Estimating Uncertainties of Theoretical Data for Electron Collisions with Atoms and Ions

Klaus Bartschat

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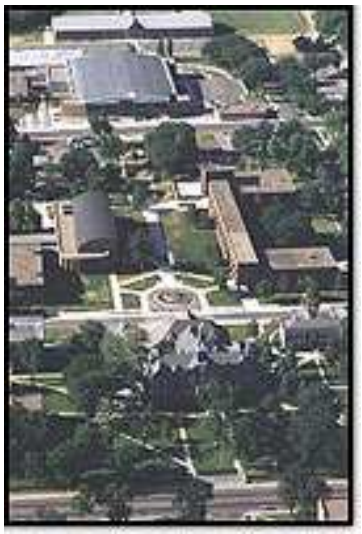

IAEA; Dec. 19–21, 2016

NSF Support: PHY-1403245, PHY-1520970, and XSEDE (PHY-090031)

Special Thanks to: Oleg Zatsarinny

OVERVIEW:

I. Production and Assessment of Atomic Data
II. Computational Methods for Electron Collisions
III. Examples for Elastic Scattering, Excitation, Ionization
IV. Conclusions

PERSPECTIVE

This might serve as some motivation ...

Electron collisions with atoms, ions, molecules, and surfaces: Fundamental science empowering advances in technology

Klaus Bartschat[a,1] and Mark J. Kushner[b]

Edited by David A. Weitz, Harvard University, Cambridge, MA, and approved May 16, 2016 (received for review April 16, 2016)

Electron collisions with atoms, ions, molecules, and surfaces are critically important to the understanding and modeling of low-temperature plasmas (LTPs), and so in the development of technologies based on LTPs. Recent progress in obtaining experimental benchmark data and the development of highly sophisticated computational methods is highlighted. With the cesium-based diode-pumped alkali laser and remote plasma etching of Si_3N_4 as examples, we demonstrate how accurate and comprehensive datasets for electron collisions enable complex modeling of plasma-using technologies that empower our high-technology–based society.

electron scattering | close coupling | ab initio | plasmas | kinetic modeling

Production and Assessment of Atomic Data

- Data for electron collisions with atoms and ions are needed for **modeling processes** in
  - **laboratory plasmas**, such as discharges in lighting and lasers
  - **astrophysical plasmas**
  - **planetary atmospheres**
- The data are obtained through
  - **experiments**
    - valuable but expensive (**$$$**) benchmarks (often differential in energy, angle, spin, ...)
    - often problematic when **absolute (cross section) normalization** is required
  - **calculations** (Opacity Project, Iron Project, ...)
    - relatively cheap
    - almost any transition of interest is possible
    - often restricted to particular energy ranges:
      - high (→ Born-type methods)
      - low (→ close-coupling-type methods)
    - cross sections may peak at "intermediate energies" (→ **???**)
  - **good (or bad ?) guesses**
- **Sometimes the results are (obviously) wrong or (more often) inconsistent !**

Basic Question: WHO IS RIGHT ? (And WHY ???)

For *complete* data sets, theory is often the "only game in town"!

IOP Publishing Journal of Physics D: Applied Physics

J. Phys. D: Appl. Phys. **49** (2016) 363002 (27pp) doi:10.1088/0022-3727/49/36/363002

Topical Review

Uncertainty estimates for theoretical atomic and molecular data

See also:
The Editors 2011 Phys. Rev. A 83 040001

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Abstract

Sources of uncertainty are reviewed for calculated atomic and molecular data that are important for plasma modeling: atomic and molecular structures and cross sections for electron-atom, electron-molecule, and heavy particle collisions. We concentrate on model uncertainties due to approximations to the fundamental many-body quantum mechanical equations and we aim to provide guidelines to estimate uncertainties as a routine part of computations of data for structure and scattering.

Choice of Computational Approaches

- **Which one is right for YOU?**
  - **Perturbative (Born-type) or Non-Perturbative (close-coupling, time-dependent, ...)**?
  - **Semi-empirical or fully ab initio**?
  - **How much input from experiment?**
  - **Do you trust that input?**
  - **Predictive power? (input $\leftrightarrow$ output)**
- **The answer depends on many aspects, such as:**
  - **How many transitions do you need?** (elastic, momentum transfer, excitation, ionization, ... how much lumping?)
  - **How complex is the target** (H, He, Ar, W, H_2, H_2O, radical, DNA, ...)?
  - **Do the calculation yourself or beg/pay somebody to do it for you?**
  - **What accuracy can you live with?**
  - **Are you interested in numbers or "correct" numbers?**
  - **Which numbers do really matter?**

Who is Doing What?

The list is NOT Complete

- "special purpose" elastic/total scattering: Stauffer, McEachran, Garcia, ...

  (some version of Potential Scattering; PS)

- inelastic (excitation and ionization): perturbative
  - Madison, Stauffer, McEachran, Dasgupta, Kim, Dong ...

    (some version of the Distorted-Wave Born Approximation; DWBA)

- inelastic (excitation and ionization): non-perturbative
  - Fursa, Bray, Stelbovics, ... (Convergent Close-Coupling, CCC)
  - Burke, Badnell, Pindzola, Ballance, Gorczyca, ... ("Belfast" R-Matrix, RM)
  - Zatsarinny, Bartschat, ... (B-spline R-Matrix, BSR)
  - Colgan, Pindzola, ... (Time-Dependent Close-Coupling, TDCC)
  - McCurdy, Rescigno, Bartlett, Stelbovics (Exterior Complex Scaling, ECS)
- Molecular Targets: You heard [some of] the main players yesterday.

Classification of Numerical Approaches

- **Special Purpose (elastic/total)**: OMP (pot. scatt.); Polarized Orbital

Optical Model Potential (Blanco, Garcia) – a "Special Purpose" Approach

Numerical Methods: OMP for Atoms

- For electron-atom scattering, we solve the partial-wave equation

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - 2V_{\rm mp}(k,r)\right) u_\ell(k,r) = k^2 u_\ell(k,r).$$

- The **local model potential** is taken as

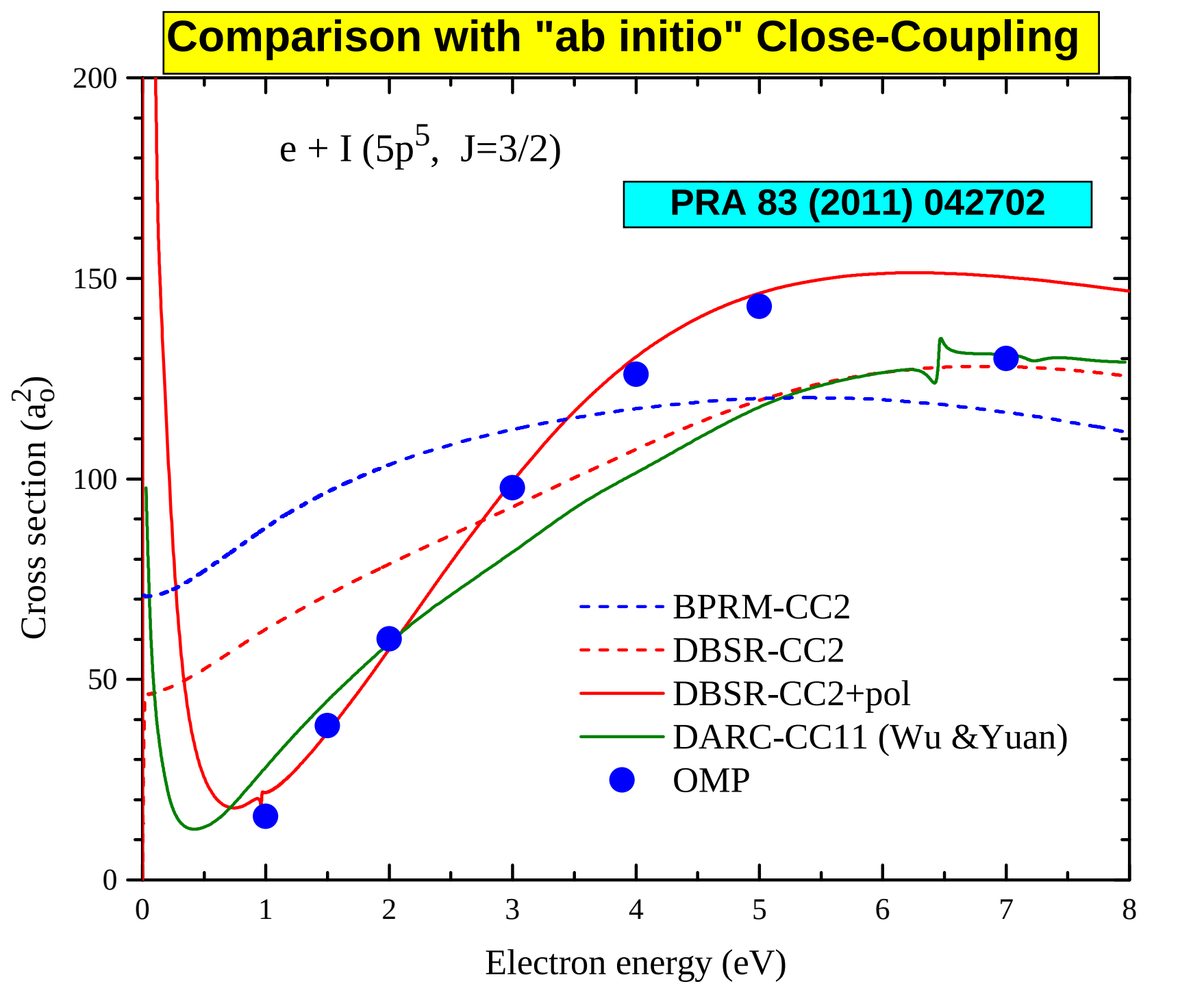
$$V_{\rm mp}(k,r) = V_{\rm static}(r) + V_{\rm exchange}(k,r) + V_{\rm polarization}(r) + iV_{\rm absorption}(k,r)$$

with

  - $V_{\rm exchange}(k,r)$ from Riley and Truhlar (J. Chem. Phys. **63** (1975) 2182);
  - $V_{\rm polarization}(r)$ from Zhang *et al.* (J. Phys. B **25** (1992) 1893);
  - $V_{\rm absorption}(k,r)$ from Staszewska *et al.* (Phys. Rev. A **28** (1983) 2740).

