(CTAMOP, Queen's University of Belfast)

Collaborators : S D Loch, C Johnson , D Ennis (Auburn University)

M O'Mullane (University of Strathclyde/JET)

Overview of talk

1. Brief reminder of the expt/theory and the capabilities of R-matrix theory and other theory results within the literature, our experimental collaborators and the interface of our results with ADAS.

2. Development of the code base to meet the challenge of heavy complex species

3. Electron-impact excitation of W I, WII

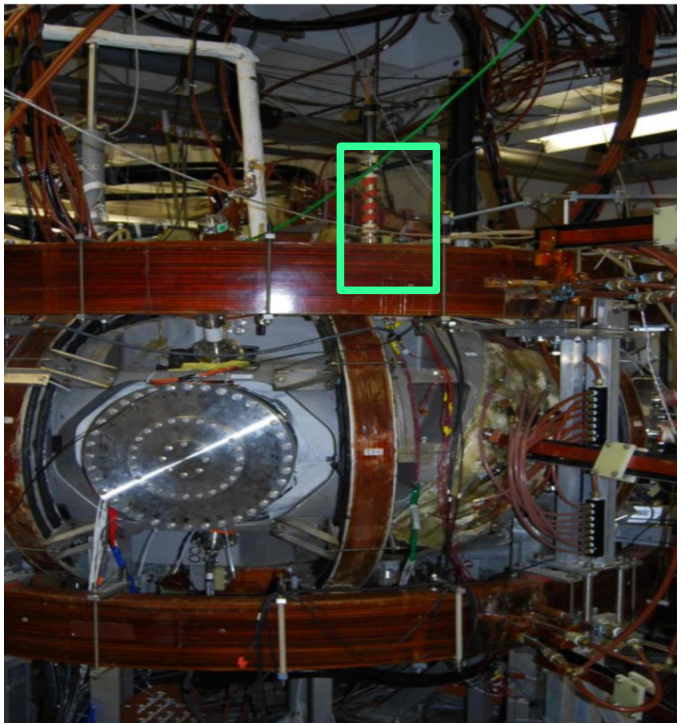
4. Electron-impact ionisation of W I

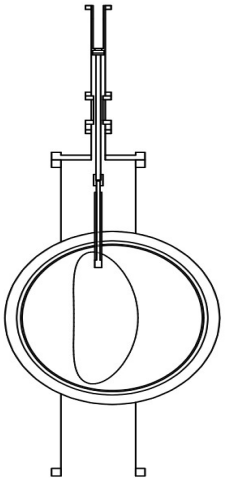
5. Uncertainty quantification work progresses

We validate our theoretical synthetic spectra against ongoing spectral measurements at CTH(Auburn University,USA) and DIID (General Atomics, CA, USA)

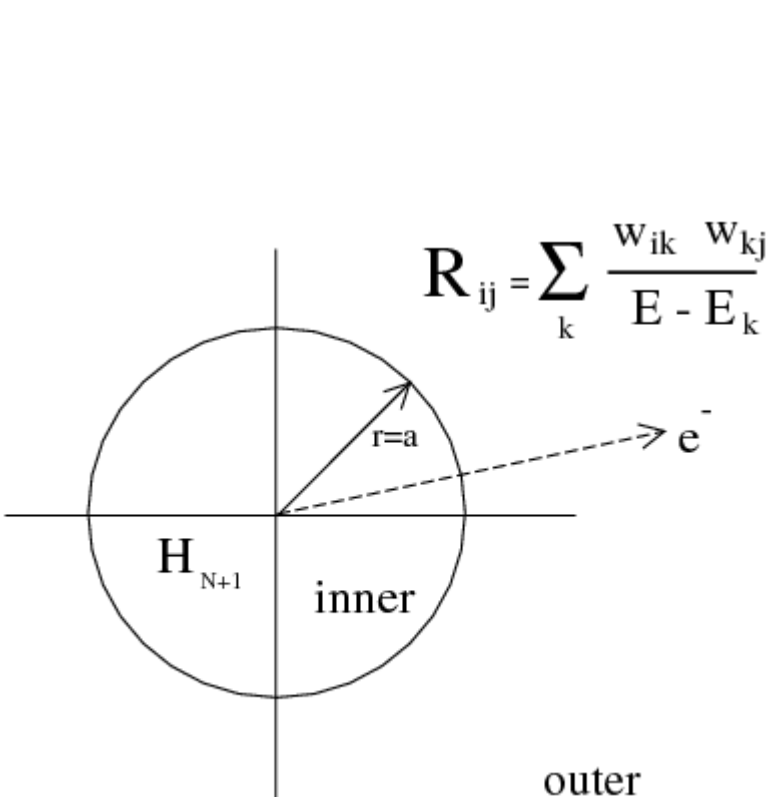
- Tungsten employed at JET, ITER, DIII-D and
- (CTH -Compact Toroidal Hybrid), Auburn University)
- Tungsten has favourable physical properties such as high thermal conductivity.

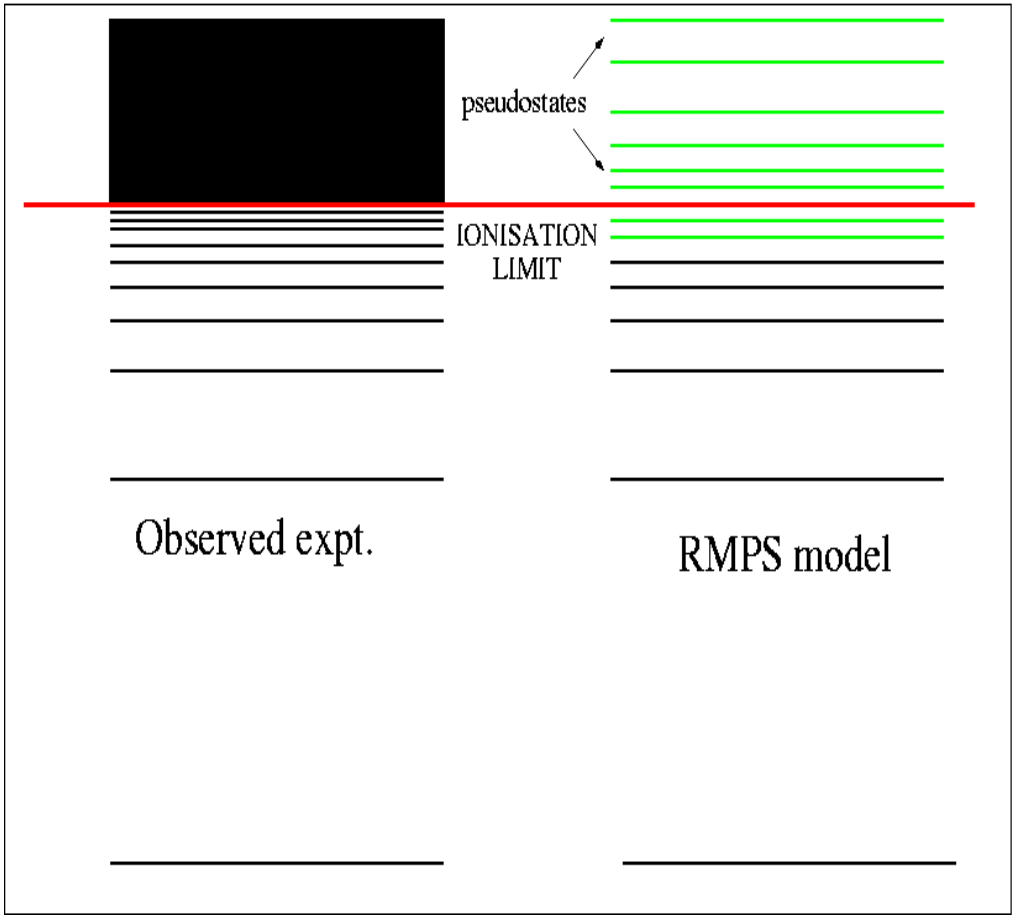
CTH (Auburn University)





R-matrix/R-matrix with Pseudostates (RMPS) review





$$\Psi_k(x_1 \ldots x_{N+1}) = A \sum_{ij} c_{ijk} \bar{\Phi}_i(x_1 \ldots x_N, \hat{r}_{N+1}\sigma_{N+1}) u_{ij}(r_{N+1}) + \sum_j d_{jk} \phi_j(x_1 \ldots x_{N+1})$$

Capabilities

- Most first order electron-impact driven processes

  connorb.freeshell.org (login and password available on request)

  Electron-impact excitation

  Electron-impact ionisation

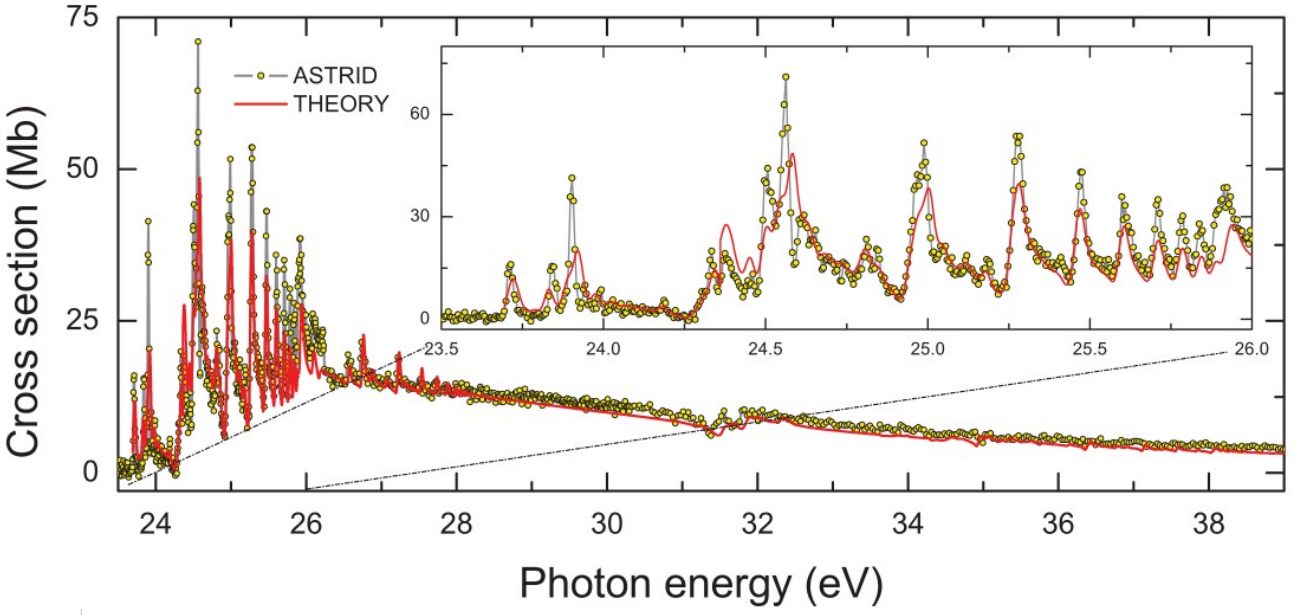
  Electron-impact recombination (DR/radiative)

