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Valdas Jonauskas

Theoretical study of electron-impact ionization in atoms and ions

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Outline

- Theory
- Single ionization
  - Convergence of the excitation-autoionization (EA) cross sections
  - Resonant excitation double autoionization (REDA)
  - Correlation effects
  - The scaled DW cross sections
- Conclusions

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Single ionization by electron impact

- $\sigma_{if}(\varepsilon) = \sigma_{if}^{\mathrm{DI}}(\varepsilon) + \sigma_{if}^{\mathrm{indir}}(\varepsilon)$
- $\sigma_{if}(\varepsilon) = \sigma_{if}^{\mathrm{DI}}(\varepsilon) + \sum_k \sigma_{ik}^{\mathrm{EXC}}(\varepsilon)\, B_{kf}^{a}(\varepsilon)$
- Autoionization branching ratio:

$$B_{kf}^{a}(\varepsilon) = \frac{A_{kf}^{a}}{\sum_n A_{kn}^{a} + \sum_{m<k} A_{km}^{r}}$$

A^a – Auger transition probability,

A^r – radiative transition probability

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The scaled DW cross sections

- DI for atoms:

$$\sigma_{if}^{\mathrm{DI}*}(\varepsilon) = \frac{\varepsilon}{\varepsilon + I + \varepsilon_k}\,\sigma_{if}^{\mathrm{DI}}(\varepsilon)$$

I is the ionization energy, ε_k is the kinetic energy of the bounded electron

- DI for ions:

$$\sigma_{if}^{\mathrm{DI}*}(\varepsilon) = \frac{\varepsilon}{\varepsilon + I}\,\sigma_{if}^{\mathrm{DI}}(\varepsilon)$$

- Excitation:

$$\sigma_{if}^{\mathrm{EXC}*}(\varepsilon) = \frac{\varepsilon}{\varepsilon + \Delta E_{if} + \varepsilon_b}\,\sigma_{if}^{\mathrm{EXC}}(\varepsilon)$$

ΔE_{if} is the transition energy, ε_b is the bounding energy of electron

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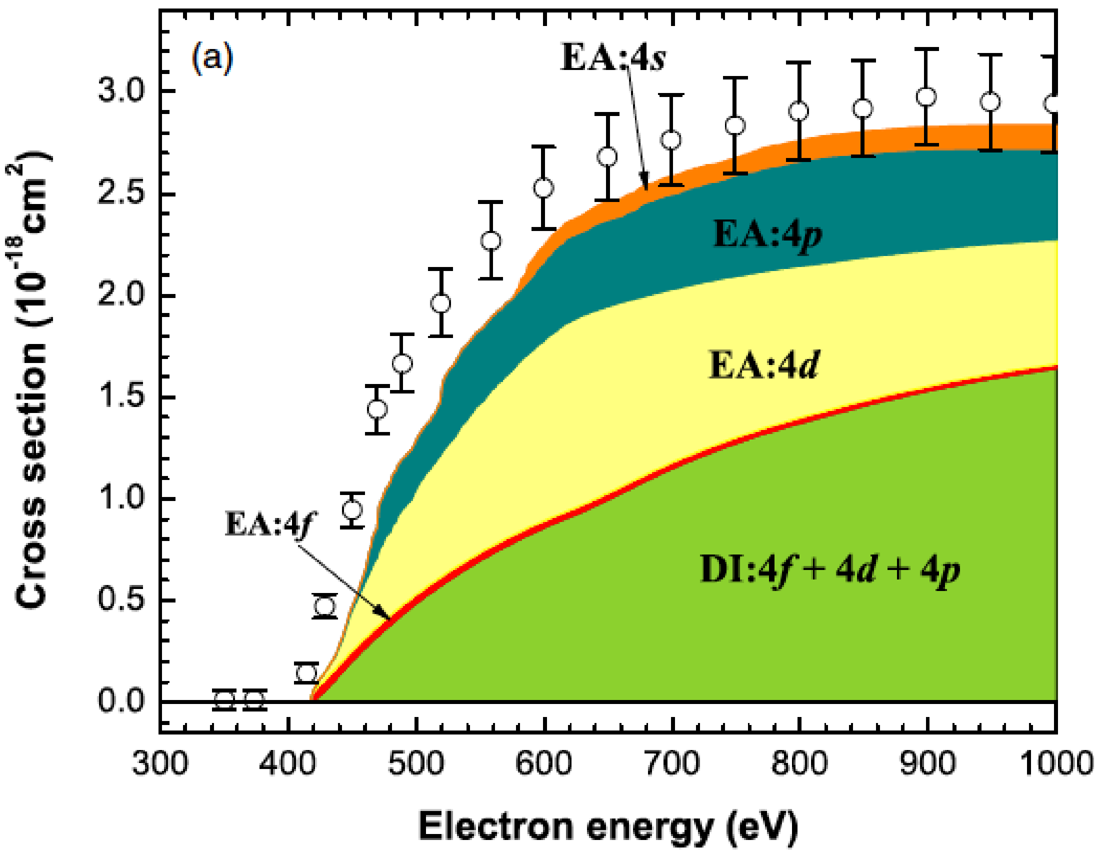
W^{17+} single ionization



J Rausch, et al, Electron-impact single and double ionization of W^{17+}, J. Phys. B 44 (2011) 165202

D-H Zhang, D-H Kwon, Theoretical electron-impact ionization of W^{17+} forming W^{18+}, J. Phys. B **47** 075202 (2014)

EA:

$4s, 4p \rightarrow nl \ (4 \leq n \leq 25)$,

$4d \rightarrow nl' \ (5 \leq n \leq 25)$,

$4f \rightarrow nl' \ (10 \leq n \leq 38)$,

where $l' \leq 5$.

