Benchmark calculations for electron collisions with complex atoms

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Benchmark calculations for electron collisions with general B-spline R-matrix package (BSR)

Benchmark results:

- maximum accuracy
- possible source of uncertainties
- convergence
- uncertainty estimations

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- **Continuum pseudo−state approach (RMPS)**

2. **Examples**

- **Scattering on neutral atoms (Ar, C, N, O, F, Be, Mg)**
- **Scattering on ions (Be-like N^{3+}, O-like Mg^{4+})**

4. **Summary**

Benchmark calculations for electron collisions with general B-spline R-matrix package (BSR)

OVERVIEW:

1. General features of BSR:
   - R−matrix method (close−coupling expansion)
   - B-splines as universal basis
   - Non-orthogonal orbitals technique
   - Continuum pseudo−state approach (RMPS)
2. Examples
   - Scattering on neutral atoms (Ar, C, N, O, F, Be, Mg)
   - Scattering on ions (Be-like N^{3+}, O-like Mg^{4+})
4. Summary

The B-Spline R-Matrix (BSR) Method

[O. Zatsarinny, Comp. Phys. Commun. 174, 273 (2006)]

- The method is based on the non-perturbative **close-coupling** expansion.

- Standard method of treating **low-energy** scattering
- Based upon an "**exact**" expansion of the total scattering wavefunction over target states

$$\Psi_E^{LS\pi}(r_1,\ldots,r_{N+1}) = A\sum_i \int \Phi_i^{LS\pi}(r_1,\ldots,r_N,\hat{r})\frac{1}{r}F_{E,i}(r) + \sum_j \Phi_j^{LS\pi}(r_1,\ldots,r_{N+1})$$

- Simultaneous results for transitions between **all states** in the expansion
- **Problems:**
  - close–coupling expansion must be **cut off**
  - accuracy (expansions) of **target** states are limited

Main source of uncertainties

The B-Spline R-Matrix (BSR) Method

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- The method is based on the non-perturbative **close-coupling** expansion.
- The close-coupling equations are solved using the **R-matrix method**.

- **Basic Idea**: indirect calculations – inner ($r < a$) and outer regions ($r > a$).
- **Complete set** of inner-region solutions is found from diagonalization of total Hamiltonian modified with Bloch operator
- **Scattering parameters** can then obtained from matching with solutions in external region − allows us obtain cross sections at many energy points rather cheaply

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- **Computer Codes:**
  - RMATRX–I : Berrington *et al* (1995)
  - PRMAT - parallelized version of RMARX-I
  - Badnell's Rmax complex - http: //amdpp.phys.strath.ac.uk/, with possibility for radiative damping
  - DARC – relativistic version, http://web.am.qub.ac.uk/DARC/
  - Enormous number of calculations

Principal ingredient: a single set of orthogonal one-electron orbitals

- $< P_{n\ell} \mid P_{n'\ell} > = 0 \rightarrow$ difficulties to achieve accurate target representation for different states
- $< P_{n\ell} \mid F_{k\ell} > = 0 \rightarrow$ large (N+1)-electron expansions needed for completeness (may lead to appearance of pseudo-resonances)

$$\Psi_E^{LS\pi}(r_1,...,r_{N+1}) = A\sum_i \int \Phi_i^{LS\pi}(r_1,...,r_N,\hat{r})\frac{1}{r}F_{E,i}(r) + \sum_j \Phi_j^{LS\pi}(r_1,...,r_{N+1})$$

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- The method is based on the non-perturbative **close-coupling** expansion.
- The close-coupling equations are solved using the **R-matrix method**.
- Atomic-structure calculations – **frozen-core approximation**

Distinctive feature:

Allows for **non-orthogonal orbital sets** to represent both bound and continuum radial functions

- **independent generation of target states** – much more accurate target representation (**term-dependence, relaxation effects, correlation**)

It allows us to considerably (almost completely) reduce the uncertainties due to the accuracy of the target states

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Distinctive feature:

Allows for **non-orthogonal orbital sets** to represent both bound and continuum radial functions

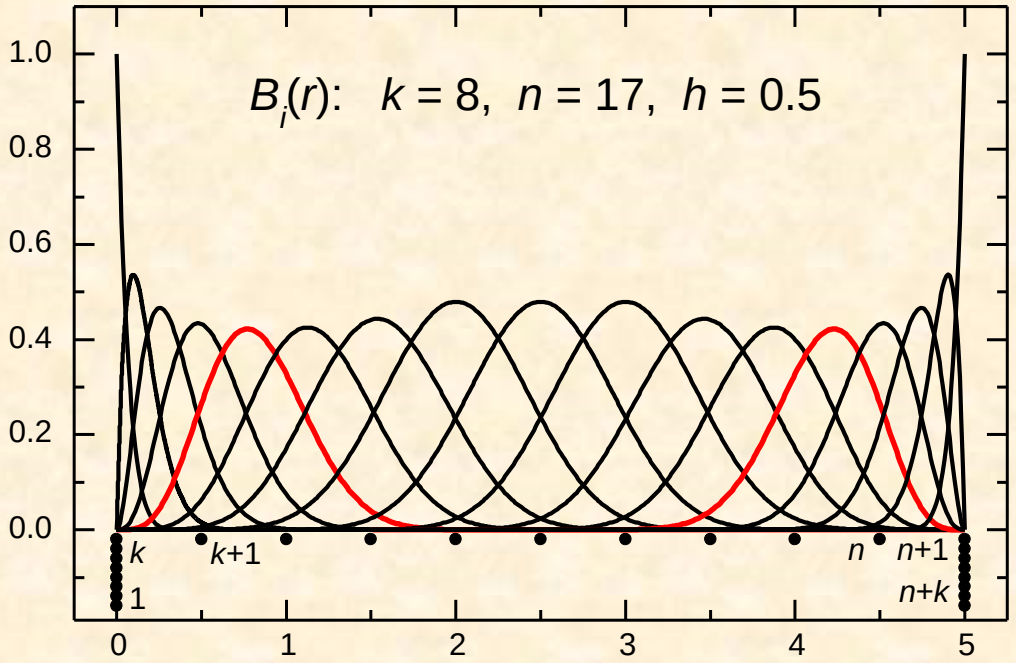
- **independent generation of target states** – much more accurate target representation (**term-dependence, relaxation effects, correlation**)

- **no artificial orthogonality constraints for continuum orbitals** – more consistent treatment of N-electron target and (N+1)-electron collision system –> (**no pseudo–resonances, improved convergence)**

Additional source of uncertainties

$$\Psi_E^{LS\pi}(r_1,\ldots,r_{N+1}) = A\sum_i \int \Phi_i^{LS\pi}(r_1,\ldots,r_N,\hat{r})\frac{1}{r}F_{E,i}(r) + \sum_j \Phi_j^{LS\pi}(r_1,\ldots,r_{N+1})$$

Why B-splines ?



- **excellent numerical properties** – machine accuracy with Gaussian quadratures.
- **flexibility** in the choice of radial grid.
- effective **completeness** of B-spline basis – no Buttle correction required;
  finite representation of whole Rydberg series or continuum spectra.
- avoid finite-difference algorithms – established **Linear Algebra packages** can be used.

$$\psi(r) = \sum_i c_i B_i(r) \qquad H\Psi = E\Psi \;\rightarrow\; \mathbf{Hc} = E\mathbf{Sc}$$

- first R-matrix calculation with B-splines: e-H scattering (van der Hart 1997)

However – scattering calculations require relatively big basis: n ~ 50–100

BSR – general B-spline R-matrix package

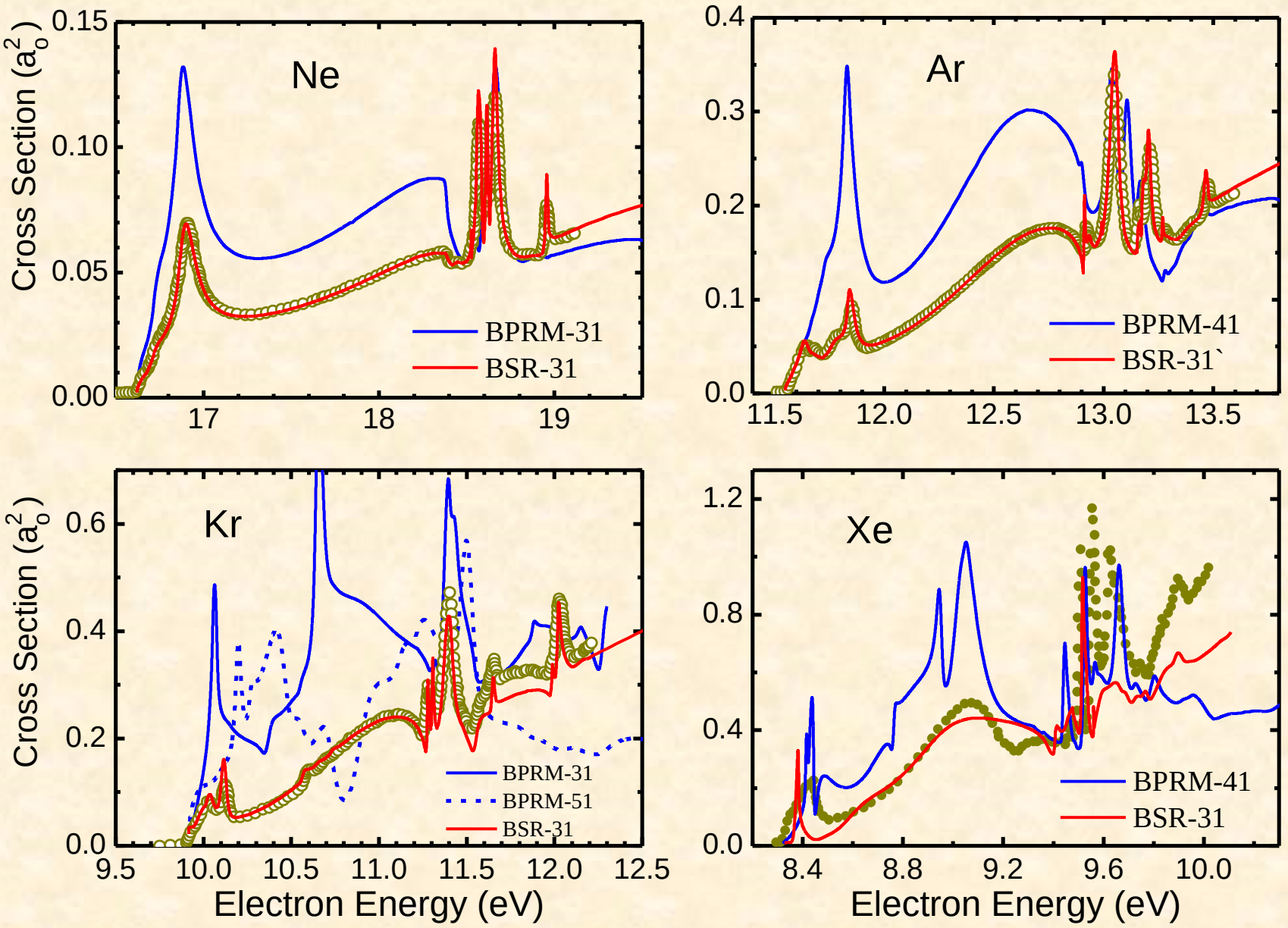
1. First implementation: Li photoionization (2000)
2. First presentation: ICPEAC XXX, Rosario, Argentina (2005)
3. First version published: Comp.Phys.Comm. (2006)
4. Fully-relativistic version: e-Cs scattering (2008)
5. RMPS extension and ionization: e-He,Ne scattering (2011-2012)
6. Topical review: J.Phys.B 46, 112001 (2013)

Calculations:

1. Electron scattering from neutrals (including inner-core excitations)
   He, Be,C, N, O, F, S, Cl, Ne, Na, Mg, Al, Si, Ar, K, Ca, Zn, Cu, I, Kr, Rb, Xe, Cs, Kr, Xe, Cs, Au, Hg, Pb
2. Electron-ion collisions (rate coefficients)
   S II, K II, Fe II, Fe VII, Fe VIII, Fe IX
3. Photodetachment and photoionization
   He-, Li-, B-, O-, Ca-, Li, K, Zn
4. Atomic structure: energies, oscillator strengths, polarizabilities
   C, Ne, S, SII, F, CL, Ar, Kr, Xe

Metastable production in Electron Collisions with noble gases

BSR calculations

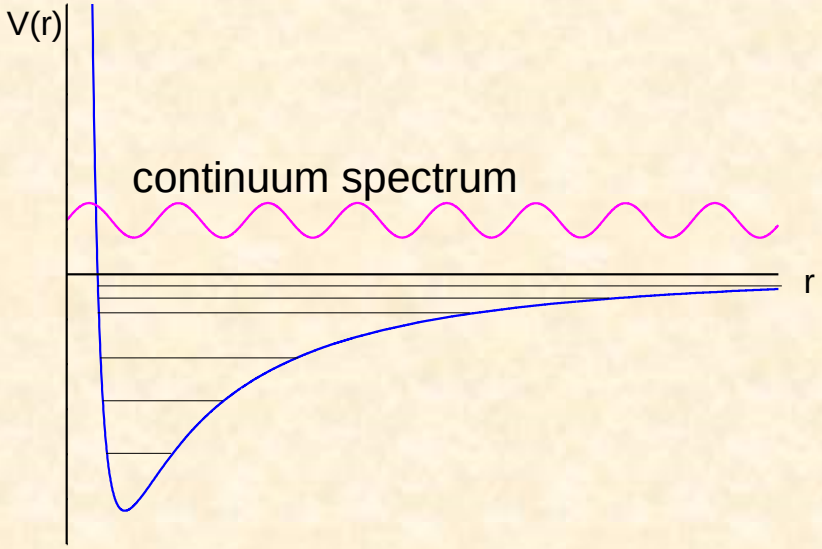


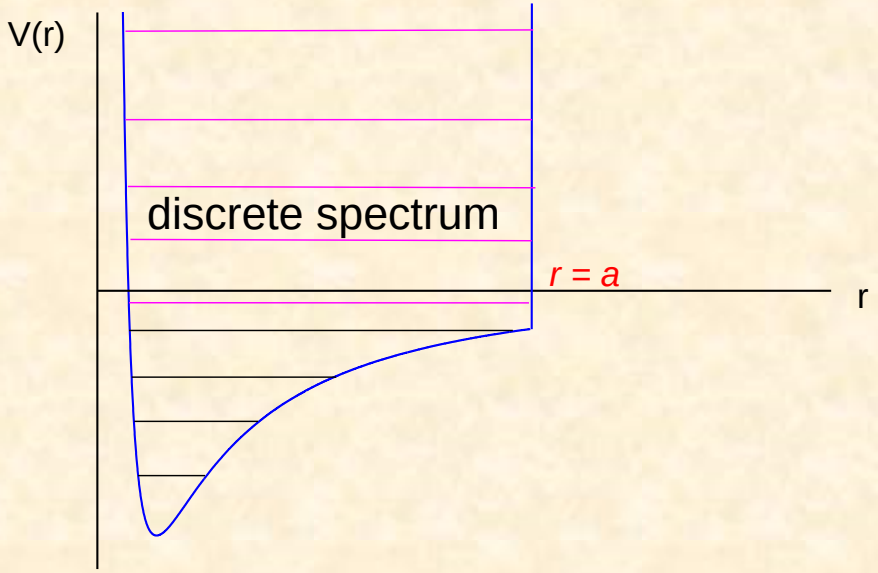
BSR with pseudo-states

$$\Psi_E^{LS\pi}(r_1,\ldots,r_{N+1}) = A\sum_i \int \Phi_i^{LS\pi}(r_1,\ldots,r_N,\hat{r}_{N+1})\frac{1}{r_{N+1}}F_{E,i}(r_{N+1}) + \sum_j \Phi_j^{LS\pi}(r_1,\ldots,r_{N+1})$$

?