- + photoionisation , photon-excitation (opacity)

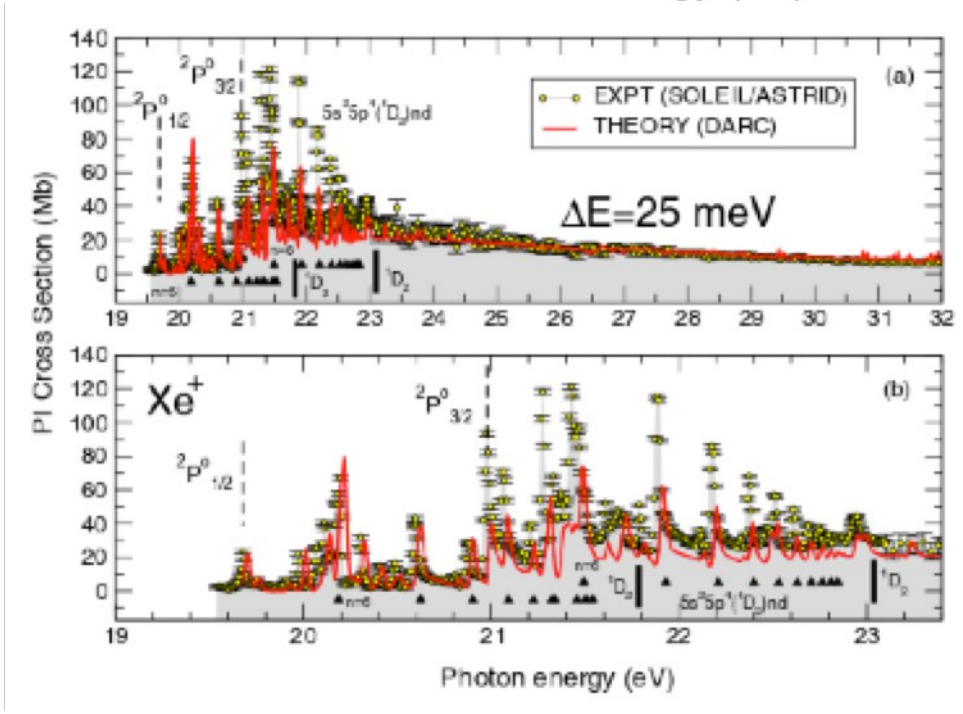
- The codes should cover most of the periodic table, and there are LS coupling (non-relativistic), Breit-Pauli (semi-relativistic) and Dirac R-matrix suites of codes. The results are stored in ADAS(O'Mullane), CLOUDY(G.Ferland), Chianti(Del Zanna) formats

Photoionisation/photo-excitation

Traditionally, we compared our results against astronomical observation and laboratory measurement. We still do, either remaining observations from the ALS (Advanced Light Source, CA,US) or the SOLEIL experiment (France)



hv + Kr II



hv + Xe II

The ability to map out the fine resonance structure and identify individual resonaces is a strength.

To provide experiments advance information is also a strength

Theory can aid by suggesting wave length windows and distinct isolated diagnostic lines

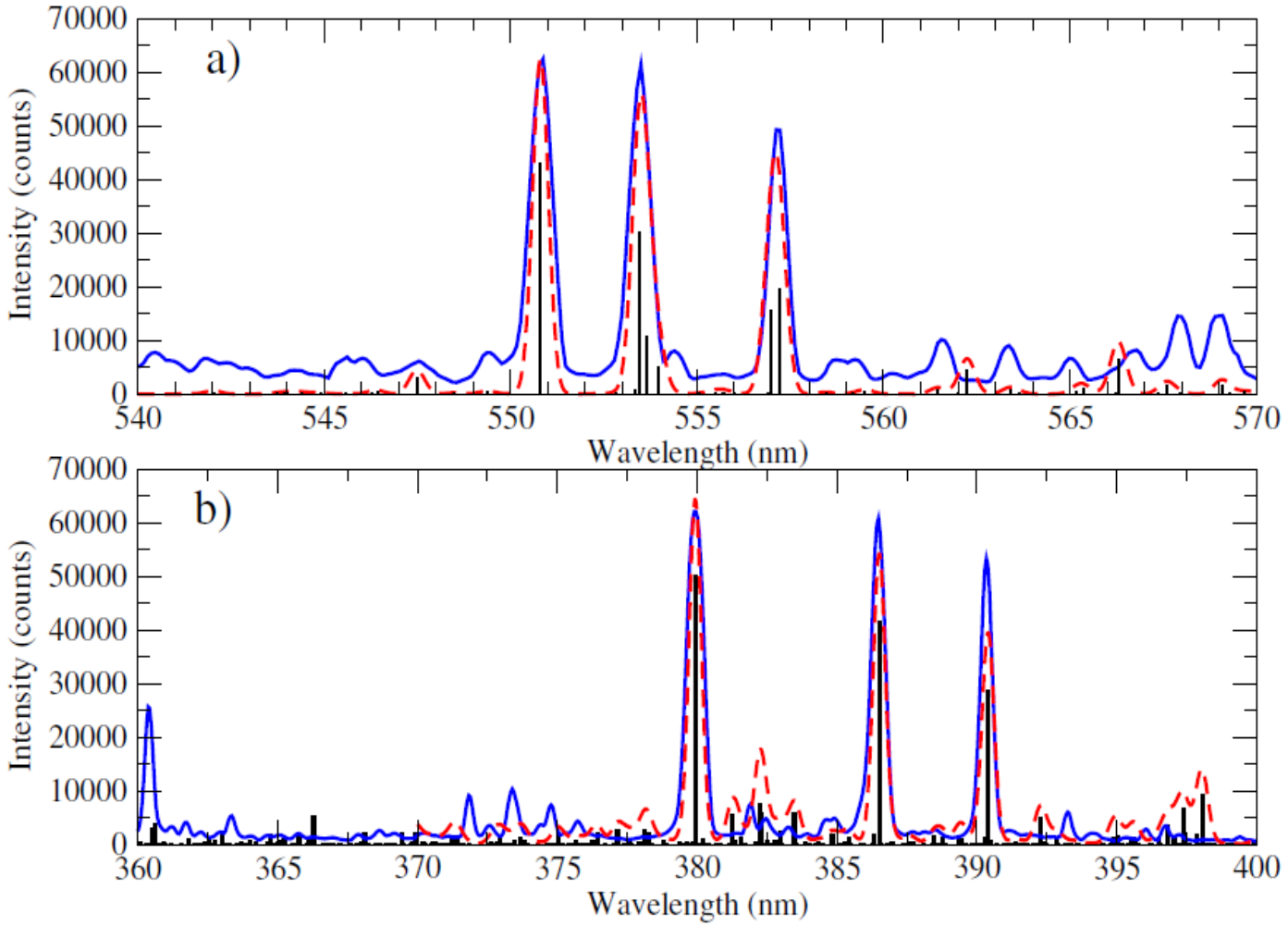
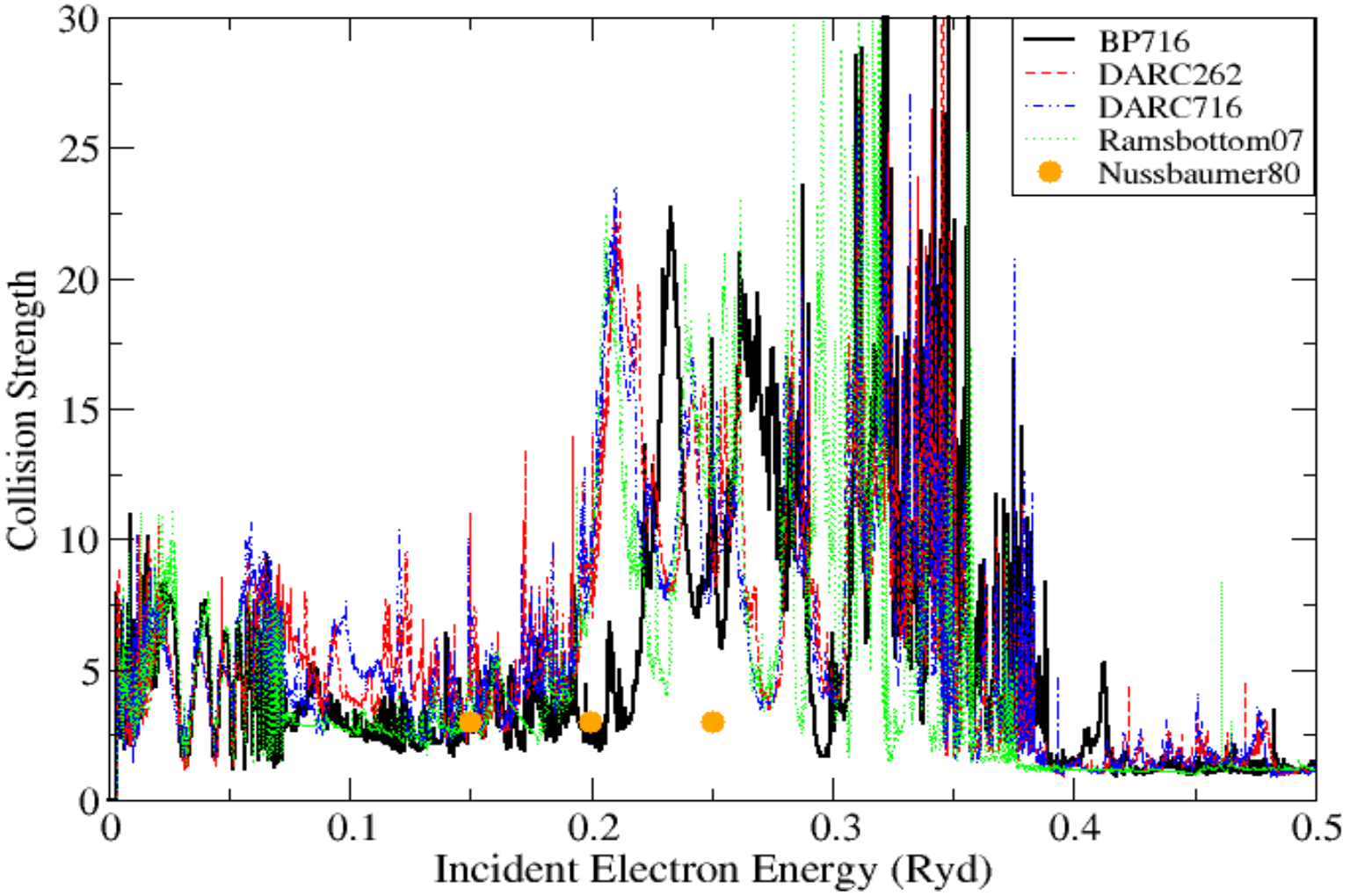


