparse very quickly.



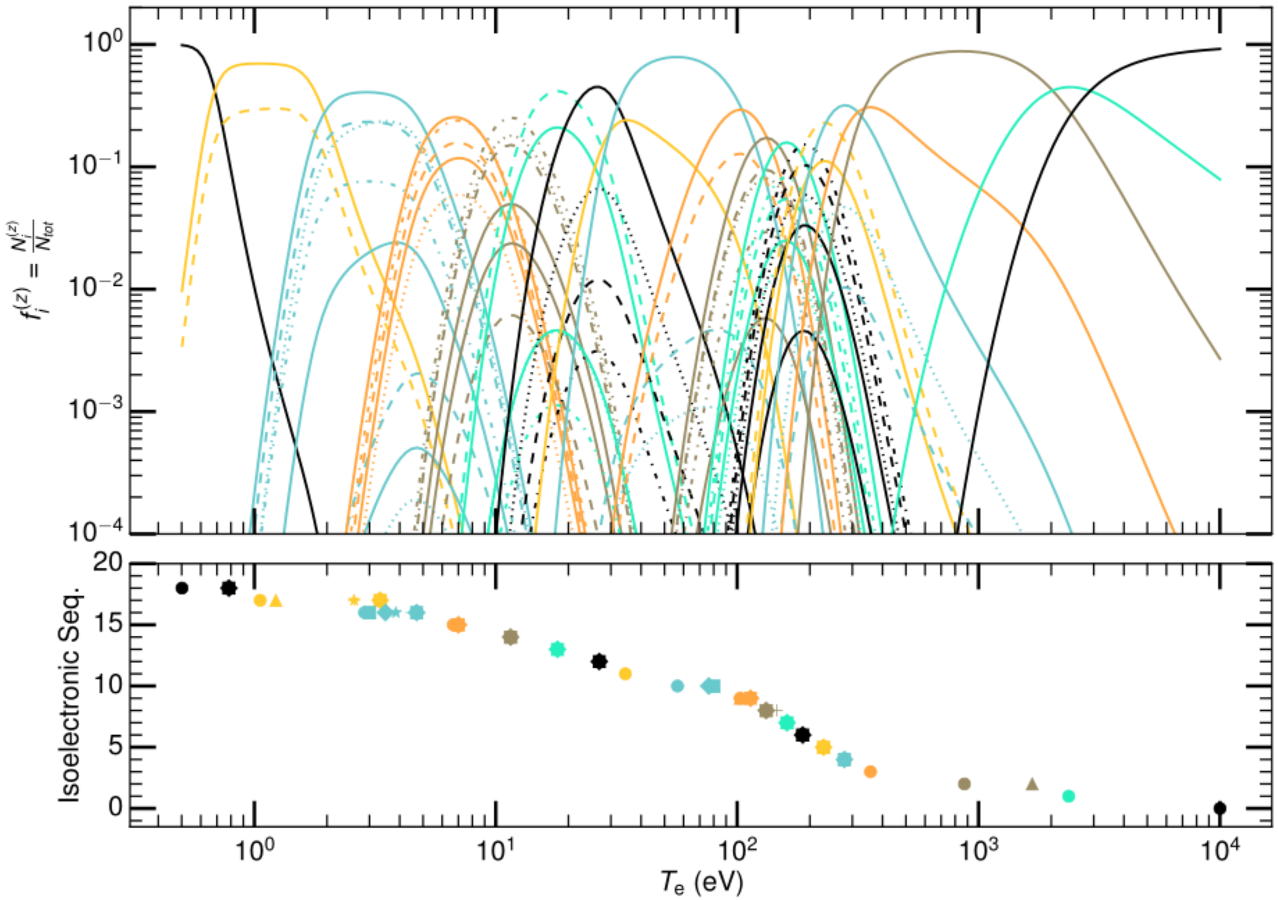
Optimizing the radiated power

- 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.

Intermediate coupling GCR – prototyped with Argon



- Required ion impact to mix closely-spaced energy levels (stored in *adf06* files)
- Increases the number of metastables.
- Raises questions on how to handle/classify these metastables. Generating derived data targeted at the plasma environment under study is necessary.

Conclusions

- Advancing the quality of atomic data required for fusion is important.
- The quantity and use of data for modelling and diagnostics is such that the *ab initio* codes used to produce these data must be validated by measured data wherever possible.
- The code validation does not necessarily need to be fusion relevant.

- The way atomic data will be used is changing, being embedded into complex analysis chains, some with machine protection implications (and responsibilities).
- Provenance of atomic data is important.
- Provenance goes hand in hand with validation.

- At ITER a measurement requirement (a diagnostic) is characterised and ranked by:
    - needed for machine protection.
    - needed for basic machine control.
    - required for advanced plasma control.
    - required for evaluation and physics studies.

- But all discharges at ITER must be modelled and verified before execution so accurate atomic data is still essential.

Spend more time on atomic data and models!

ADAS

Atomic Data and Analysis Structure

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ADAS Workshop 2018

The 2018 ADAS Workshop will be held 9–11 December at *Physikzentrum Bad Honnef* in Germany.

The Institute of Energy and Climate Research (IEK-4) of Forschungszentrum Jülich **FZJ** are kindly hosting the 2018 meeting. It has been five years since we last held the ADAS workshop in Germany and we are delighted that the venue will be the **Physikzentrum** in Bad Honnef.

http://adas.ac.uk/