$W^{17+} : 4f^{11}$

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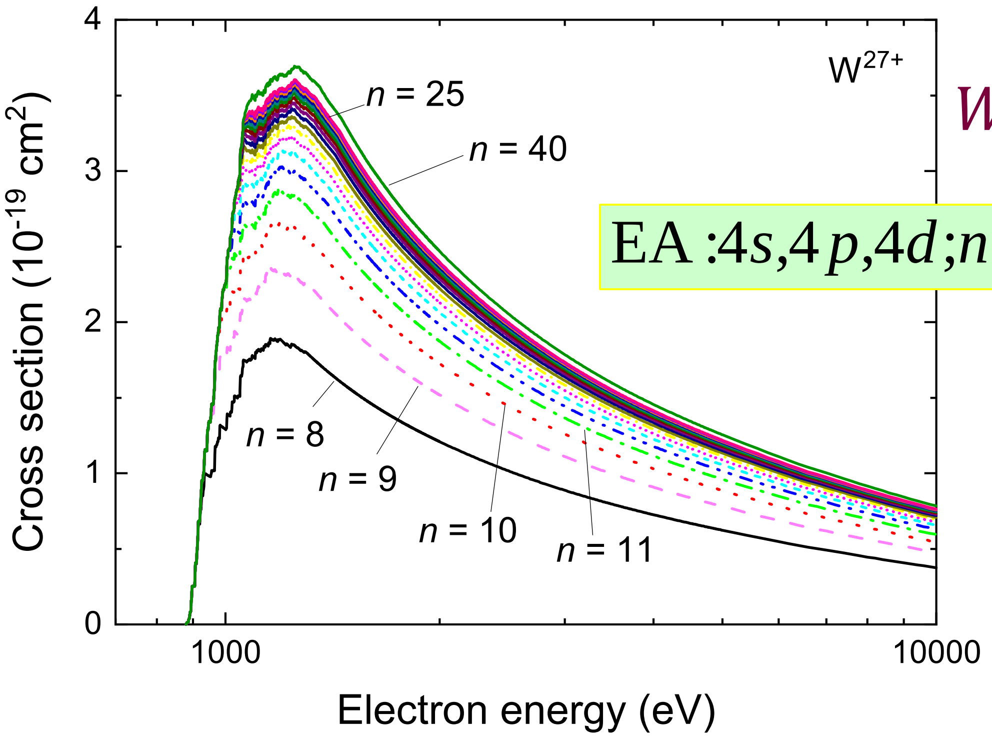
W^{27+} EA channels: convergence



$W^{27+}: 4d^{10}4f$

$\mathrm{EA}: 4s, 4p, 4d; n \leq 40, l \leq 6$

Jonauskas et al, Phys. Rev. A 91, 012715 (2015)

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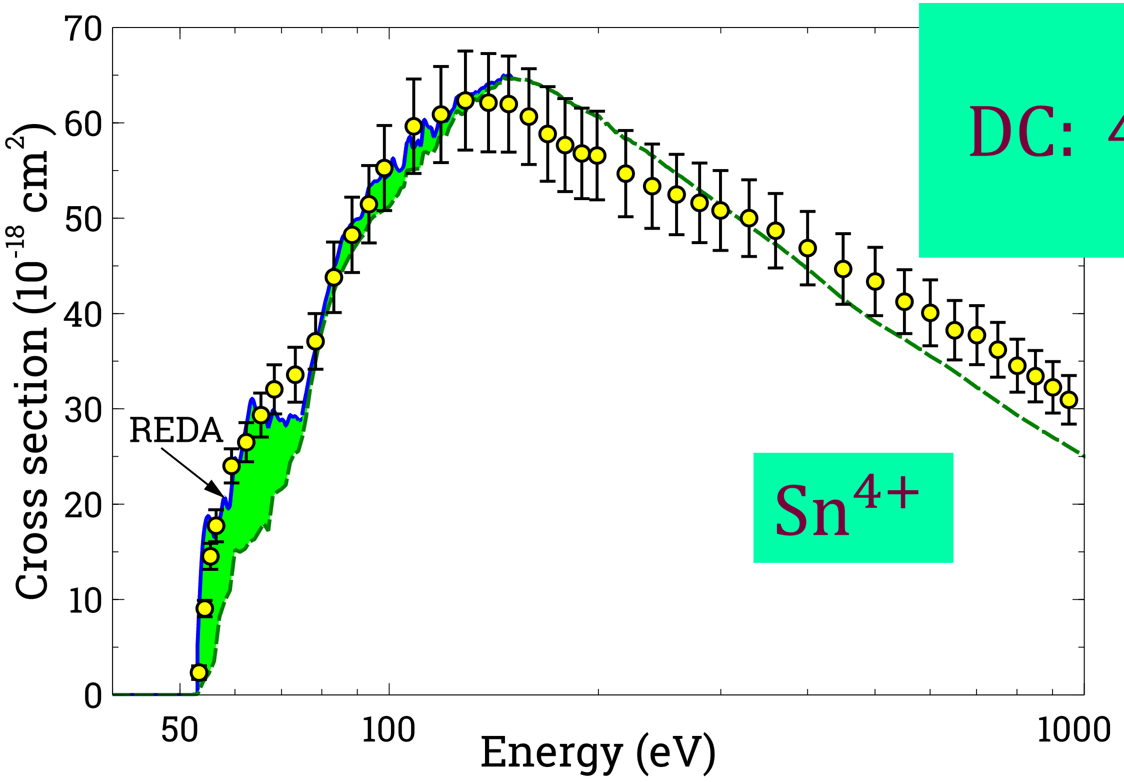
REDA