We use the **box-based** approach:





Both physical and pseudo-states are found by **direct** solving the close-coupling (frozen-cores) equations for **N-electron** atomic wavefunctions with zero boundary conditions.

How many pseudo-states do we need in this approach to simulate the target continuum?

Electron-impact excitation of neon at intermediate energies

(PHYSICAL REVIEW A 86, 022717, 2012)

Target states:

$$\Phi(2s^2 2p^5 nl, J) = A\sum_{ij,LS} a_{ij}\{\varphi(2s^2 2p^5;^2\mathrm{P}) \bullet B_i(r)\,|\,l_j s>, LS\}^J$$
$$+ A\sum_{ij,LS} a_{ij}\{\varphi(2s2p^6;^2\mathrm{S}) \bullet B_i(r)\,|\,l_j s>, LS\}^J$$

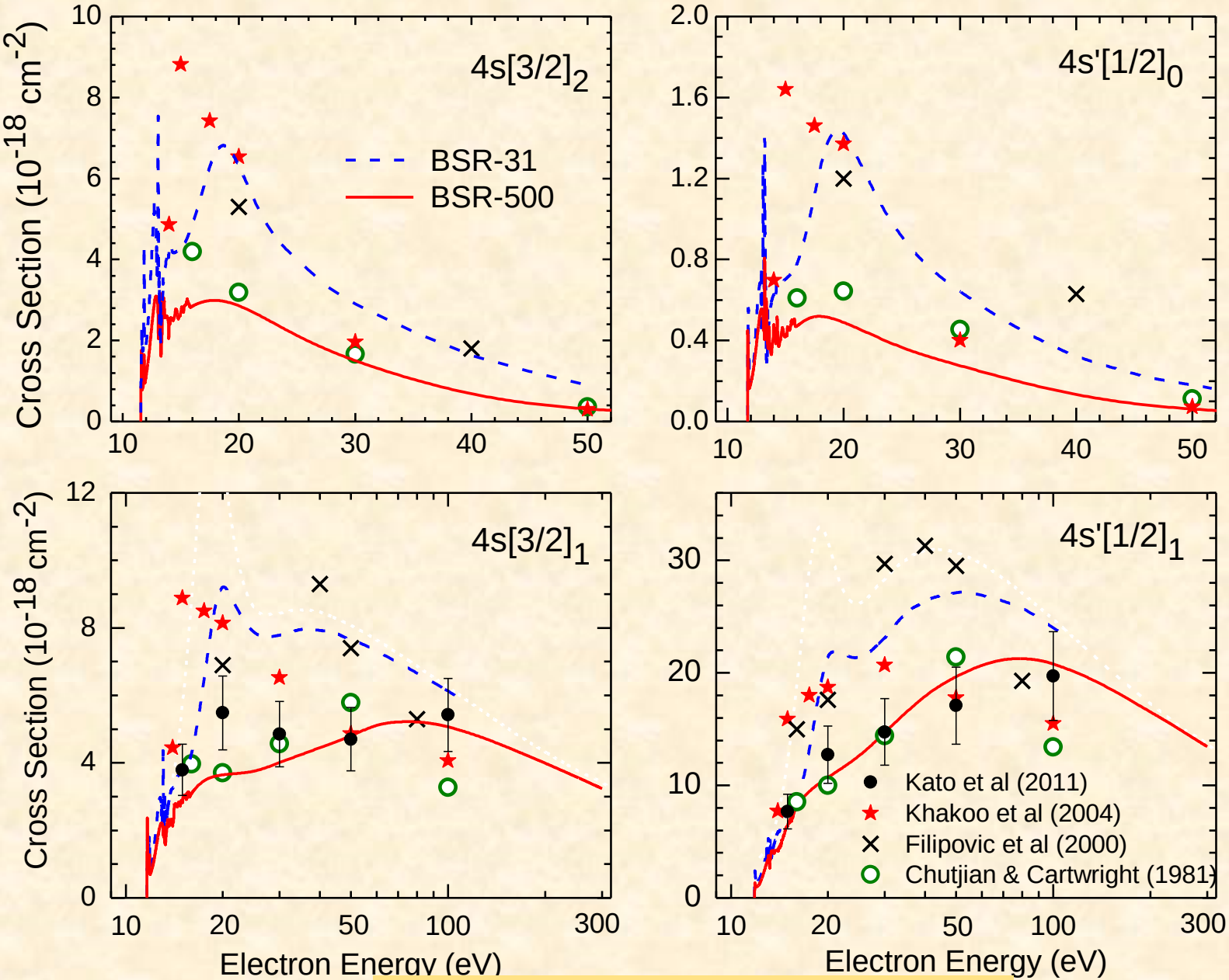
Total number of states	**–**	**457**
Bound states	**–**	**87**
Continuum pseudostates	**–**	**370**
(l = 0 – 3)		
Continuum energy coverage	**–**	**40eV**
Number of channels	**–**	**2260**
R-matrix radius	**–**	**$30a_o$**
Number of *B*-splines	**–**	**70**
Hamiltonian matrix	**–**	**150000**

Number of processors used – up to 1000

Resources used – **200000 PU** (1 hour x 1 processor)
(for 50 partial waves)

Do we really need such big computational efforts?

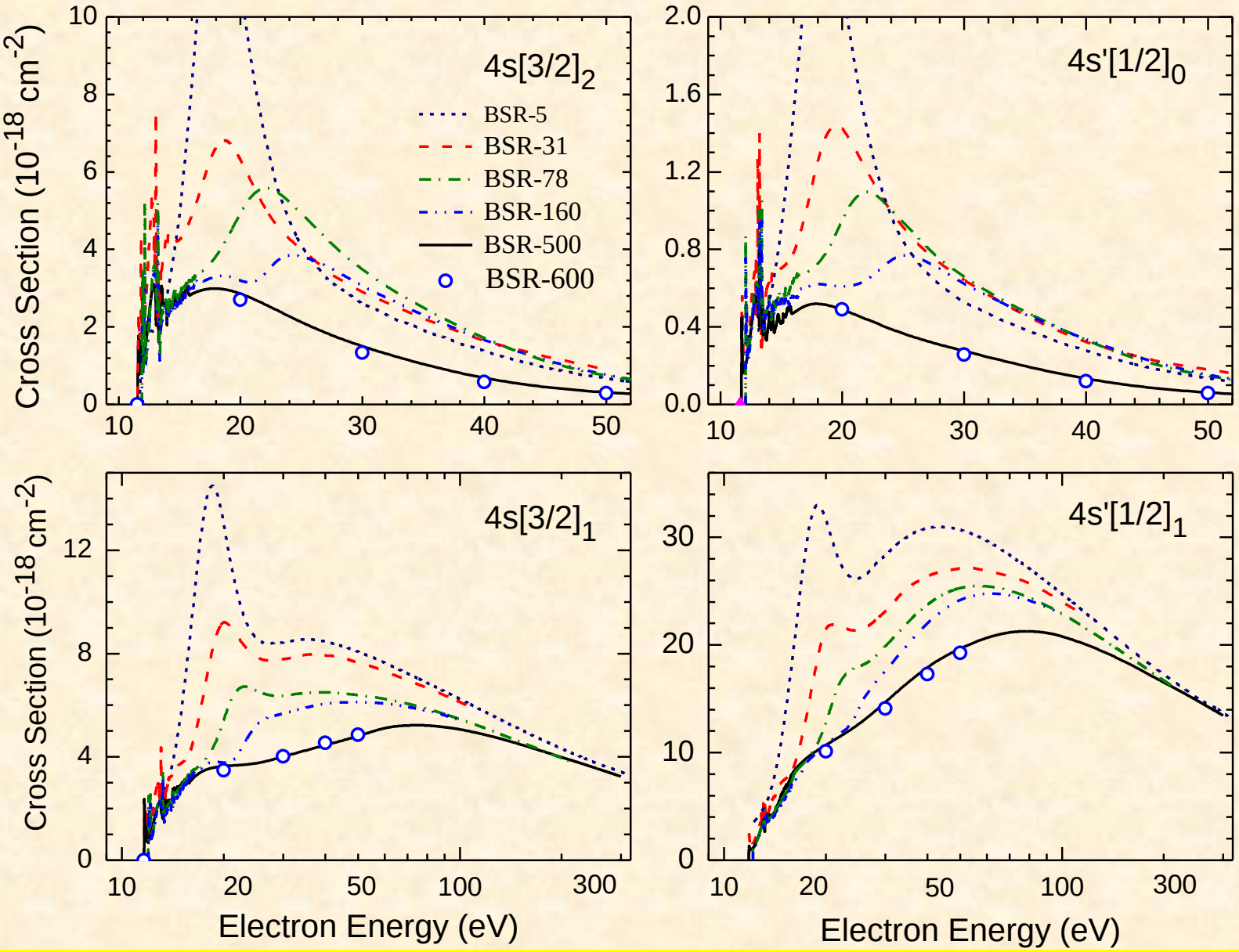
Effect of Channel Coupling to Discrete and Continuum spectrum in Ar



How to estimate uncertainties here?

Total Cross Section for Electron Impact Excitation of Argon

Convergence study

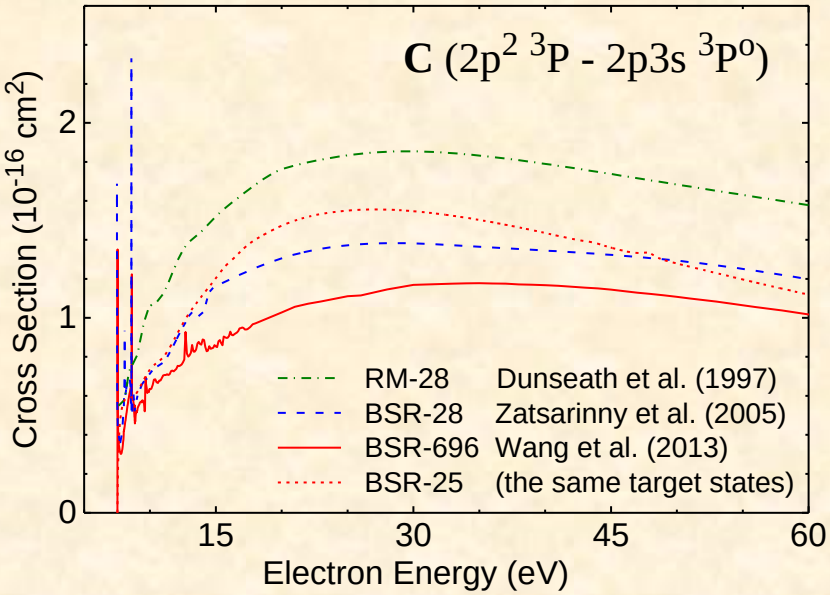


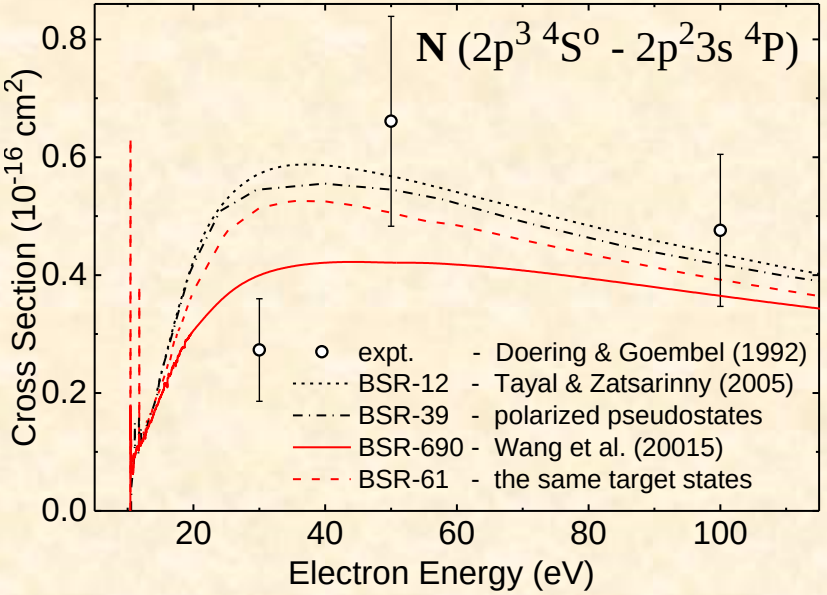
Final uncertainty within 5−10 percent, just based on the convergence study.

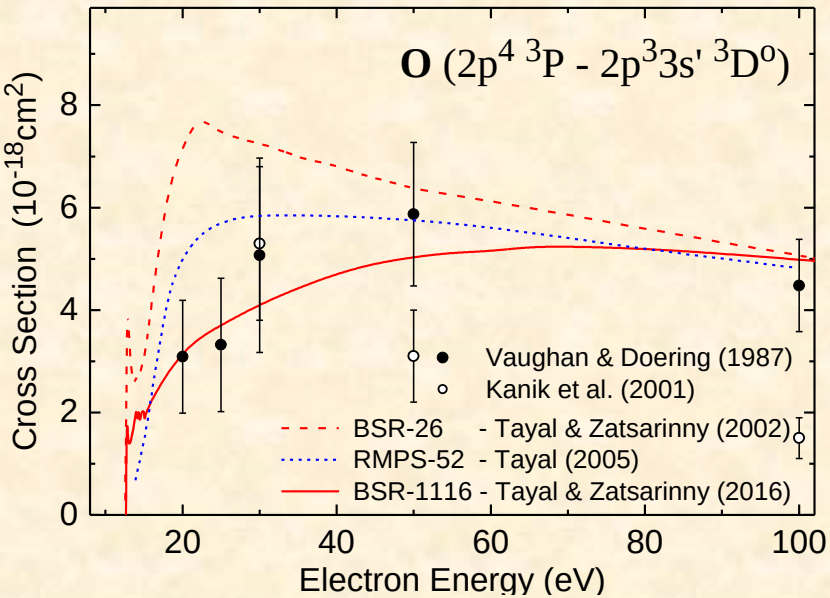
- Ne($2p^6$) , Ar($3p^6$) - extremely big influence of target continuum.

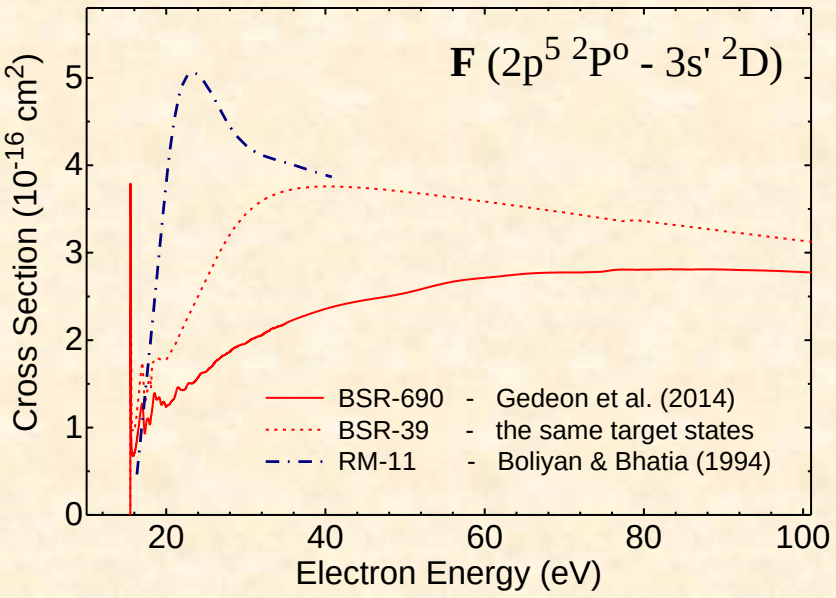
- What about other atoms with open p-shells:

  B(2p), C($2p^2$), N($2p^3$), O($2p^4$), F($2p^5$) - ?









