Recent progress on SXB coefficients for complex species and electron-impact excited state ionization for light species

Stuart Loch, Jonathan Pearce, Mitch Pindzola,
Don Griffin, Teck Lee,
Shahin Abdel-Naby, Connor Ballance,

Auburn University, Auburn, AL
Rollins College,Winter Park, FL

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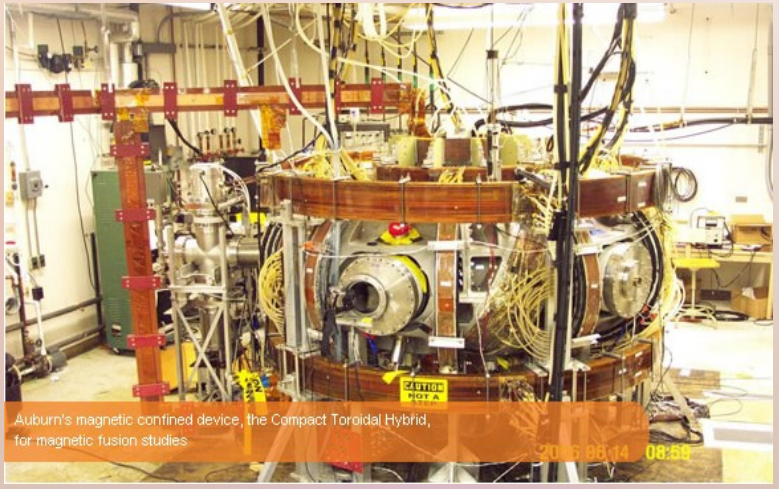
Outline

- Brief update on SXBs for Mo^{+} and W^{3+}
- Brief review of excited state ionization, progress for light species.
  - An interesting case for neutral nitrogen
- Future plans



ADAS course, 2011

ALEXIS

MDPX

Impurity influx diagnostics using SXB coefficients

The intensity of a spectral line can be related to its influx rate [Behringer PPCF **31** 2059 (1989)]. The number of 'ionizations per photon' (or SXB) is directly proportional to the impurity influx (Γ).

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

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

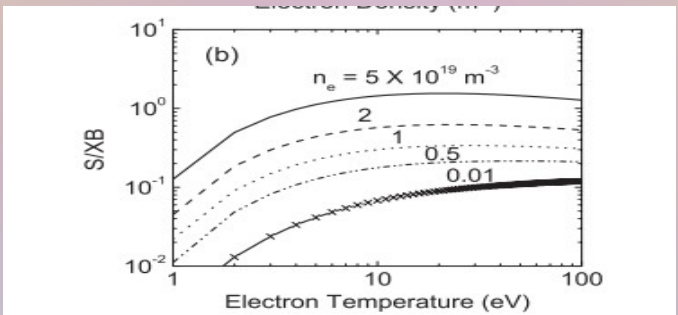


Figure 2. (*a*) S/XB dependence on electron density parametrized with electron temperature for lithium. (*b*) S/XB dependence on electron temperature parametrized with electron density. The S/XB ratio is obtained from the ADAS collisional–radiative atomic rate calculation package [19].