- Due to the imaginary absorption potential, **the OMP method**
  - yields a complex phase shift $\delta_\ell = \lambda_\ell + i\mu_\ell$
  - allows for the calculation of ICS and DCS for
    - elastic scattering
    - inelastic scattering (all states together)
    - the sum (total) of the two processes

It can be great if this is all you want.


Comparison with "ab initio" Close-Coupling
e + I (5p5, J=3/2)
PRA 83 (2011) 042702
BPRM-CC2
DBSR-CC2
DBSR-CC2+pol
DARC-CC11 (Wu &Yuan)
OMP
Cross section (a02)
Electron energy (eV)
0
50
100
150
200
0
1
2
3
4
5
6
7
8

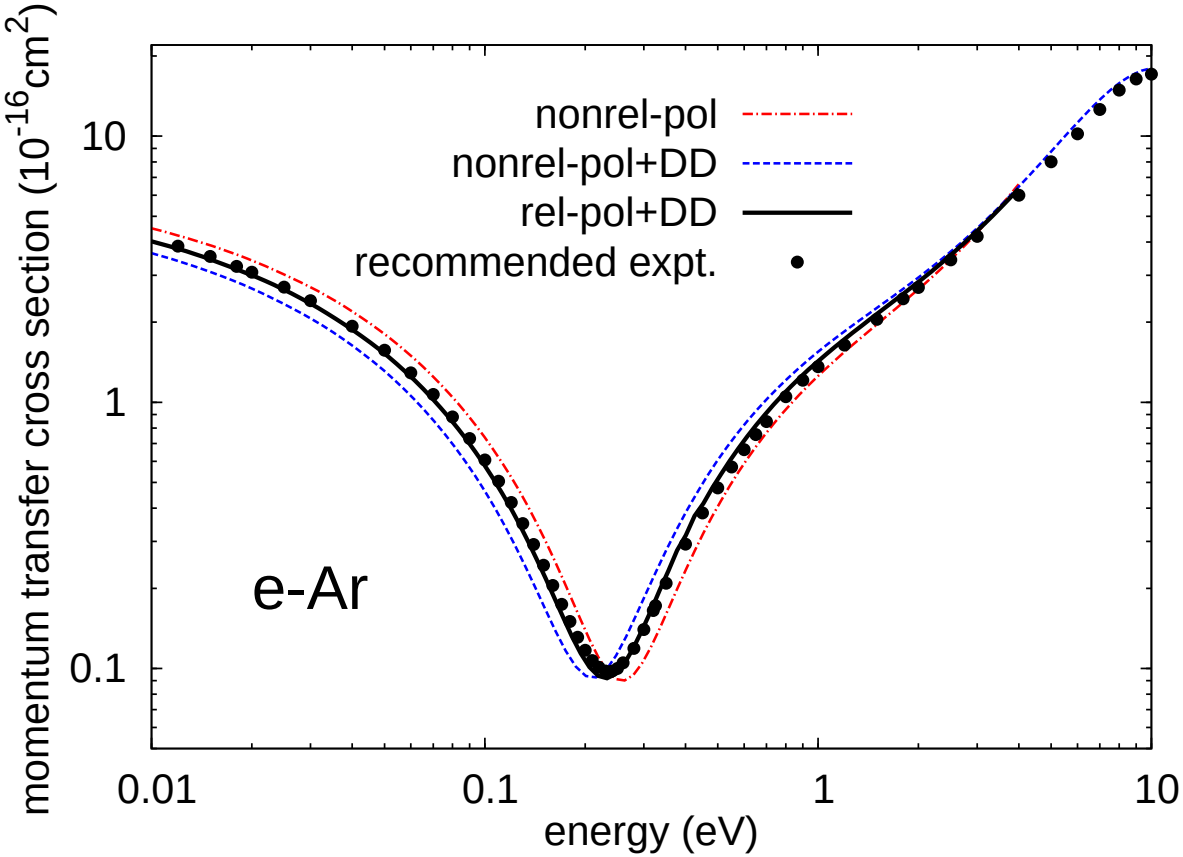
Polarized Orbital – an "Ab Initio Special Purpose" Approach

Aust. J. Phys., 1997, **50**, 511–24

Relativistic Effects in Low-energy Electron–Argon Scattering*

R. P. McEachran[A,B] *and A. D. Stauffer*[B]

We have performed a relativistic treatment at low energy of electron–argon scattering which includes both polarisation and dynamic distortion effects. Our results are in excellent agreement with the experimentally derived momentum transfer cross section and scattering length, as well as with very recent measurements of the elastic differential cross section.



Extension to account for inelastic effects:
J. Phys. B 42 (2009) 075202

Classification of Numerical Approaches

- **Special Purpose (elastic/total)**: OMP (pot. scatt.); Polarized Orbital
- **Born-type methods**
  - PWBA, DWBA, FOMBT, PWBA2, DWBA2, ...
  - fast, easy to implement, flexible target description, test physical assumptions
  - two states at a time, no channel coupling, problems for low energies and optically forbidden transitions, results depend on the choice of potentials, unitarization

Semi-Relativistic DWBA

PHYSICAL REVIEW A, VOLUME 61, 022701

Excitation of Ar $3p^5 4s$-$3p^5 4p$ transitions by electron impact

C. M. Maloney,[1] J. L. Peacher,[1] K. Bartschat,[2] and D. H. Madison[1]
[1]*Physics Department, University of Missouri–Rolla, Rolla, Missouri 65409-0640*
[2]*Physics Department, Drake University, Des Moines, Iowa 50311*

Electron-impact excitation of argon from the $3p^5 4s$ ($J=0,2$) metastable states to the $3p^5 4p$ ($J=0,1,2,3$) manifold has been investigated in the semirelativistic first-order distorted-wave and plane-wave Born approximations. The results are compared with recent experimental data of Boffard *et al.* [Phys. Rev. A **59**, 2749 (1999)] and *R*-matrix predictions by Bartschat and Zeman [Phys. Rev. A **59**, R2552 (1999)]. In cases for which perturbative approaches are expected to be valid, the plane-wave Born approximation is found to be sufficiently accurate and thus allows for an efficient calculation of results over a wide range of collision energies.

The first-order distorted-wave T matrix for atomic excitation is given by

$$T_{fi}=(n+1)\langle \chi_f^-(r_0)\Psi_f(\xi)|V-U_f(r_0)|A\Psi_i(\xi)\chi_i^+(r_0)\rangle .$$

$$(K+U_f-E_f)\chi_f^-=0$$

$$U_f=\gamma V_f-\tfrac{1}{4}(\alpha V_f)^2-\frac{(j+1)}{r}\frac{\eta'}{\eta}+\frac{3}{4}\left(\frac{\eta'}{\eta}\right)^2-\frac{1}{2}\frac{\eta''}{\eta'},$$

$$\gamma=\sqrt{1+\alpha^2 E_f}, \qquad \eta=1+\gamma-\tfrac{1}{2}\alpha^2 V_f$$

polarization and absorption potentials may also be included

Ar $3p^5 4s$ –> $3p^5 4p$: DWBA vs. R-matrix

unitarization problem!

(can be fixed; e.g., LANL Codes)

MALONEY, PEACHER, BARTSCHAT, AND MADISON

Phys. Rev. A 61 (2000) 022701

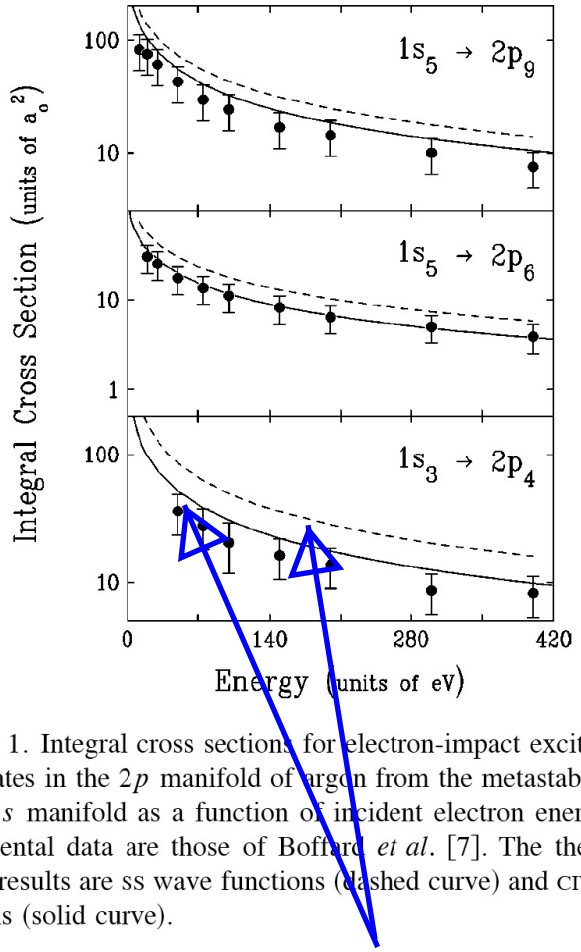


FIG. 1. Integral cross sections for electron-impact excitation of three states in the $2p$ manifold of argon from the metastable states in the $1s$ manifold as a function of incident electron energy. The experimental data are those of Boffard *et al.* [7]. The theoretical SRDW results are SS wave functions (dashed curve) and CIV3 wave functions (solid curve).

