Atomic Collision Data for Light Atoms and Ions

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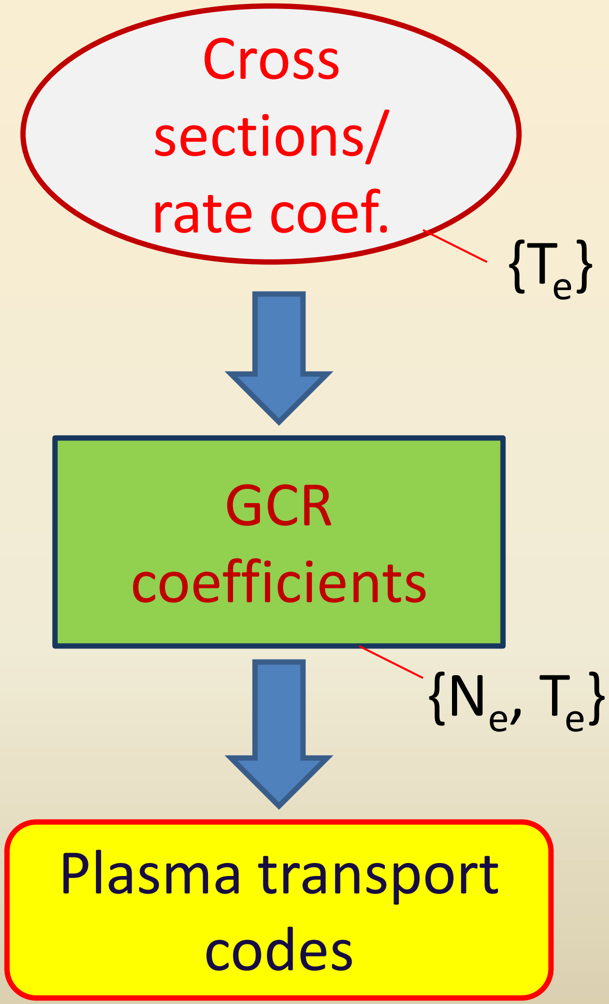
Overview

- Outline of theoretical methods
- Quick review on H, He, Li and Be data.
- Recent results
  - Ionization of B, B^{+} and B^{2+}
  - Ionization of C^{3+}, C^{+}
  - Double ionization of B^{+}
  - Dielectronic recombination of C^{3+}
- Summary and future plan.

Theoretical methods

- *Perturbation theory*
  - Distorted-wave (mainly for ionization process)
- *Non-perturbative methods*
  - R-matrix close-coupling (RM, RMPS)
  - Time-dependent close-coupling (TDCC)
  - Convergent close coupling (CCC)
  - Exterior complex scaling (ECS)
- Collisional-radiative codes from ADAS



Generalized collisional-radiative (GCR) coefficients

- Effective ionization rates

Ionization rates

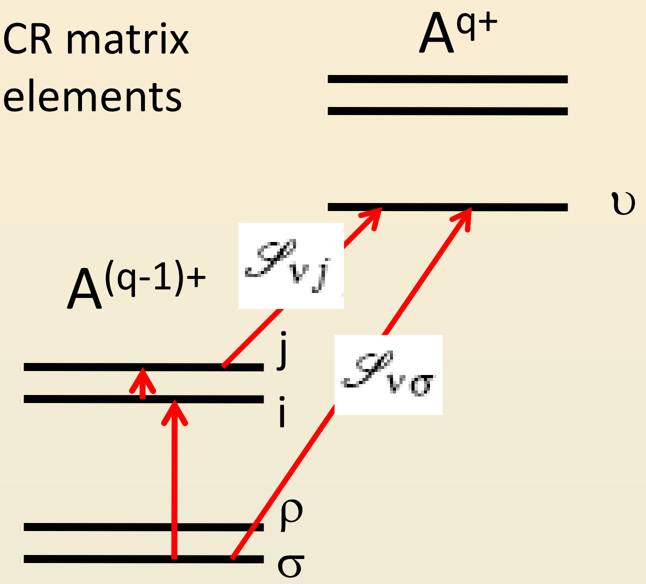
CR matrix elements

$$S_{CD,\sigma\to\nu} = \mathscr{S}_{\nu\sigma} - \sum_{j=1}^{O} \mathscr{S}_{\nu j} \sum_{i=1}^{O} \mathscr{C}_{ji}^{-1} \mathscr{C}_{i\sigma}$$