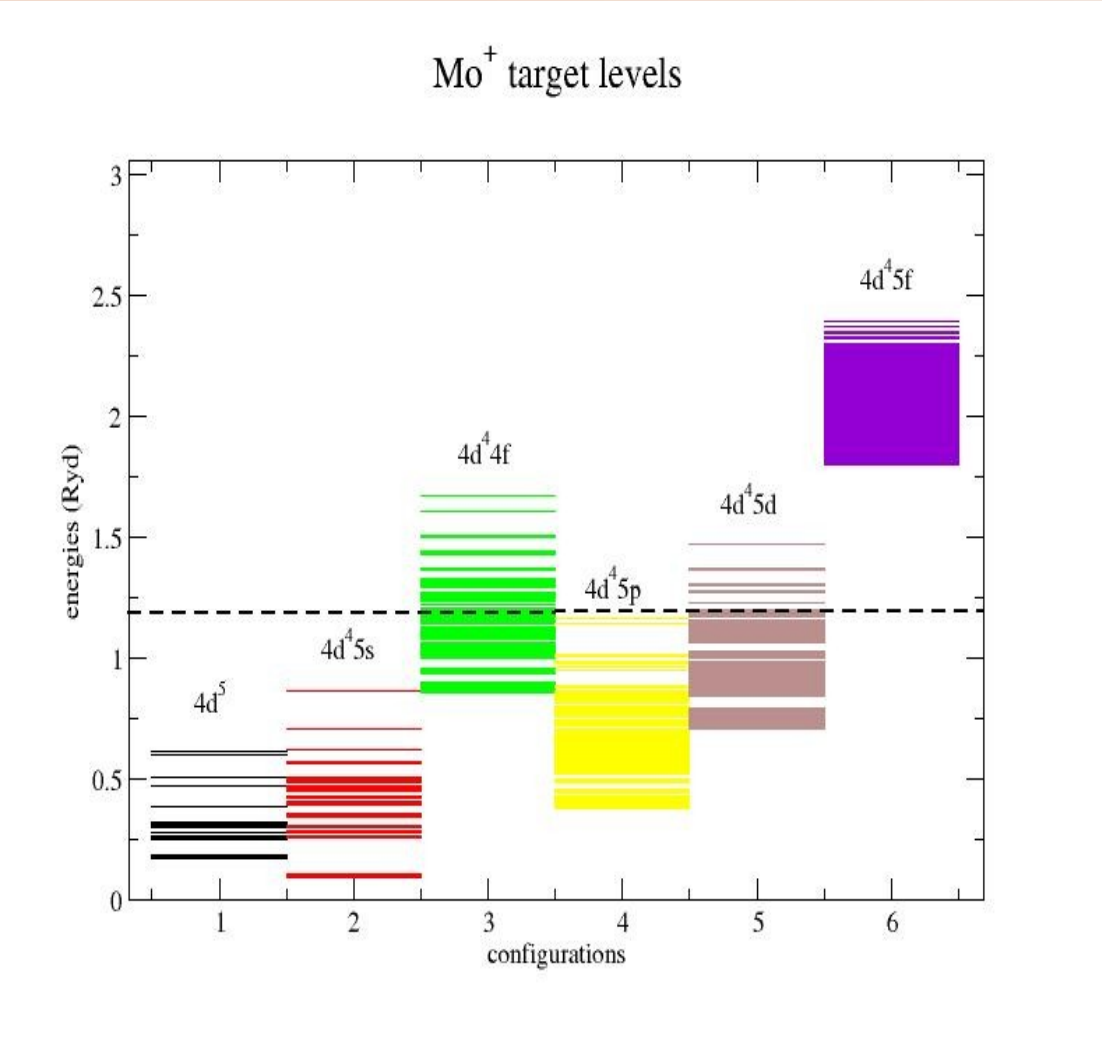
where

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

*Taken from Allain et al. Nucl. Fusion **44** 655 (2004)*

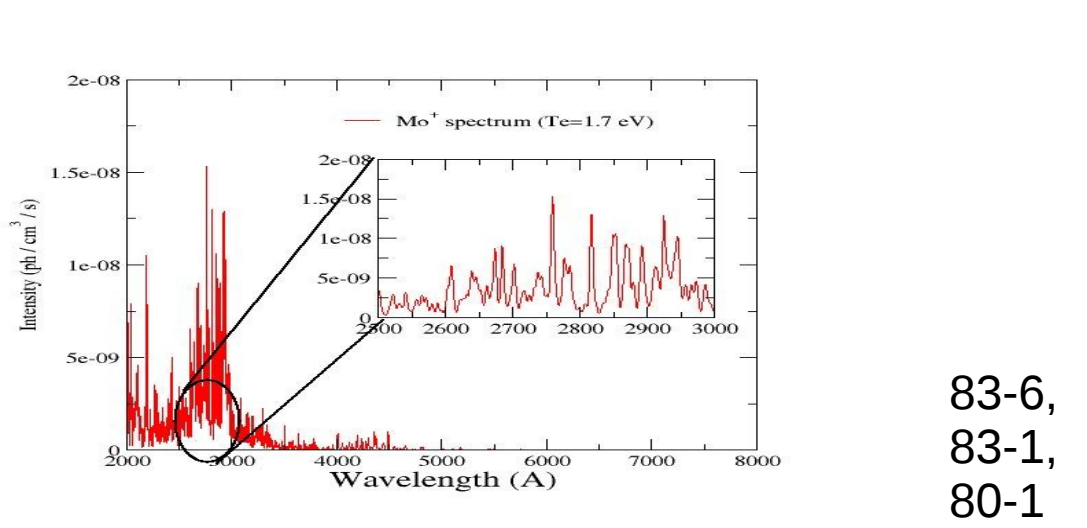
The atomic structure for our Mo^+ excitation calculation

- Recently, SXB values for **neutral Mo** were measured at PISCES-B [Nishijima et al. *J. Phys. B* **43** 225701 (2010)].
  - Factors of 2-5 difference in their measurements compared with the existing ADAS. data.
- We decided to start with Mo^+, to develop a method for non-perturbative calculations for complex systems.
  - Atomic structure from Dirac-Hartree-Fock program (GRASP0).
  - included $4d^5$, $4d^45s$, and $4d^45p$.(280 levels)
  - Strong mixing.

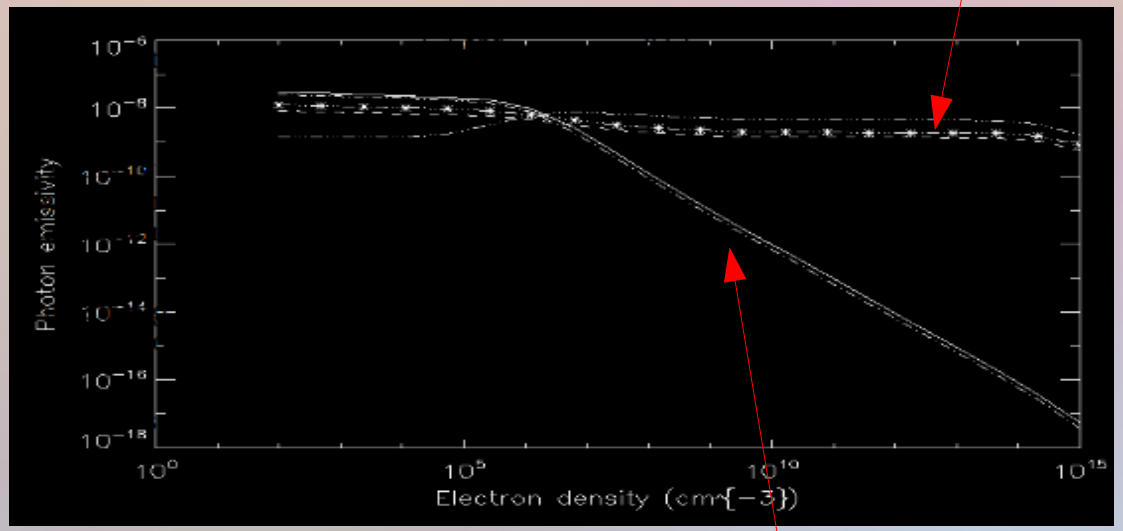


The calculation of SXBs for Mo^+

- Our Mo^+ calculation included.
  - LS R-matrix with pseudostates calculations for the ionization.
  - Dirac R-matrix calculations for the excitation data.
- There were no strong lines in the visible, but many in the UV.
- **The key lesson was the value of shifting to NIST energies during the R-matrix calculation.**