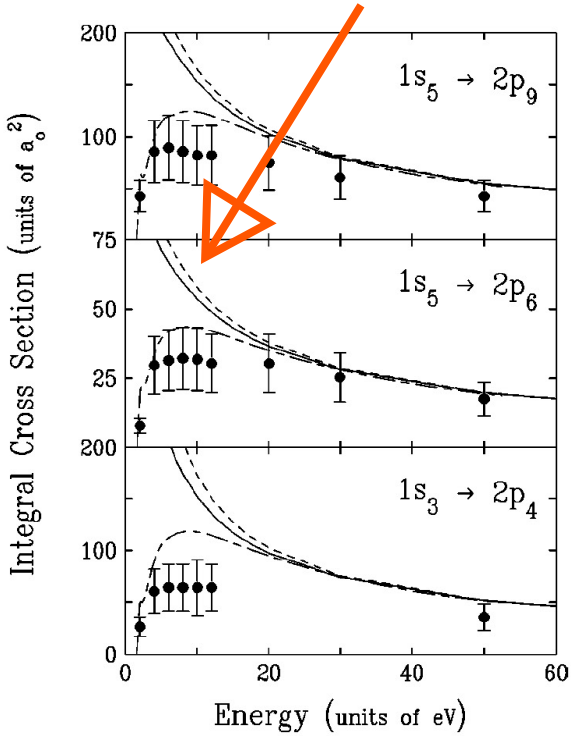


FIG. 2. Integral cross sections for electron-impact excitation of three states in the $2p$ manifold of argon from the metastable states in the $1s$ manifold as a function of incident electron energy. The experimental data are those of Boffard *et al.* [7]. The theoretical results are PWBA (dashed curve); 15-state R-matrix results (long-short dash); and SRDW with CIV3 wave functions (solid curve).

Theoretical results depend on wavefunctions and potentials.

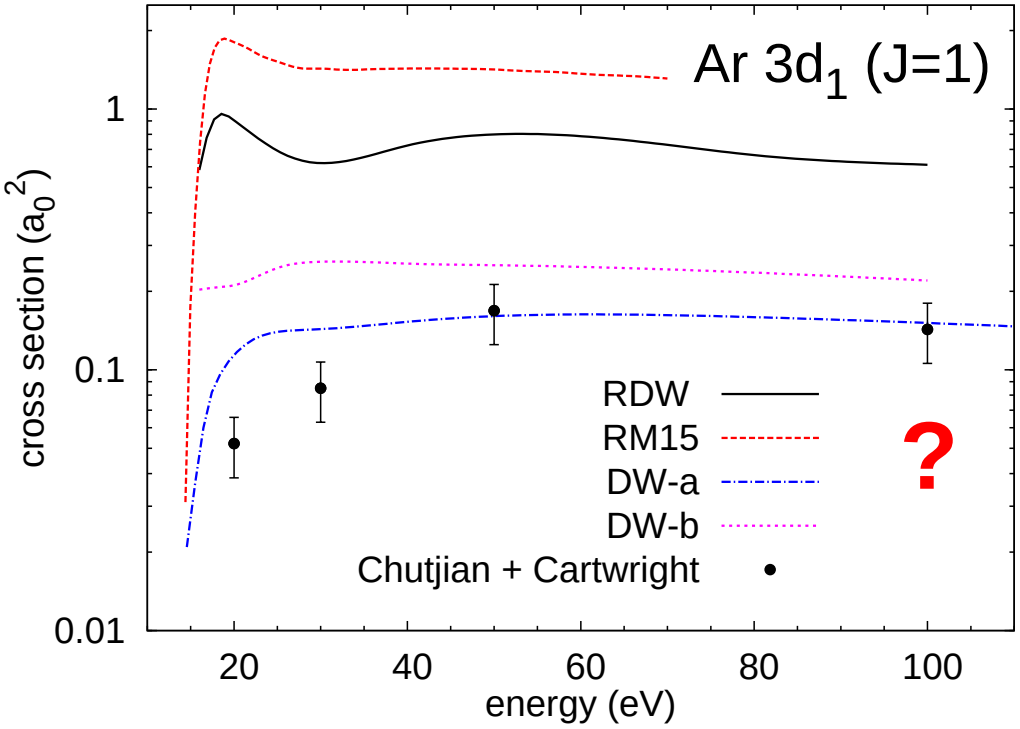
The target description is ALWAYS an issue.

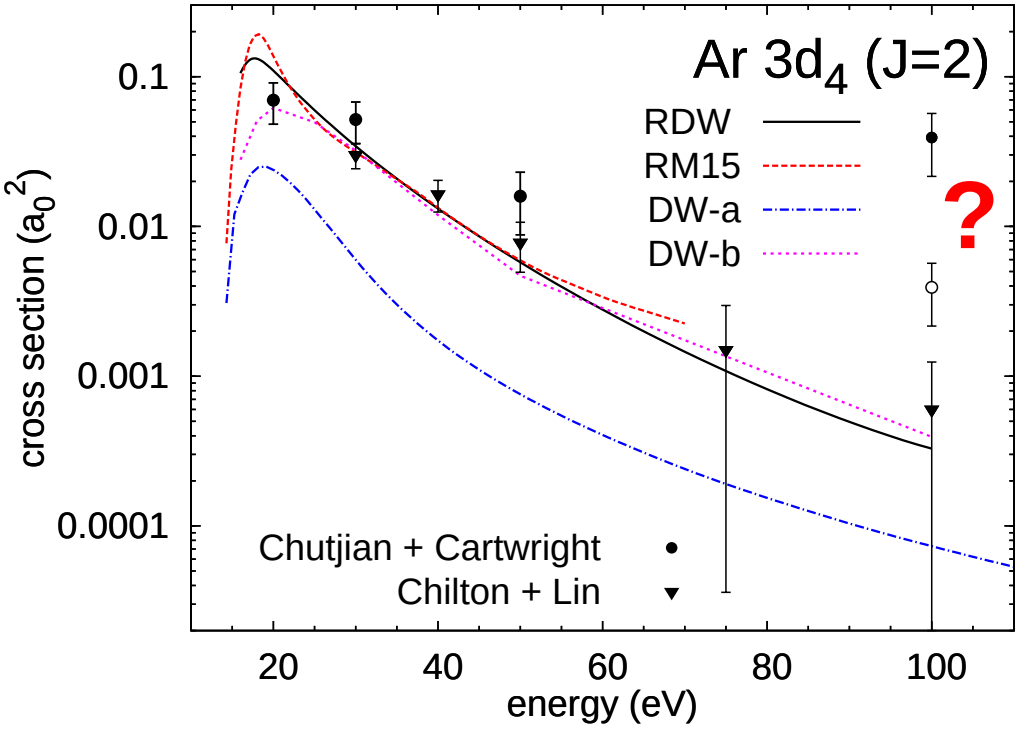
Relativistic DWBA; Semi-Relativistic DWBA; R-Matrix; Experiment

PHYSICAL REVIEW A **81**, 052707 (2010)

Electron-impact excitation of argon: Cross sections of interest in plasma modeling

R. K. Gangwar,[1] L. Sharma,[2] R. Srivastava,[1] and A. D. Stauffer[3]





Key Message:
Sometimes BIG Differences between Theories and HUGE Experimental Error Bars!

Which model, if any, can we trust?

Classification of Numerical Approaches

- **Special Purpose (elastic/total)**: OMP (pot. scatt.); Polarized Orbital
- **Born-type methods**
  - PWBA, DWBA, FOMBT, PWBA2, DWBA2, ...
  - fast, easy to implement, flexible target description, test physical assumptions
  - two states at a time, no channel coupling, problems for low energies and optically forbidden transitions, results depend on the choice of potentials, unitarization
- **(Time-Independent) Close-coupling-type methods**
  - CCn, CCO, CCC, RMn, IERM, RMPS, DARC, BSR, ...
  - Standard method of treating low-energy scattering; based upon the expansion

$$\Psi_E^{LS\pi}(\mathbf{r}_1,\ldots,\mathbf{r}_{N+1}) = \mathcal{A}\sum_i \Phi_i^{LS\pi}(\mathbf{r}_1,\ldots,\mathbf{r}_N,\hat{\mathbf{r}})\,\frac{1}{r}\,F_{E,i}(r)$$

  - simultaneous results for transitions between **all states** in the expansion; sophisticated, publicly available codes exist; results are **internally consistent**
  - expansion must be cut off (→ **CCC, RMPS, IERM**)
  - **usually, a single set of mutually orthogonal one-electron orbitals is used for all states in the expansion** (→ **BSR with non-orthogonal orbitals**)
- **Time-dependent and other direct methods**
  - TDCC, ECS
  - solve the Schrödinger equation directly on a grid
  - very expensive, only possible for (quasi) one- and two-electron systems.