- Effective recombination rates

$$R_{CD,\nu\to\sigma} = \mathscr{R}_{\sigma\nu} + \sum_{j=1}^{O} \mathscr{C}_{\sigma j} \sum_{i=1}^{O} \mathscr{C}_{ji}^{-1} \mathscr{R}_{i\nu}$$

RR and DR rates



- Total Line Power Loss

$$P_{LT,\sigma} = \sum_{k,j} \Delta E_{kj} A_{j\to k} F_{j\sigma}^{exc}$$

excitation rates

spontaneous emission rates

j->k transition energy

*Summers et al., Plasma Phys. Control. Fusion, **48** 263 (2006)*

Elements, Processes and Methods

Elements/Proc	Excitation (n<=5)	Ionization (n<=2)	RR	DR
H	RMPS	TDCC, RMPS, CCC	DW	DW
He	RMPS	TDCC, RMPS, CCC	DW	DW
He+	RMPS	TDCC, RMPS, CCC	DW	DW
Li isonuclear sequence	RMPS	TDCC, RMPS, CCC, ECIP	DW	DW
Be isonuclear sequence	RMPS	TDCC, RMPS, CCC, ECIP, DW	DW	DW
B isonuclear sequence	RMPS	TDCC, RMPS, CCC, ECIP, DW	DW	DW

In good shape, agrees with CCC & TDCC

In good shape

In good shape, compare well with expt.

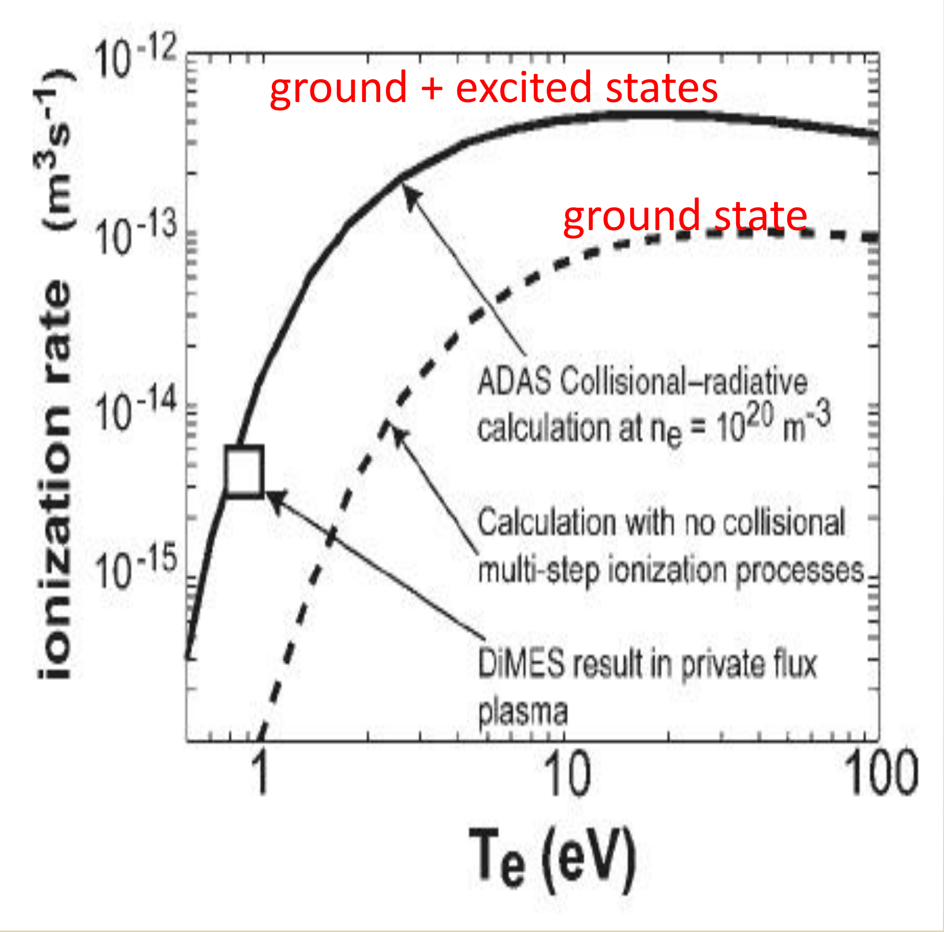
GCR data

- H & He : *Loch et al., Plasma Phys. Control. Fusion,* ***51*** *105006 (2009)*
- Li: *Loch et al., ADNDT,* ***92*** *813 (2006)*
- Be: *Loch et al., ADNDT,* ***94*** *257 (2008)*

Measurements of Li ionization rates at DIII-D

• Plasma transport studies on the DIII-D tokamak measured the density dependent ionization rate to be more than an order of magnitude larger than the ground Li.