$$\text{DC: } 4s^2 4p^6 4d^{10} + e \rightarrow \begin{cases} 4s\,4p^6 4d^{10} n_1 l_1 n_2 l_2 \\ 4s^2\,4p^5 4d^{10} n_1 l_1 n_2 l_2 \end{cases}$$

$$n_1 = 4{,}5, n_2 = 4 - 40, l_1 l_2 < 5$$

Jonauskas, JQSRT 239,106659 (2019)

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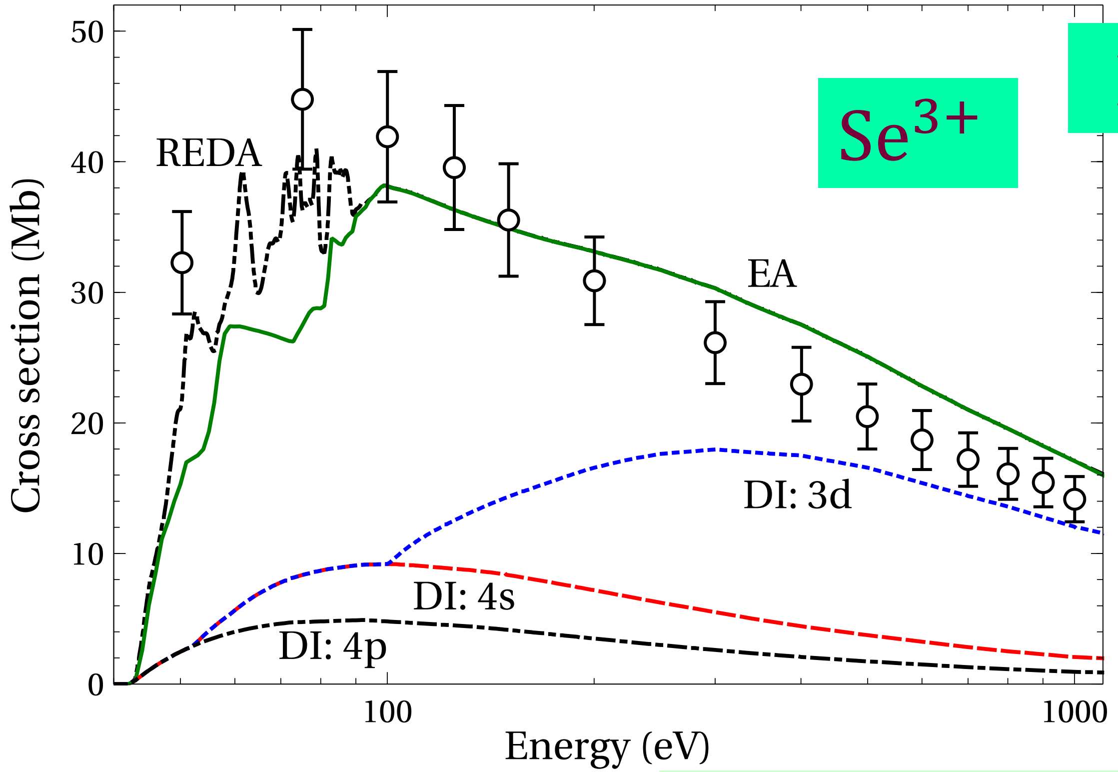
REDA



Se^{3+}

DC: $3d^{10}4s^2 4p + e \rightarrow 3d^9 4s^2 4p\, n_1 l_1 n_2 l_2$

$n_1 = 4 - 6, n_2 = n_1 - 50, l_1 l_2 < 5$

Pakalka et al, PRA 97, 012708 (2018)