Inclusion of Target Continuum (Ionization)

- **imaginary absorption potential (OMP)**
- **final continuum state in DWBA**
- **directly on the grid and projection to continuum states (TDCC, ECS)**
- **add square-integrable pseudo-states to the CC expansion (CCC, RMPS, ...)**

Inclusion of Relativistic Effects

- **Re-coupling** of non-relativistic results (problematic near threshold)
- Perturbative (**Breit-Pauli**) approach; matrix elements are calculated between **non-relativistic wavefunctions**
- **Dirac-based approach**

Time-Independent Close-Coupling

- Standard method of treating low-energy scattering
- Based upon an expansion of the total wavefunction as

H Ψ = E Ψ

$$\Psi_E^{LS\pi}(\mathbf{r}_1,\ldots,\mathbf{r}_{N+1}) = \mathcal{A}\sum_i \Phi_i^{LS\pi}(\mathbf{r}_1,\ldots,\mathbf{r}_N,\hat{\mathbf{r}})\,\frac{1}{r}\,F_{E,i}(r)$$

- Target states Φ_i diagonalize the N-electron target Hamiltonian according to

$$\langle \Phi_{i'} \mid H_T^N \mid \Phi_i \rangle = E_i\,\delta_{i'i}$$

good start – remember your QM course?

- The unknown radial wavefunctions $F_{E,i}$ are determined from the solution of a system of coupled integro-differential equations given by

$$\left[\frac{d^2}{dr^2} - \frac{\ell_i(\ell_i+1)}{r^2} + k^2\right] F_{E,i}(r) = 2\sum_j V_{ij}(r)\,F_{E,j}(r) + 2\sum_j W_{ij}\,F_{E,j}(r)$$

with the direct coupling potentials

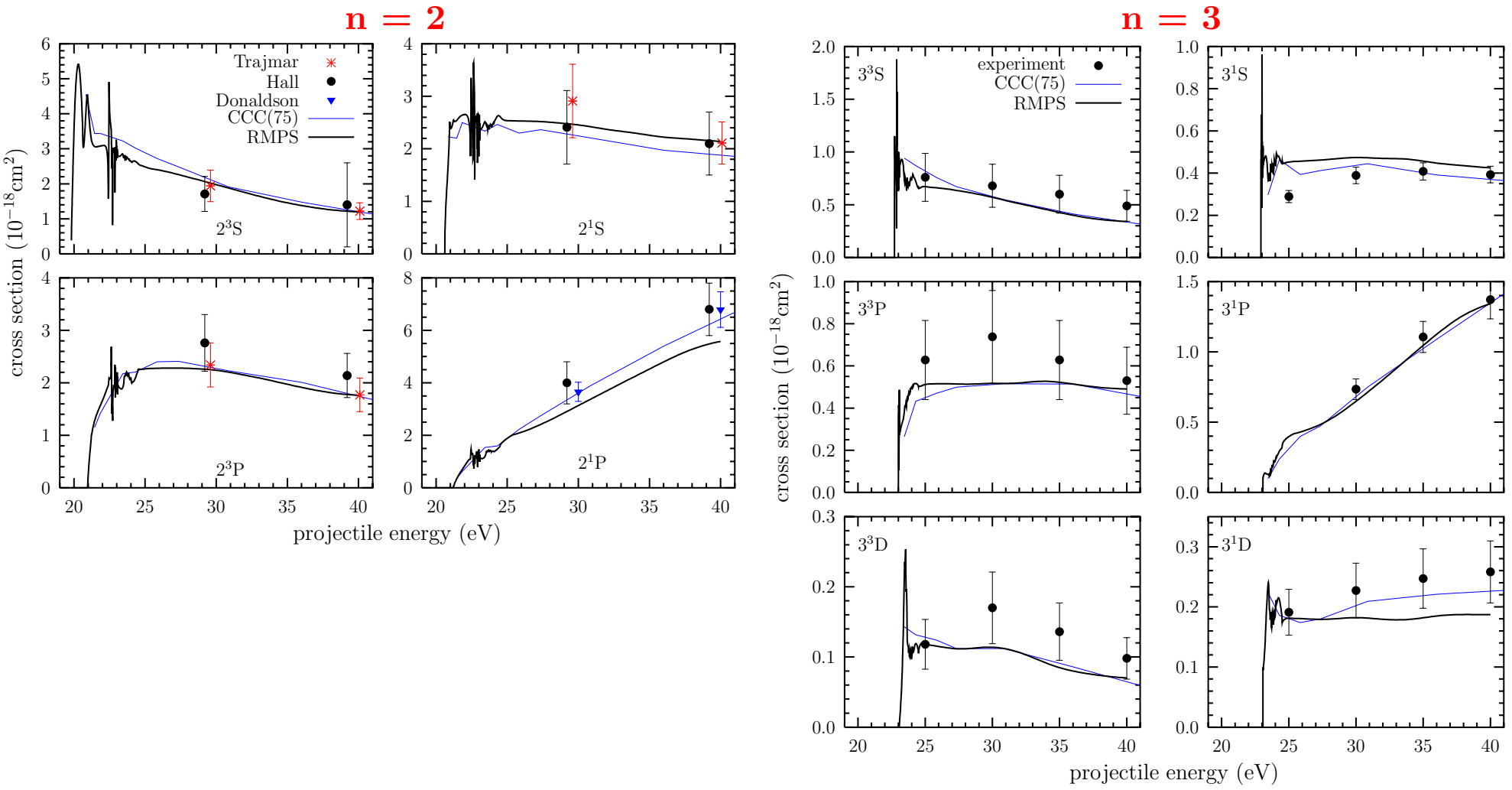
$$V_{ij}(r) = -\frac{Z}{r}\,\delta_{ij} + \sum_{k=1}^{N}\langle \Phi_i \mid \frac{1}{|\mathbf{r}_k - \mathbf{r}|} \mid \Phi_j \rangle$$

and the exchange terms

$$W_{ij}F_{E,j}(r) = \sum_{k=1}^{N}\langle \Phi_i \mid \frac{1}{|\mathbf{r}_k - \mathbf{r}|} \mid (\mathcal{A}-1)\,\Phi_j F_{E,j}\rangle$$

Close-coupling can yield *complete* data sets, and the results are *internally consistent* (unitary theory that conserves total flux)!

Total Cross Sections for Electron-Impact Excitation of Helium
K. Bartschat, J. Phys. B 31 (1998) L469