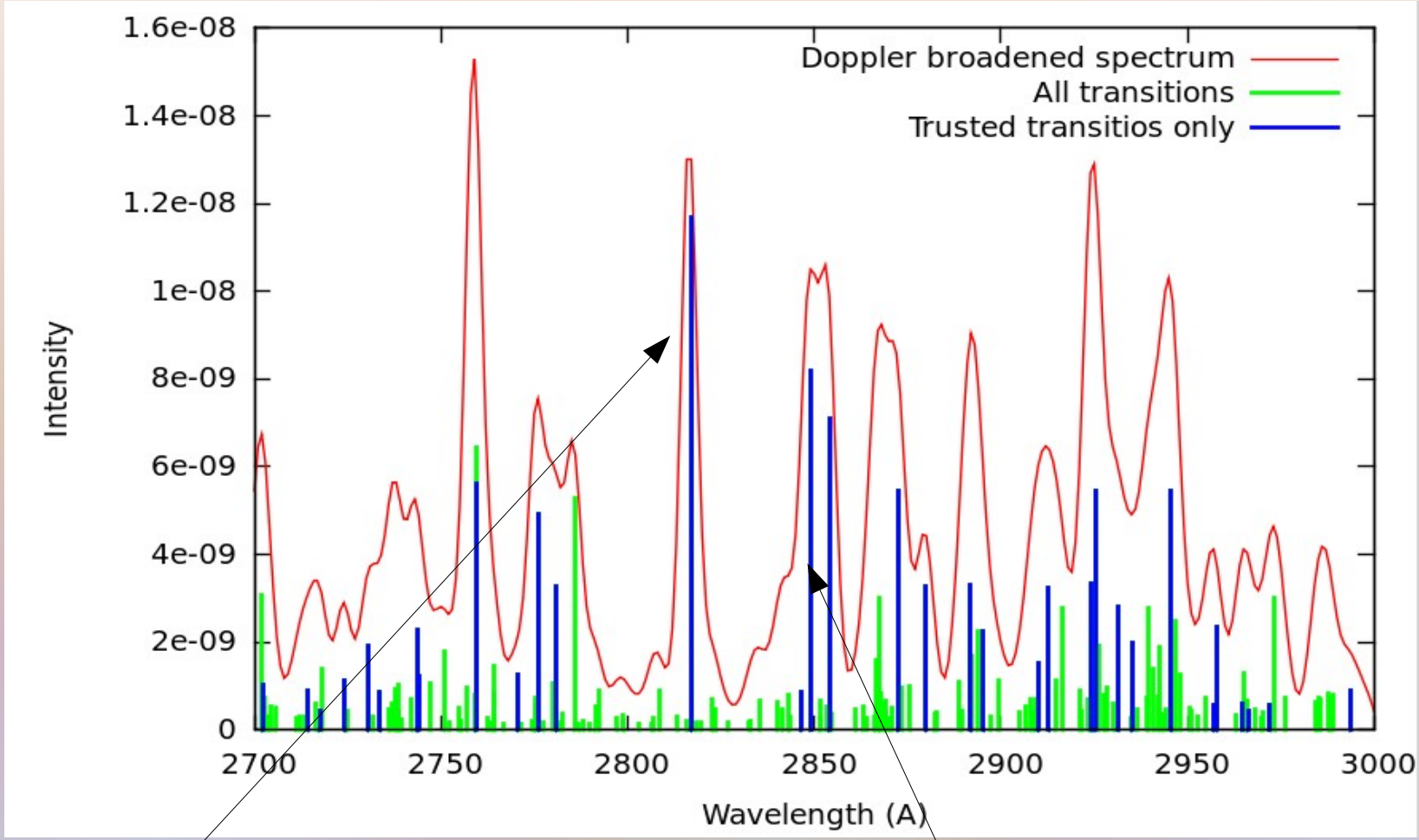


83-6, 83-1, 80-1



6-1 and 5-1

Identifying the 'trusted' spectral lines

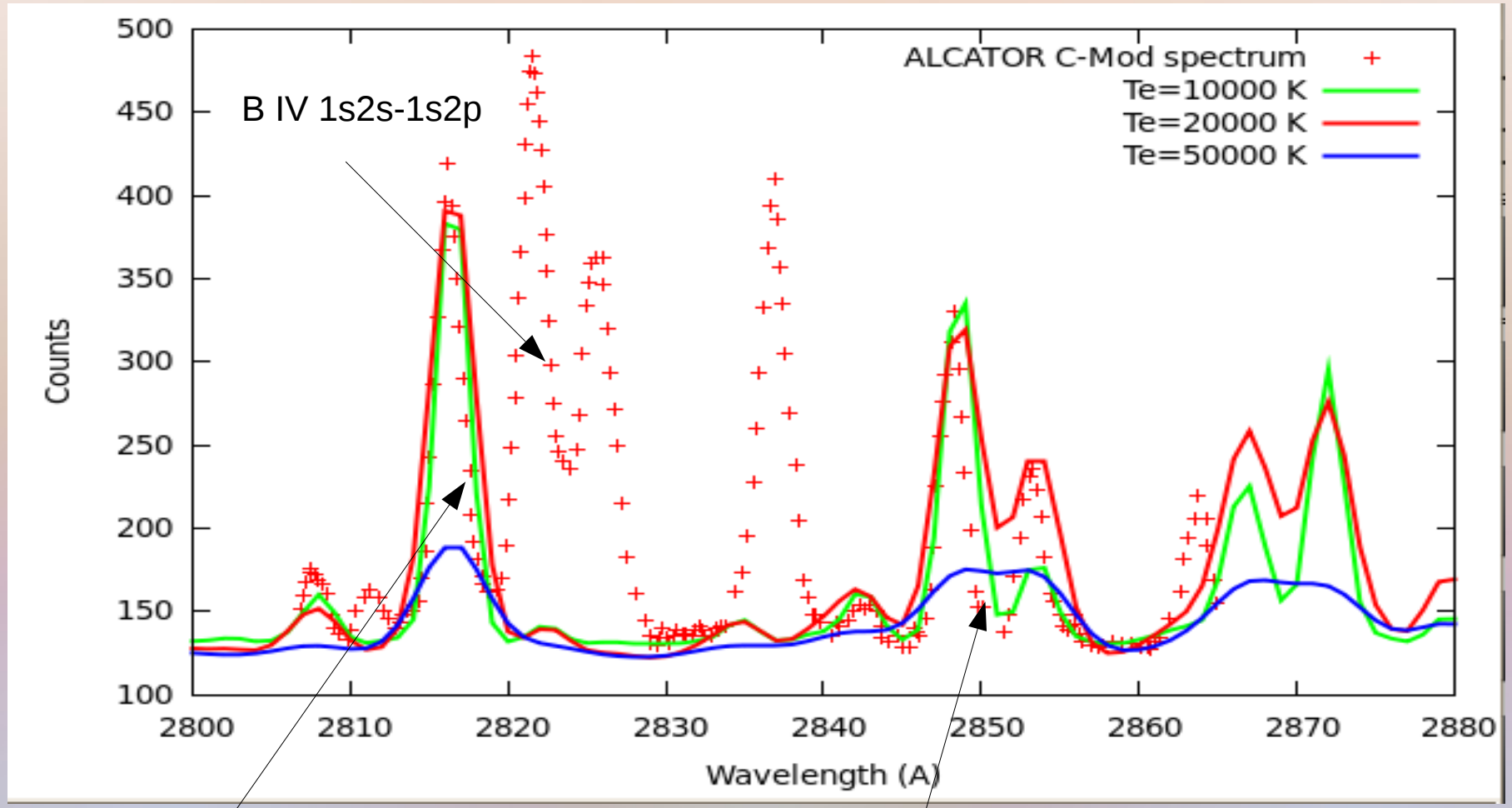


$4d^4\ 5p\ (^6F_{5.5}) – 4d^4\ 5s\ (^6D_{4.5})$

$4d^4\ 5p\ (^6F_{4.5}) – 4d^4\ 5s\ (^6D_{3.5})$

$4d^4\ 5p\ (^4I_{7.5}) – 4d^4\ 5s\ (^4H_{6.5})$

Comparison with ALCATOR C-Mod spectrum (at MIT)