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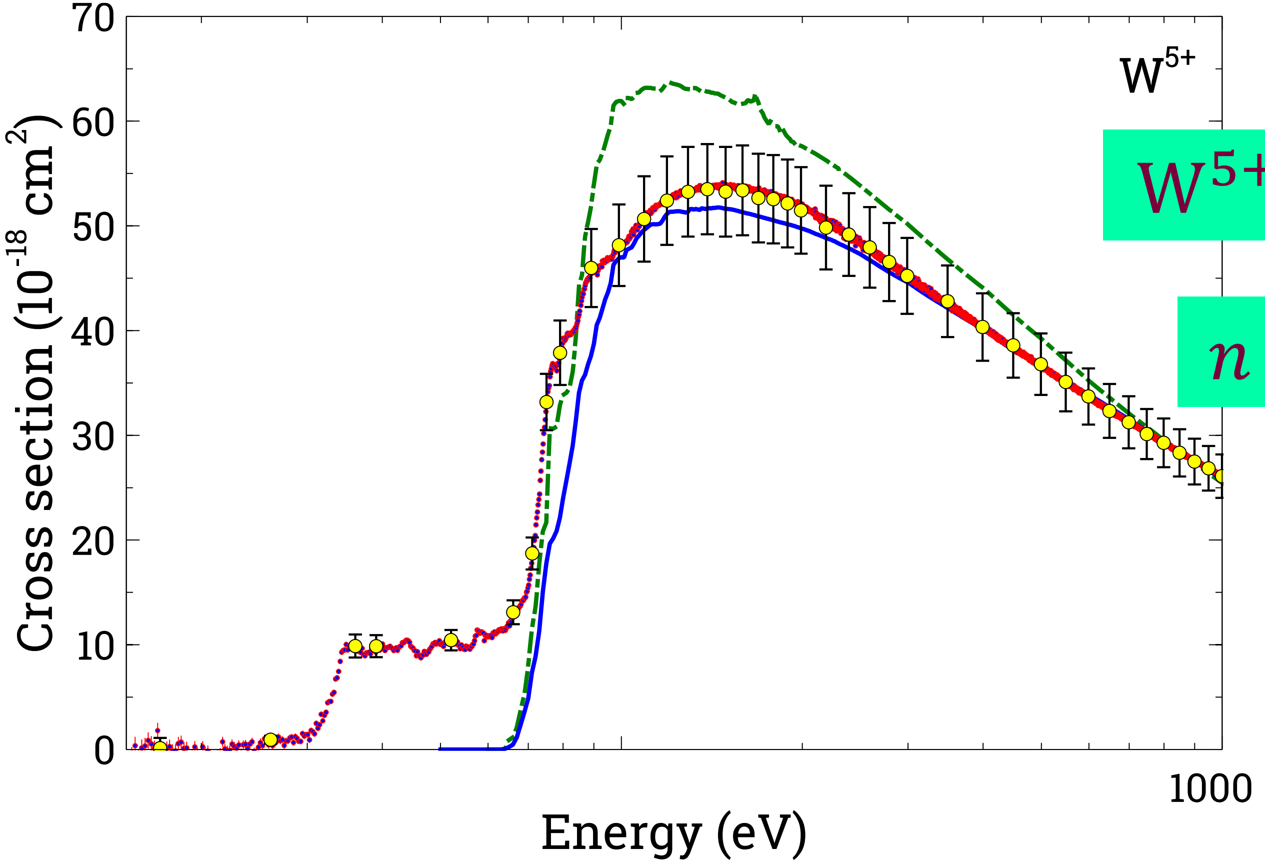
Correlation effects: W^{5+}



$W^{5+}\ 4f^{14}5s^2\,5p^6\,5d$

$n \leq 12$

Jonauskas *et al*, PRA 100, 062701 (2019)

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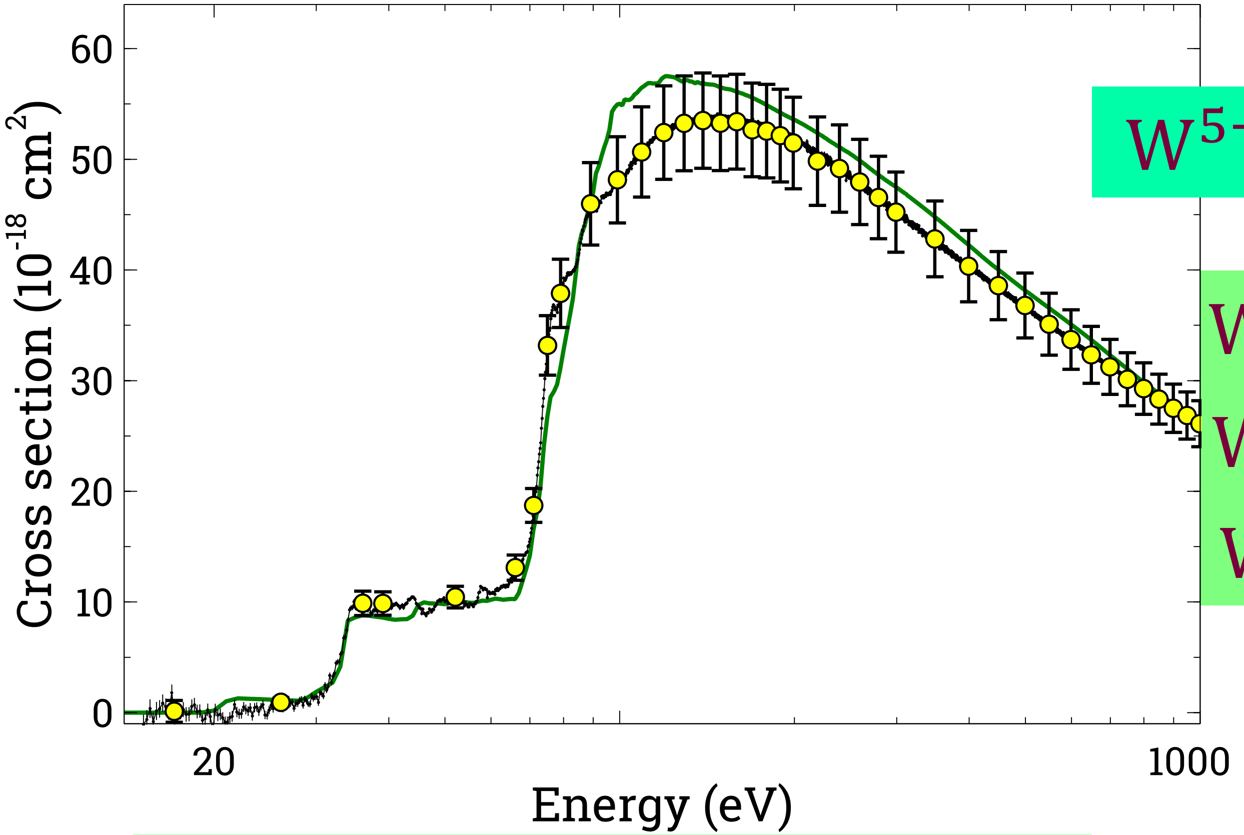
Correlation effects: W^{5+}