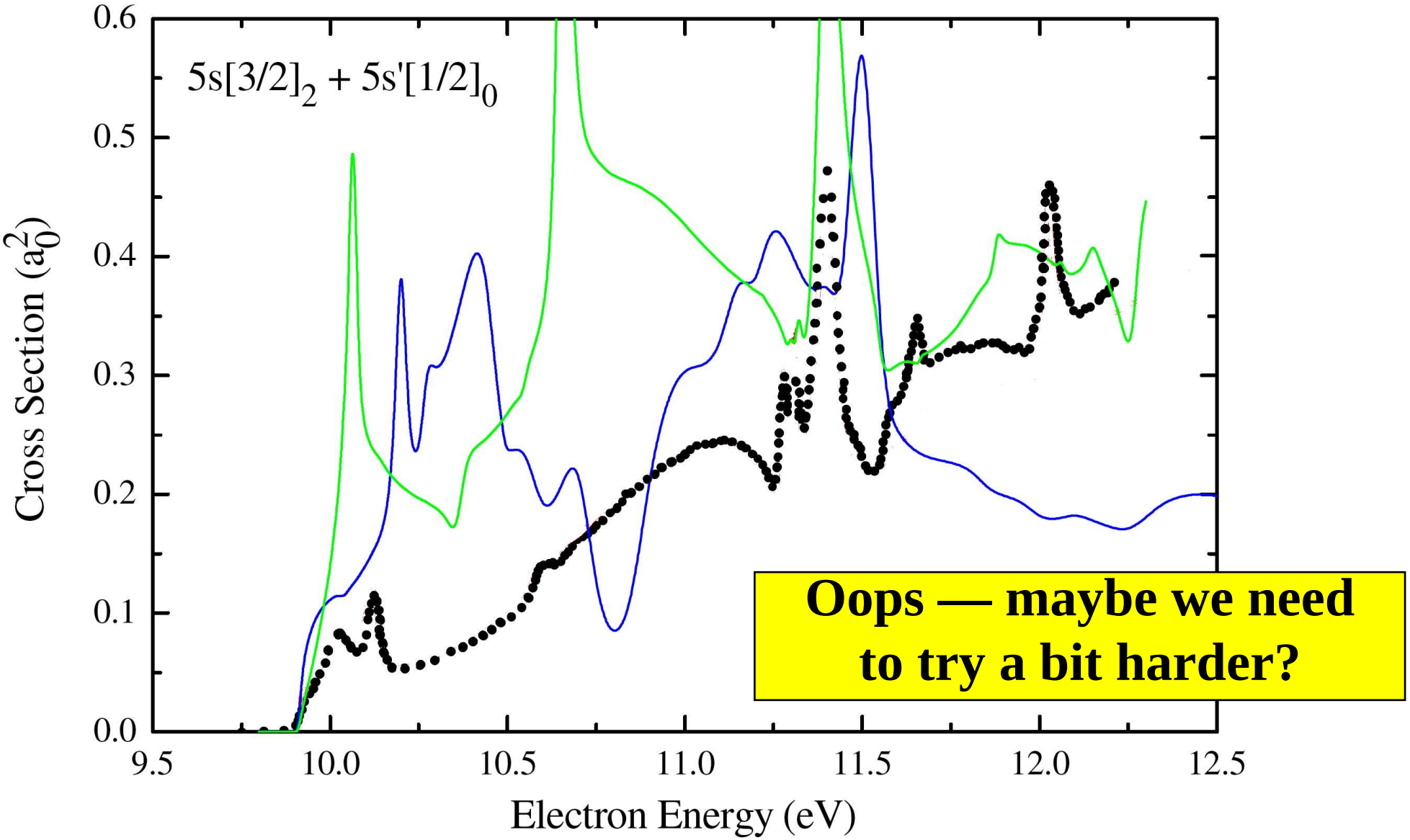


In 1998, de Heer recommends 0.5 x (CCC+RMPS) for uncertainty of 10% — independent of experiment!

Metastable Excitation Function in Kr

Experiment: Buckman *et al* (1983), multiplied by 0.67

Theories: 31-state Breit-Pauli R-matrix (Zeman & Bartschat 1998)
51-state Breit-Pauli R-matrix (Bartschat & Grum-Grzhimailo 2000)



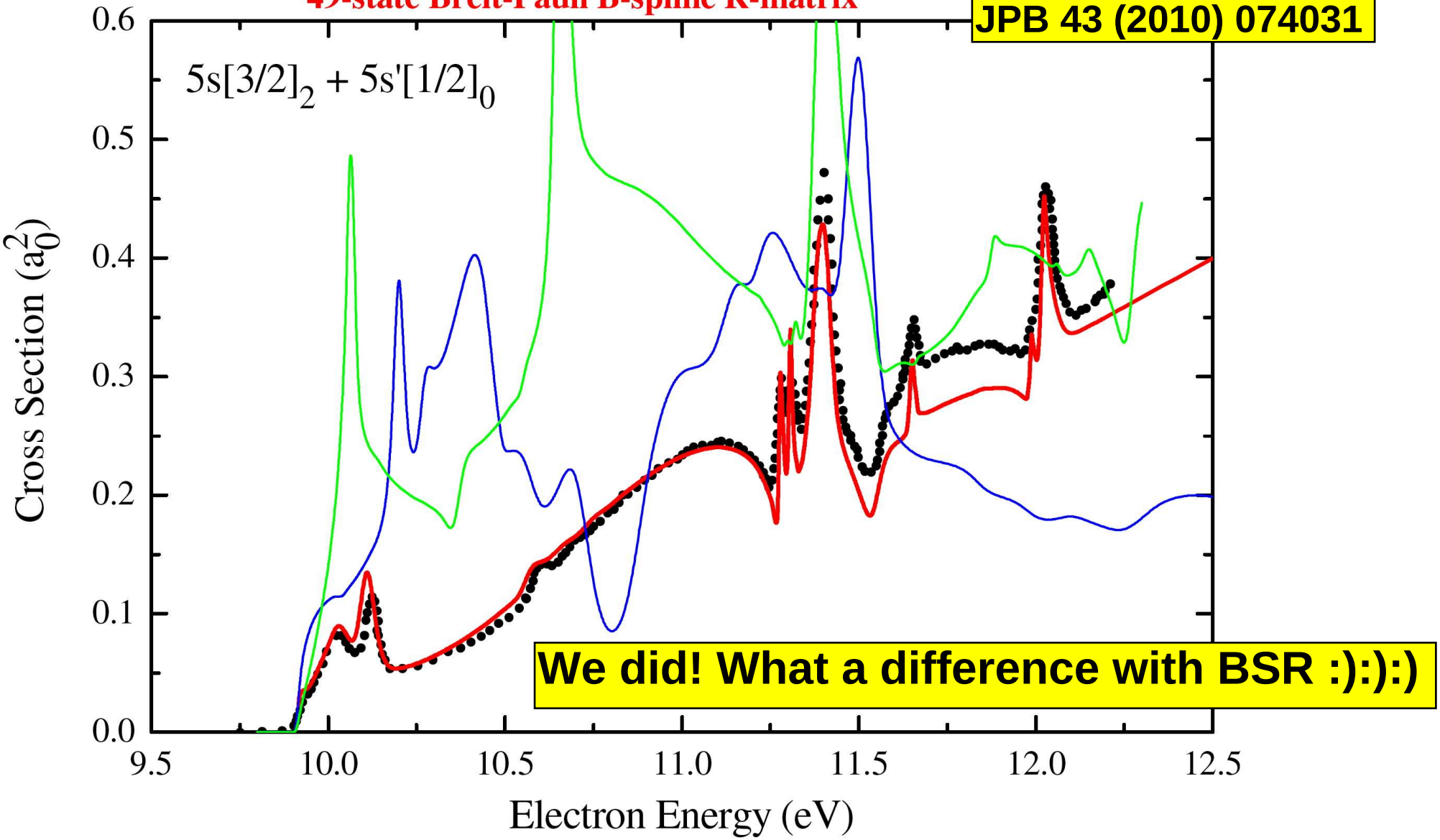
Oops — maybe we need to try a bit harder?

Metastable Excitation Function in Kr

Experiment: Buckman *et al* (1983), multiplied by 0.67

Theories: 31-state Breit-Pauli R-matrix (Zeman & Bartschat 1998)
51-state Breit-Pauli R-matrix (Bartschat & Grum-Grzhimailo 2000)
49-state Breit-Pauli B-spline R-matrix

JPB 43 (2010) 074031



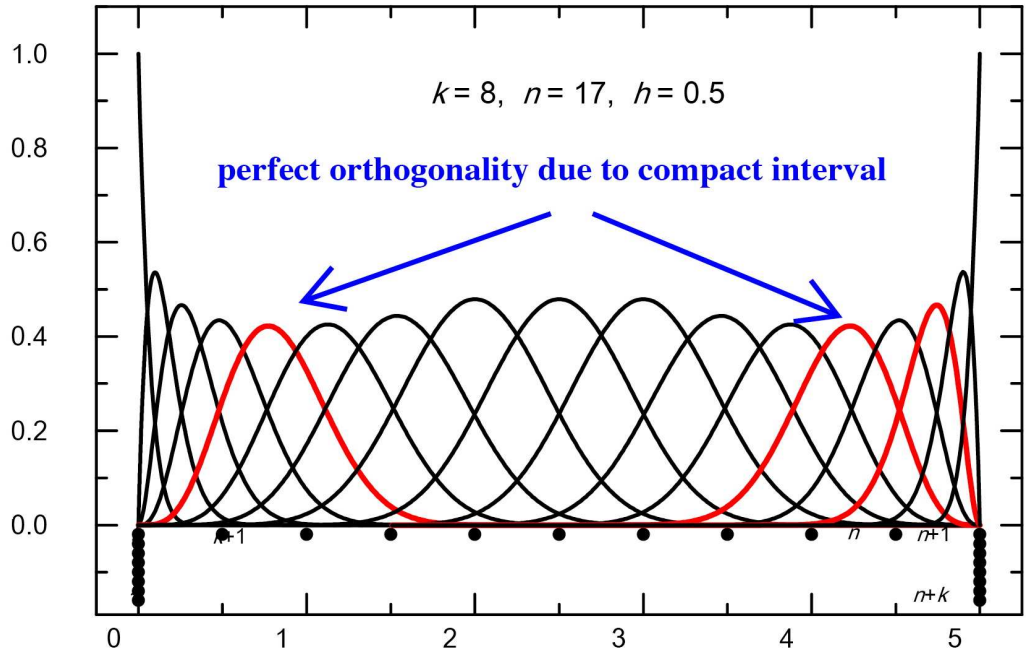
We did! What a difference with BSR :):):)

We have a great program now :):):) -> Zatsarinny talk

General B-Spline R-Matrix (Close-Coupling) Programs (D)BSR

- **Key Ideas:**
  - Use *B*-**splines as universal basis** set to represent the continuum orbitals
  - Allow **non-orthogonal orbital sets** for bound and continuum radial functions

not just the numerical basis!



O. Zatsarinny, CPC 174 (2006) 273

- **Consequences:**
  - **Much improved target description possible with small CI expansions**
  - **Consistent description of the *N*-electron target and (*N*+1)-electron collision problems**
  - No "Buttle correction" since *B*-spline basis is effectively complete
- **Complications:**
  - Setting up the Hamiltonian matrix can be very complicated and lengthy
  - Generalized eigenvalue problem needs to be solved
  - Matrix size typically **100,000 or more** due to size of *B*-spline basis
  - Rescue: Excellent numerical properties of *B*-splines; use of (SCA)LAPACK *et al.*

record:200,000 to do 50-100 times; 0.5 - 1.0 MSU (1 MSU = $50,000 in NSF Accounting)

We also have to solve the problem outside the box for each energy (from 100's to 100,000's).