- Inclusion of the target continuum – mandatory condition for the neutral atoms, at least.
- But first check target − then CC convergence !
- **Uncertainties** – the upper limit – may be estimated as difference between CC models with the **same target w.f**.

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Calculations for electron-impact excitation and ionization of beryllium

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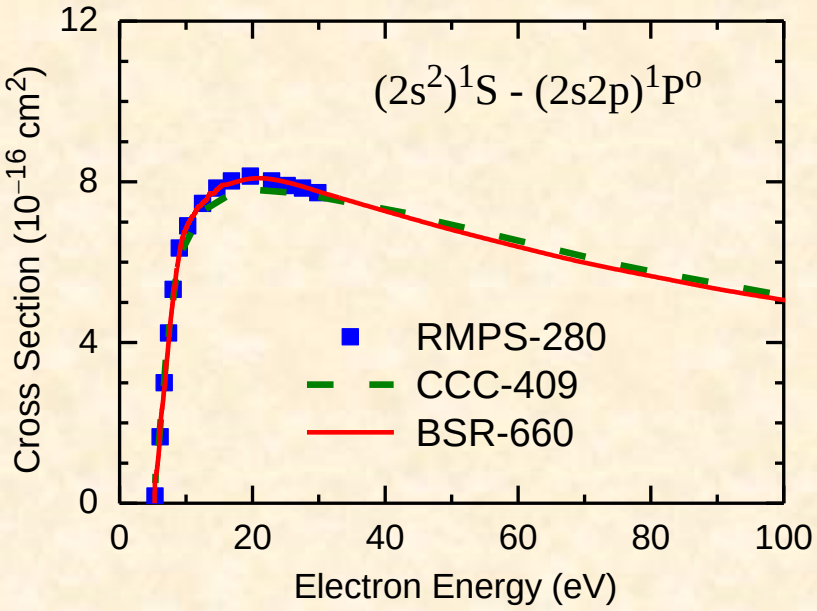
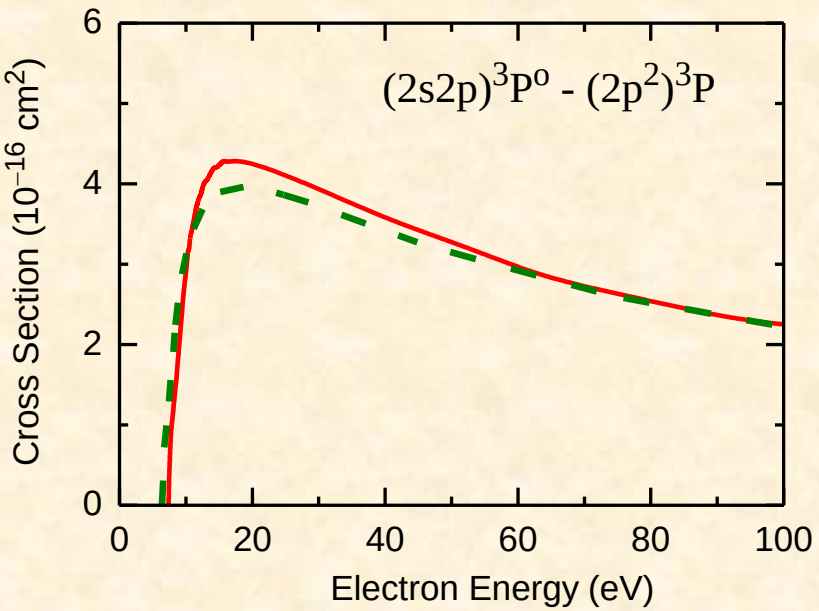
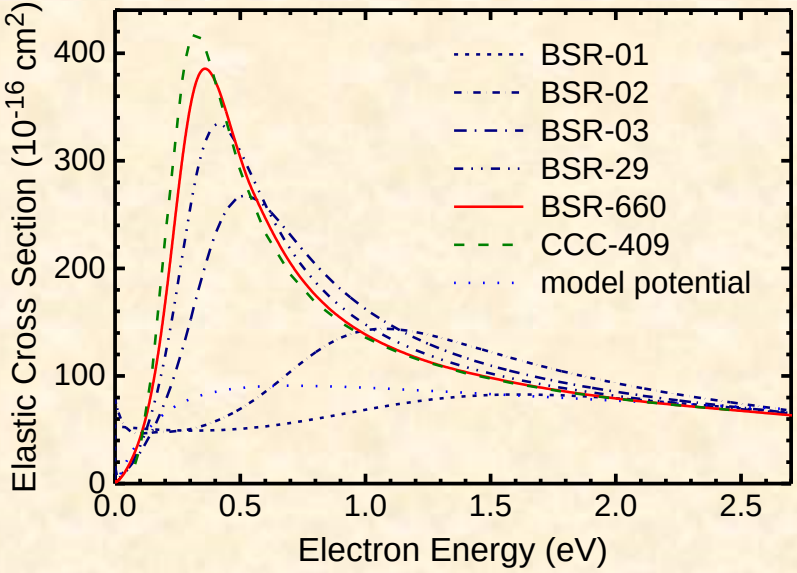
[2] Curtin Institute for Computation and Department of Physics, Astronomy and Medical Radiation Science, Curtin University, GPO Box U1987, Perth, WA 6845, Australia

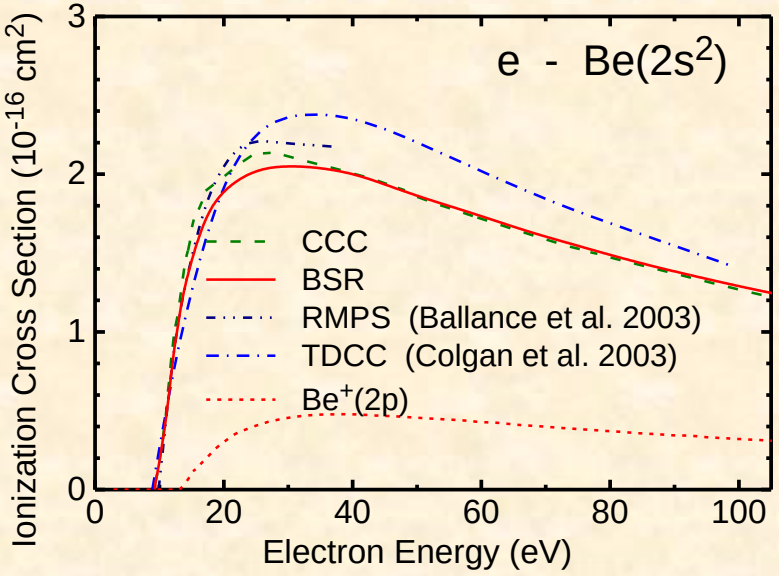
Motivation:

1. Big interest in plasma applications (JET project, ITER).
2. No experimental data.
3. What accuracy can be achieved for this ‘simple’ system?
4. Complete set of scattering data (first 21 levels).
5. Joint work of CCC and BSR teams.



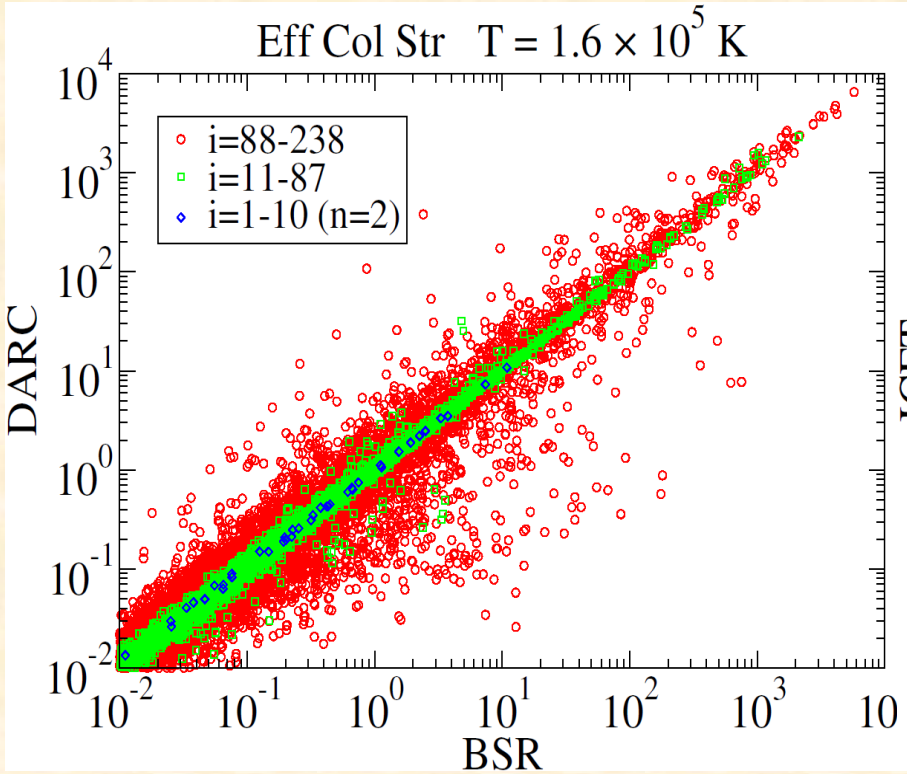


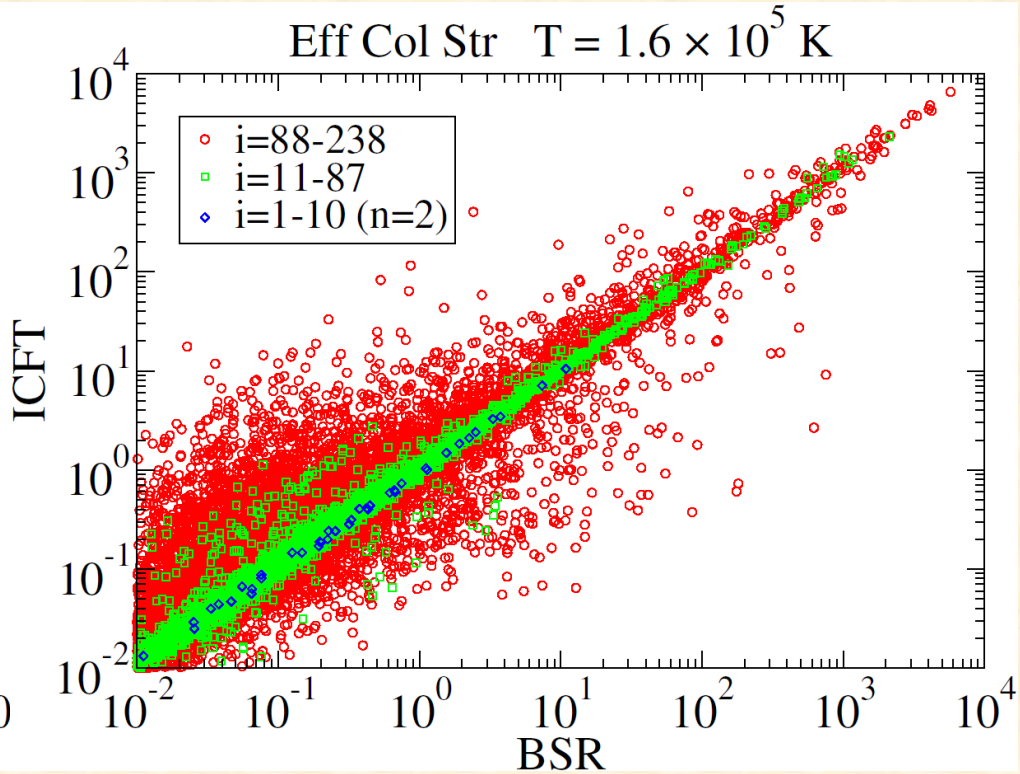




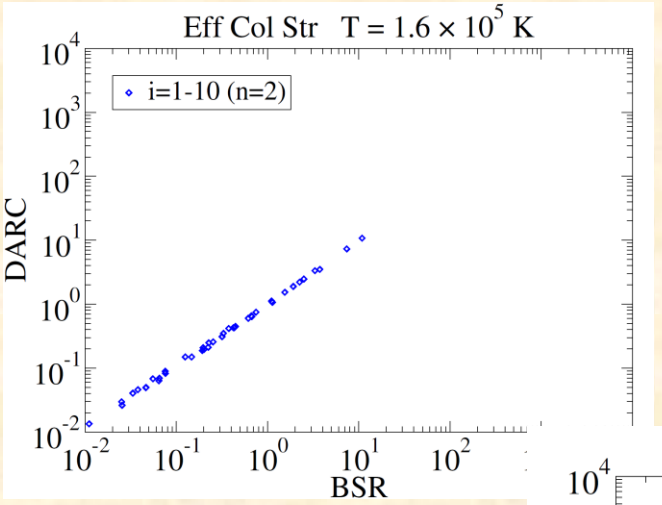
- A complete and consistent set of scattering data for Be, with a high level of confidence in a small uncertainty (5-10 %).
- A good example of team work (CCC + BSR) to get accurate results.
- New similar calculations for e-Mg are now in progress

Electron-impact excitation of N^{3+} ($2s^2$) ($2snl$, $2pnl$, $n \leq 8$)

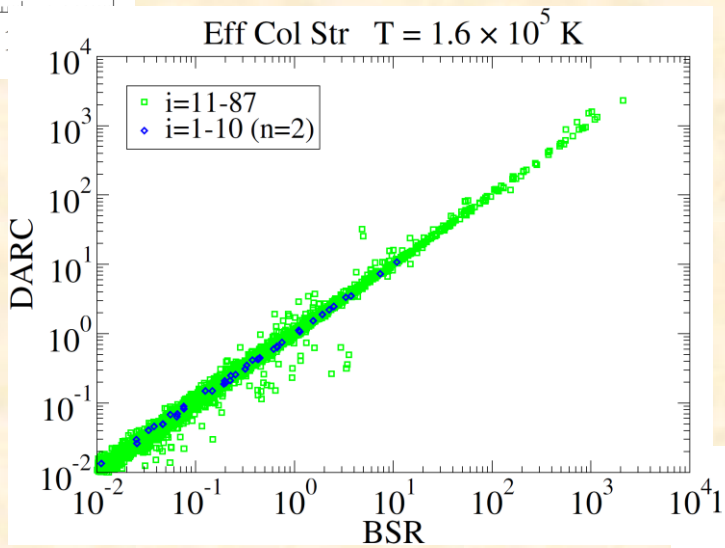




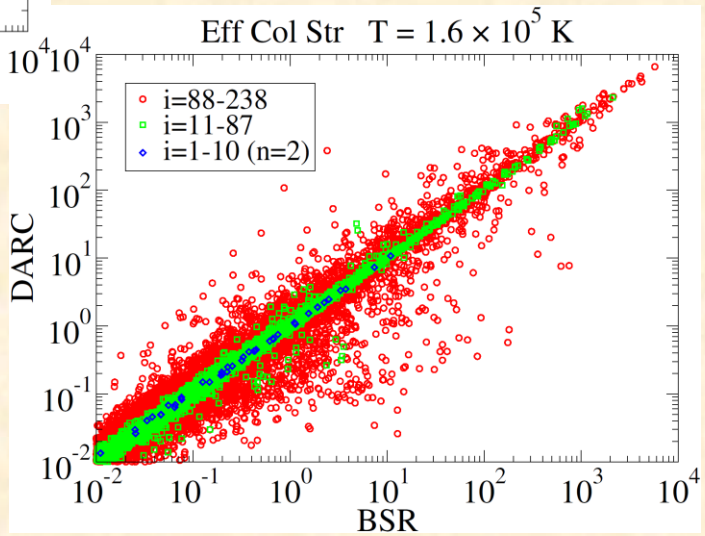
- **RM-238** (**ICFT** - Intermediate Coupling Frame Transformation) Fernandez-Menchero *et al*. 2014, Astron. Astroph. 566 A104)
- **DARC-238** (Dirac Atomic R-matrix Code) Aggarwal et al. 2016 Mon. Not. R. Astr. Soc. 461 3997)
- **BSR-238** with improved structure description (submitted to J.Phys.B)



n=2 transitions



n=2 -> higher levels



All transitions

Electron-impact excitation of Mg^{4+} ($2p^4$)