W^{5+} $4f^{14} 5s^2\, 5p^6\, 5d$

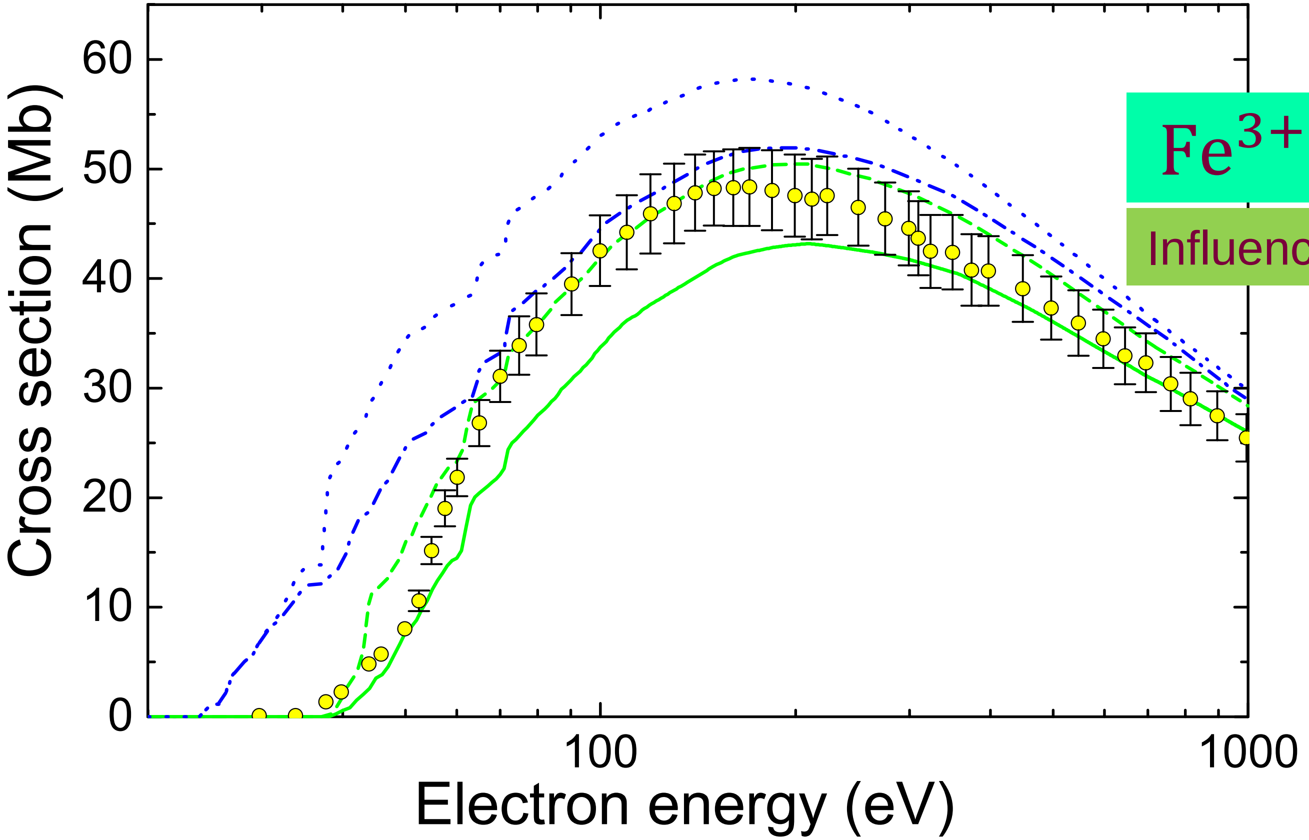
W^{5+} $4f^{14} 5s^2\, 5p^5\, 5d^2$

W^{5+} $4f^{13} 5s^2\, 5p^6\, 5d^2$

W^{5+} $4f^{14} 5s^2\, 5p^6\, 6s$

Jonauskas *et al*, PRA 100, 062701 (2019)

Correlation effects: Fe^{3+}



$Fe^{3+}\ 3s^2 3p^6 3d^4 4s$

Influence of correlation effects

Kynienė *et al*, PRA 100, 052705 (2019)