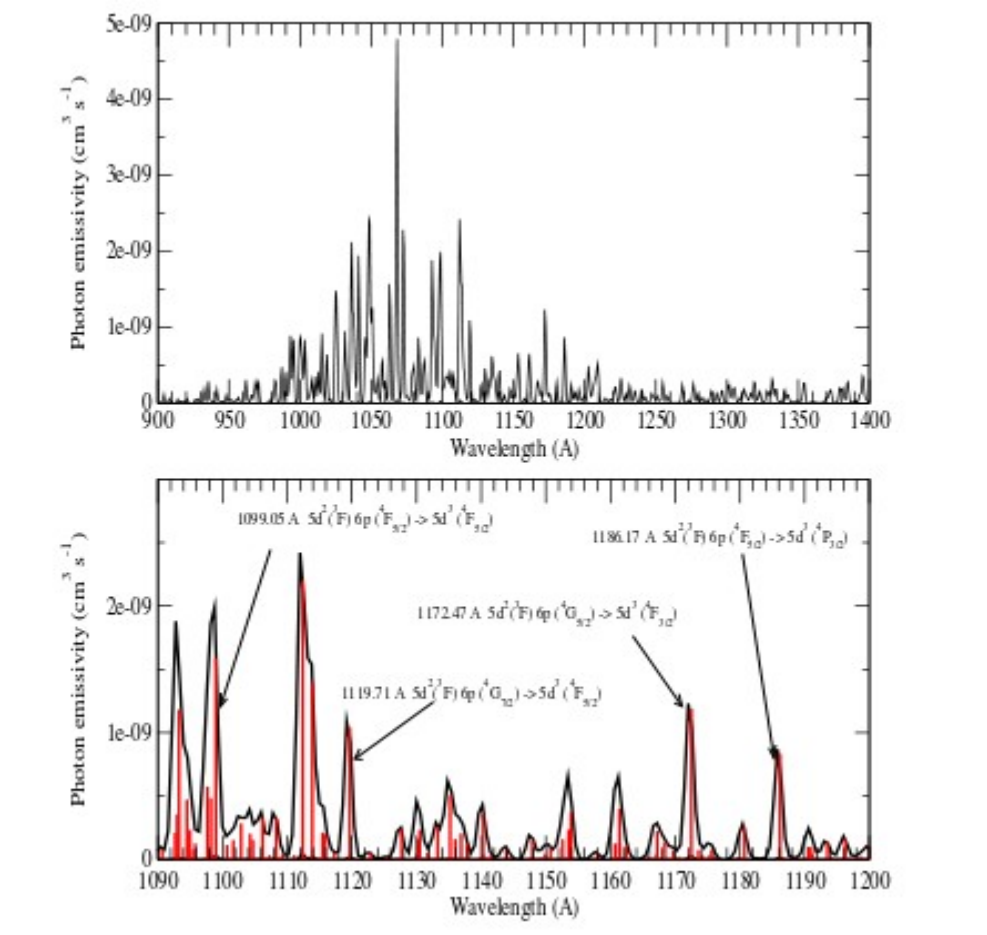
$4d^4\ 5p\ (^6F_{5.5}) - 4d^4\ 5s\ (^6D_{4.5})$ **[98-6]**

$4d^4\ 5p\ (^6F_{4.5}) - 4d^4\ 5s\ (^6D_{3.5})$ **[95-5]**

$4d^4\ 5p\ (^4I_{7.5}) - 4d^4\ 5s\ (^4H_{6.5})$ **[147-38]**

W^{3+} SXBs

- We used our methodology from Mo^{+}, and calculated data for W^{3+}.



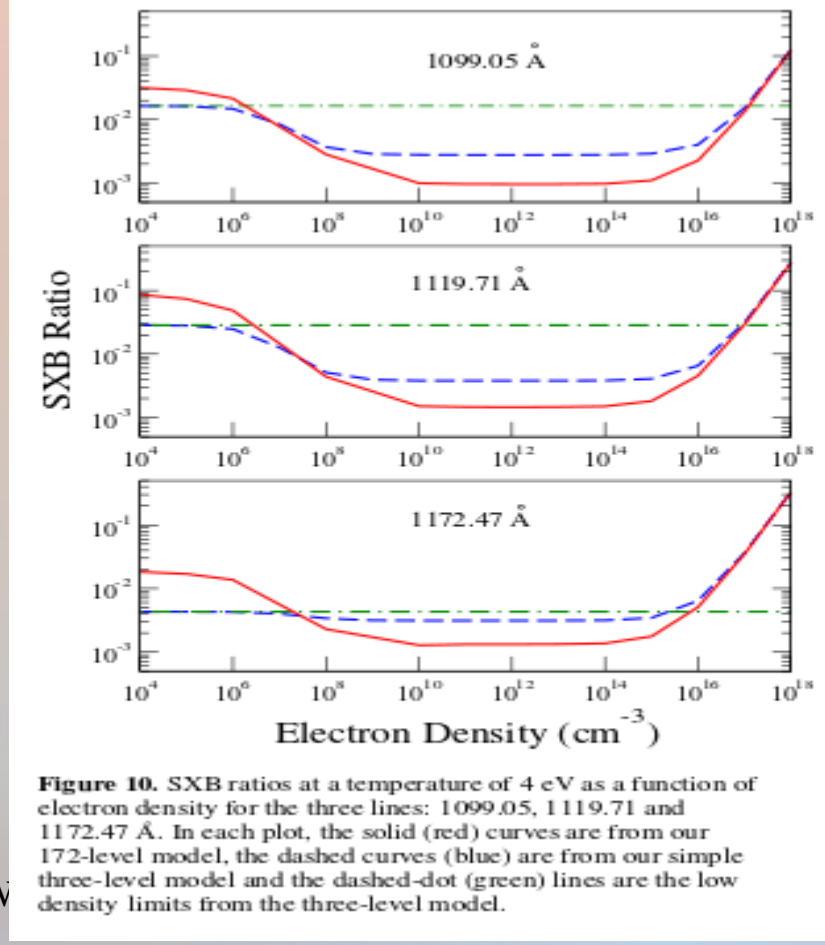
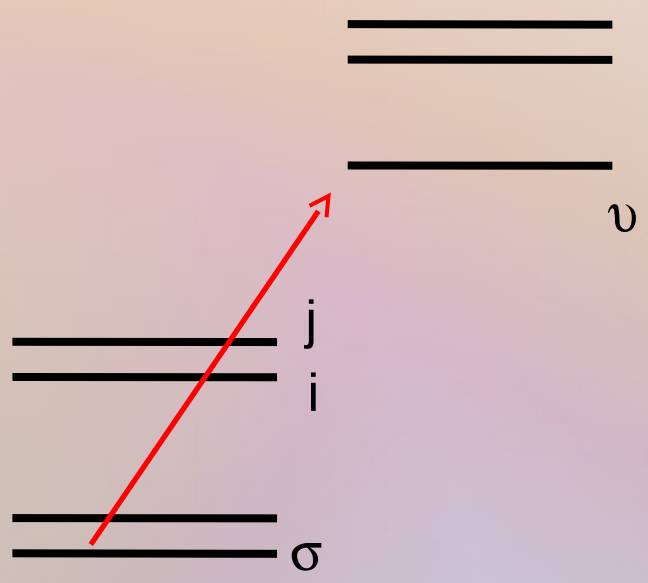