• For moderate densities plasma (10^{10} – 10^{15} cm^{-3}), ionization from excited states (ES) may be significant.



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

Boron isonuclear sequence data source

- **Dielectronic Recombination**
  - ✓ B^{4+} : *Badnell et al., Astron. Astrophys.* ***447*** *389 (2006)*
  - ✓ B^{3+} : *Bautista et al., Astron. Astrophys.* ***466*** *755 (2007)*
  - ✓ B^{2+} : *Colgan et al., Astron. Astrophys.* ***417*** *1183 (2004)*
  - ✓ B^{+} : *Colgan et al., Astron. Astrophys.* ***412*** *597 (2003)*
- **Excitation**
  - ✓ B^{4+} : RMPS – *Ballance et al., J. Phys. B* ***36*** *3707 (2003)*
  - ✓ B^{3+} : RMPS – *Ballance (unpublished) – available at ADAS*
  - ✓ B^{2+} : RMPS – *Griffin et al., J. Phys. B* ***33*** *1013 (2000)*
  - ✓ B^{+} : RMPS – *Badnell et al., J. Phys. B* ***36*** *1337 (2003)*
  - ✓ B: RMPS – *Ballance et al., J. Phys. B* ***40*** *1131 (2007)*
- **Ionization**
  - ✓ B^{4+} : RMPS+DW – *Griffin et al., J. Phys. B* ***38*** *L199 (2005)*
  - ✓ B^{3+} : CCC + Expt – *Renwick et al., J. Phys. B* ***42*** *175203 (2009)*
  - ✓ B^{2+} : RMPS – *Badnell & Griffin., J. Phys. B* ***33*** *2955 (2000)*
  - ✓ B^{+} : TDCC, RMPS, DW + Expt – *Berrengut et al., Phys. Rev. A* ***78*** *012704 (2008)*
  - ✓ B: TDCC, RMPS, DW + BEB – *Berrengut et al., Phys. Rev. A* ***76*** *042704 (2007)*
  - ✓ ES ionization for B, B^{+} and B^{2+} – *Lee et al., Phys. Rev. A* ***82*** *042721 (2010)*
- ➢ GCR data production

Excited states ionization of neutral Boron

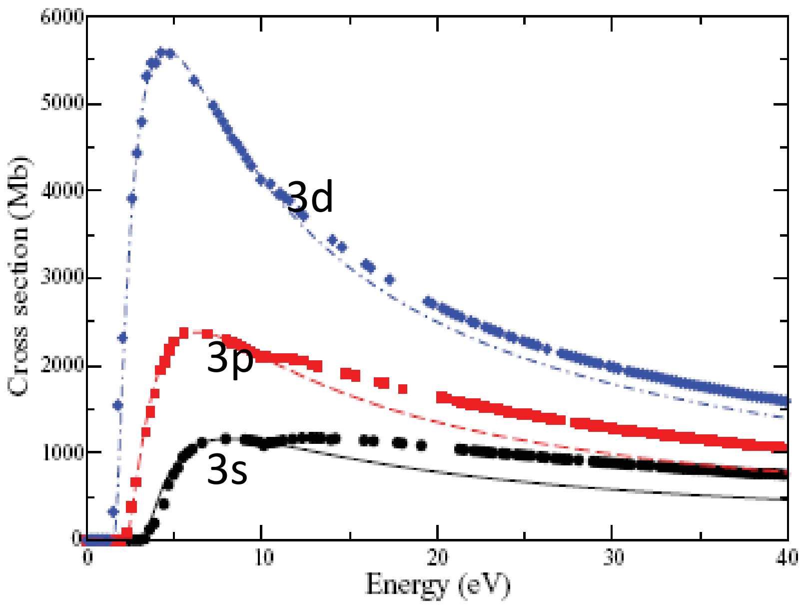


FIG. 1. (Color online) Total electron-impact-ionization cross sections for the $3l$ excited states of B. Circles, raw RMPS for $1s^2 2s^2 3s$; squares, raw RMPS for $1s^2 2s^2 3p$; diamonds, raw RMPS for $1s^2 2s^2 3d$. Solid line, fit to low-energy raw RMPS data for $1s^2 2s^2 3s$; dashed line, fit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

- Configurations in CC: $1s^2 2s^2 2p$, $1s^2 2s^2 nl$, $1s^2 2s 2p^2$, $1s^2 2s 2p nl$, $1s^2 2p^3$ and $1s^2 2p^2 nl$
- Excitation-autoionization from $1s^2 2s 2p^2$, $1s^2 2s 2p 3l$, $1s^2 2s 2p 4l$ and $1s^2 2s 2p 5l$.
- Excitation-autoionization contributions become less pronounced as n increases.
- Same analysis was done for B^+ and B^{2+}.