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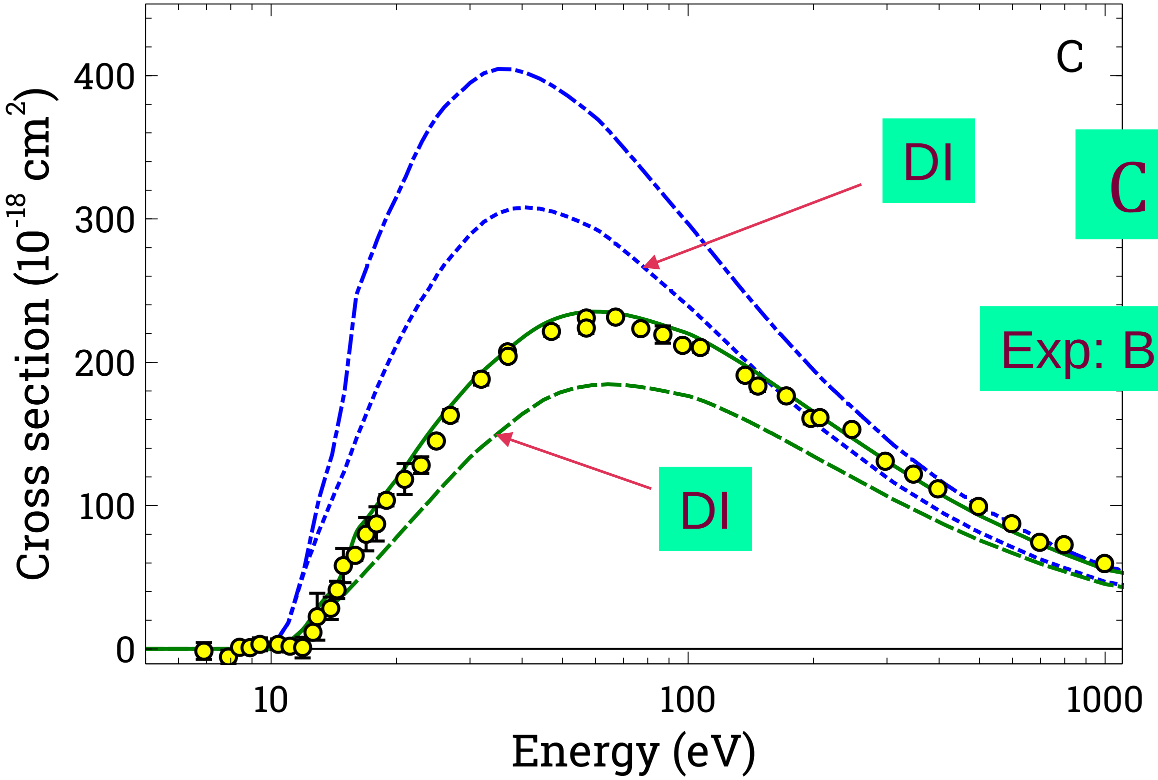
Scaling of DW cross sections: C



$C\ 2s^2\,2p^2$

Exp: Brook *et al* 1978, J. Phys. 11, 3115

Jonauskas, AA 620, A188 (2018)

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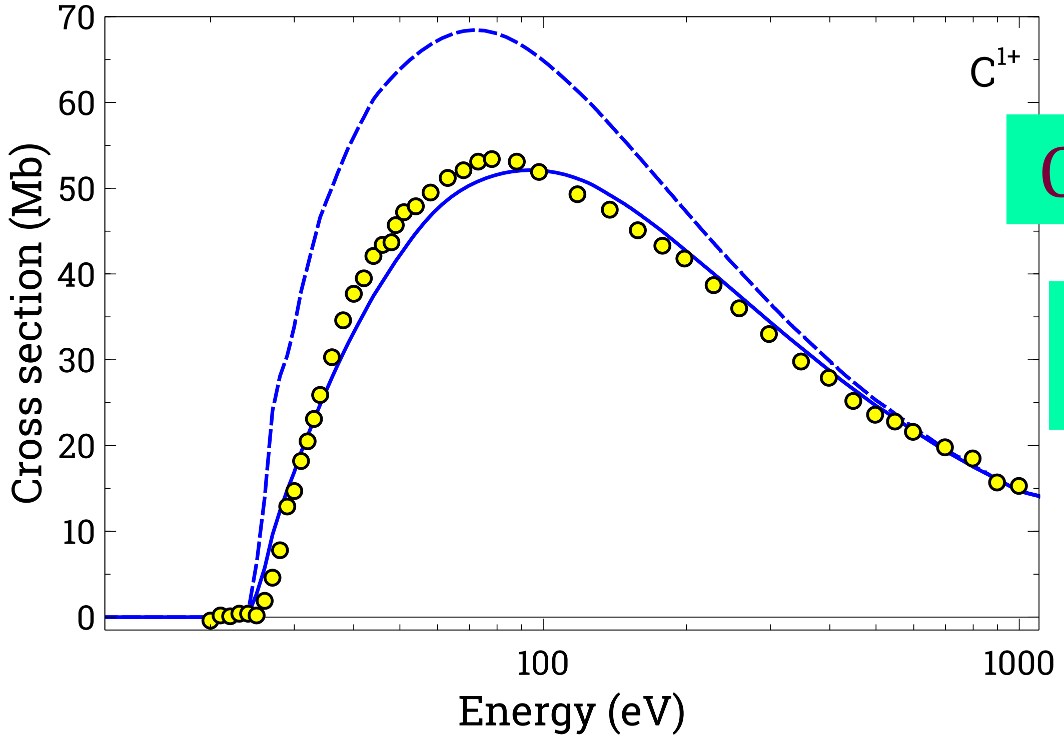
Scaling of DW cross sections: C^+



$C^+ \ 2s^2\, 2p$

Exp: Yamada et al. 1989,
J. Phys. Soc. Jpn., 58, 1585

Jonauskas, AA 620, A188 (2018)