Figure 10. SXB ratios at a temperature of 4 eV as a function of electron density for the three lines: 1099.05, 1119.71 and 1172.47 Å. In each plot, the solid (red) curves are from our 172-level model, the dashed curves (blue) are from our simple three-level model and the dashed-dot (green) lines are the low density limits from the three-level model.

The GCR ionization rate coefficients for light species

The GCR ionization coefficient accounts for both direct ionization, excitation-autoionization, and stepwise ionization, including collisional redistribution effects.

$$S_{CD,\sigma\to\upsilon} = \left(\mathscr{S}_{\upsilon\sigma} - \sum_{j=1}^{O} \mathscr{S}_{\upsilon j} \sum_{i=1}^{O} \mathscr{C}_{ji}^{-1} \mathscr{C}_{i\sigma}\right)$$



GCR ionization

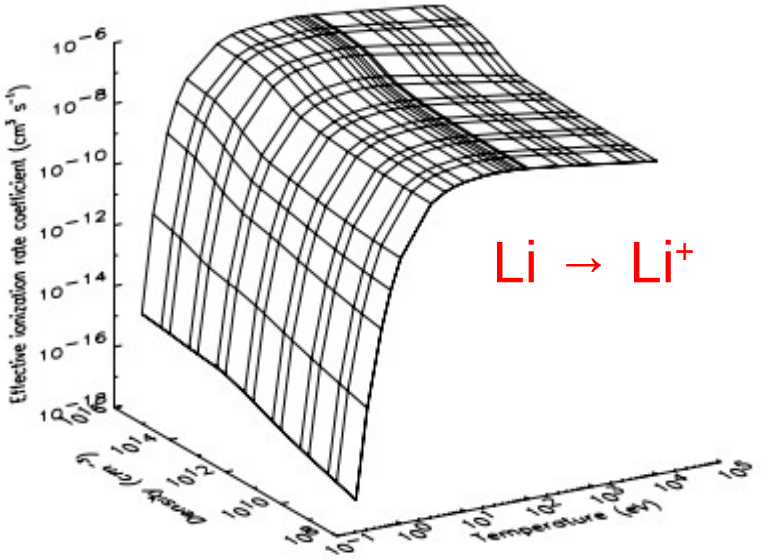
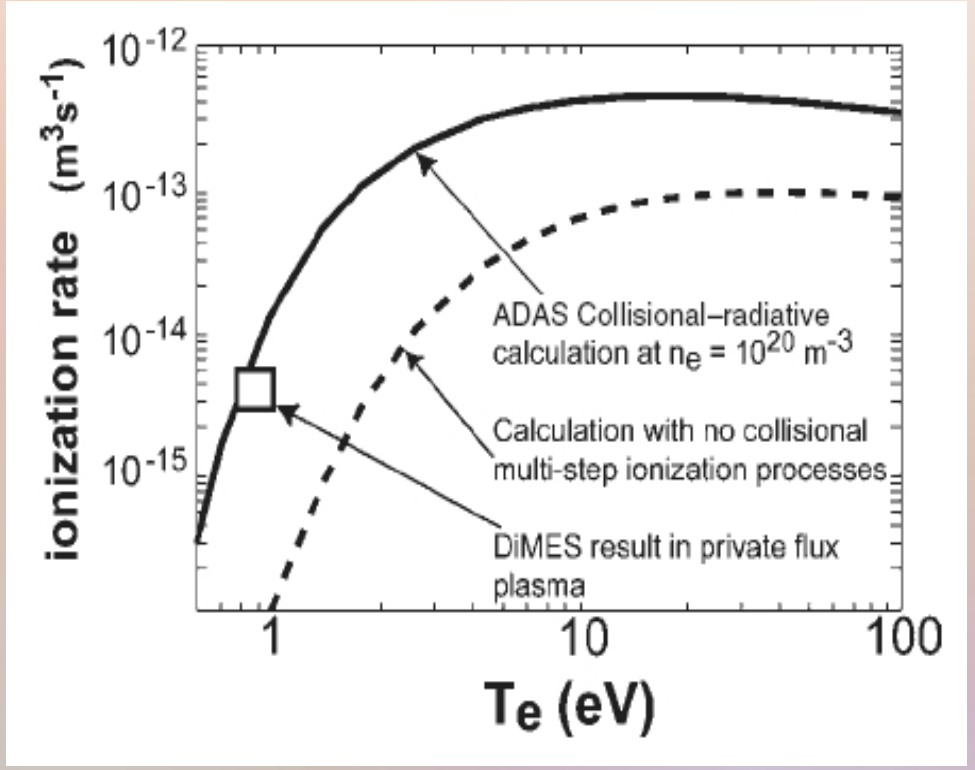


Fig. 8. Effective ionization rate coefficient for the ionization process $e + Li(1s^2\,2s\,^2S) \rightarrow Li^+(1s^2\,^2S) + 2e$ as a function of electron temperature and density. Note that the density dependence comes in through the role of ionization from excited states.