Bundled-n of ionization data for B, B^+ and B^{2+}

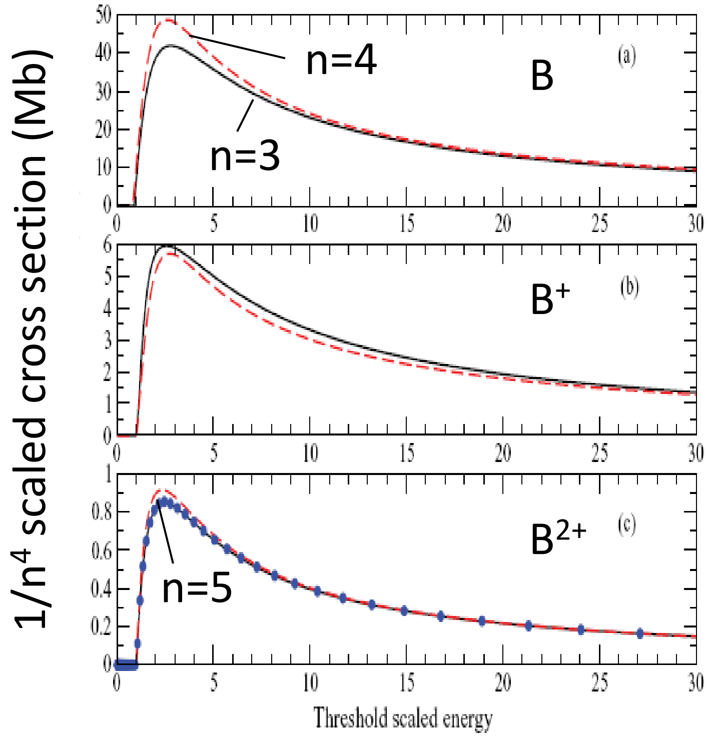


FIG. 5. (Color online) n-scaled electron-impact-ionization cross sections vs threshold scaled energy, that is, cross section divided by n^4 for the n-bundled excited states of (a) B, (b) B^+, and (c) B^{2+}. In all plots the solid line shows the $n = 3$ RMPS data, the dashed line shows the $n = 4$ RMPS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

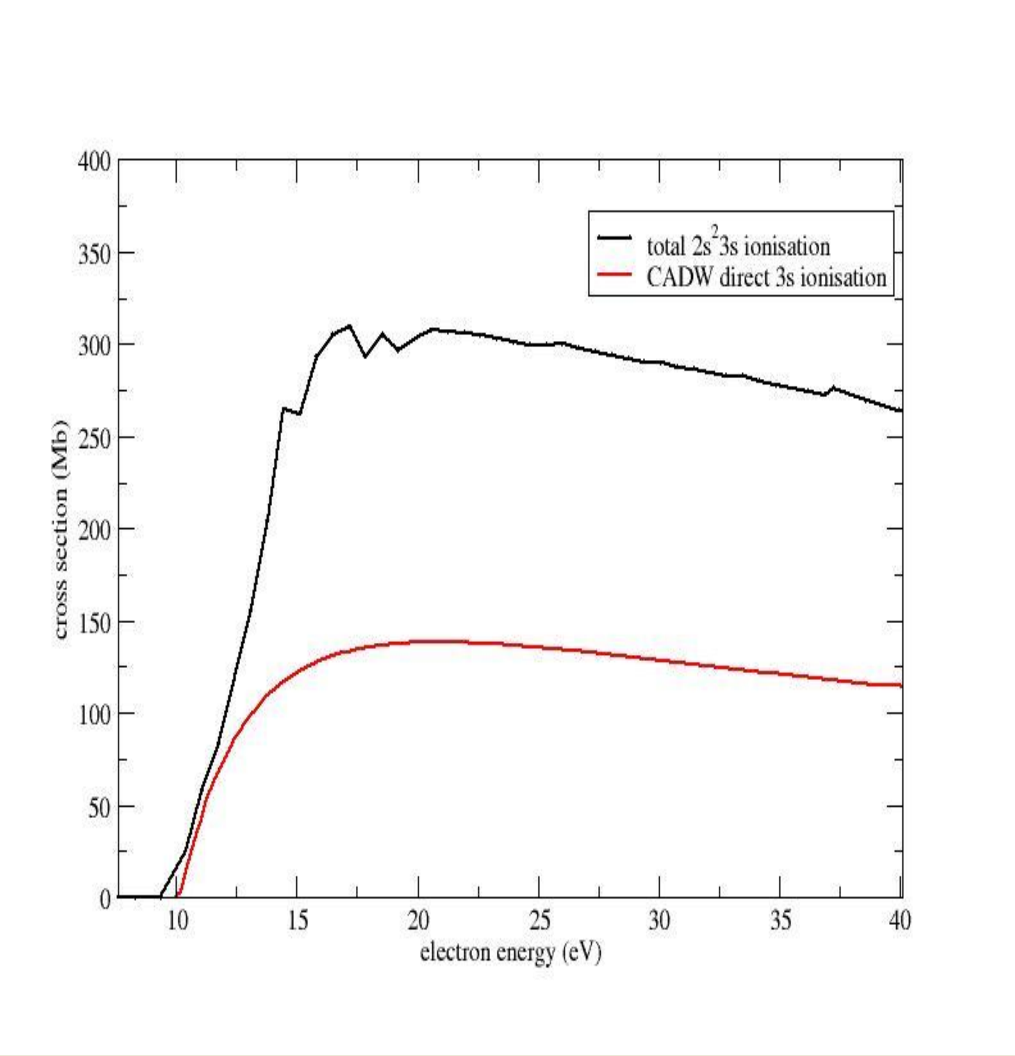
- Semi-empirical method (ECIP) can be fitted to the RMPS results and used to scale to even higher n shells, i.e., n = 6 and 7.