Big difference between existing datasets:

- **RM-37** (Hudson et al., 2009, A \& A 494, 729)
- **BSR-86** (Tayal & Sossah, 2015, A&A, 574, 87) **{ $2s^2 2p^4$, $2s 2p^5$, $2s^2 2p^3 3l$ }**
- **DARC-86** (Aggarwal & Keenan, 2016, Can. J. Phys., online)

statement: DARC calculations are much more accurate;
BSR results are completely wrong (possibly because
BSR code is not able to avoid pseudo resonances)

Electron-impact excitation of Mg^{4+} ($2p^4$)

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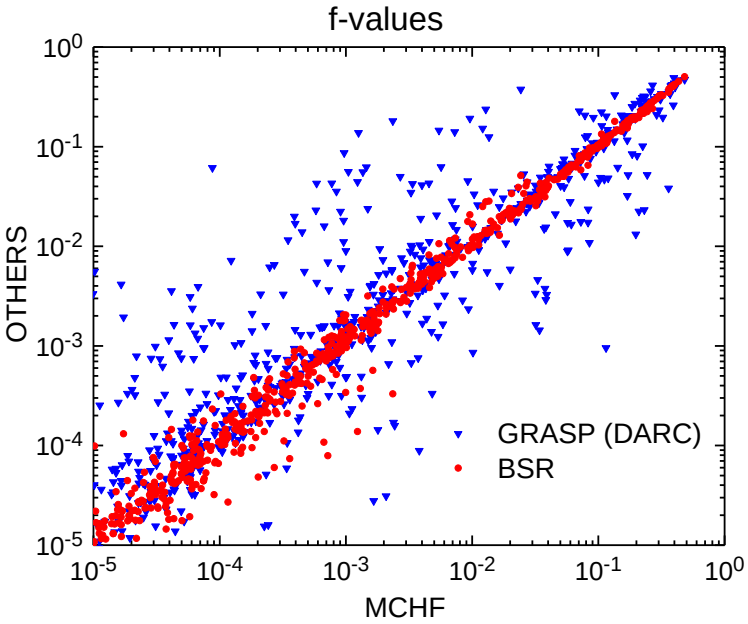
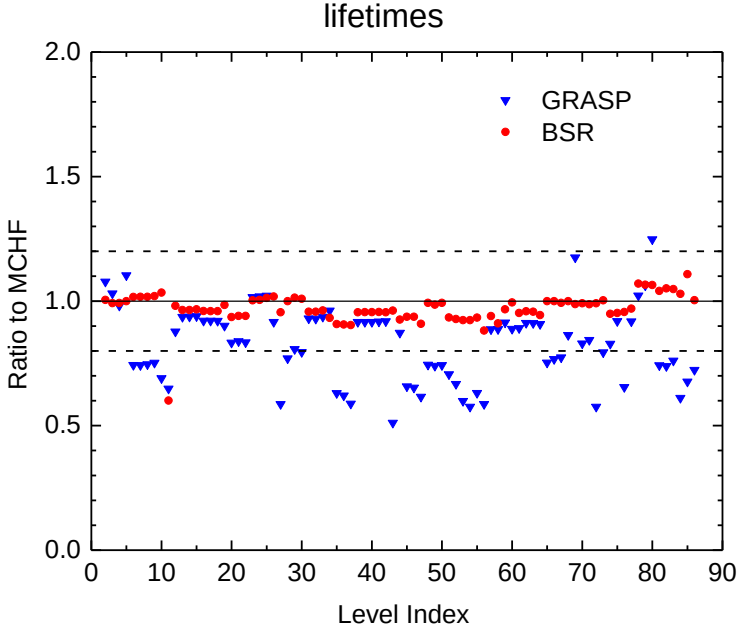
Really ???

New calculations:

- **BSR-86** with improved structure description
- **BSR-316** with additional **$2s^2 2p^3 4l$** and **$2s 2p^5 3l$** states

f-values and lifetimes of Mg^{4+} ($2p^4$)



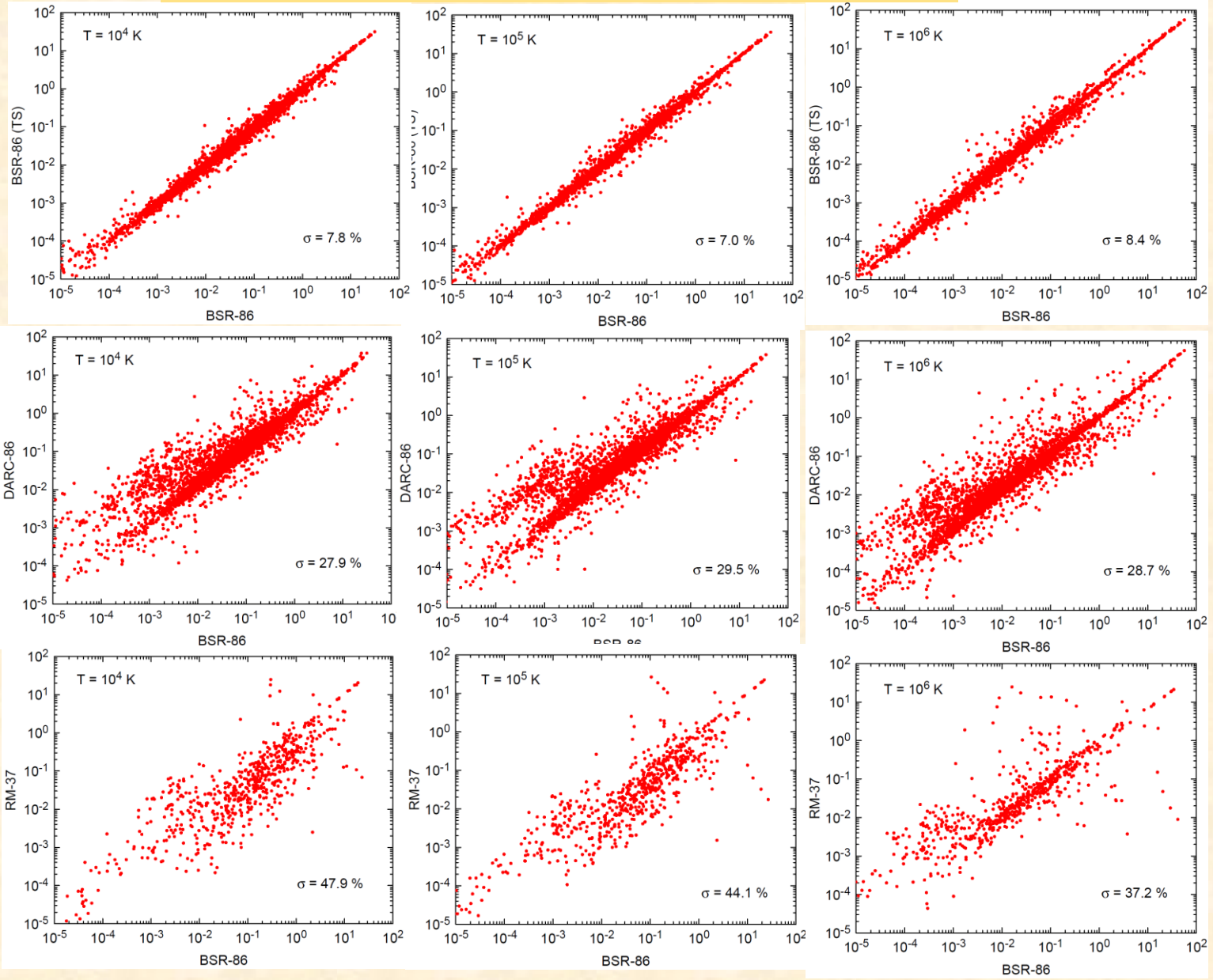


MCHF - Tachiev & Froese Fischer (2004)

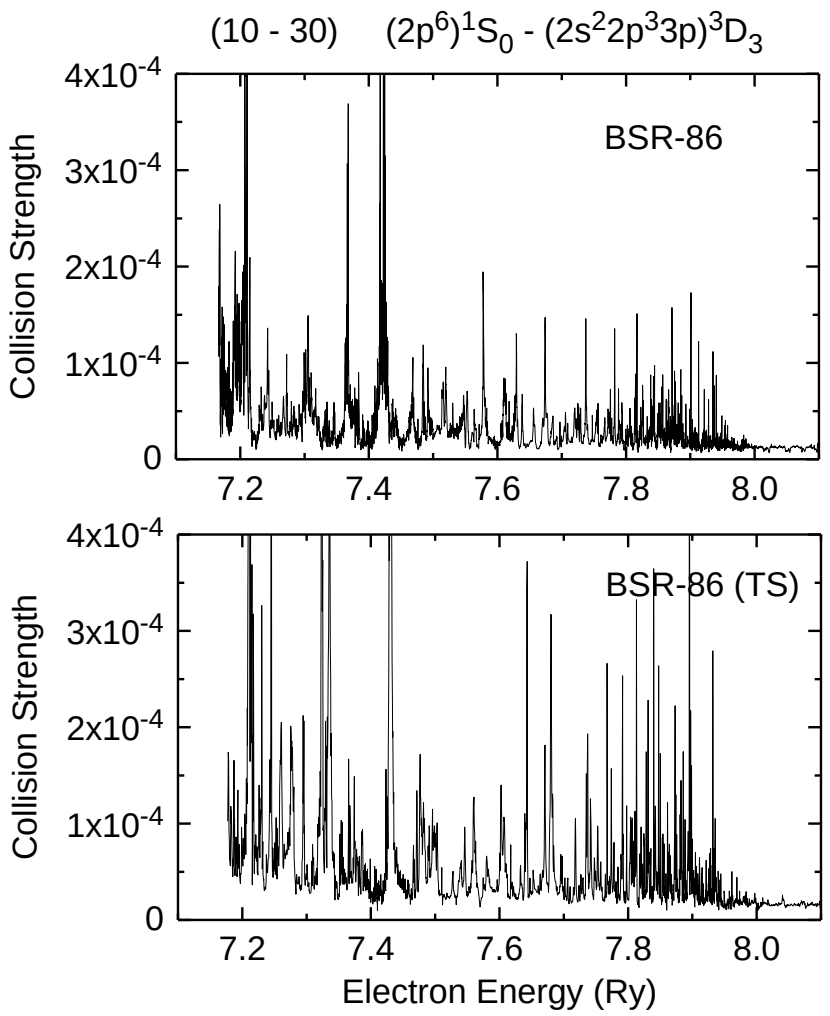
GRASP - Aggarwal & Keenan (2016), DARC-86

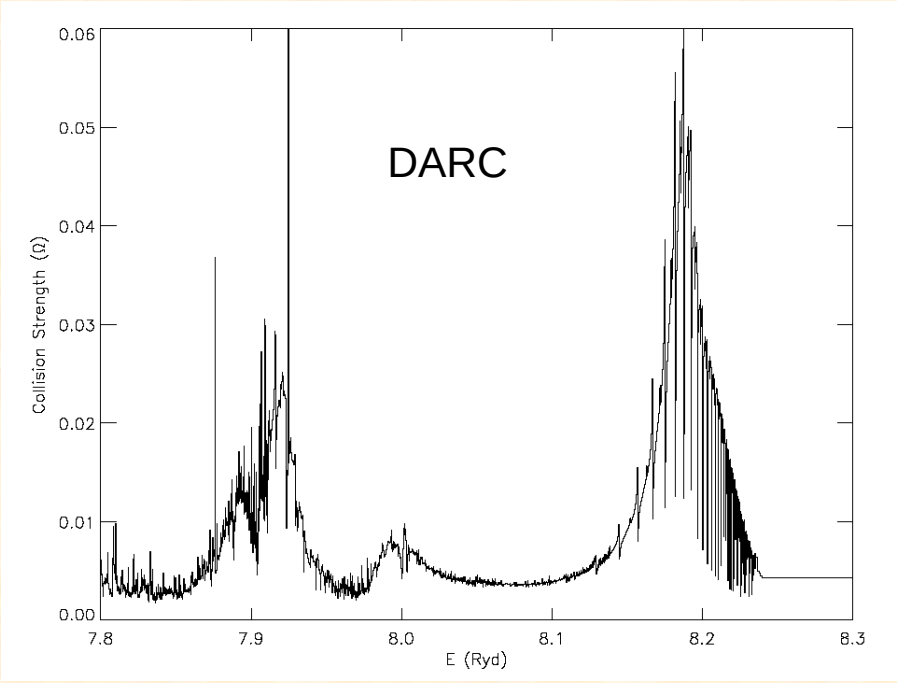
Effective collision strengths of Mg^{4+} ($2p^4$)

BSR-86 vs. BSR-86(TS), DARC-86, RM-37



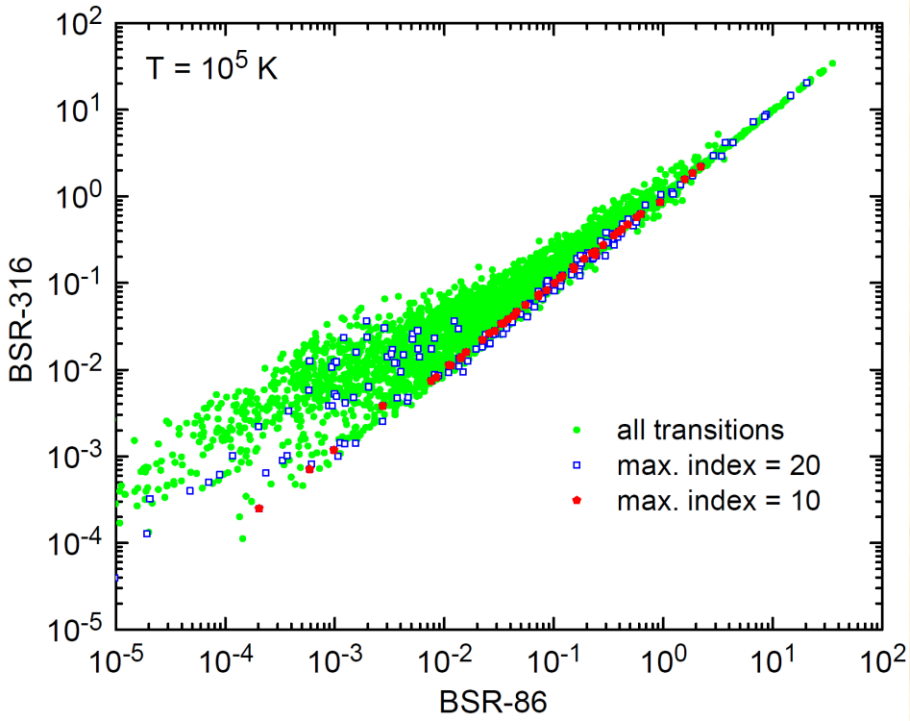
Electron-impact excitation of Mg^{4+} ($2p^4$)