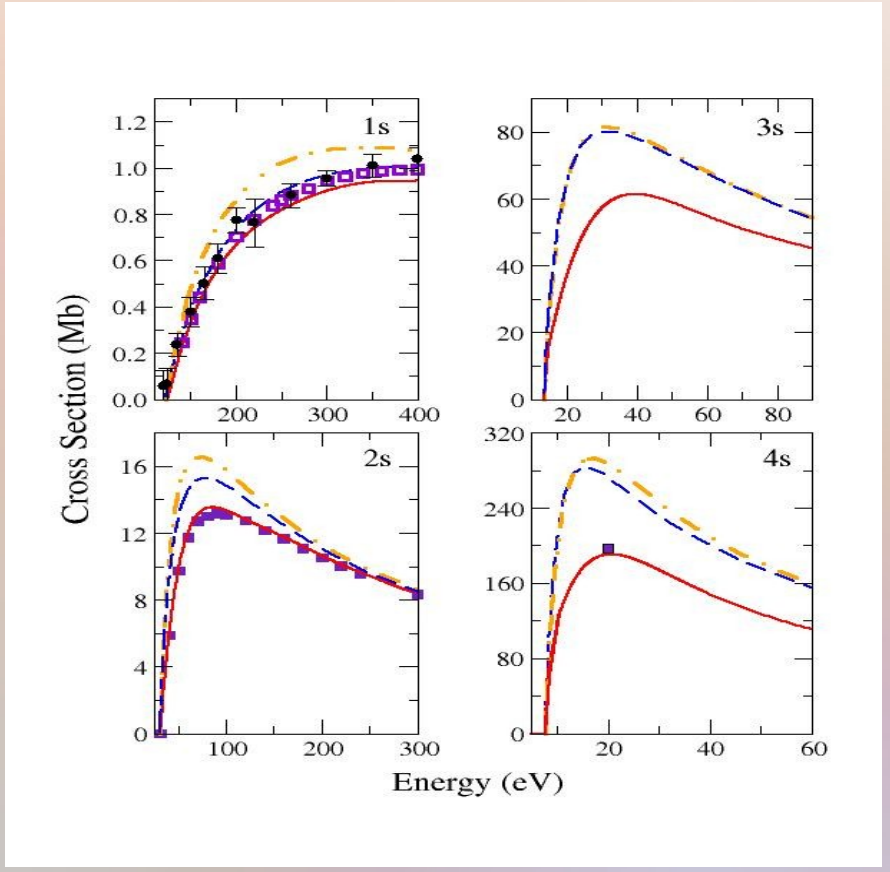
*Loch et al. ADNDT **92** 818 (2006)*



Allain et al., Nucl. Fusion, **44** 655 (2004)

The problem of ionization from excited states

- So one needs data for ionization from the excited levels. However,
- ***Perturbative methods overestimate the ionization cross section for near neutral systems. This gets worse for excited states.***
- Calculations using non-perturbative methods (TDCC, RMPS, CCC) become increasingly difficult for higher n-shells.
- There is a need to calculate data up to quite high n-shells.



*Griffin et al., J. Phys. B, **38** L199 (2005)*

Excited states ionization of neutral Boron

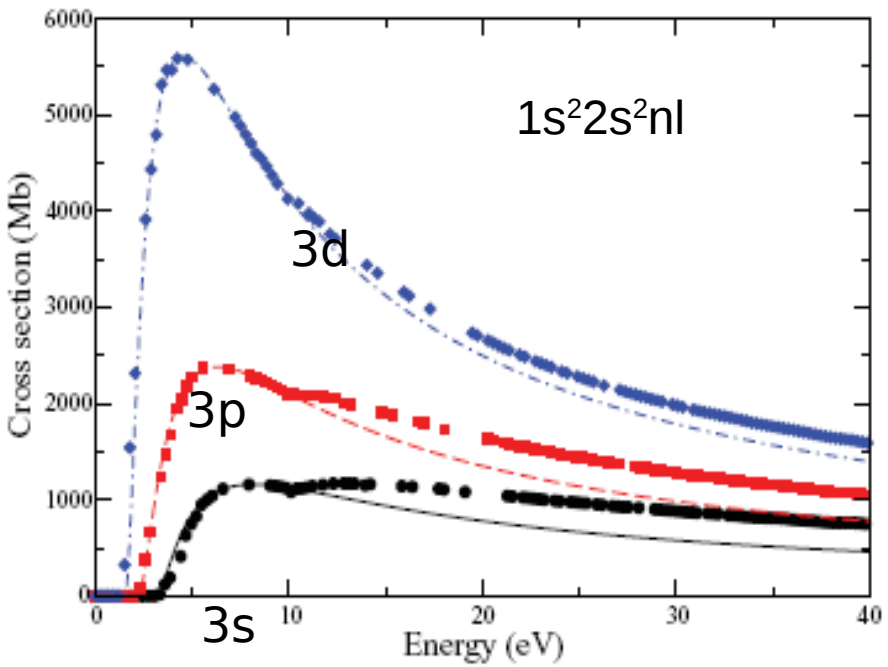


FIG. 1. (Color online) Total electron-impact-ionization cross sections for the $3l$ excited states of B. Circles, raw RMPS for $1s^2 2s^2 3s$; squares, raw RMPS for $1s^2 2s^2 3p$; diamonds, raw RMPS for $1s^2 2s^2 3d$. Solid line, fit to low-energy raw RMPS data for $1s^2 2s^2 3s$; dashed line, fit to low-energy raw RMPS data for $1s^2 2s^2 3p$; dot-dashed line, fit to low-energy raw RMPS data for $1s^2 2s^2 3d$ (1 Mb = 10^{-18} cm^2).

*Lee et al., Phys. Rev. A **82** 042721 (2010)*

- Consider the ionization cross sections (RMPS) for the n=3 shell in neutral B.
  - Excitation-autoionization starts to contribute above about 10 eV and becomes smaller for the higher n-shells.
  - By fitting the direct ionization part we can see if there is an n-scaling in the cross sections.
  - *If it was a purely classical calculation the scaling would go as n^4.*
- We repeated the same study for B^+, and B^{2+}.