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

Carbon isonuclear sequence data source

- **Dielectronic Recombination**
  - ✓ C^{5+} : *Badnell et al., Astron. Astrophys.* ***447*** *389 (2006)*
  - ✓ C^{4+} : *Bautista et al., Astron. Astrophys.* ***466*** *755 (2007)*
  - ✓ C^{3+} : *Colgan et al., Astron. Astrophys.* ***417*** *1183 (2004)*
  - ✓ C^{2+} : *Colgan et al., Astron. Astrophys.* ***412*** *597 (2003)*
  - ✓ C^{+} : *Altun et al., Astron. Astrophys.* ***420*** *775 (2004)*
- **Excitation**
  - ✓ C^{5+} : RMPS – *Ballance et al., J. Phys. B* ***36*** *3707 (2003)*
  - ✓ C^{4+} : RMPS – *Loch & Ballance, (unpublished) – available at ADAS*
  - ✓ C^{3+} : RMPS, TDCC + DW – *Griffin et al., J. Phys. B 33, 1013 (2000)*
  - ✓ C^{2+} : RMPS – *Mitnik et al., J. Phys. B* ***36*** *717 (2003)*
  - o C^{+} : Work in progress.
  - o C: Work in progress.
- **Ionization**
  - ✓ C^{3+} :RMPS– *Badnell & Griffin., J. Phys. B* ***33*** *2955 (2000)*
  - ✓ C^{2+} : TDCC, CCC, RMPS, DW + Expt – *Loch et al., Phys. Rev. A* ***71*** *012716 (2005)*
  - ✓ C^{+} : TDCC, RMPS, DW + Expt –*Ludlow et al., Phys. Rev. A* ***78*** *1 (2008)*
  - ✓ C: TDCC, DW + Expt – *Pindzola et al., Phys. Rev. A* ***62*** *042705 (2000)*.
  - ✓ Ionization from excited states of C^{3+} – *Pindzola et al., Phys. Rev. A* ***XX*** *XXXXXX (2011)*
  - o Ionization from excited states of C^{2+}, C^{+} and C: Work in progress.
- ➢ GCR data production.