FIG. 6. Measured spectrum from the CTH plasma (solid blue line), compared with theoretical results. The solid black sticks show the PEC coefficients for the Mo I transitions, while the dashed red curve shows a theoretical spectrum based upon Gaussian convolved PEC data. A FWHM for the Gaussian convolution of 0.15 nm was used, based upon the instrument resolution, and the PECs are shown for an electron temperature of 6 eV and an electron density of 1×10^{12} cm^{-3}.

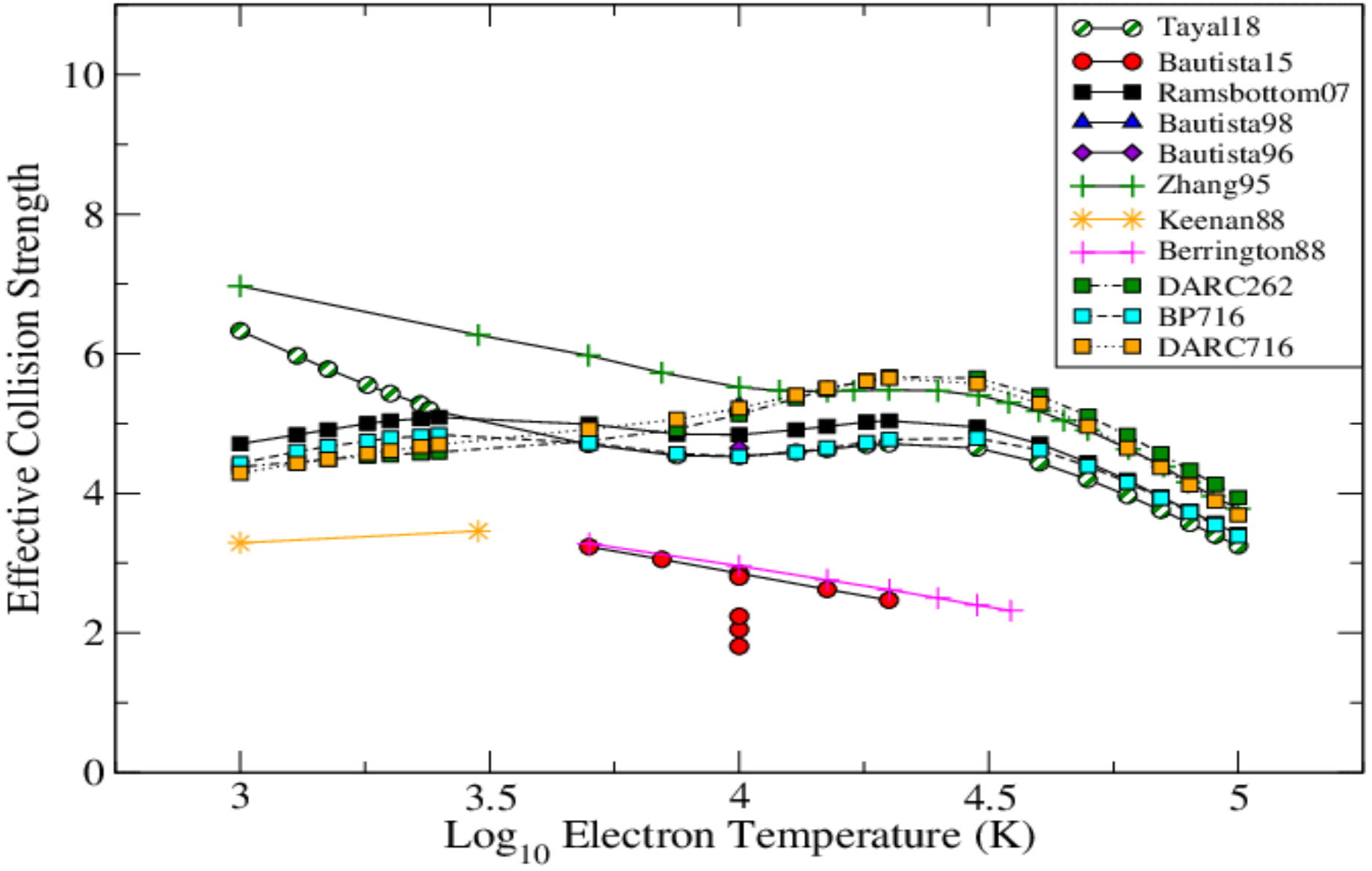
Electron-impact excitation

R-matrix strength is near neutral open shell systems such as Fe II (3d^4,4s^2) (Rosetta Stone), which has a long history ….

Smyth et al, Monthly Notices of the Royal Astronomical Society. 483, 1, p. 654-663 2019



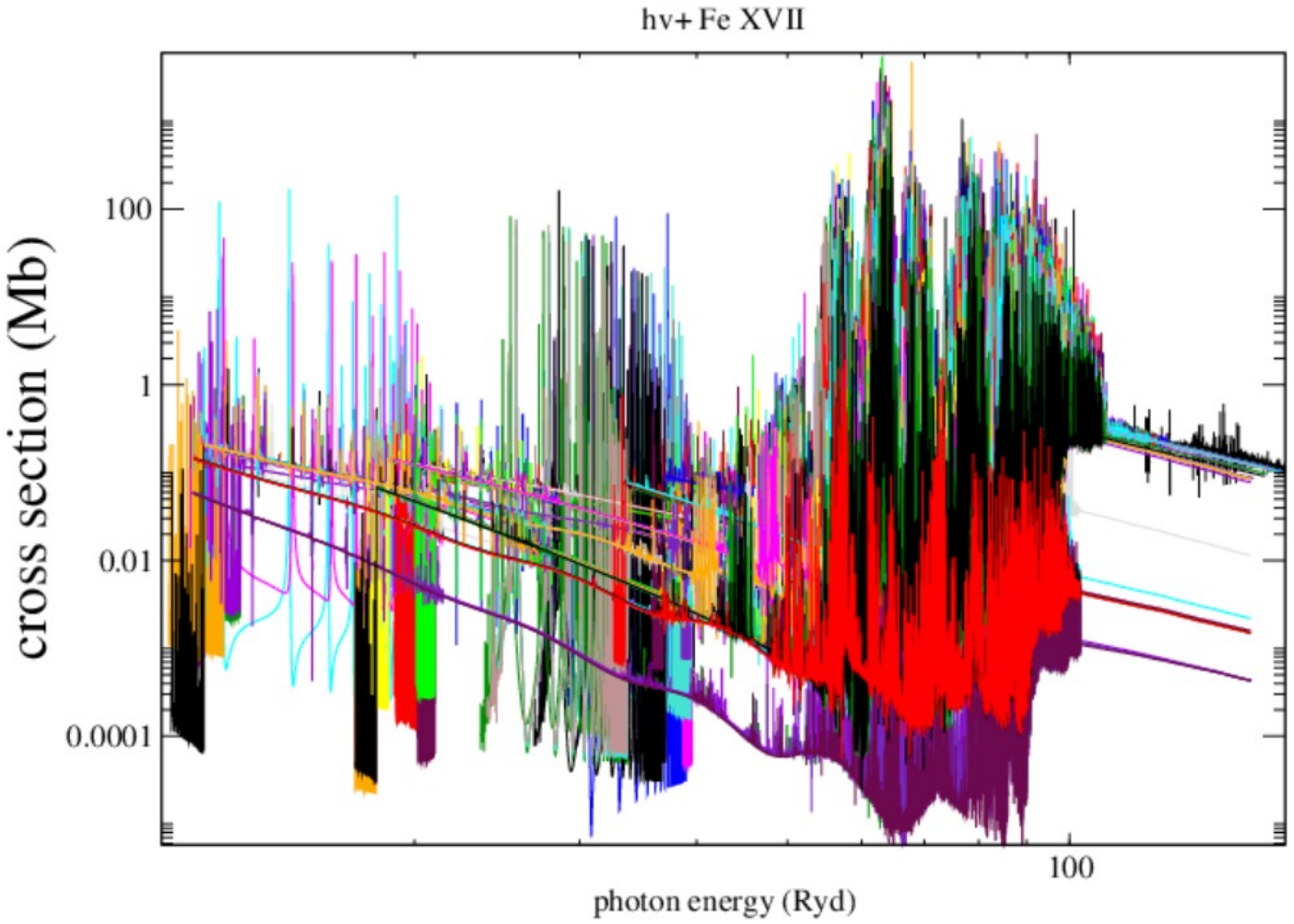
Various Calculations for the 1-2 transition in Fe II (^6D groundstate) J=9/2-7/2)



Stellar Opacities

High performance computing + scripting = comprehensive data sets (bound-bound, bound-free, free-free transitions)

i.e. total photoionisation of every Fe XVII level



All the R-matrix codes,but in particular the Dirac R-matrix codes required major revision.