n-scaling data for B, B^{+} and B^{2+}

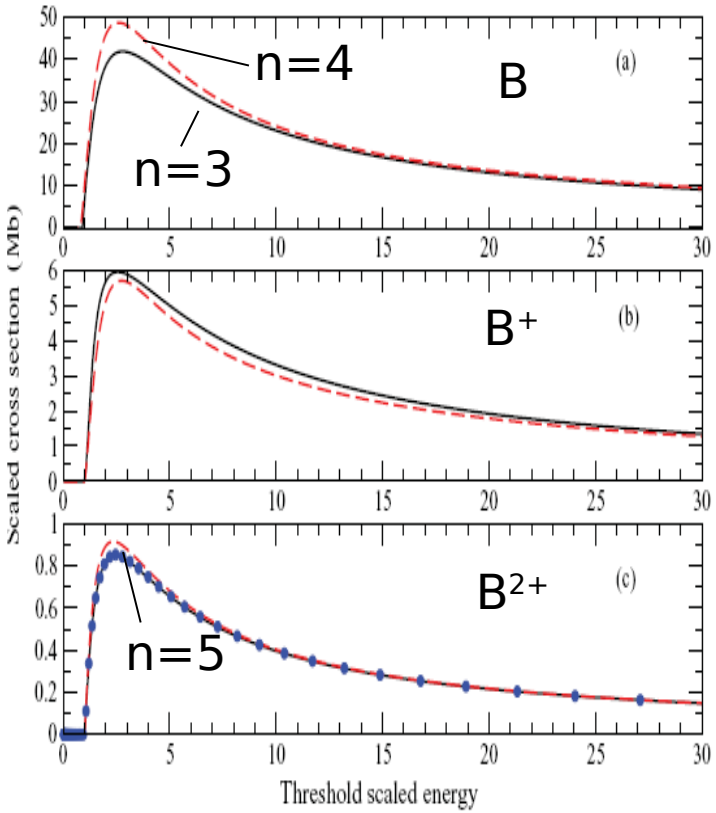
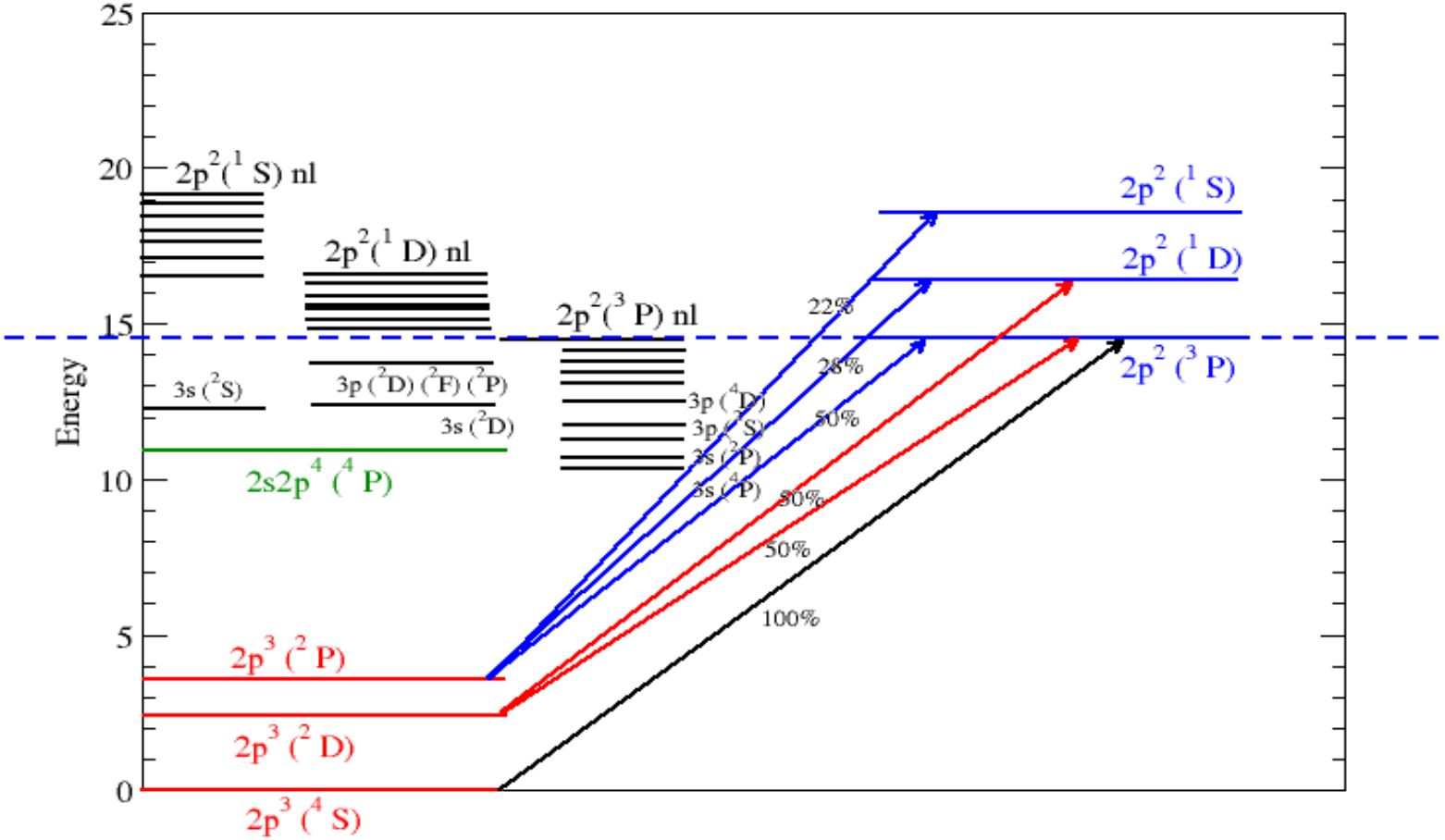


FIG. 5. (Color online) n-scaled electron-impact-ionization cross sections vs threshold scaled energy, that is, cross section divided by n^4 for the n-bundled excited states of (a) B, (b) B^+, and (c) B^{2+}. In all plots the solid line shows the $n = 3$ RMPS data, the dashed line shows the $n = 4$ RMPS data and in panel (c) the solid circles show the $n = 5$ RMPS data (1 Mb = 10^{-18} cm^2).