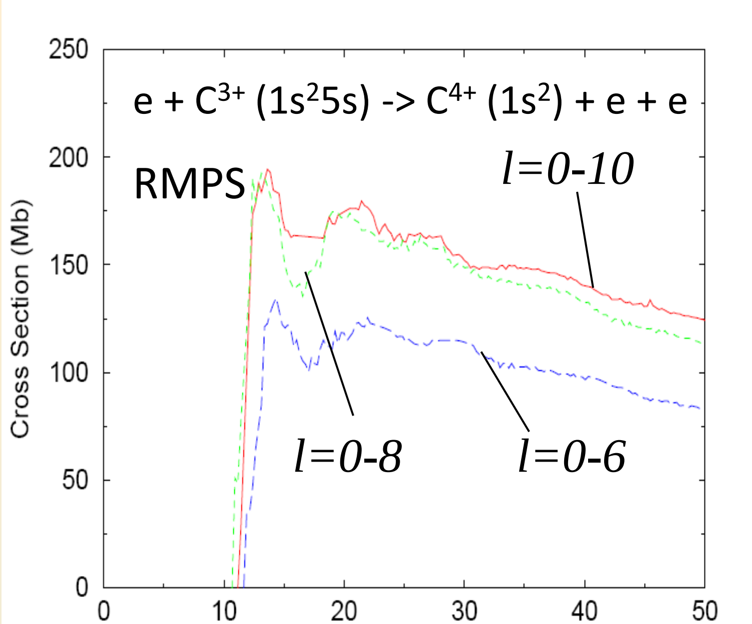
Excited state ionization of C^+ ($2s^23s$) ions



- Including
  - 3s direct ionization
  - 2s direct ionization
  - excitation-autoionization from
    - ✓ $1s^22s2p3l$
    - ✓ $1s^22s2p4l$
    - ✓ $1s^22s2p5l$

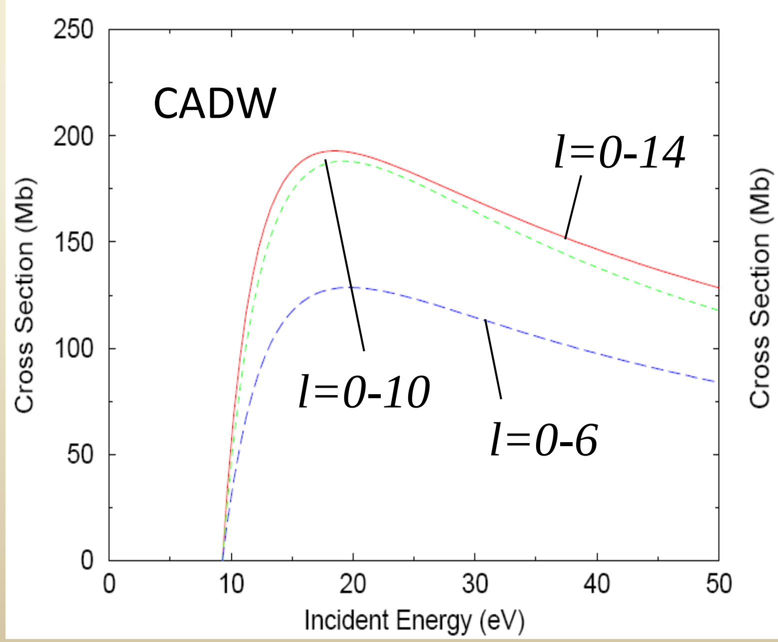
- CADW model includes only one configuration.

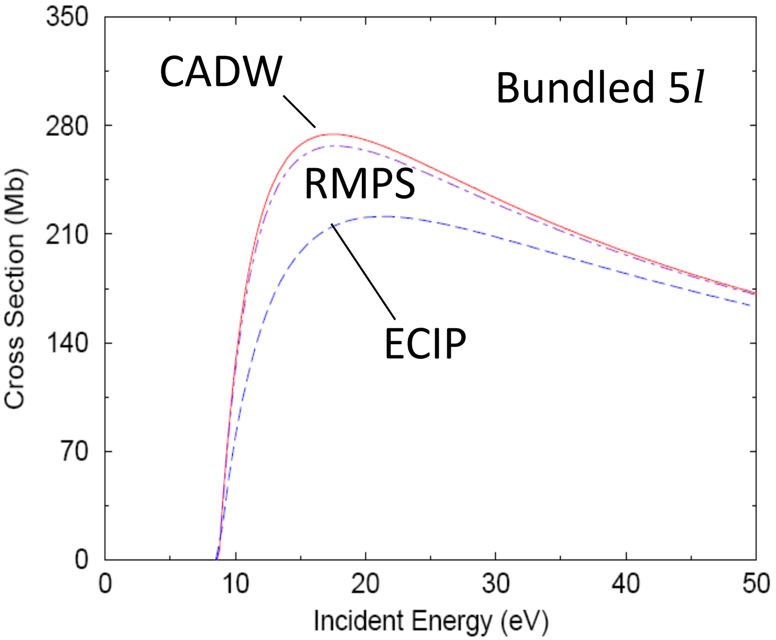
Excited state ionization of C^{3+} ($1s^25s$) ions