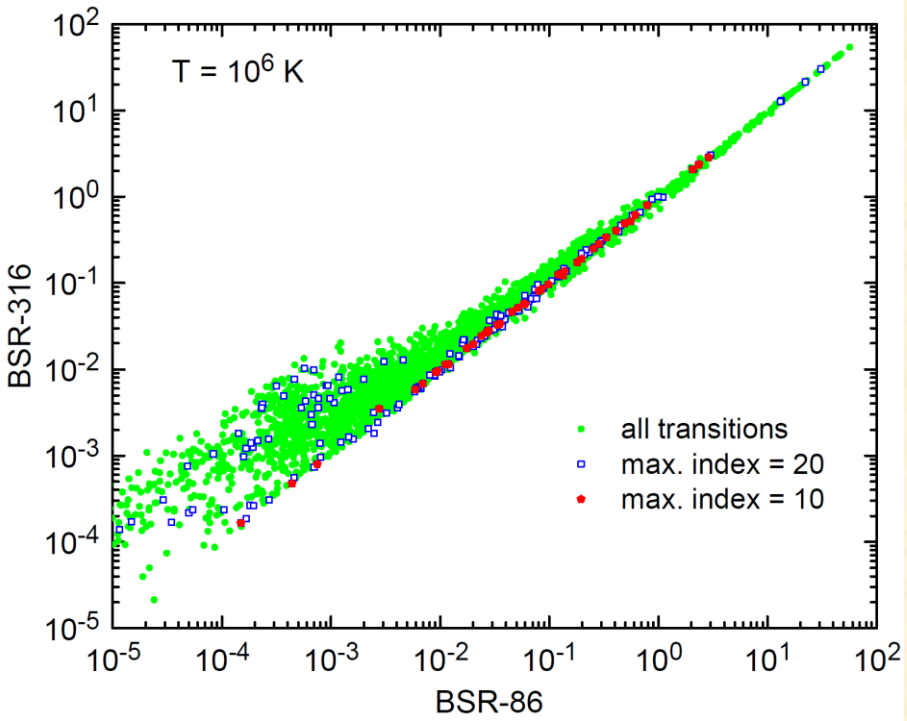




Effective collision strengths of Mg^{4+} ($2p^4$)

CC – convergence: BSR-86 vs. BSR-316





The **$2s^22p^4 \rightarrow 2s^22p^33l$** are mainly converged.

Difference mainly for weak two-electron transitions **$2s2p^5$, $2p^6 \rightarrow 2s^22p^33l$** or for transitions between close-lying levels

Electron-impact excitation of Mg^{4+} ($2p^4$)

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- **BSR-86** (Tayal & Sossah, 2015, A&A, 574, 87) **{ $2s^22p^4$, $2s2p^5$, $2s^22p^33l$ }**
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  statement: DARC calculations are much more accurate and the best;
  BSR results are completely wrong
  BSR code is not able to avoid pseudo resonances

New calculations

- **BSR-86** with improved structure description
- **BSR-316** with additional **$2s^22p^34l$ and $2s2p^53l$** states

Our conclusions:

- Good agreement our oscillator strengths with the extensive MCHF calculations indicate that our target description is more accurate than used before.
- We essentially confirm the previous BSR calculations by Tayal & Sossah (2015) (except #10 and #86 levels – computational bugs)
- Big disagreement with DARC calculations is mainly due to the target description (and possible pseudo resonances).
- RM-37 calculations of Hudson et al. (2009) for some transitions are clearly wrong due to evident appearance of pseudo resonances.
- Comparison of BSR-86 and BSR-316 indicate convergence for the lower levels.

Summary

❖ For complex targets, the **BSR method with non-orthogonal orbitals** has advantages:

- highly **accurate** target description
- more **consistent** description of (N+1)-electron scattering system
- considerable improvement for **low-energy region** and **near-threshold resonance** phenomena
- improvement for **intermediate** energies with **RMPS approach** (MPI version)
- BSR code is able to provide **benchmark** results for uncertainty estimation
  - ► considerable reduction (elimination) of **target description** uncertainty
  - ► absence of pseudo resonances
  - ► systematic check of **convergence** (including target continuum)

❖ requires **large-scale** computations using supercomputers (i.e., extensive and expensive)

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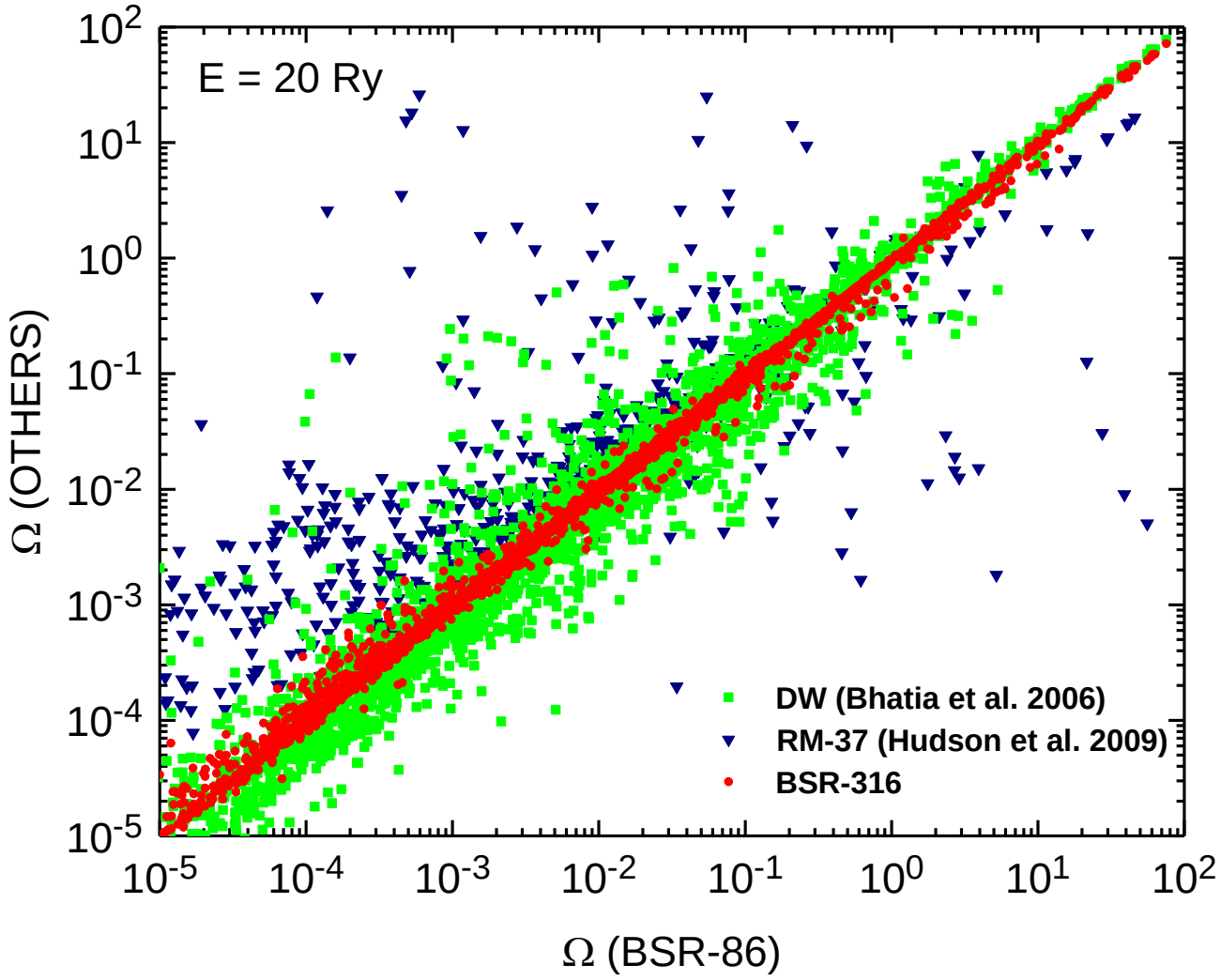
❖ My main point: The importance of accurate target descriptions is highly **underestimated** in most scattering calculations.
This leads to lower accuracy and larger uncertainties.

THANK YOU
For Your Attention!

Electron-impact excitation of Mg^{4+} ($2p^4$)

Background collision strengths: BSR-86 vs. DW, RM, BSR-316



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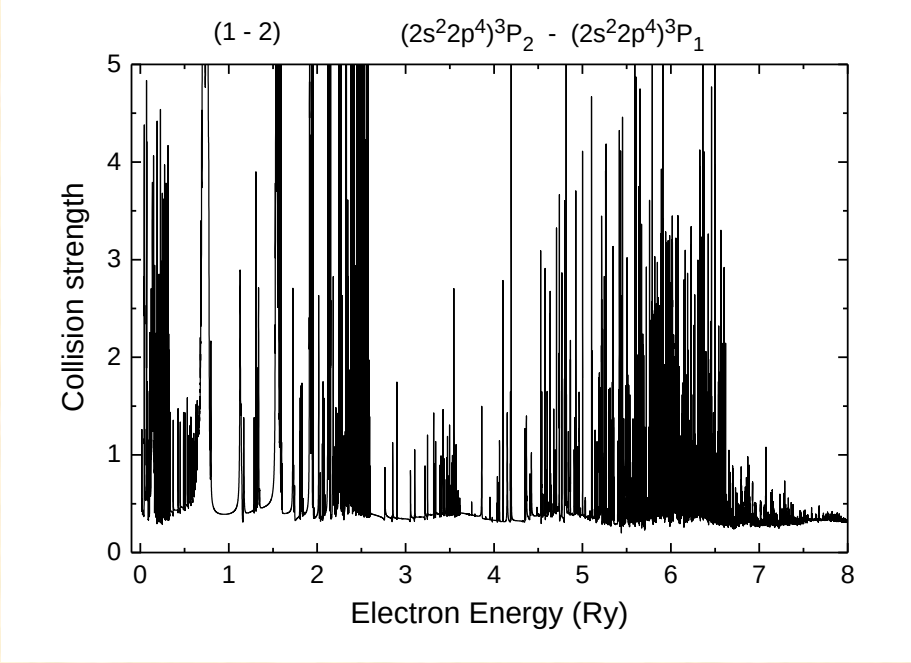
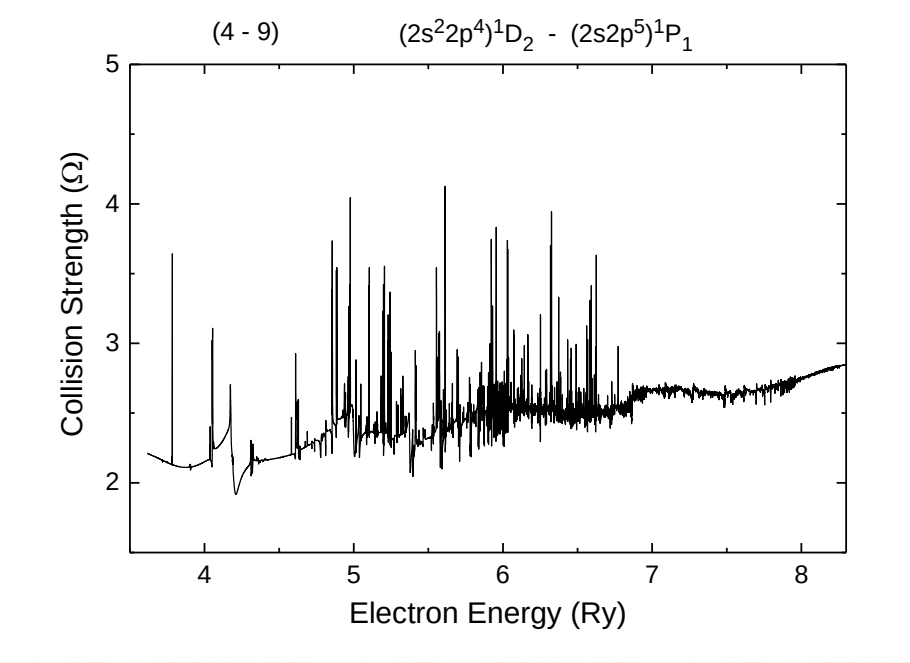
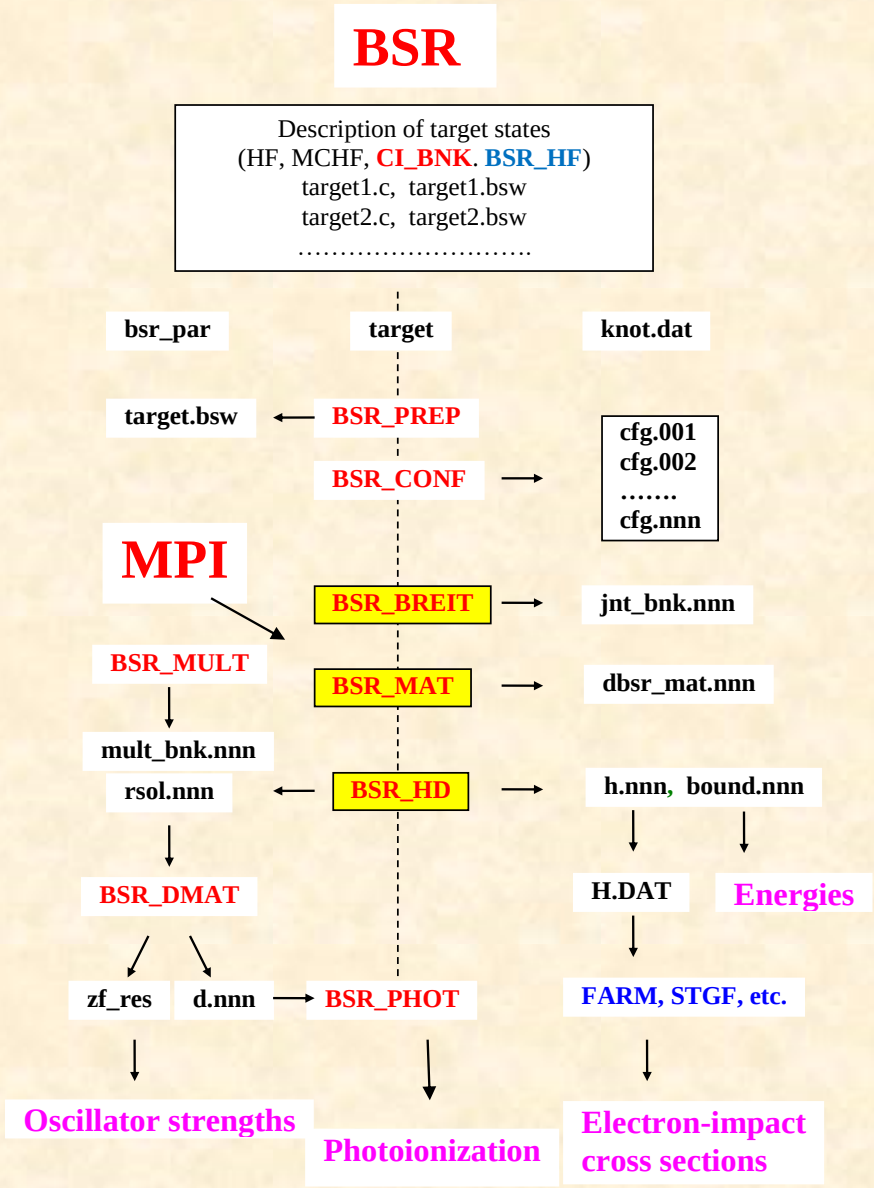
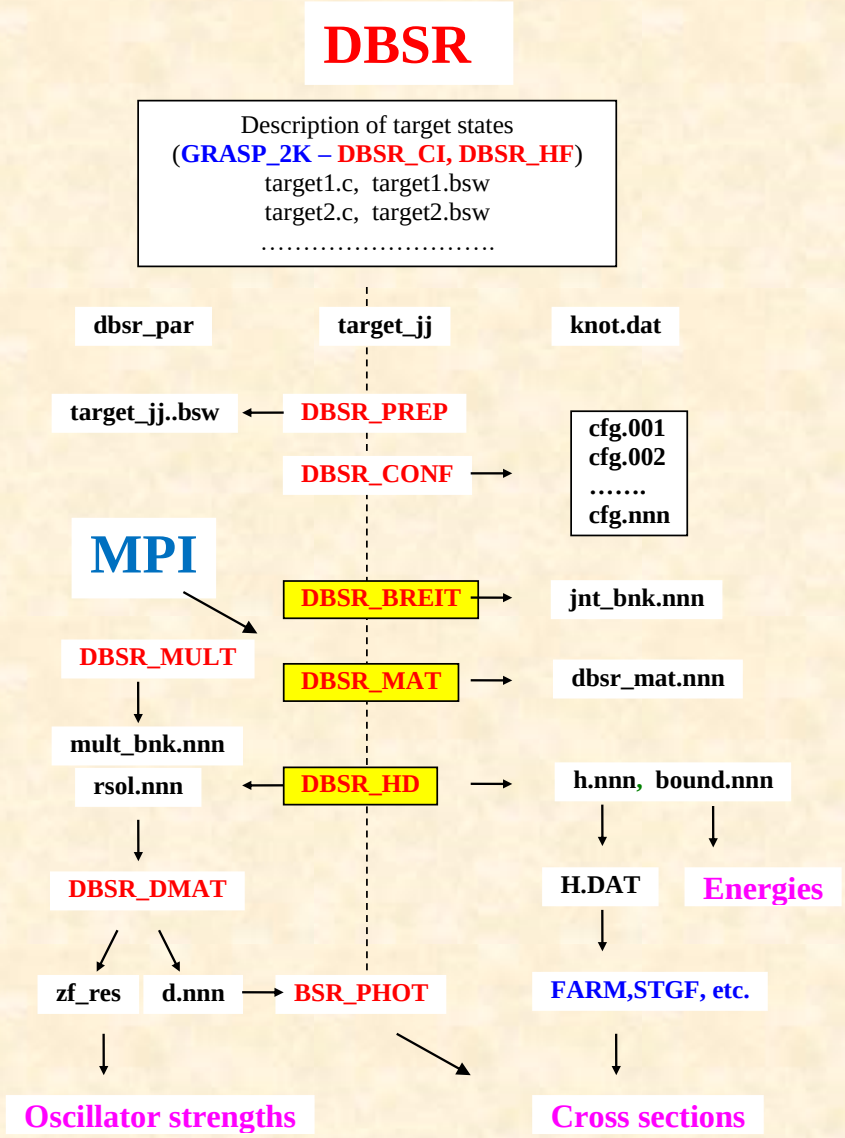