List of early calculations with the BSR code (rapidly growing)

***hν* + Li**	Zatsarinny O and Froese Fischer C *J. Phys. B* **33** 313 (2000)
***hν* + He**	Zatsarinny O, Gorczyca T W and Froese Fischer C *J. Phys. B.* **35** 4161 (2002)
***hν* + C**	Gibson N D *et al.* Phys. Rev. A **67**, 030703 (2003)
***hν* + B**	Zatsarinny O and Gorczyca T W Abstracts of XXII ICPEAC (2003)
***hν* + O**	Zatsarinny O and Bartschat K *Phys. Rev. A* **73** 022714 (2006)
***hν* + Ca**	Zatsarinny O *et al. Phys. Rev. A* **74** 052708 (2006)
e + He	Stepanovic *et al. J. Phys. B* **39** 1547 (2006)
	Lange M *et al. J. Phys. B* **39** 4179 (2006)
e + C	Zatsarinny O, Bartschat K, Bandurina L and Gedeon V *Phys. Rev. A* **71** 042702 (2005)
e + O	Zatsarinny O and Tayal S S *J. Phys. B* **34** 1299 (2001)
	Zatsarinny O and Tayal S S *J. Phys. B* **35** 241 (2002)
	Zatsarinny O and Tayal S S As. J. S. S. **148** 575 (2003)
e + Ne	Zatsarinny O and Bartschat K *J. Phys. B* **37** 2173 (2004)
	Bömmels J *et al.* Phys. Rev. A **71**, 012704 (2005)
	Allan M *et al. J. Phys. B* **39** L139 (2006)
e + Mg	Bartschat K, Zatsarinny O, Bray I, Fursa D V and Stelbovics A T *J. Phys. B* **37** 2617 (2004)
e + S	Zatsarinny O and Tayal S S *J. Phys. B* **34** 3383 (2001)
	Zatsarinny O and Tayal S S *J. Phys. B* **35** 2493 (2002)
e + Ar	Zatsarinny O and Bartschat K *J. Phys. B* **37** 4693 (2004)
e + K (inner-shell)	Borovik A A *et al. Phys. Rev. A,* **73** 062701 (2006)
e + Zn	Zatsarinny O and Bartschat K *Phys. Rev. A* **71** 022716 (2005)
e + Fe^+	Zatsarinny O and Bartschat K *Phys. Rev. A* **72** 020702(R) (2005)
e + Kr	Zatsarinny O and Bartschat K *J. Phys. B* **40** F43 (2007)
e + Xe	Allan M, Zatsarinny O and Bartschat K *Phys. Rev. A* 030701(R) (2006)
Rydberg series in C	Zatsarinny O and Froese Fischer C *J. Phys. B* **35** 4669 (2002)
osc. strengths in Ar	Zatsarinny O and Bartschat K *J. Phys. B: At. Mol. Opt. Phys.* **39** 2145 (2006)
osc. strengths in S	Zatsarinny O and Bartschat K *J. Phys. B: At. Mol. Opt. Phys.* **39** 2861 (2006)
osc. strengths in Xe	Dasgupta A *et al. Phys. Rev. A* **74** 012509 (2006)

at least 80 more since 2006

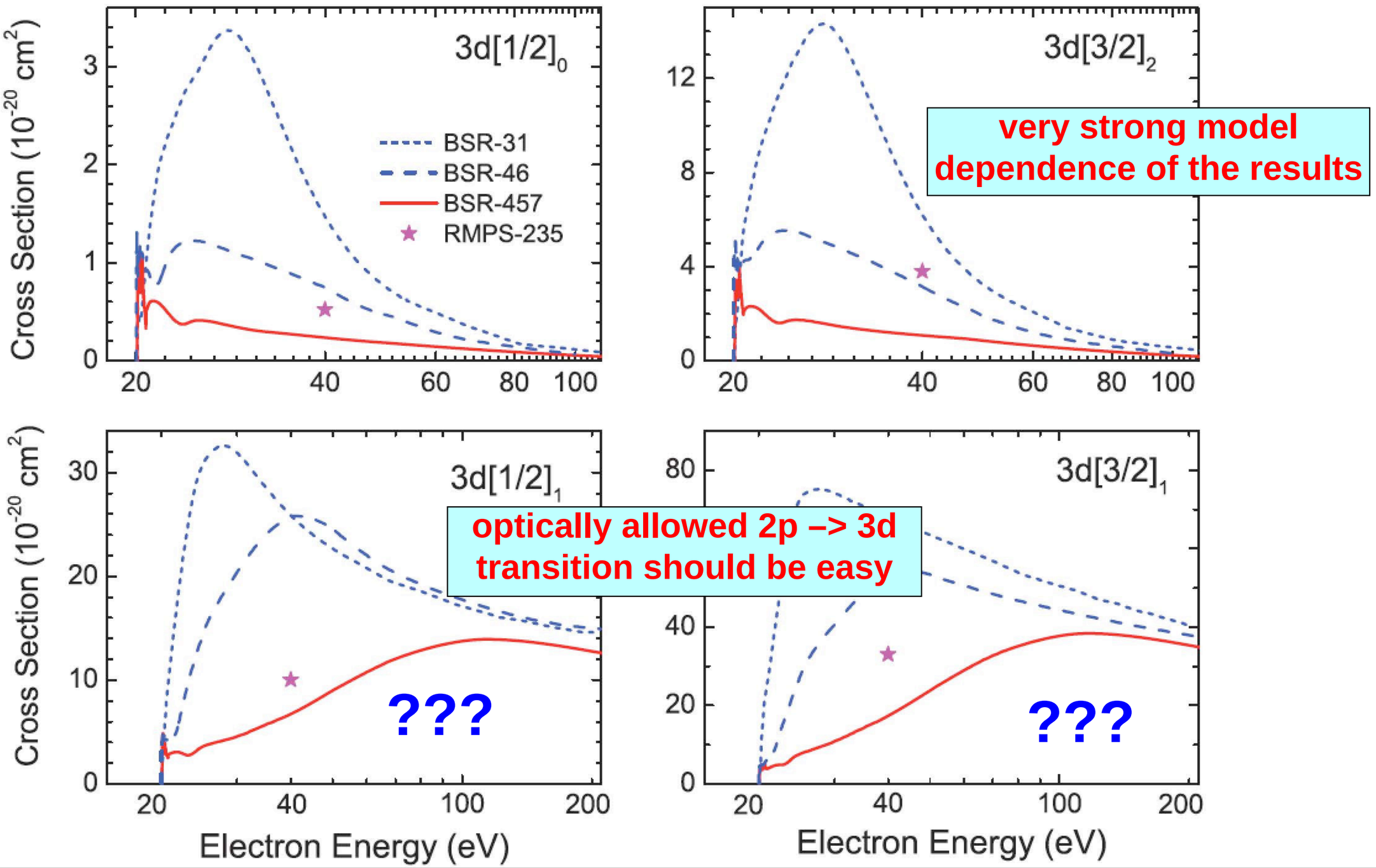
Topical Review: J. Phys. B 46 (2013) 112001

PHYSICAL REVIEW A **86**, 022717 (2012)

Electron-impact excitation of neon at intermediate energies

Oleg Zatsarinny and Klaus Bartschat

BIG SURPRISE (discovered through a GEC collaboration):
This is not what I learned in "Introduction to Atomic Collision Theory".



Collisions at "intermediate energies":
Coupling to the continuum can be very, very important.