1. Tungsten excitation/ionisation for many ion stages involves open d and shell systems, which requires a target description of several hundred of thousand levels.

2. From the scattering perspective (whether excitation or ionisation) involves thousands of scattering channels. Unlike perturbative methods these channels are are all coupled.

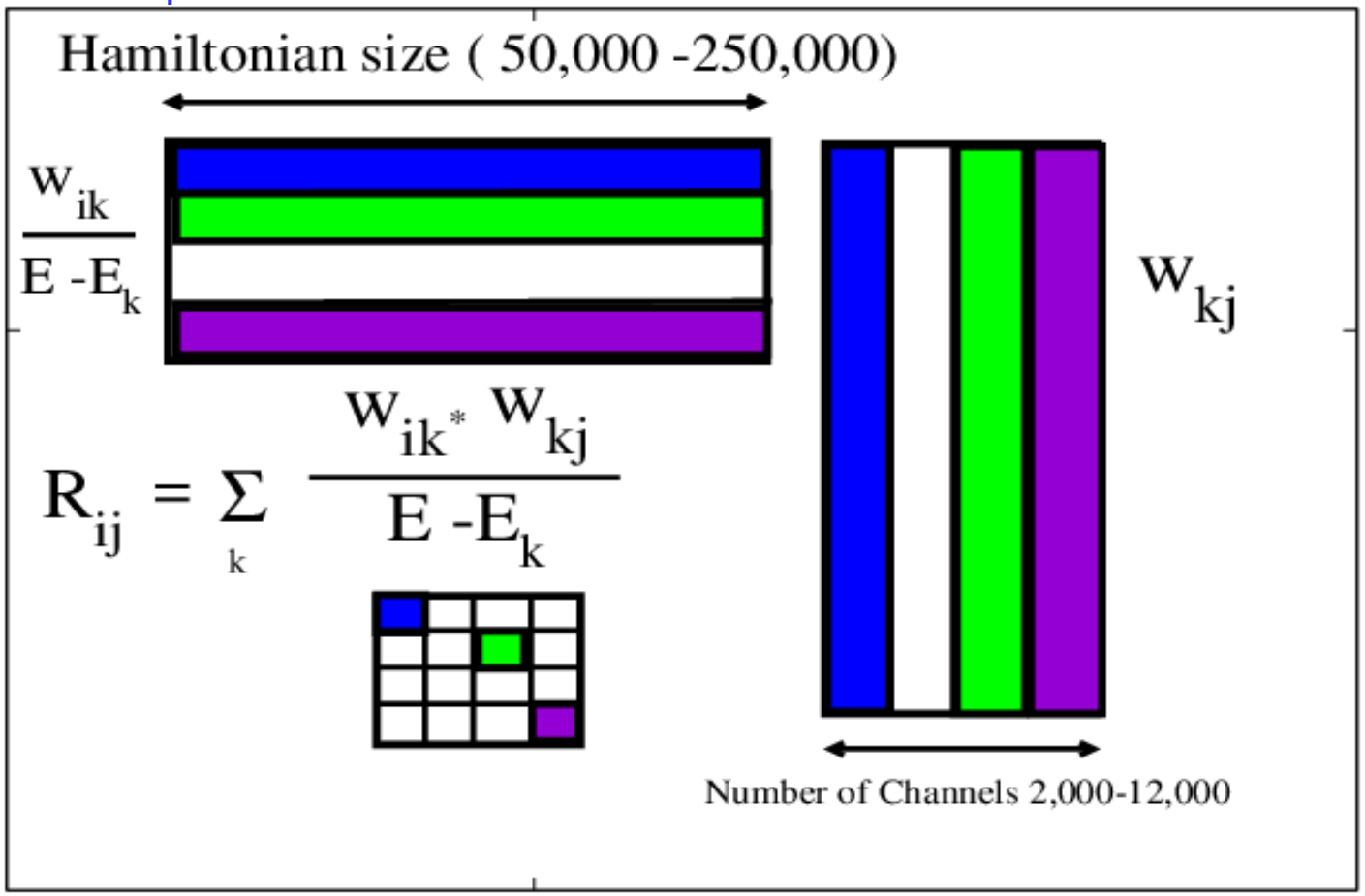
3. Extensive work (in terms of multi-level MPI) is required if we are to build Hamiltonian matrices in excess of 250K by 250 K in a finite period of time.

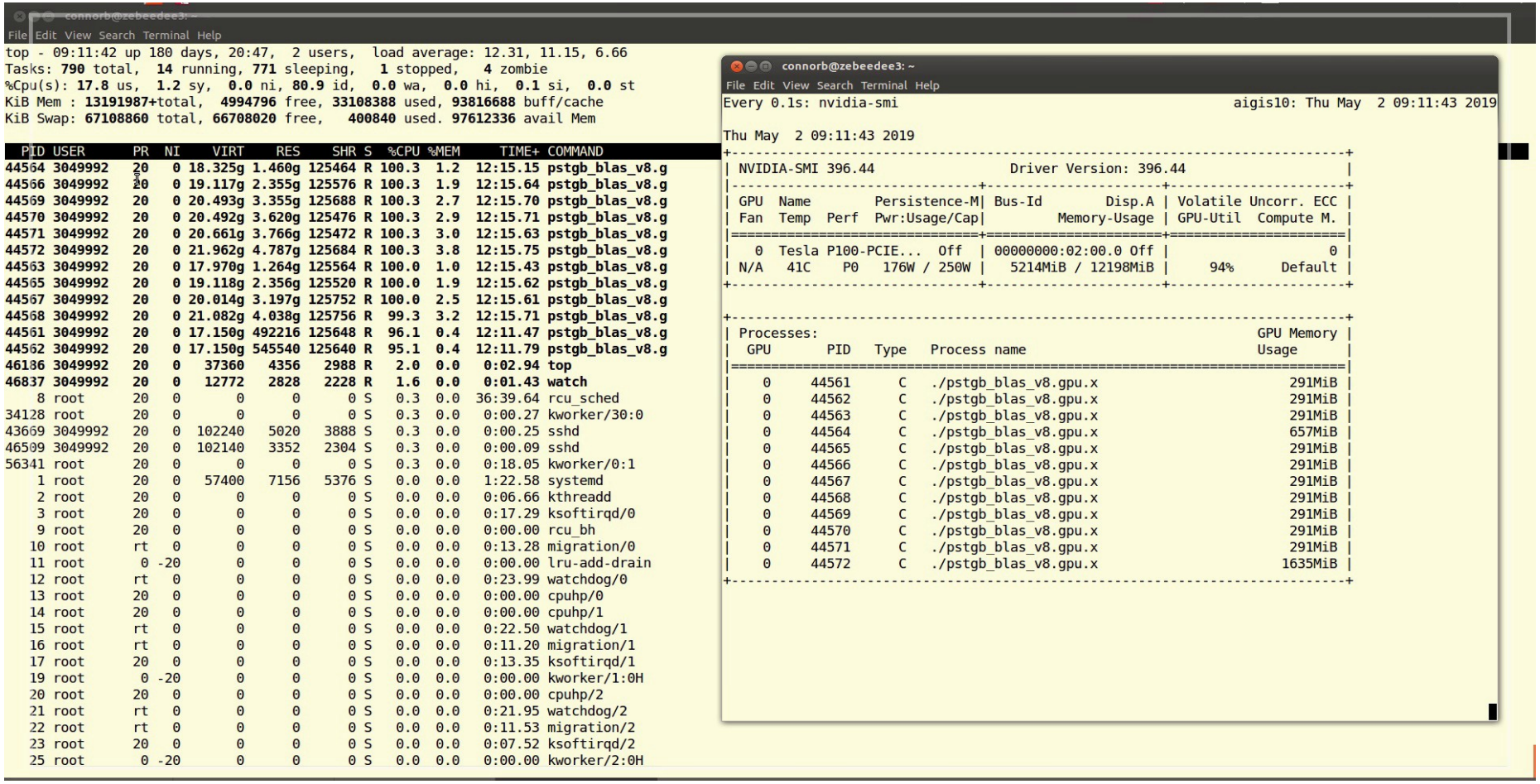
4. Of particular note is the inclusion of GPU (Graphical Processing Units), that assist greatly with dense matrix multiplies

You have mentioned 10,000 channels and matrices exceeding 100 K by 100 K, but does not the R-matrix have to be calculated for every energy ?

10,000*10,000*100,000= 10^13 operations ….. and modern CPUs only are of the order 10^9 operations per sec. Do you wait an hour per energy point ?