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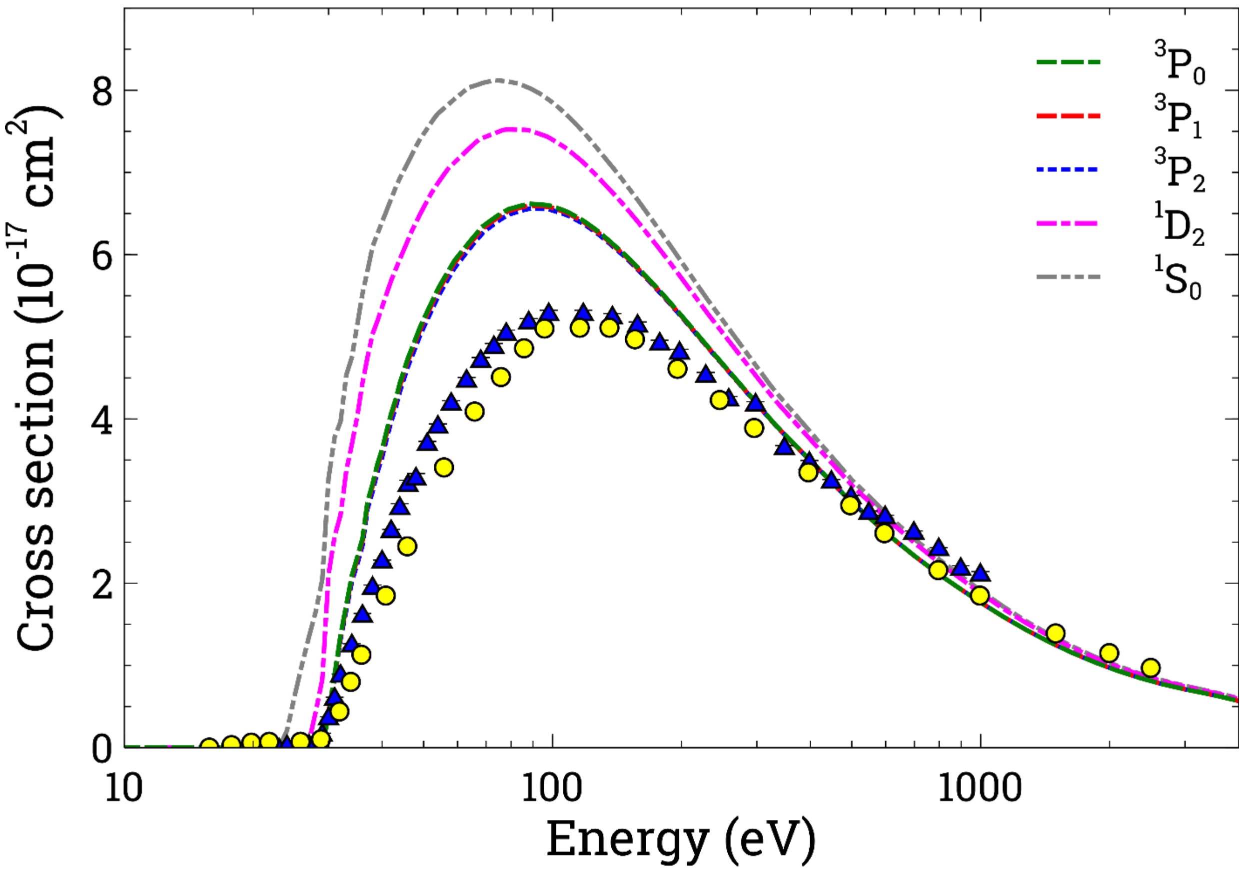
DW cross sections: N^+



$N^+ \ 2s^2 \ 2p^2$

Experiments:
Lecointre et~al. 2013,
J. Phys. B, 46, 205201
Yamada et~al. 1989,
J. Phys. Soc. Jpn, 58, 1585

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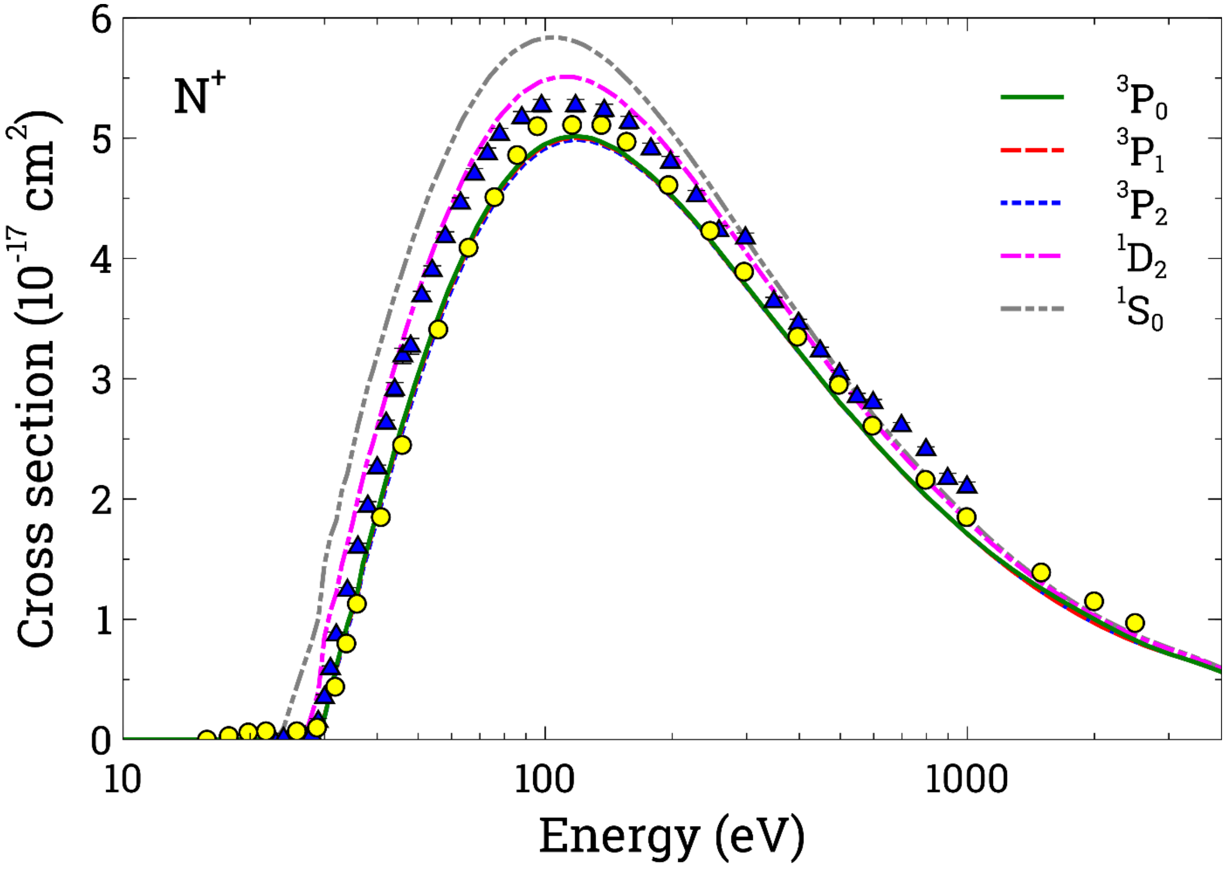
Scaling of DW cross sections: N^+