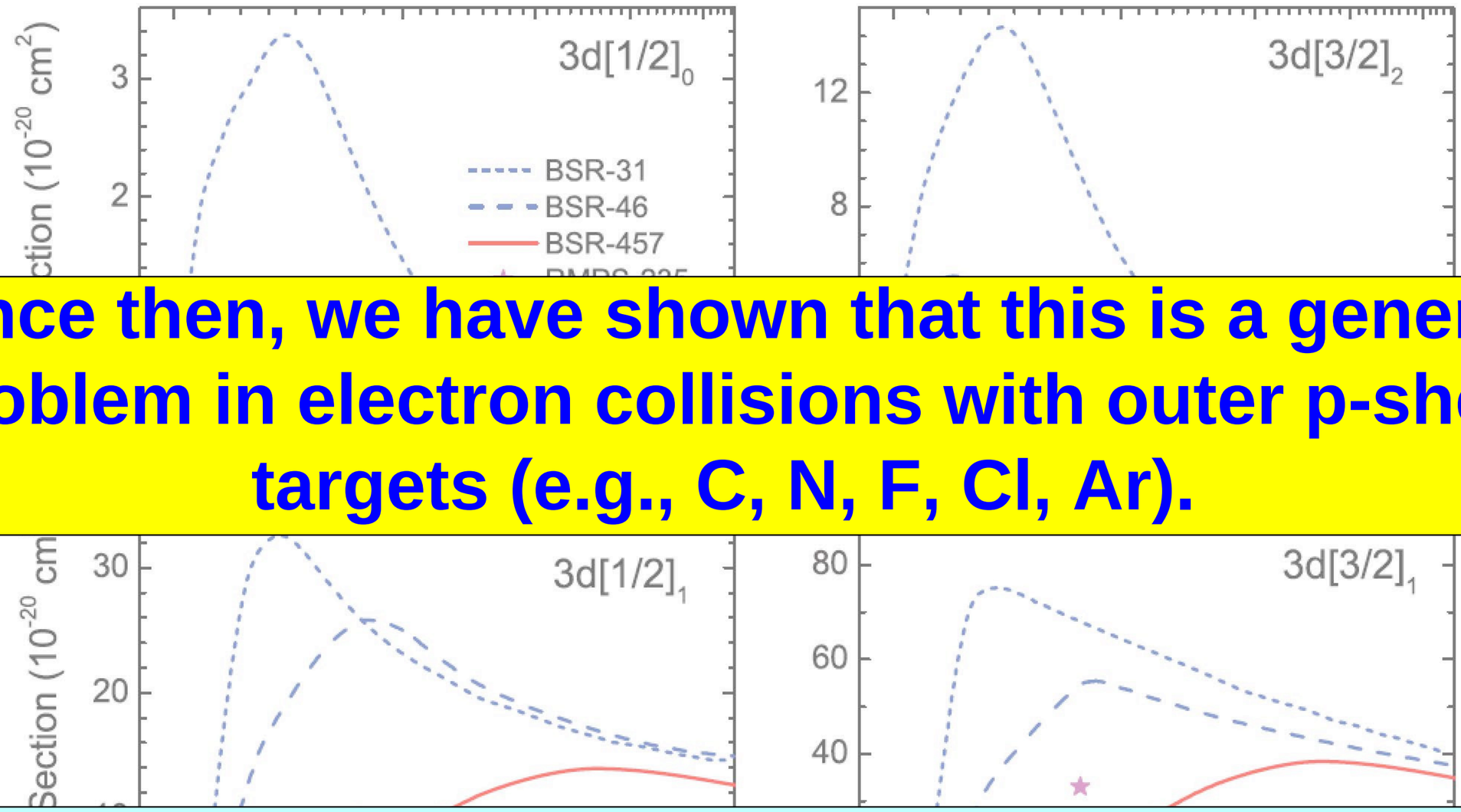
PHYSICAL REVIEW A **86**, 022717 (2012)

Electron-impact excitation of neon at intermediate energies

Oleg Zatsarinny and Klaus Bartschat

Department of Physics and Astronomy, Drake University, Des Moines, Iowa 50311, USA

(Received 18 July 2012; published 30 August 2012)



Since then, we have shown that this is a general problem in electron collisions with outer p-shell targets (e.g., C, N, F, Cl, Ar).

Convergence and sensitivity studies provide a systematic way to assign some uncertainty to theoretical predictions, which is becoming an increasingly "hot" topic. (PRA editorial 2011, IAEA/ITAMP workshop 2014, ...)

In fact, that's why we are here today.

DOI: 10.1002/ppap.201600093

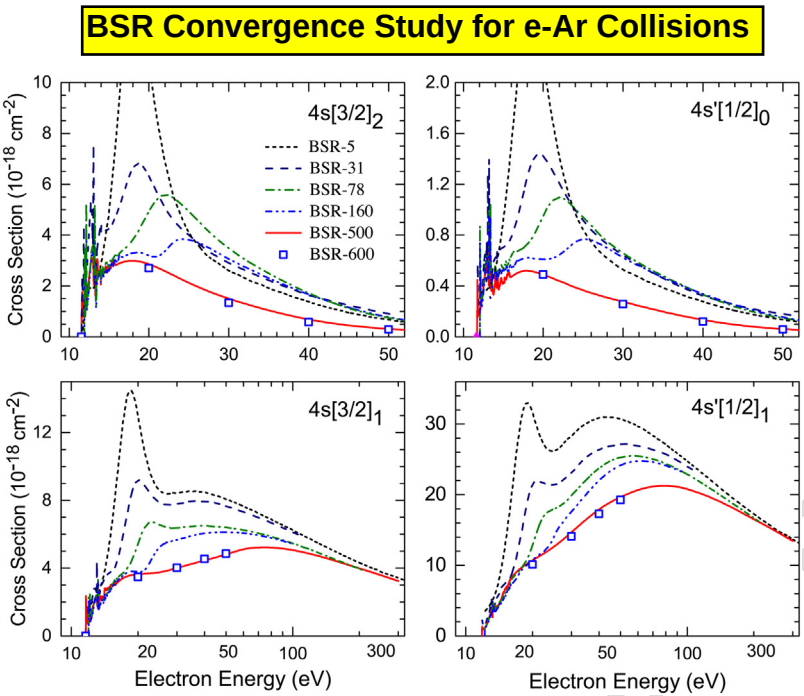


Figure 5. Cross sections for electron-impact excitation of the individual states of the $3p^5 4s$ manifold in argon from the ground state $(3p^6)\,^1S_0$. The results from a number of BSR calculations with a varying number of states shows the convergence of the CC expansion.

Trust Theory or Experiment?

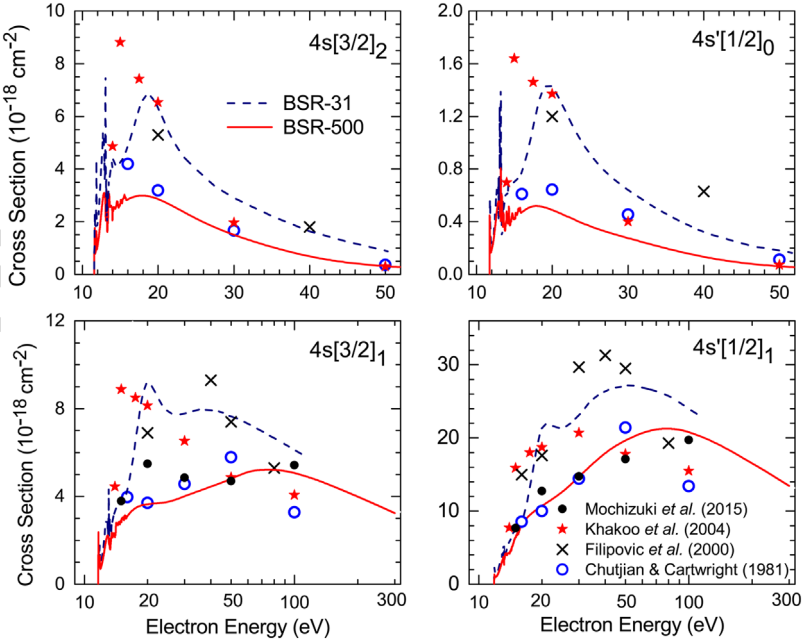


Figure 6. Cross sections for electron-impact excitation of the individual states of the $3p^5 4s$ manifold in argon from the ground state. The BSR-31 and BSR-500 predictions[48] are compared with a variety of experimental data.[73–76]

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Calculations for electron-impact excitation and ionization of beryllium

e-Be: Since there is no experiment, which theory?

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As we will see, the answer seems clear. Now you just have to use these results!