No fortunately, we can employ GPUs (Graphical Processing Units) for the dense matrix multiplies




connorb@zebeedee3: ~
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top - 09:11:42 up 180 days, 20:47, 2 users, load average: 12.31, 11.15, 6.66
Tasks: 790 total, 14 running, 771 sleeping, 1 stopped, 4 zombie
%Cpu(s): 17.8 us, 1.2 sy, 0.0 ni, 80.9 id, 0.0 wa, 0.0 hi, 0.1 si, 0.0 st
KiB Mem : 13191987+total, 4994796 free, 33108388 used, 93816688 buff/cache
KiB Swap: 67108860 total, 66708020 free, 400840 used. 97612336 avail Mem
PID USER PR NI VIRT RES SHR S %CPU %MEM TIME+ COMMAND
44564 3049992 20 0 18.325g 1.460g 125464 R 100.3 1.2 12:15.15 pstgb_blas_v8.g
44566 3049992 20 0 19.117g 2.355g 125576 R 100.3 1.9 12:15.64 pstgb_blas_v8.g
44569 3049992 20 0 20.493g 3.355g 125688 R 100.3 2.7 12:15.70 pstgb_blas_v8.g
44570 3049992 20 0 20.492g 3.620g 125476 R 100.3 2.9 12:15.71 pstgb_blas_v8.g
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44572 3049992 20 0 21.962g 4.787g 125684 R 100.3 3.8 12:15.75 pstgb_blas_v8.g
44563 3049992 20 0 17.970g 1.264g 125564 R 100.0 1.0 12:15.43 pstgb_blas_v8.g
44565 3049992 20 0 19.118g 2.356g 125520 R 100.0 1.9 12:15.62 pstgb_blas_v8.g
44567 3049992 20 0 20.014g 3.197g 125752 R 100.0 2.5 12:15.61 pstgb_blas_v8.g
44568 3049992 20 0 21.082g 4.038g 125756 R 99.3 3.2 12:15.71 pstgb_blas_v8.g
44561 3049992 20 0 17.150g 492216 125648 R 96.1 0.4 12:11.47 pstgb_blas_v8.g
44562 3049992 20 0 17.150g 545540 125640 R 95.1 0.4 12:11.79 pstgb_blas_v8.g
46186 3049992 20 0 37360 4356 2988 R 2.0 0.0 0:02.94 top
46837 3049992 20 0 12772 2828 2228 R 1.6 0.0 0:01.43 watch
8 root 20 0 0 0 0 S 0.3 0.0 36:39.64 rcu_sched
34128 root 20 0 0 0 0 S 0.3 0.0 0:00.27 kworker/30:0
43669 3049992 20 0 102240 5020 3888 S 0.3 0.0 0:00.25 sshd
46509 3049992 20 0 102140 3352 2304 S 0.3 0.0 0:00.09 sshd
56341 root 20 0 0 0 0 S 0.3 0.0 0:18.05 kworker/0:1
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2 root 20 0 0 0 0 S 0.0 0.0 0:06.66 kthreadd
3 root 20 0 0 0 0 S 0.0 0.0 0:17.29 ksoftirqd/0
9 root 20 0 0 0 0 S 0.0 0.0 0:00.00 rcu_bh
10 root rt 0 0 0 0 S 0.0 0.0 0:13.28 migration/0
11 root 0 -20 0 0 0 S 0.0 0.0 0:00.00 lru-add-drain
12 root rt 0 0 0 0 S 0.0 0.0 0:23.99 watchdog/0
13 root 20 0 0 0 0 S 0.0 0.0 0:00.00 cpuhp/0
14 root 20 0 0 0 0 S 0.0 0.0 0:00.00 cpuhp/1
15 root rt 0 0 0 0 S 0.0 0.0 0:22.50 watchdog/1
16 root rt 0 0 0 0 S 0.0 0.0 0:11.20 migration/1
17 root 20 0 0 0 0 S 0.0 0.0 0:13.35 ksoftirqd/1
19 root 0 -20 0 0 0 S 0.0 0.0 0:00.00 kworker/1:0H
20 root 20 0 0 0 0 S 0.0 0.0 0:00.00 cpuhp/2
21 root rt 0 0 0 0 S 0.0 0.0 0:21.95 watchdog/2
22 root rt 0 0 0 0 S 0.0 0.0 0:11.53 migration/2
23 root 20 0 0 0 0 S 0.0 0.0 0:07.52 ksoftirqd/2
25 root 0 -20 0 0 0 S 0.0 0.0 0:00.00 kworker/2:0H
connorb@zebeedee3: ~
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Every 0.1s: nvidia-smi aigis10: Thu May 2 09:11:43 2019
Thu May 2 09:11:43 2019
| NVIDIA-SMI 396.44 Driver Version: 396.44 |
GPU Name Persistence-M	Bus-Id Disp.A	Volatile Uncorr. ECC
Fan Temp Perf Pwr:Usage/Cap	Memory-Usage	GPU-Util Compute M.
0 Tesla P100-PCIE... Off	00000000:02:00.0 Off	0
N/A 41C P0 176W / 250W	5214MiB / 12198MiB	94% Default
Processes: GPU Memory
GPU PID Type Process name Usage
0 44561 C ./pstgb_blas_v8.gpu.x 291MiB
0 44562 C ./pstgb_blas_v8.gpu.x 291MiB
0 44563 C ./pstgb_blas_v8.gpu.x 291MiB
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0 44572 C ./pstgb_blas_v8.gpu.x 1635MiB

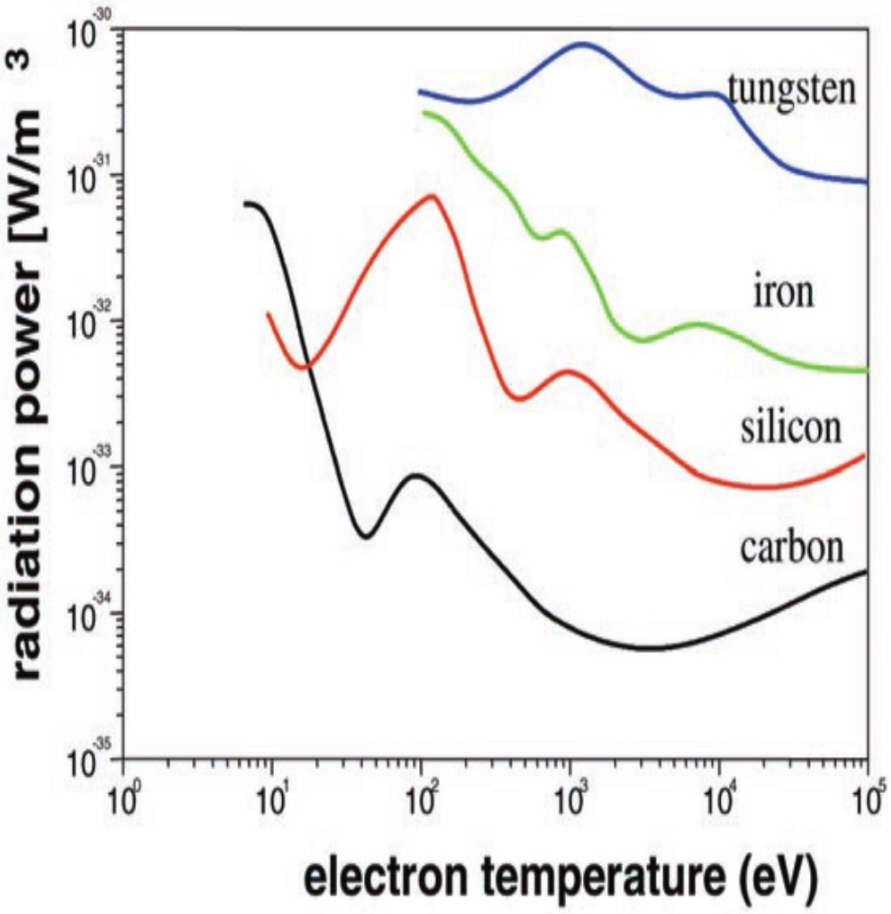
… I will talk about R-matrix results, but I'm aware of other approaches Duck-Hee Kwon (BEB), M S Pindzola (TDCC: configuration-average), Murakami (DWA: Cowan & Hullac)

Neutral Tungsten Excitation/Ionization

why tungsten ?

The merits of various wall-facing materials, from carbon to tungsten

- ***Allowable impurity concentration lower for high-Z materials***
  - High-Z materials radiate much more than previously used materials
  - Radiation significant enough to denigrate plasma performance
    - Concentration needs to be less than ~1E-4 (Putterich)
  - Need to accurately quantify and minimize erosion of wall



V. Philipps

Impurity influx diagnostics using SXB coefficients

The intensity of a spectral line can be related to its influx rate [Behringer PPCF **31** 2059 (1989)] . However it must be corrected for the fact that some of the impurity has already ionized

- The number of 'ionizations per photon' (or SXB) is directly proportional to the impurity influx (Γ).

$$\Gamma = \int_0^\infty N_e S^{z \to z+1} N^z \, dx$$

$$\Gamma = \int_0^\infty N_e \frac{S^{z \to z+1}}{A_{i \to j} \frac{N_i}{N^z}} \left(A_{i \to j} \frac{N_i}{N^z} \right) N^z \, dx = \int_0^\infty N_e SXB^z_{i \to j} \left(A_{i \to j} \frac{N_i}{N^z} \right) N^z \, dx$$

Effective ionisation rate (includes ground and excited state ionisation, and shall prove troublesome)

$$SXB^z_{i-j} = \frac{S^{z \to z+1}(Ne, Te)}{A_{i \to j} \frac{N_i}{N_z}(Ne, Te)}$$

Neutral Tungsten

Atomic Structure

- Large scale structure calculations carried out by Mons group (Palmeri/Quinet) using Cowan code (i.e. HFR Hartree Fock Relativistic)
- We have employed (GRASP0): MCDF approach, but tungsten is not perfectly known

TABLE I. Fine-structure energies of W I, in Rydbergs, obtained from the GRASP^0 model (relative to the ground state) compared to the experimental values compiled by Kramida and Shirai [31]. Absolute energy differences are given in the final column.