$N^+ \ 2s^2 \ 2p^2$

Experiments:
Lecointre et~al. 2013,
J. Phys. B, 46, 205201
Yamada et~al. 1989,
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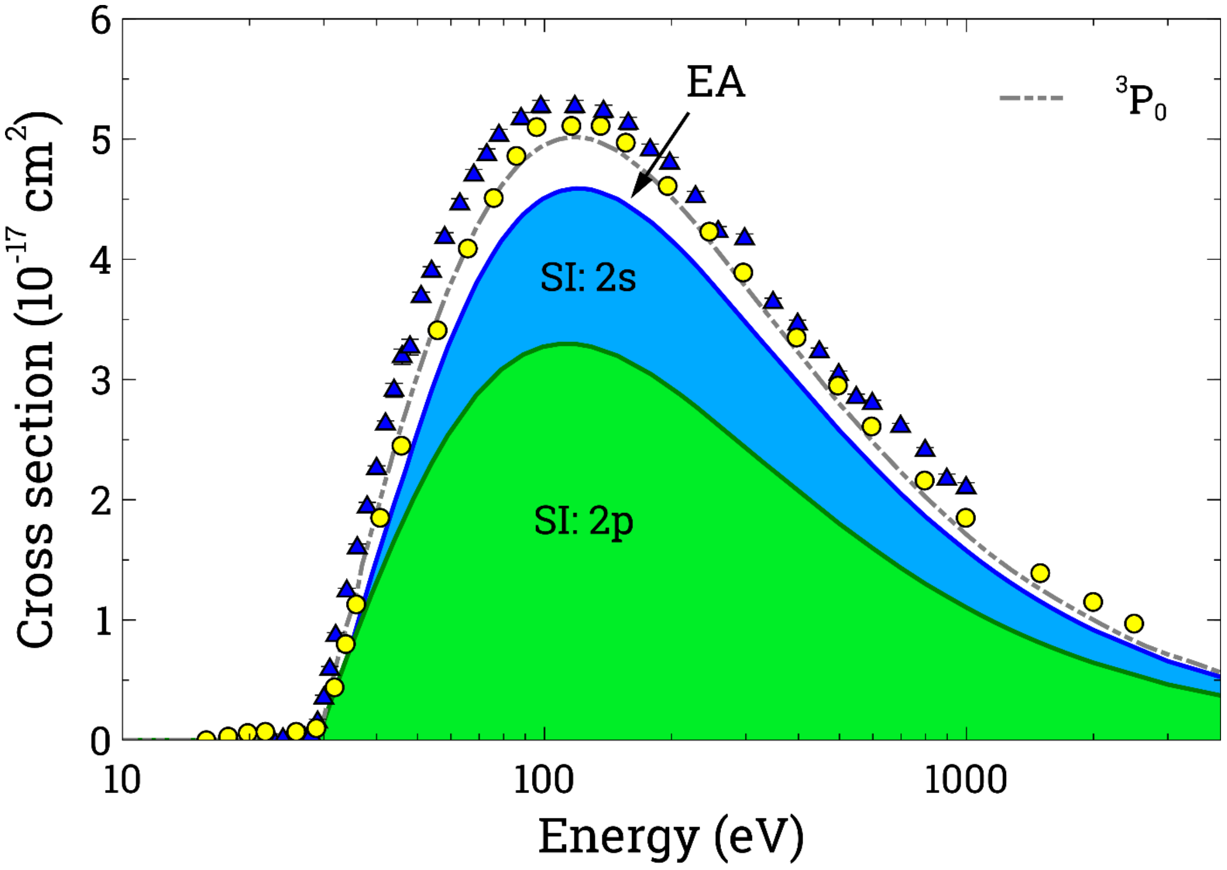
Scaling of DW cross sections: N^+



$N^+ \ 2s^2\, 2p^2$

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Conclusions

- Convergence of the EA cross sections has to be studied to provide reliable data for single ionization process
- Resonant excitation double autoionization can produce important contribution at the lower energies of electrons.
- Correlation effects diminish single ionization cross sections.
- The scaled DW cross sections can be important in the analysis of the measurements for the neutral atoms and near neutral ions.

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Thank you!