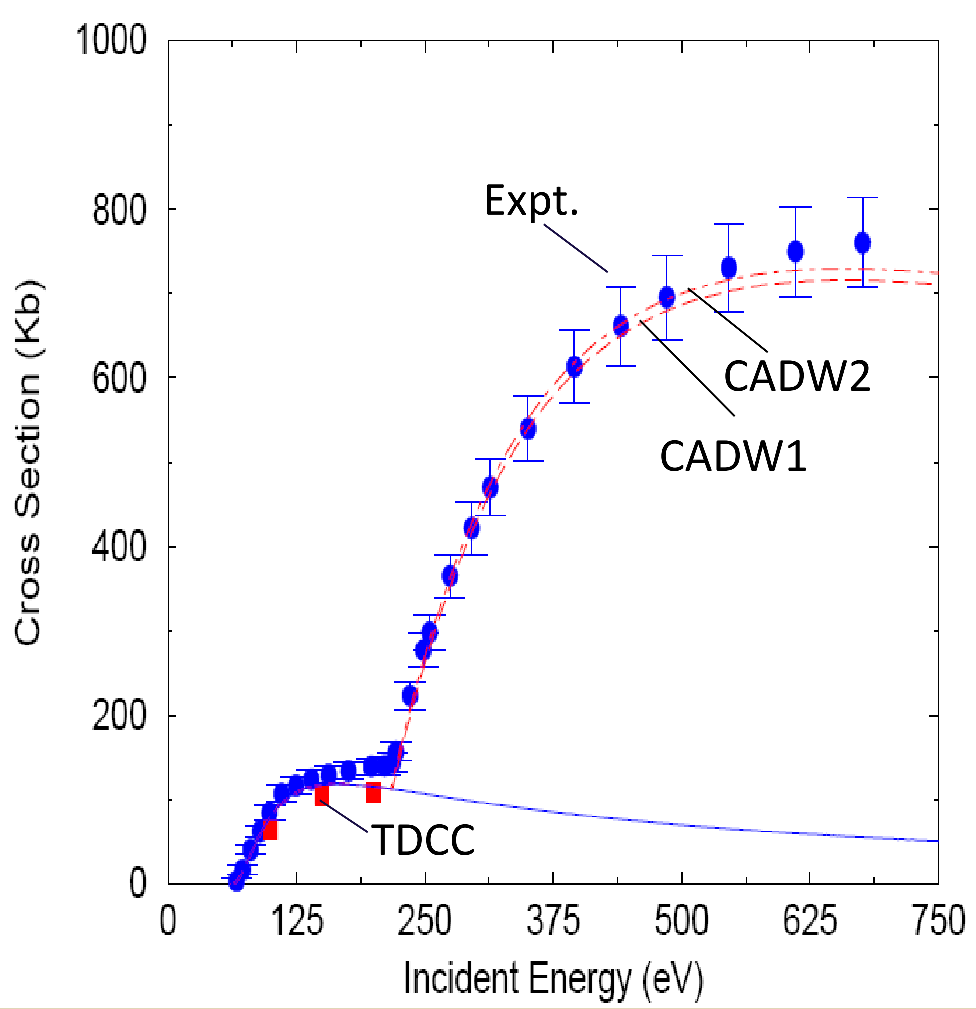
- Necessary to include higher partial waves and higher multipoles in scattering calculations to ensure convergence results.

- With *fitting parameter = 1.2* , the ECIP method may be used to extrapolate the n=5 CADW cross section data to higher n shells.