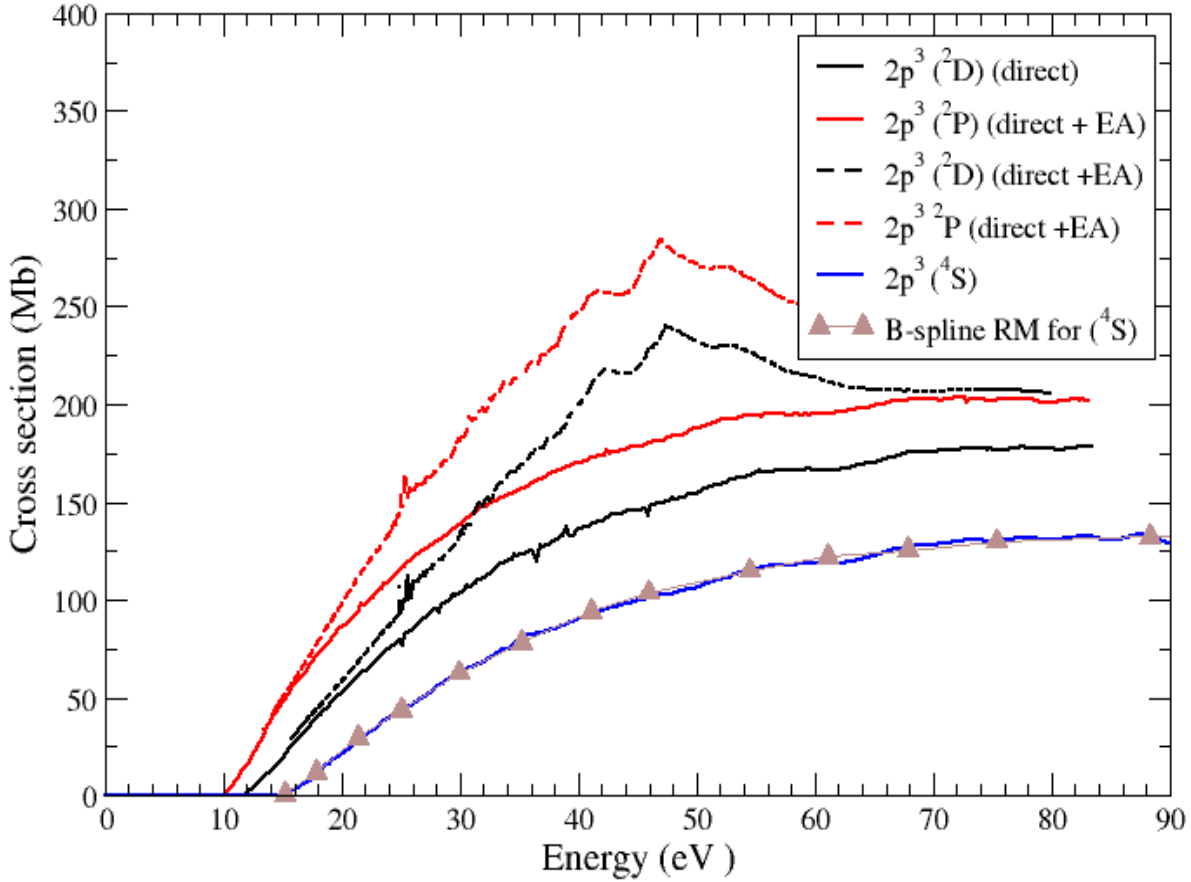
- **For each of the ions a scaling very close to n^4 was found.**
- So the recommendation would be to
  - Evaluate your non-perturbative calculation until scales as n^4, then extrapolate to higher n.
  - Or fit semi-empirical data (e.g. ECIP) to the RMPS results and used the same scaling factor to scale to even higher n shells.
- Note that the bundled-nS data can be extrapolated.

*Lee et al., Phys. Rev. A **82** 042721 (2010)*

N ionization

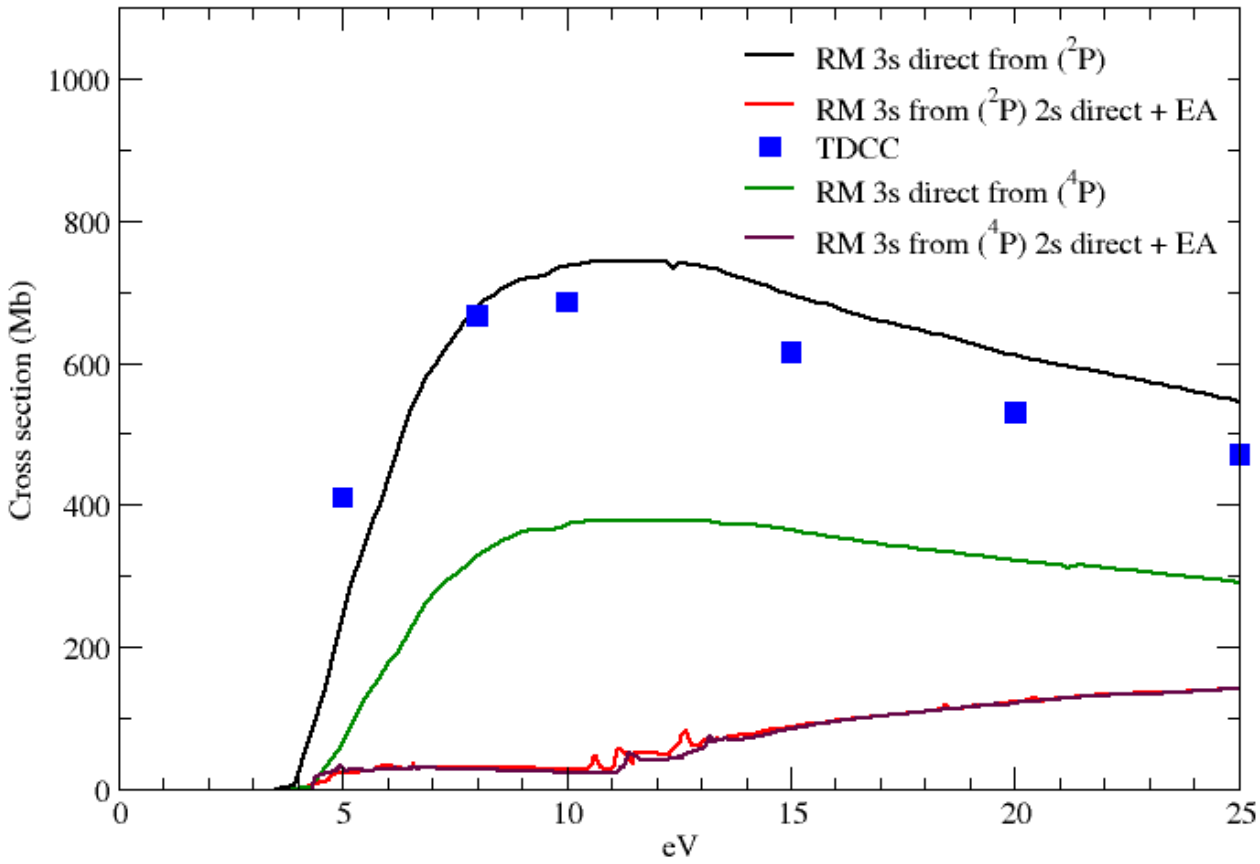


The ground configuration



- Good agreement between the new RM calculations and the recently published data of Wang et al. PRA **89** 06714 (2014)
- How do we metastable resolve the final state? Use the Sampson angular factors?
  - ^{4}S mostly goes to the ground (^{3}P)
  - (^{2}D) and (^{2}S) split can go to multiple places?

N $2s^2 2p^2(^3P)3s$ (^4P and ^2P)



- Implies that the angular coefficients could be used to resolve the final terms.
  - If mixing coefficients are also included
  - The (^{4}P) mixes very strongly with the $2s2p^4$ (^{4}P)
- 2s-2p excitation starts at 5eV.

Conclusions

- We have new SXB data for Mo^{+} and W^{3+}.
  - We are moving on to the lower charge states
- The new N ionization work will hopefully provide a road-map for metastable resolved excited state ionization calculations.
- We have all of the data for GCR calculations for C^{+} through to C^{5+}. We are completing the remaining calculations for neutral C.
  - Any interest in an intermediate GCR data-release for carbon?