No	Level	Expt [31]	GRASP^0	$\|\Delta E\|$
1	$5d^4 6s^2\ ^5D_0$	0.00000	0.00000	0.00000
2	$5d^4 6s^2\ ^5D_1$	0.01522	0.00936	0.00586
3	$5d^5(^6S)6s\ ^7S_3$	0.02689	0.02983	0.00294
4	$5d^4 6s^2\ ^5D_2$	0.03030	0.02152	0.00878
5	$5d^4 6s^2\ ^5D_3$	0.04401	0.03477	0.00924
6	$5d^4 6s^2\ ^5D_4$	0.05667	0.04876	0.00791
7	$5d^4 6s^2\ ^3P_0$	0.08683	0.10237	0.01555
8	$5d^4 6s^2\ ^3H_4$	0.11083	0.13697	0.02614
9	$5d^4 6s^2\ ^3P_1$	0.12126	0.13705	0.01579
10	$5d^4 6s^2\ ^3G_3$	0.12164	0.14721	0.02577
11	$5d^4 6s^2\ ^3F_2$	0.12555	0.15237	0.02682
12	$5d^4 6s^2\ ^3D_2$	0.13647	0.16166	0.02519
13	$5d^4 6s^2\ ^3H_5$	0.13733	0.16179	0.02446
14	$5d^4 6s^2\ ^3D_3$	0.14088	0.17371	0.03283
15	$5d^4 6s^2\ ^3G_4$	0.14973	0.17926	0.02953
16	$5d^4 6s^2\ ^3H_6$	0.15499	0.17959	0.02460
17	$5d^4 6s^2\ ^3F_4$	0.15589	0.17179	0.01590
18	$5d^4 6s^2\ ^3F_3$	0.16131	0.18253	0.02122
19	$5d^4 6s(^6D)6p\ ^7F^o_0$	0.17669	0.15519	0.02150
20	$5d^4 6s(^6D)6p\ ^7F^o_1$	0.18284	0.16060	0.02224
21	$5d^4 6s(^6D)6p\ ^7F^o_2$	0.19546	0.17048	0.02498
22	$5d^4 6s(^6D)6p\ ^7D^o_1$	0.19550	0.17862	0.01689
23	$5d^4 6s(^6D)6p\ ^7F^o_3$	0.21002	0.18382	0.02620
24	$5d^4 6s(^6D)6p\ ^7D^o_2$	0.21838	0.19354	0.02484

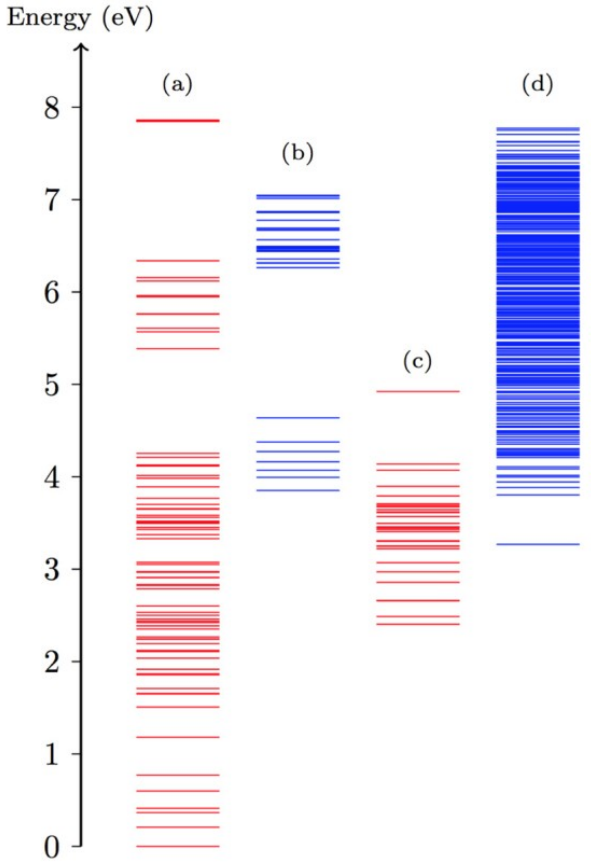


FIG. 1. Energy level spectrum of neutral tungsten with each horizontal line representing an observed fine-structure level. (a) Even parity levels with a configuration and term classification; (b) unclassified even levels; (c) classified odd levels; (d) unclassified odd levels.

Electron-impact excitation of W I/II

- Neutral tungsten (adf04-excitation only) exists

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Dirac *R*-matrix calculations for the electron-impact excitation of neutral tungsten providing noninvasive diagnostics for magnetic confinement fusion

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(Received 13 February 2018; published 7 May 2018)

Neutral tungsten is the primary candidate as a wall material in the divertor region of the International Thermonuclear Experimental Reactor (ITER). The efficient operation of ITER depends heavily on precise atomic physics calculations for the determination of reliable erosion diagnostics, helping to characterize the influx of tungsten impurities into the core plasma. The following paper presents detailed calculations of the atomic structure of neutral tungsten using the multiconfigurational Dirac-Fock method, drawing comparisons with experimental measurements where available, and includes a critical assessment of existing atomic structure data. We investigate the electron-impact excitation of neutral tungsten using the Dirac *R*-matrix method, and by employing collisional-radiative models, we benchmark our results with recent Compact Toroidal Hybrid measurements. The resulting comparisons highlight alternative diagnostic lines to the widely used 400.88-nm line.

DOI: 10.1103/PhysRevA.97.052705

Representative collision strengths for W I using DARC code

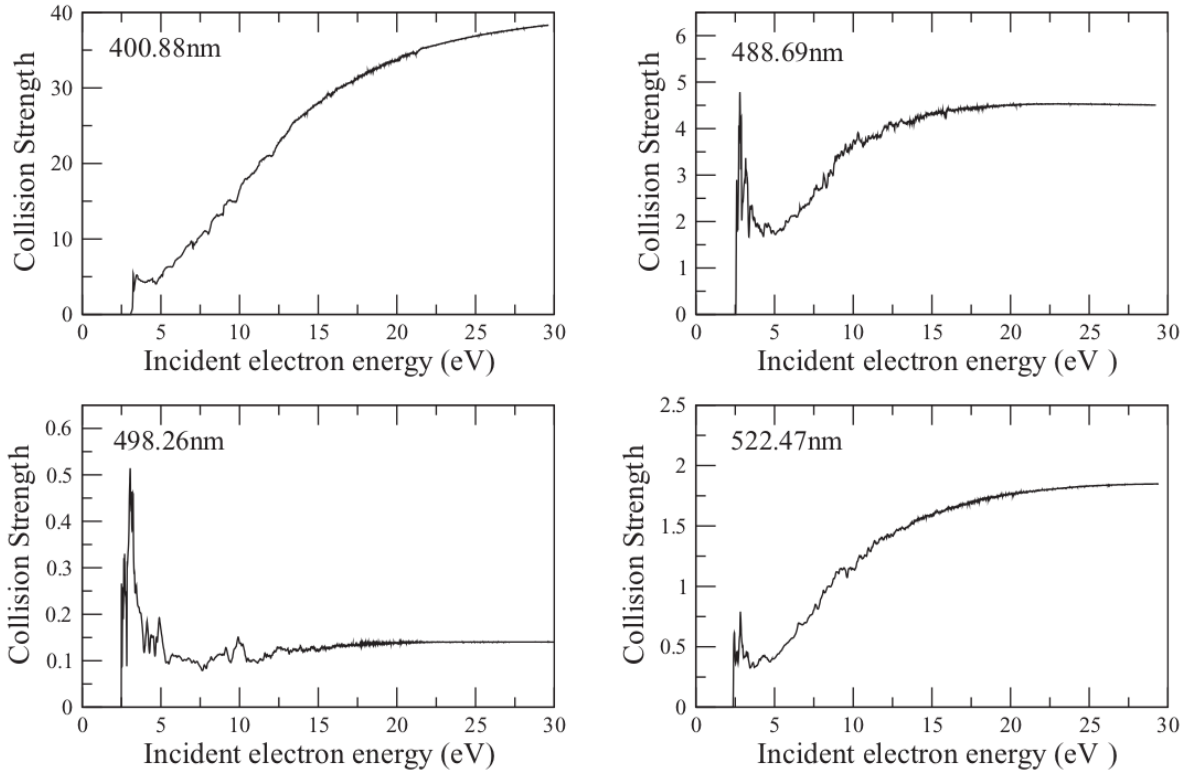
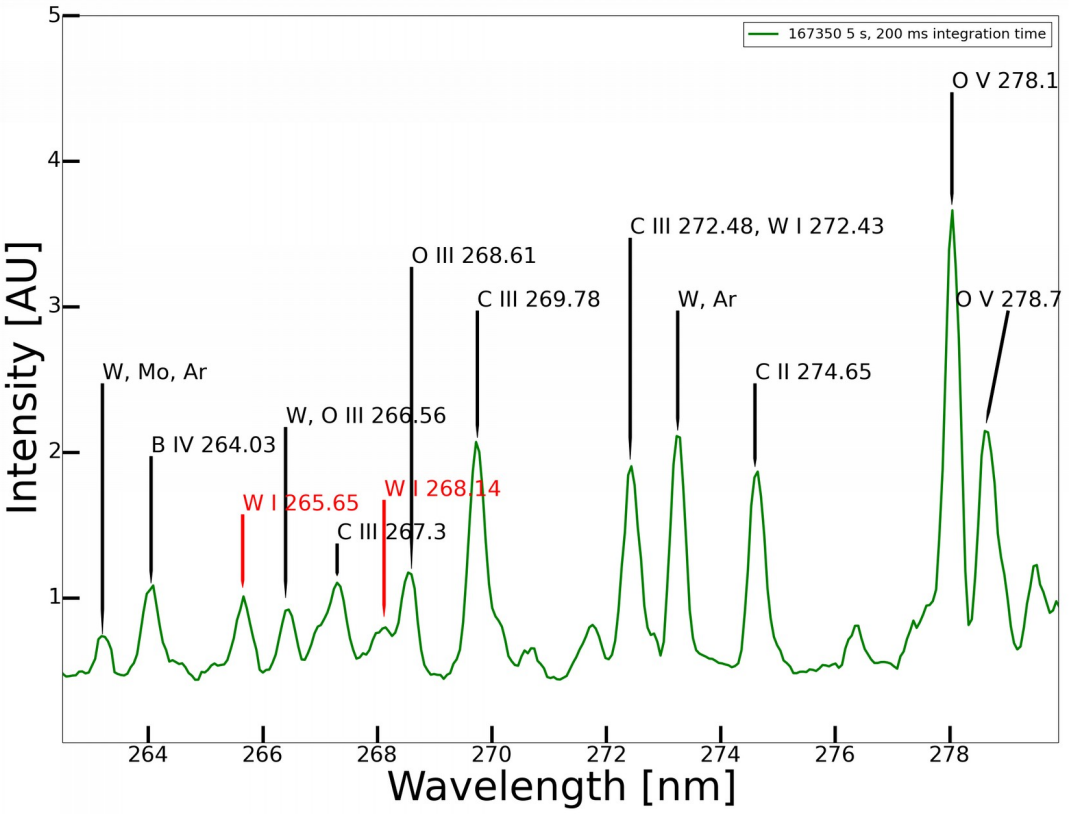


FIG. 2. Plot showing collision strengths for the $5d^4 6s 6p\ ^7P^o_4 \rightarrow 5d^5 6s\ ^7S_3$ (400.88 nm), $5d^4 6s 6p\ ^7F^o_5 \rightarrow 5d^4 6s^2\ ^5D_4$ (488.69 nm), $5d^4 6s 6p\ ^7F^o_1 \rightarrow 5d^4 6s^2\ ^5D_0$ (498.26 nm), and $5d^4 6s 6p\ ^7D^o_2 \rightarrow 5d^4 6s^2\ ^5D_3$ (522.47 nm) transitions from the present *R*-matrix calculation.