- We used 71000 energy points to resolve resonance structure





[O. Zatsarinny, Comp. Phys. Commun. 174, 273 (2006)]

Uncertainty's questions

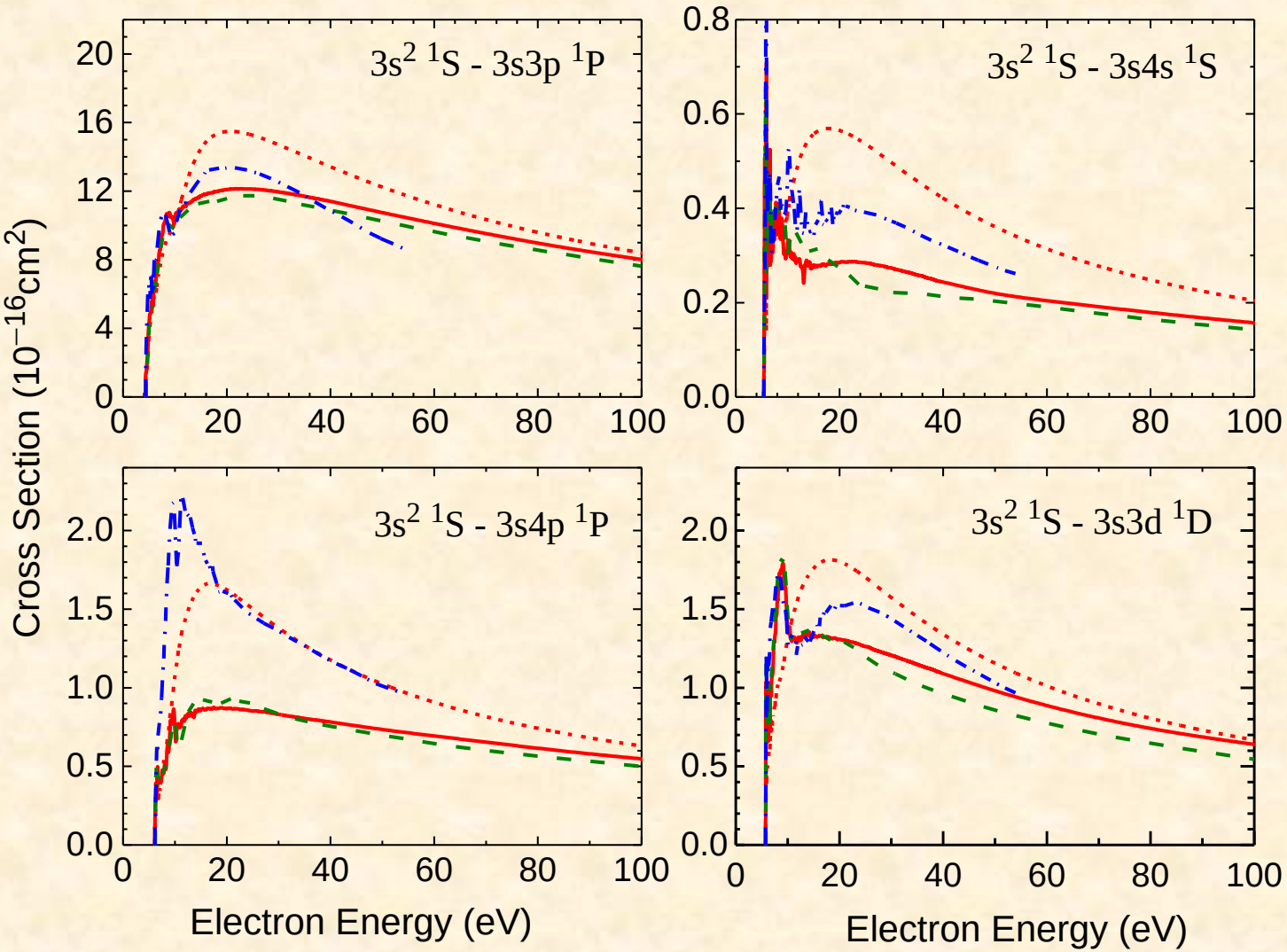
- Many existing databases for neutrals should **be re−evaluated**
- Comparison of different **codes** and **models** is crucial.
  - Repeating calculations are encouraged.
  - Non−critical using the existing codes − expert proof is still important.
- Each atom − unique!
  (the automatic calculations for whole iso-electronic or iso−nuclear series can be deceptive)
- Comparison of published results or different databases is very time consuming:
  (It is desirable to encourage development of **new software** for extracting and comparison of data in different databases and sharing the results)
- For more confident results - comprehensive comparison with included **ALL** transitions, not just the selected ones.

- My main point: The importance of accurate target descriptions is very much underestimated in most scattering calculations. This leads to lower accuracy and larger uncertainties.

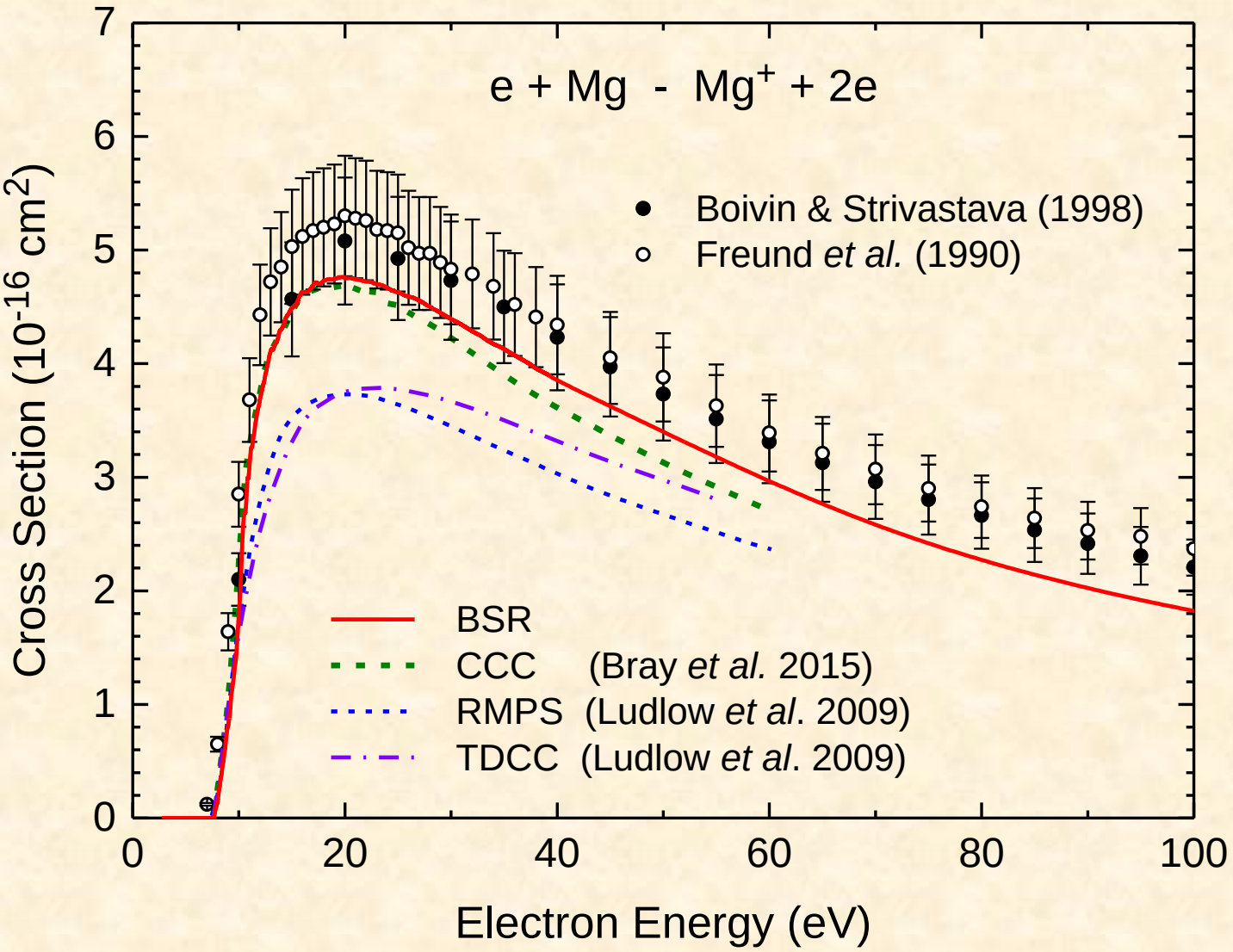
Electron-impact excitation of Mg ($3s^2$) (in progress)

- Numerous measurements and calculations but for selected transitions or energies (DCS)
- Modeling of non-equilibrium plasma requires complete set of data (Mauas *et al*. 1988 - collection from different sources with unclear uncertainties)
- BSR-37 (Zatsarinny et al. 2009) - most complete set of data for all transitions between first 37 levels ($n \leq 8$) except triplet-triplet transitions
- Merle *et al.* (2015) - rate coefficients based on BSR-37
- Osorio *et al.* (2015) – new RMPS calculations for transitions between first 10 levels (noticeable differences with existing results)
- 2016, new project – parallel CCC and BSR-712 (RMPS) calculations to get complete set with uncertainty estimations

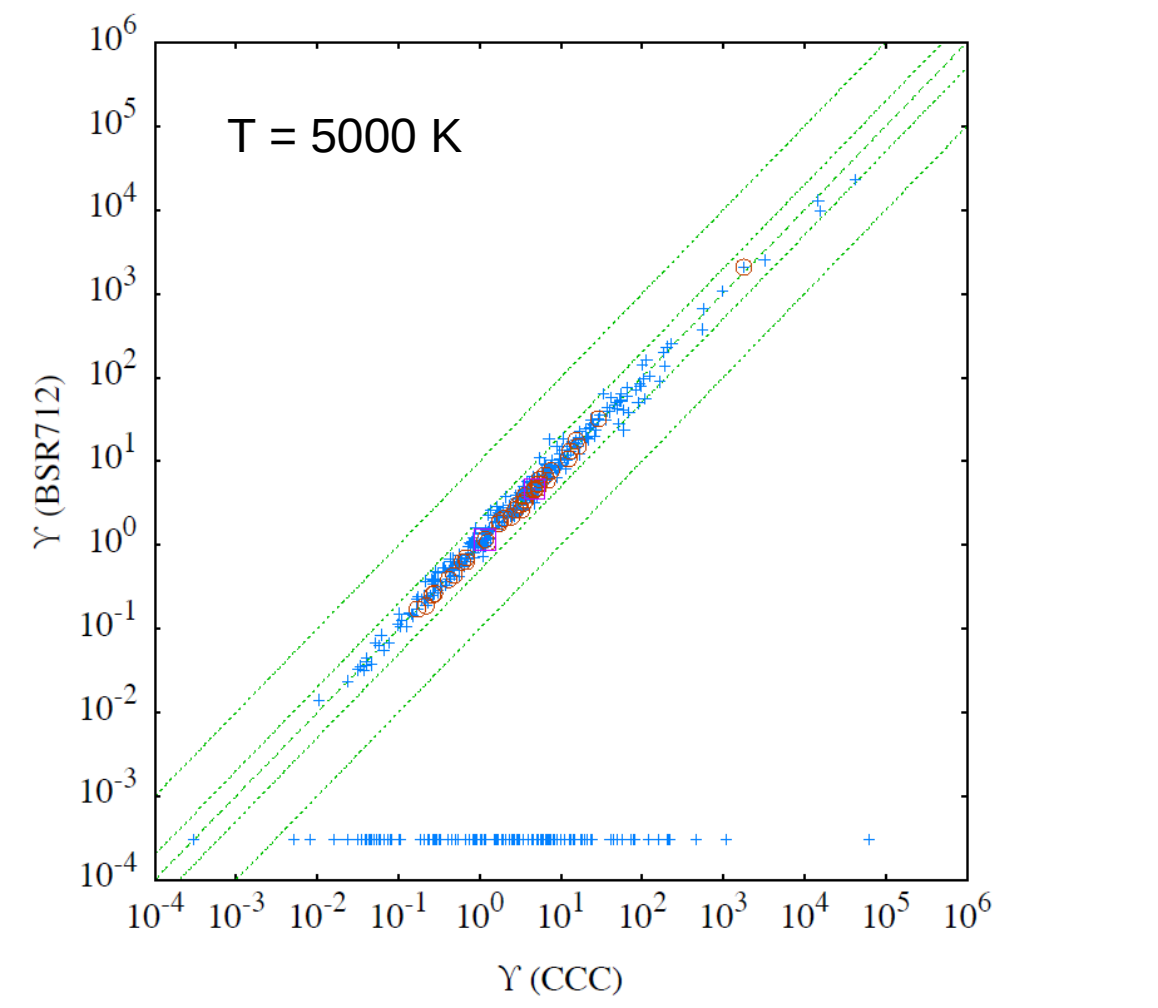
Electron-impact excitation of Mg ($3s^2$)



Electron-impact ionization of Mg ($3s^2$)



Electron-impact excitation of Mg ($3s^2$)



- The agreement between the CCC and BSR712 calculations differ by on average only 6%, with a scatter of 27% for ALL transitions between first 25 levels.
- Another example of team work to get accurate results from independent calculations

Summary

Goal: can we finally get accurate cross sections for complex atoms?