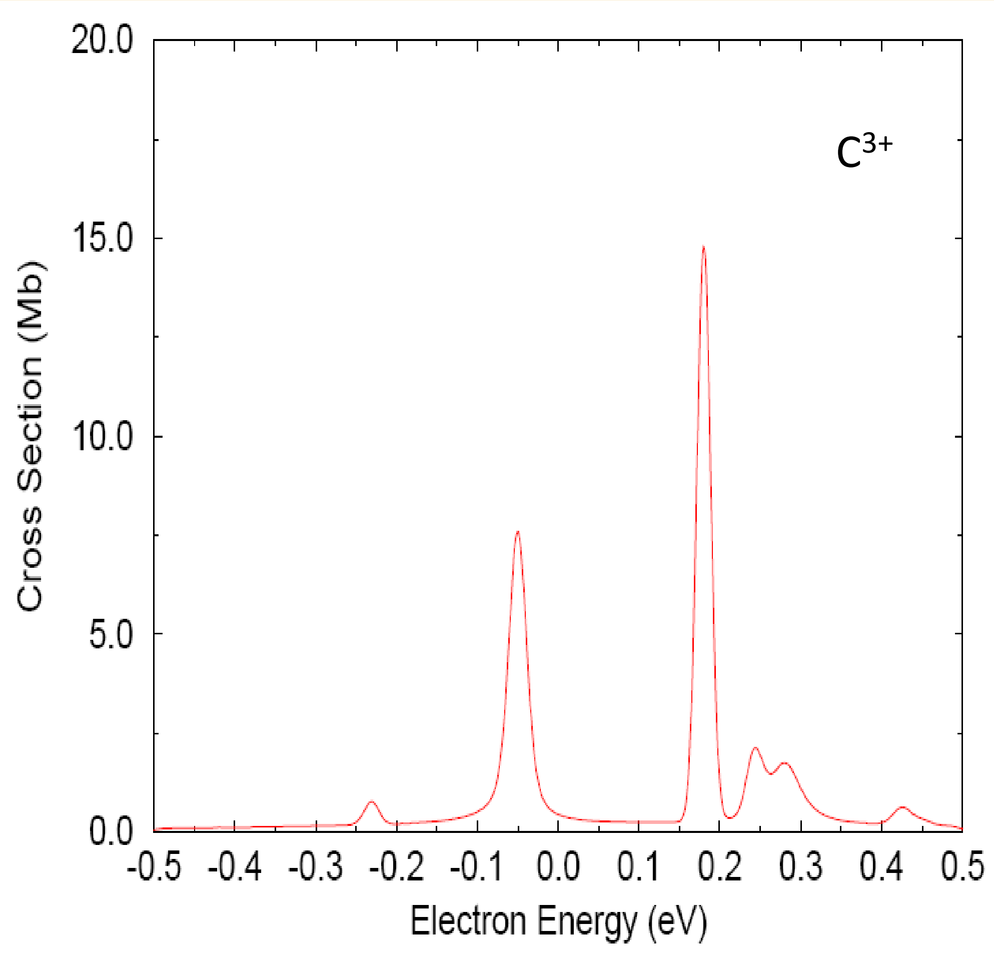
Electron-impact double ionization of B^+ ions



- Stringent test for the TDCC method.
- Double ionization of B^+ is 50 times smaller than the single ionization. So, it is not needed for fusion plasma modeling.
- But this may not be true for heavier elements, like W ions.

Pindzola et al., J. Phys. B 44, xxxxxx (2011)

Negative energy resonance states contribution to DR in C^{3+} (low temperature plasma)



- DR data for fusion is in good shape.
- Robicheaux, Loch, Pindzola & Ballance, *Phys. Rev. Lett.* 233201 (2010) finds strong resonance feature below the threshold for Mg^{8+}.
- Pindzola, Loch & Robicheaux, *Phys. Rev. A* 002700 (2011) finds strong resonance feature below the threshold for C^{3+}.

Heavy particle collision data

Charge transfer

- p + H: *Kolakowska et al., Phys. Rev. A 58, 2872 (1998)*
- p + He: *Minami et al., J. Phys. B 37, 4025 (2004)*
- p + Li: *Pindzola, Phys. Rev. A 60, 3764 (1999)*
- p + H(2s): *Pindzola et al., Phys. Rev. A 72, 062703 (2005)*
- Be^{4+} + H: *Minami et al., J. Phys. B 39, 2877 (2006)*
- p + He^{+} & α + Li^{2+}: *Minami et al., J. Phys. B 40, 3629 (2007)*
- α + H: *Minami et al., J. Phys. B 41, 135201 (2008)*

Summary

- The R-matrix, TDCC and DW methods have been used to study electron-impact ionization of neutral atomic and low-charged ionic B and C in their excited states.
- For moderate densities plasma (10^{10} –10^{15} cm^{-3}), ionization from excited states (ES) can be significant.
- The direct ionization can scaled up to higher n shells.
- But be careful with the excitation-autoionization (EA) contributions in scaling procedure.
  - ❑ B: n=3 EA is small.
  - ❑ C^+: n=3 EA is large.
- EA contributions could be even larger for heavier atoms and ions.

Future Plan

- Identifying the gaps. For examples, which light elements needed to be recalculated.
- Electron-impact excitation of C in ground state using the RMPS is ongoing.
- Electron-impact ionization of C in ground state using the RMPS is ongoing.
- Electron-impact ionization of C, C^{+} and C^{2+} in their excited states using the RMPS is ongoing.
- Produce GCR data for boron isonuclear sequence.
- Produce GCR data for carbon isonuclear sequence.
- Ne isonuclear sequence is next.