Overview of CTH measurements for Tungsten

Looking for multiple ion stages of Tungsten within the same wavelength window

- W I 265.65 nm observed to be on the order of the widely used 400.89 line:
  - Atomic calculations using ADAS confirm that W I 265.65 nm is strong for divertor temperatures and densities ~1E19 m^3 ~ 10eV
- Multiple W I lines in the region around 265.65 region:
  - High density of lines in this region motivates higher resolution spectrometer/instrument



Tungsten ground and excited state ionisation (problematic)

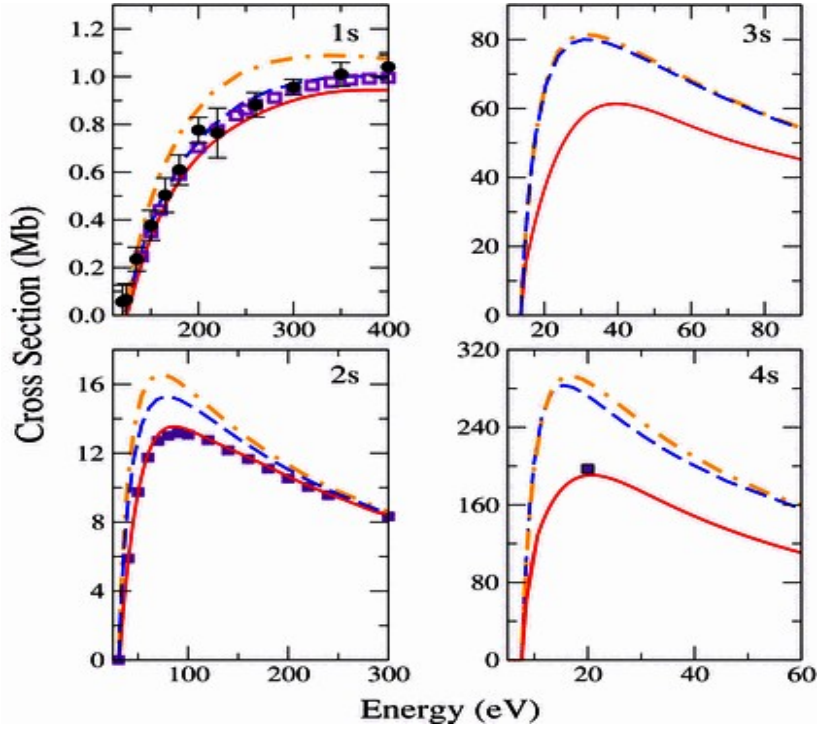
A little context for RMPS ionisation

R-matrix/RMPS : ionisation

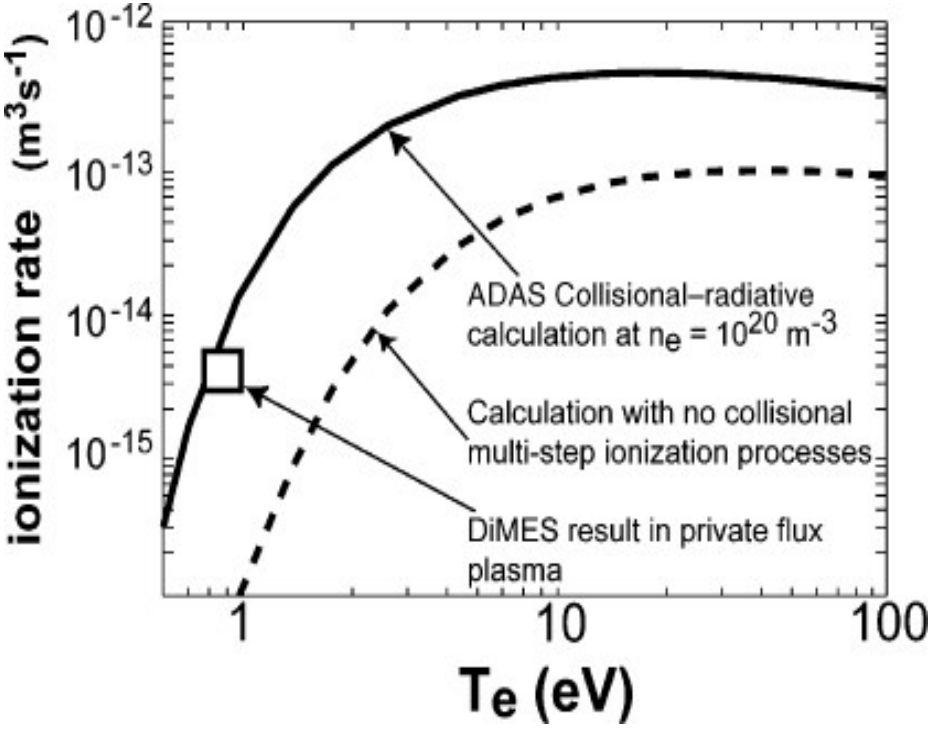
We have the capability to calculate electron-impact ionisation (ground & metastable) for light to mid-Z elements. With the availability of Prof Badnell's DRMPS (Dirac R-matrix with Pseudo-States) code, the heavier elements are now feasible.

It is the accuracy of the excited states that can prove problematic

Neutral Hydrogen



Neutral Lithium Effective Ionisation



Total electron-impact ionisation of neutral and singly ionised Tungsten

… the R-matrix results are close to the Distorted Wave results

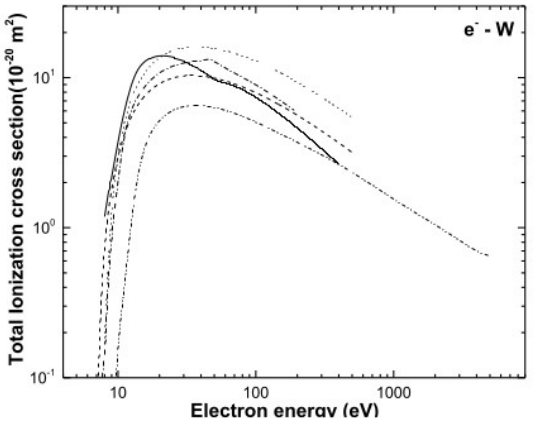


Fig. 1 Total ionization cross sections of W atoms plotted as a function of incident electron energy, solid curve: present DWA results in HULLAC [19], dashed and dotted curves: present DWA results in Cowan formalism with fine-structure and configuration mode; dash-dotted curve: results of [12] and dash-dot-dotted curve: results of [11].

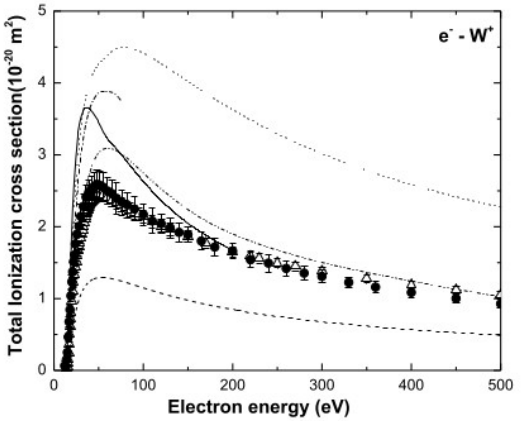
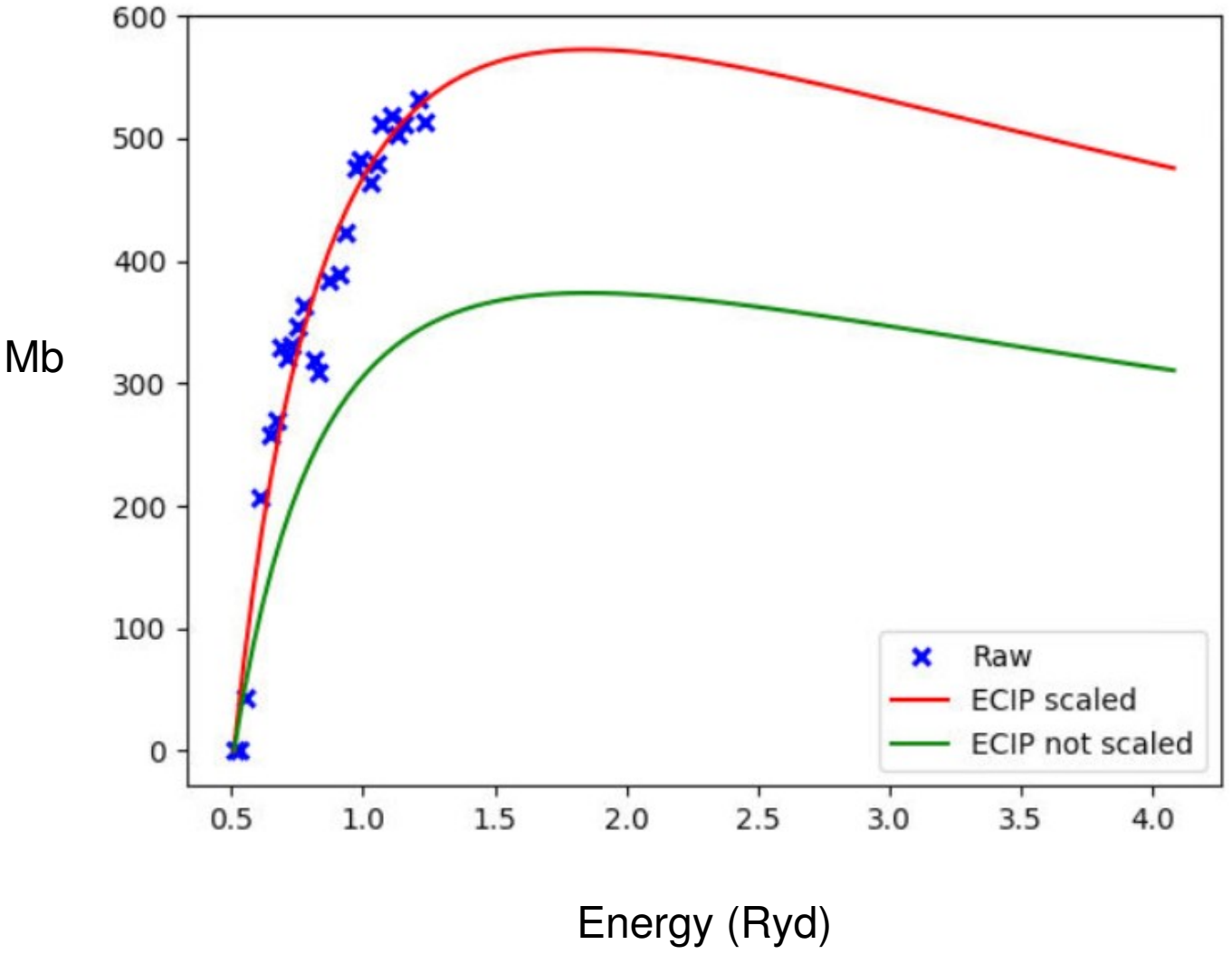