❖ For complex targets, the **BSR method with non-orthogonal orbitals** has advantages:

- highly **accurate** target description
- more **consistent** description of (N+1)-electron scattering system
- considerable improvement for **low-energy region** and **near-threshold resonance** phenomena
- improvement for **intermediate** energies with **RMPS approach** (MPI version)
- BSR code is able to provide **benchmark** results for uncertainty estimation
  - ► considerable reduction (elimination) of **target description** uncertainty
  - ► absence of pseudo resonances
  - ► systematic check of **convergence** (including target continuum)

❖ my main point: the important of accurate target description is very underestimated in the most scattering calculations and leads to lower accuracy and big uncertainties

Electron-impact excitation of N^{3+} ($2s^2$)

Big difference between existing datasets:

- Fernandez-Menchero *et al*. 2014, Astron. Astroph. 566 A104

  RM-238 (**ICFT** - Intermediate Coupling Frame Transformation)

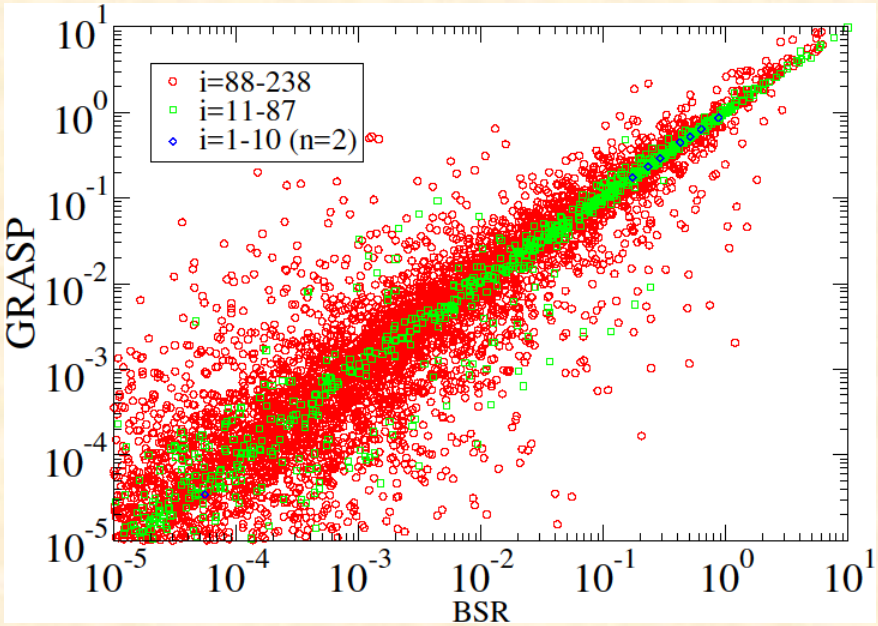
- Aggarwal et al. 2016 Mon. Not. R. Astr. Soc. 461 3997)

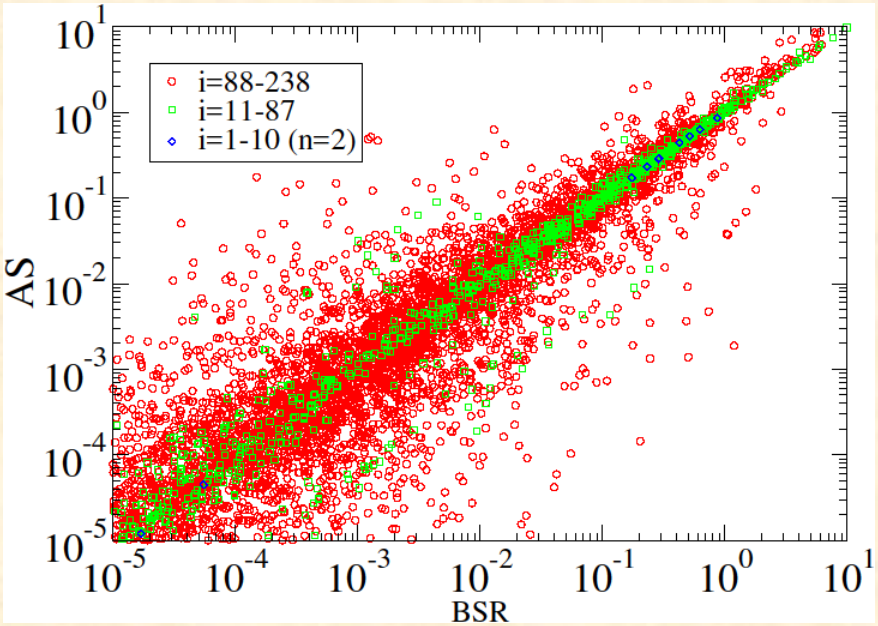
  DARC -238 (Dirac Atomic R-matrix Code)

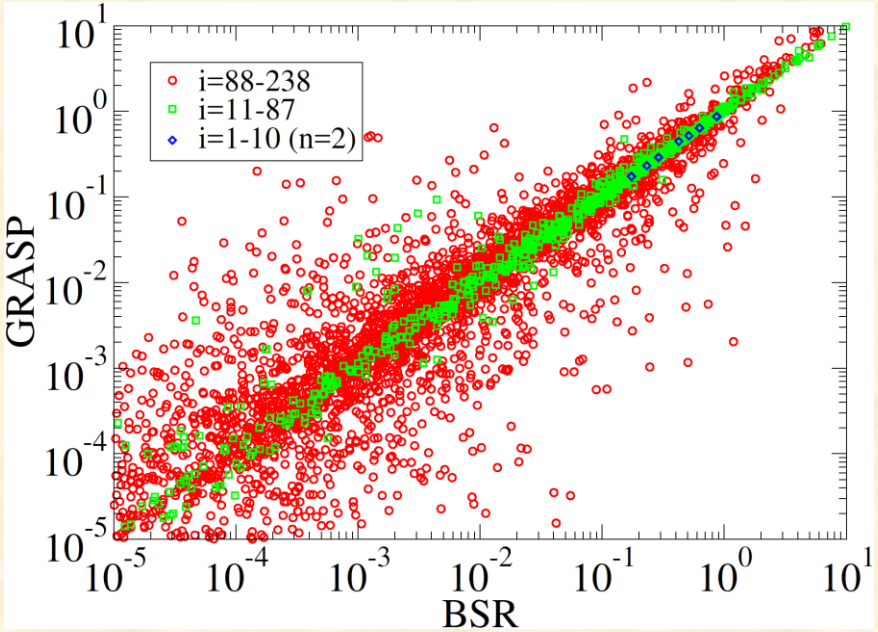
  statement: DARC calculations are much more accurate and the ICFT results might even be wrong

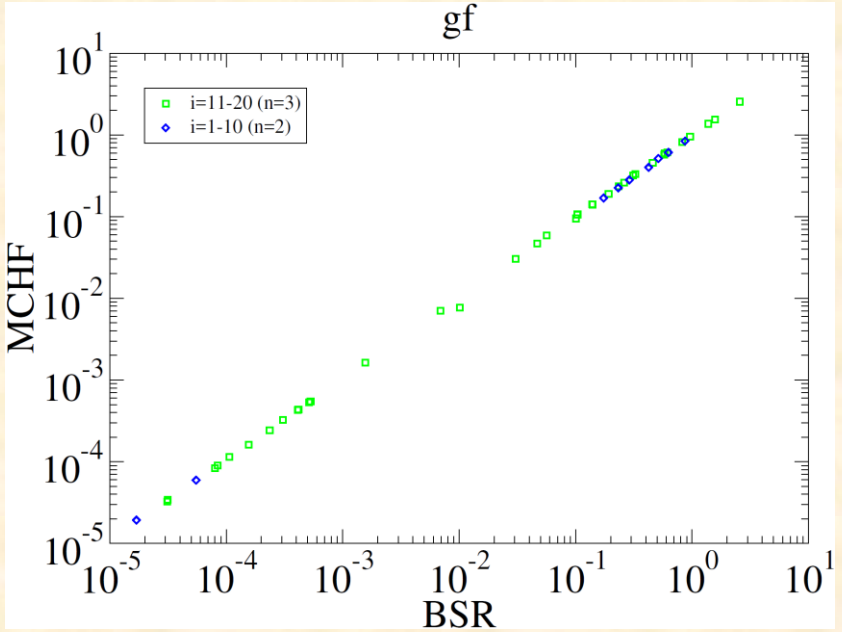
- **BSR-238** with improved structure description ($2snl$, $2pnl$, $n \leq 8$)

N^{3+} - comparison of oscillator strengths

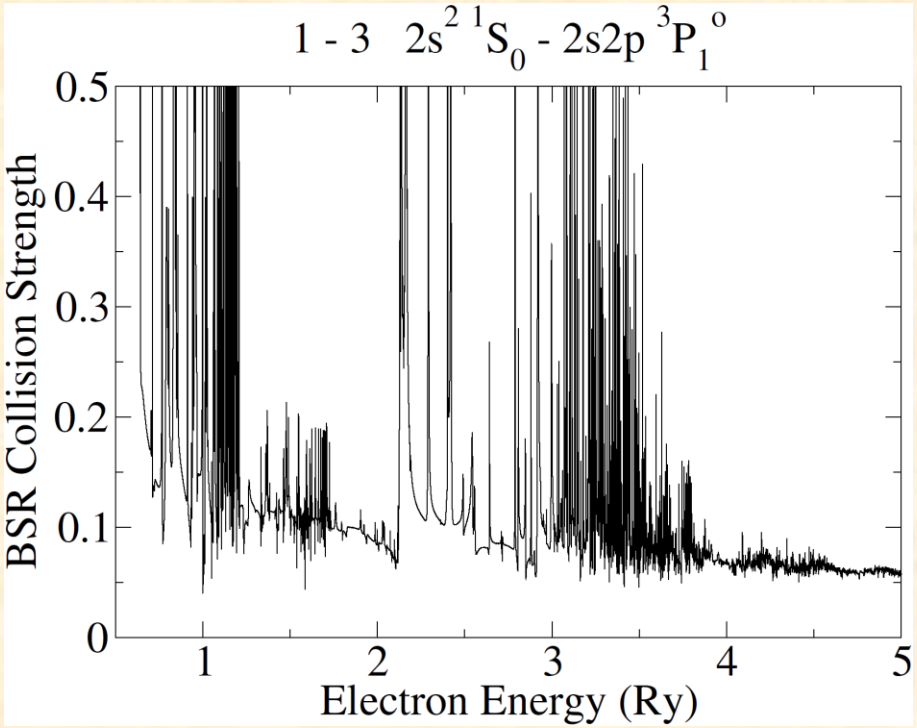


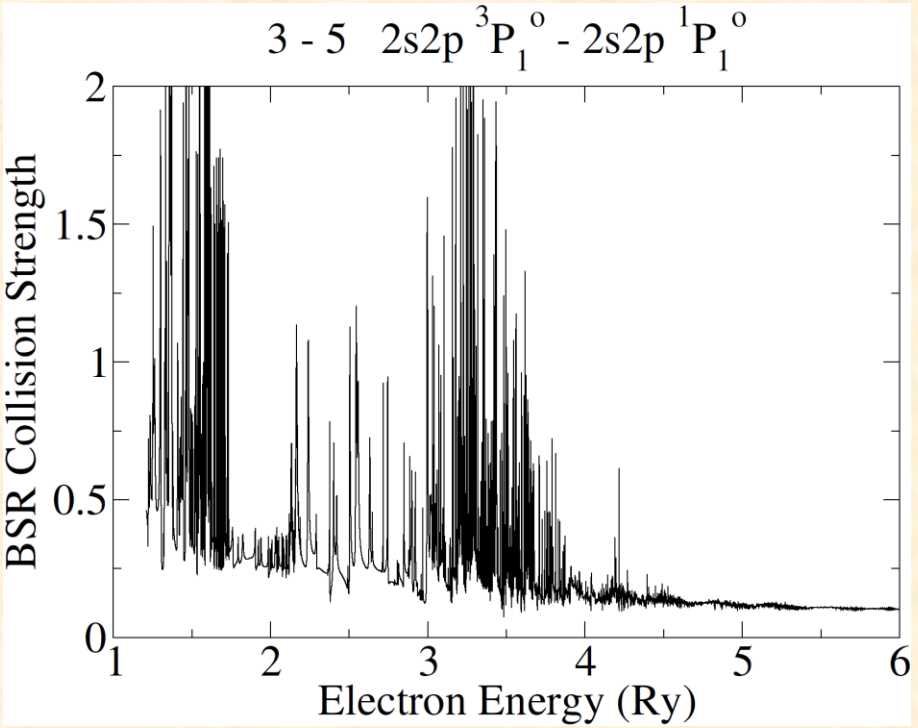






Electron-impact excitation of N^{3+} ($2s^2$)





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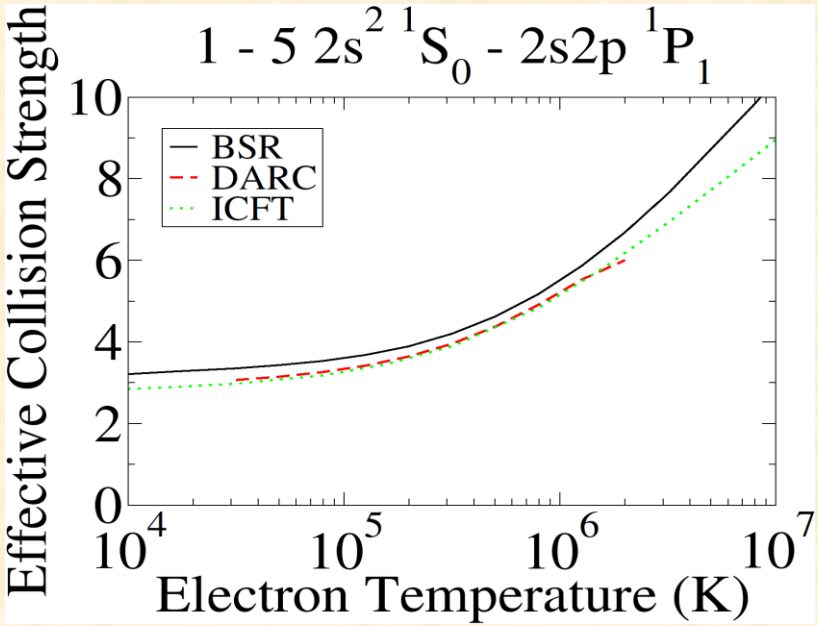

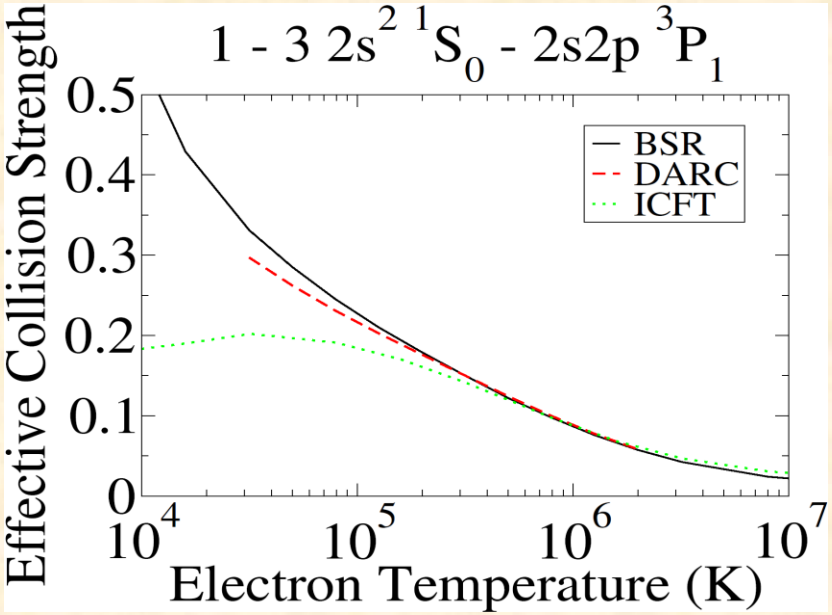

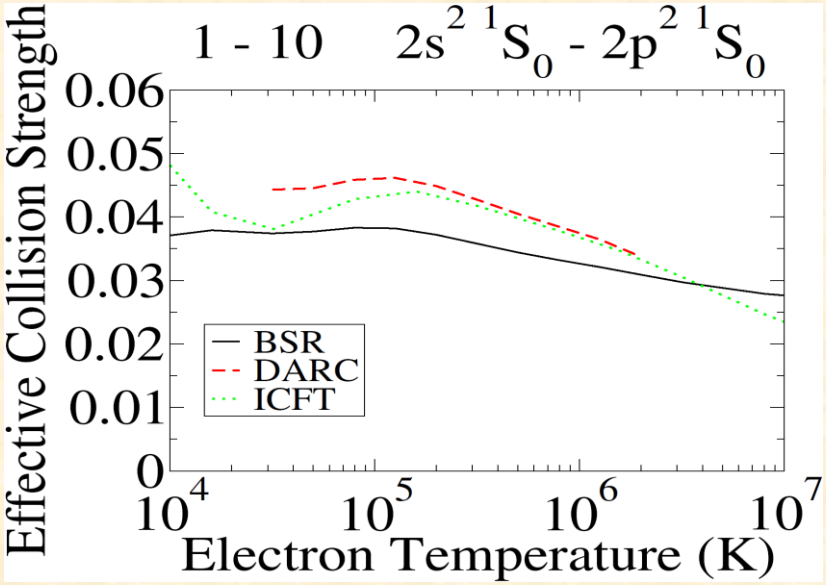

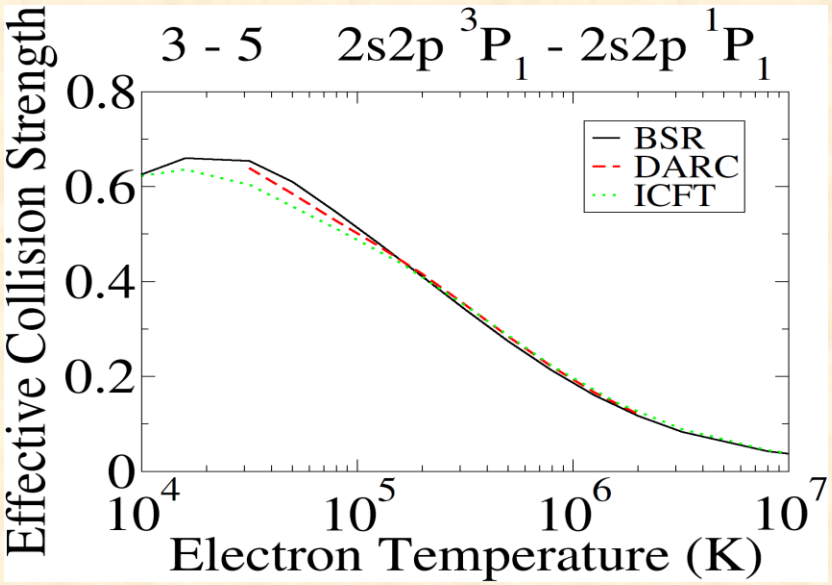

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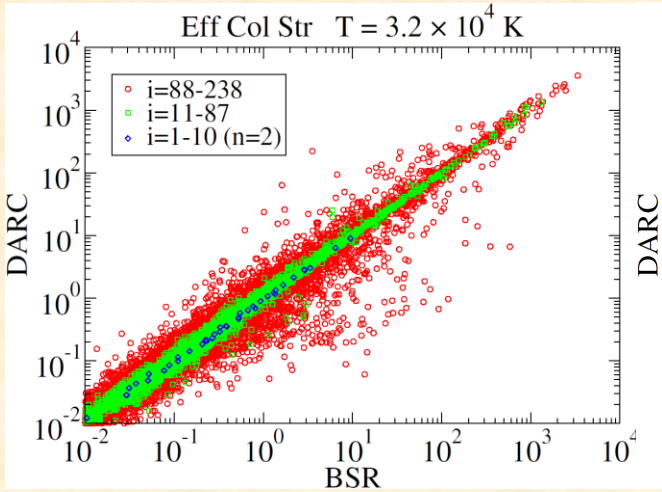

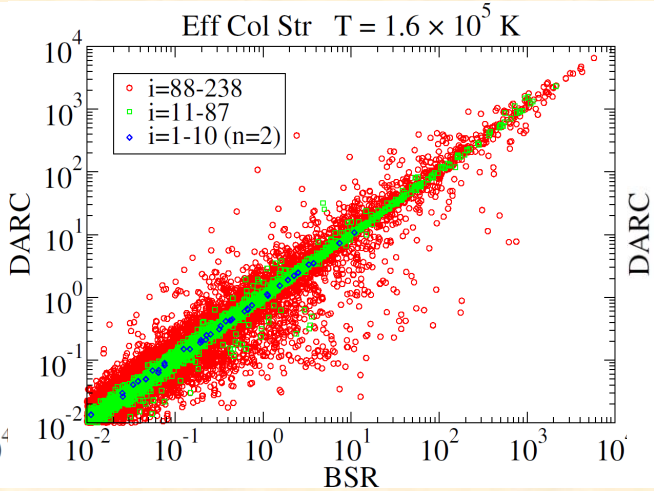

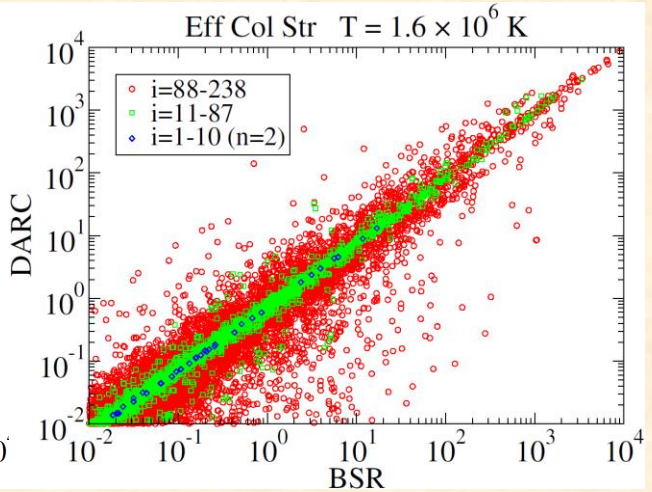

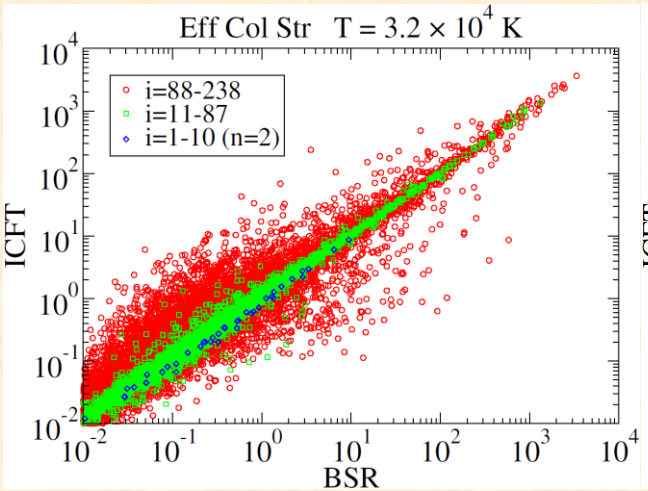

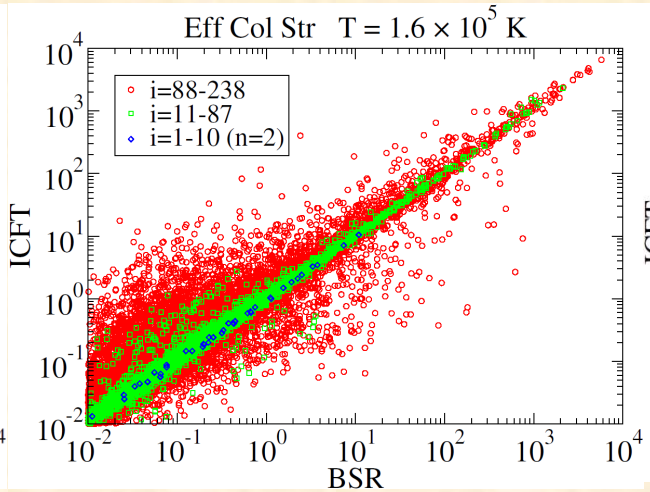

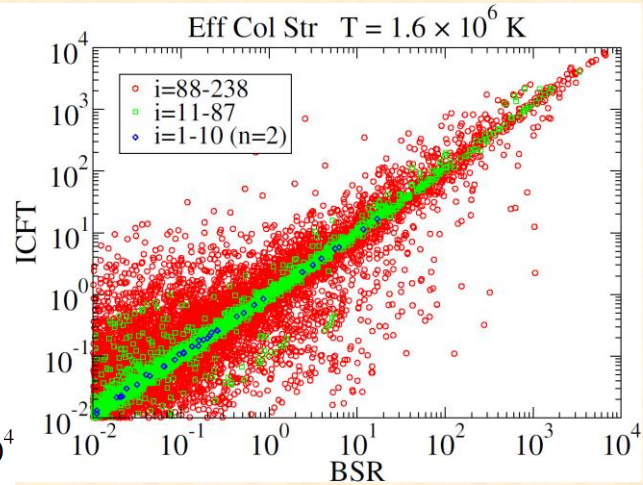

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statement: DARC calculations are much more accurate and the ICFT results might even be wrong

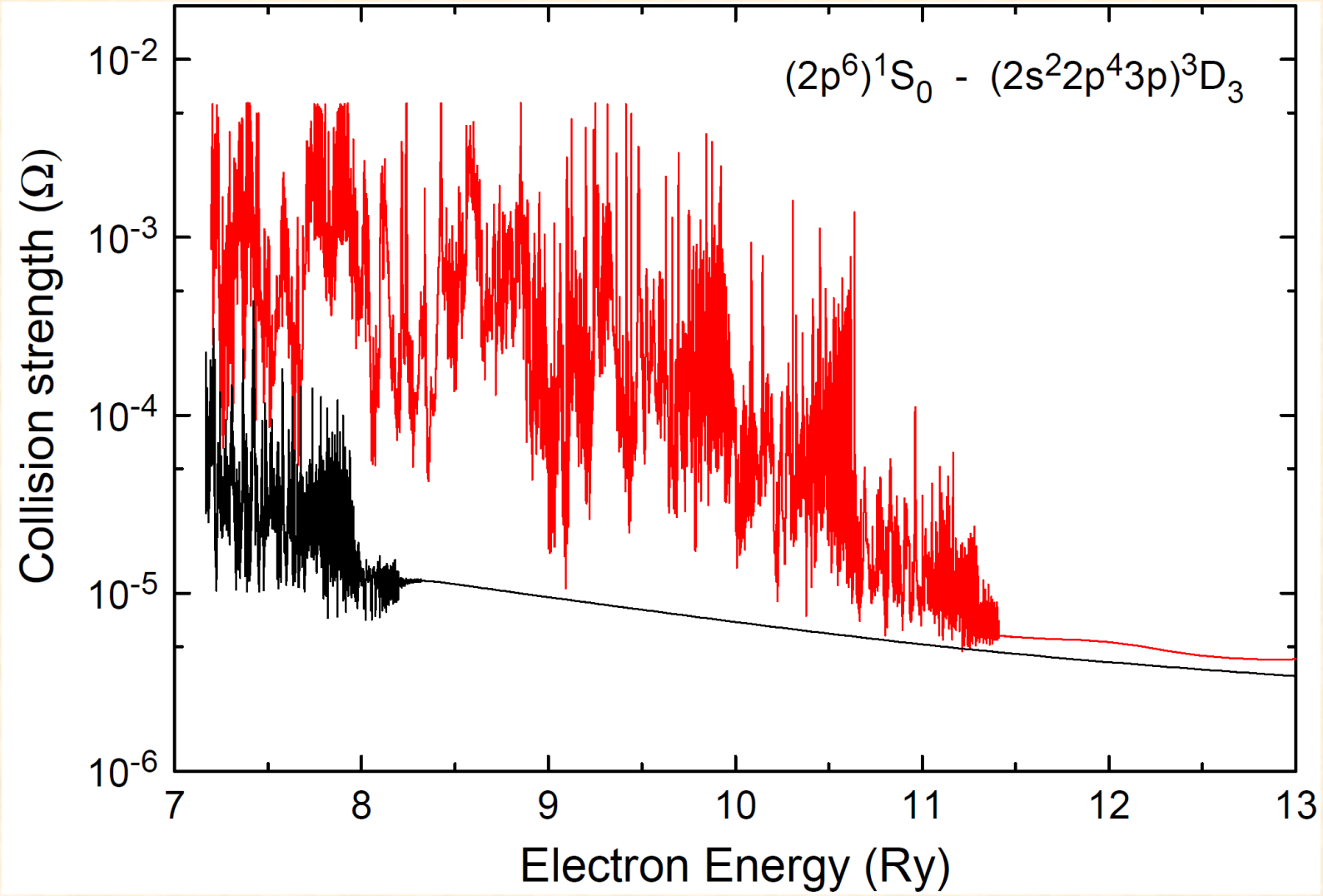
Our conclusions:

- The differences in the final results for the collision strengths are mainly due to differences in the **structure description,** specifically the inclusion of correlation effects, rather than the treatment of relativistic effects.

- Hence there is no indication that one approach is superior to another, until the **convergence** of both the target configuration and the close-coupling expansions have been fully established.

- Due to the **superior target structure** generated, we believe the BSR results are the currently best for electron collisions with N^{+3} .

- The differences between the BSR and the DARC / ICFT results may in fact serve as an **uncertainty estimate** for the available excitation rates.


$(2p^6)^1S_0$ - $(2s^22p^43p)^3D_3$
Collision strength (Ω)
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
7
8
9
10
11
12
13
Electron Energy (Ry)

Goal: can we finally get accurate cross sections for complex atoms?