Fig. 3 Total ionization cross sections of W^+ ions plotted as a function of incident electron energy, dash-dot-dotted curve: results of [10]; dash-dotted curve: results of [8]; solid circles and hollow triangles: measurements [14] and [13]; other curves are the same as Fig. 1.

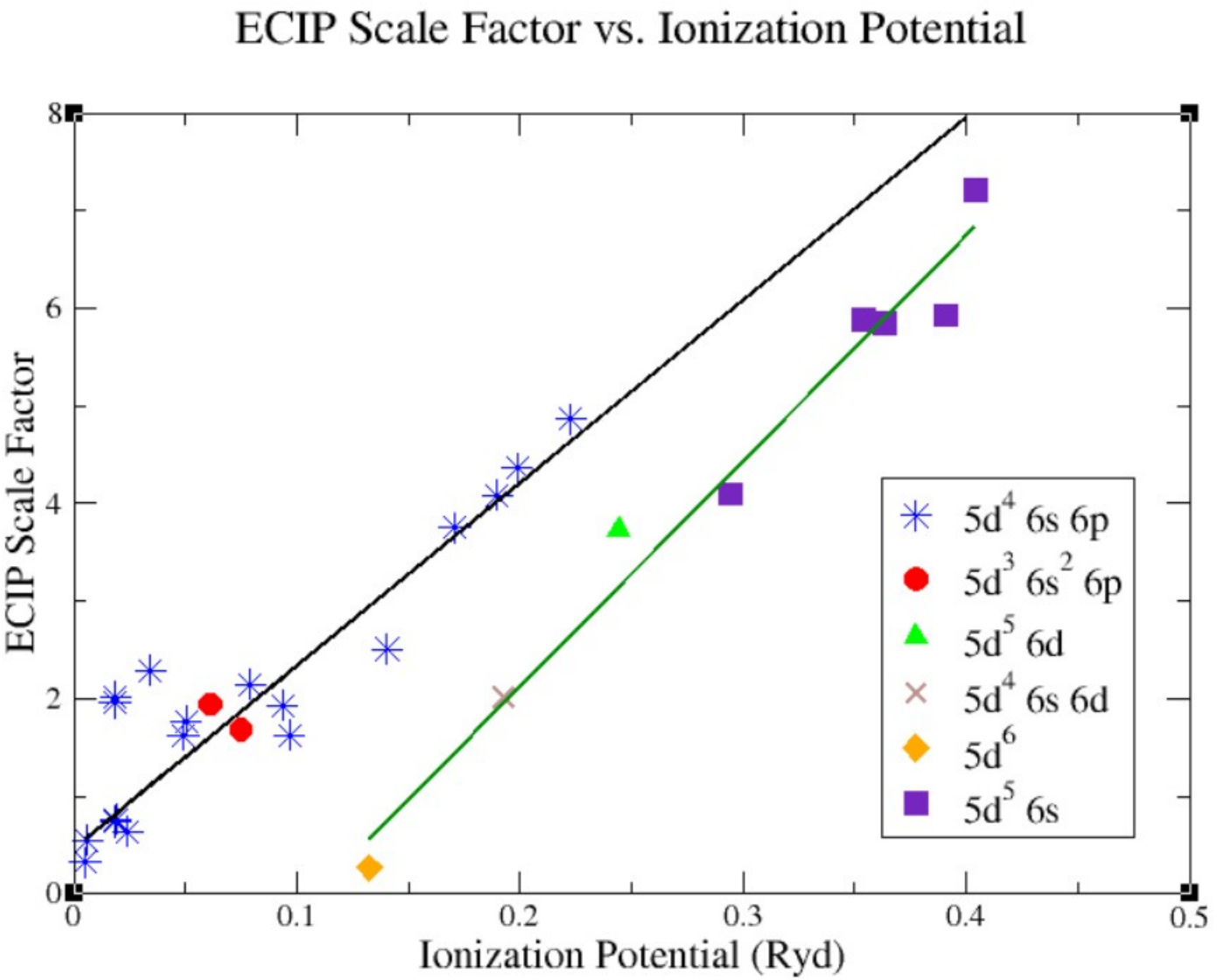
However, these are not the ionisation cross sections we should be concerned about (metastables !)

We may have to rely on the ECIP method to account for the excited state ionisation



(slide kindly provided by Connor Favreau)

There may be a linear scaling factor based upon the RMPS results for the ECIP

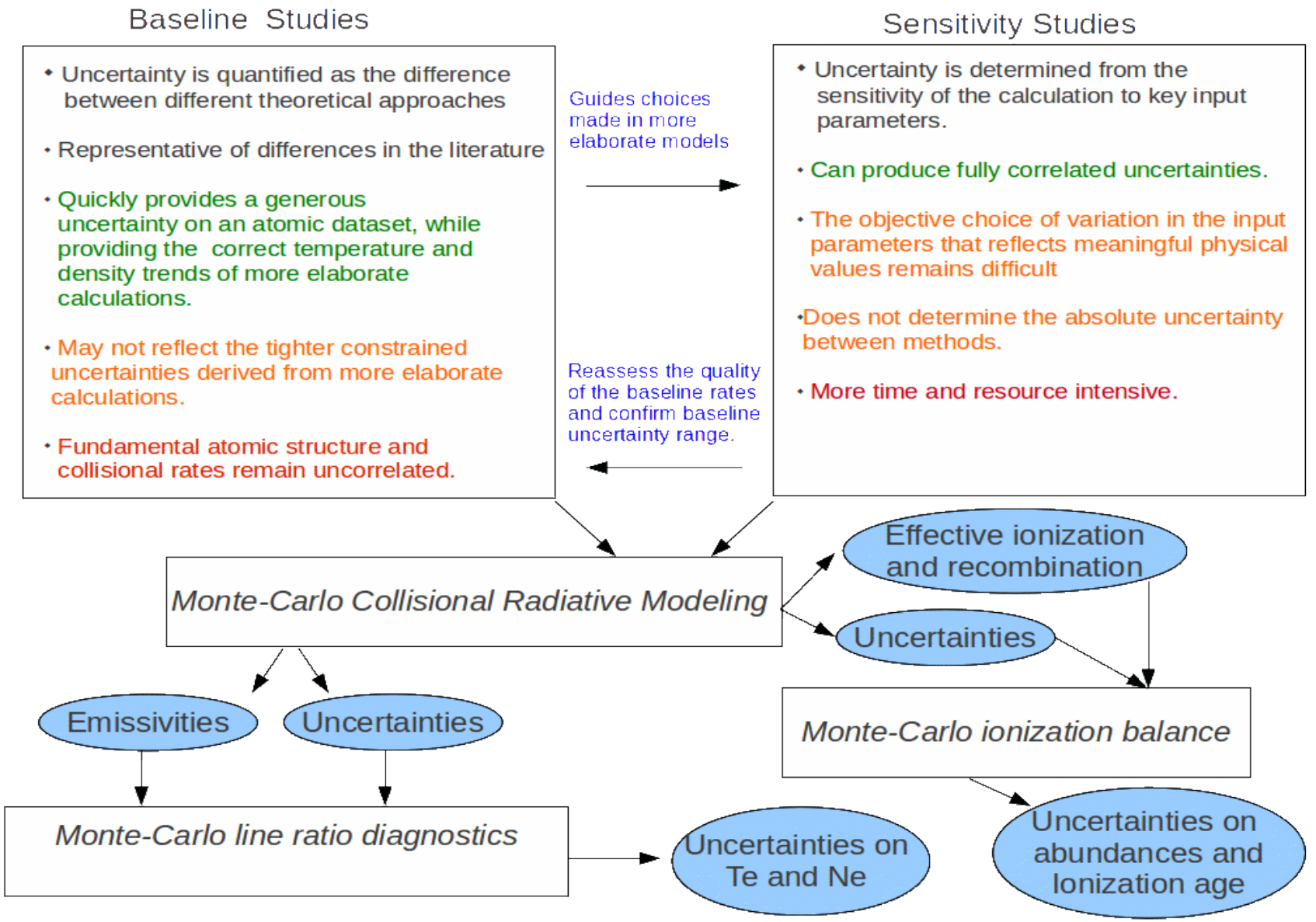


Uncertainty quantification

(progress on light fusion related elements, heavier elements require substantial resources)

Uncertainty in Theoretical Calculations

ICFT script



Thank-you for your attention