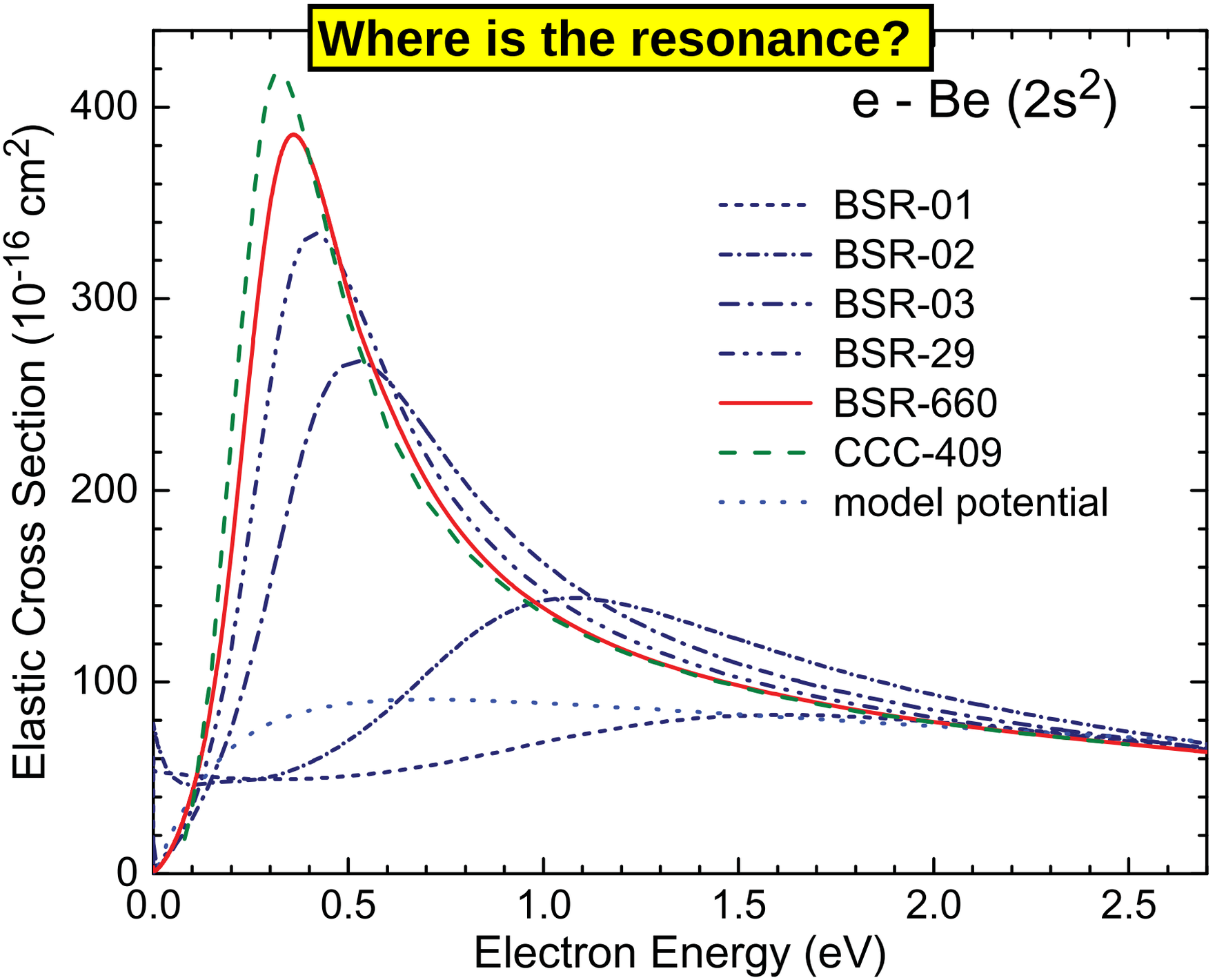


Figure 1. Cross sections for elastic electron scattering from beryllium atoms in their $(2s^2)^1S$ ground state at low energies in the region of the shape resonance. We present several BSR calculations to illustrate the convergence pattern. Also shown are the model-potential calculations by Reid and Wadehra [27].

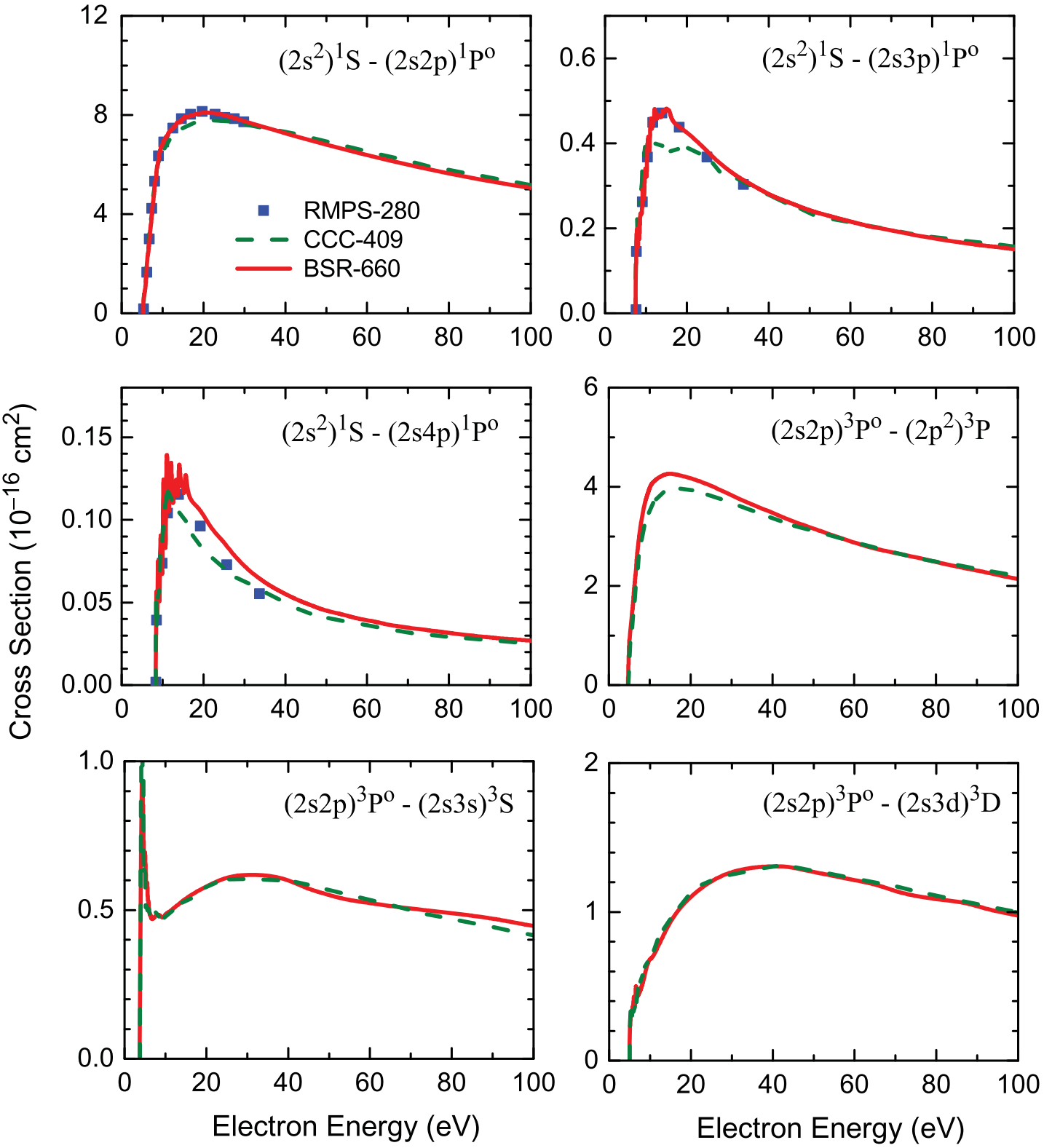
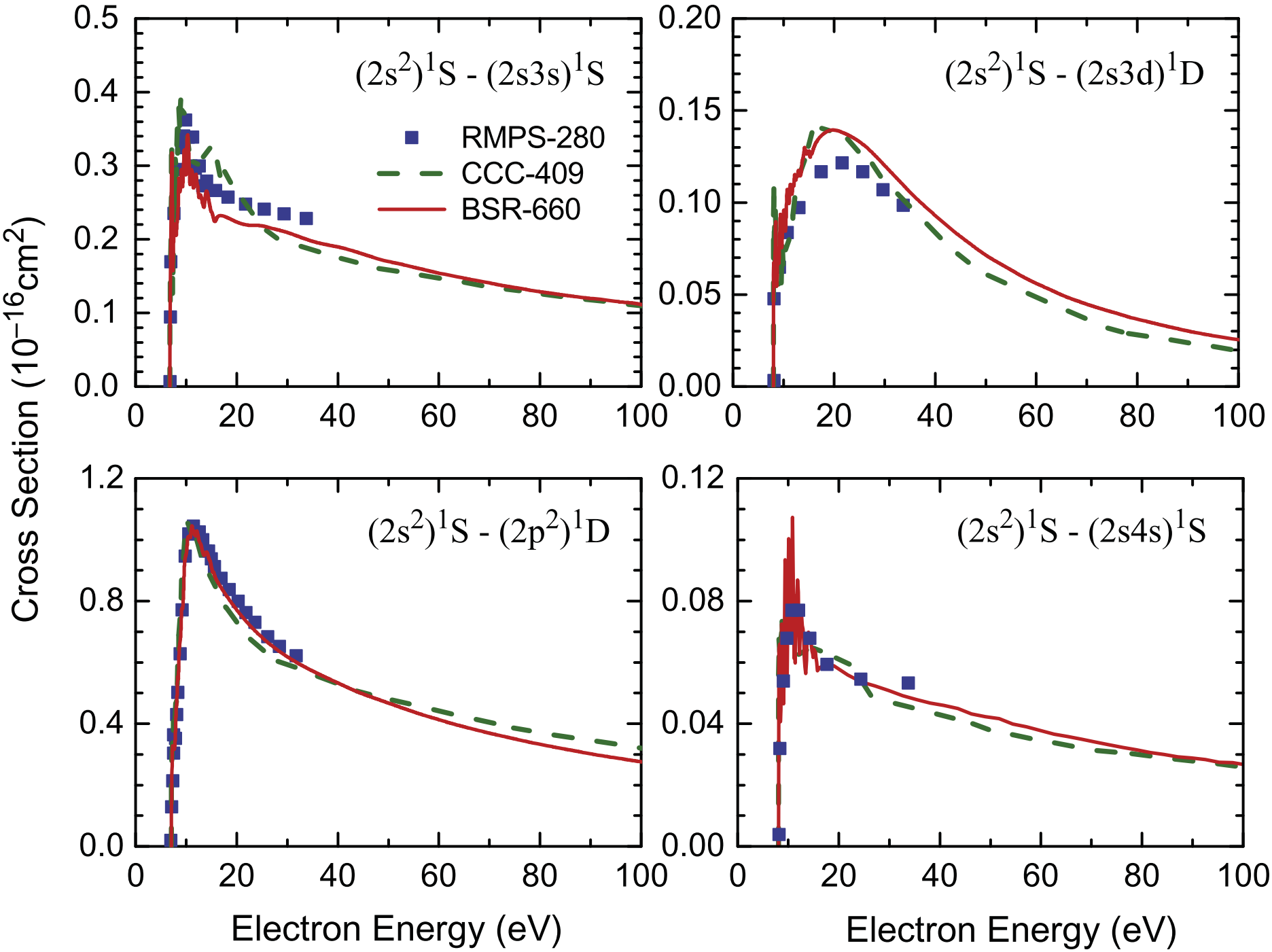


Figure 3. Cross sections as a function of collision energy for selected dipole
results
calcula

Excellent agreement between CCC, BSR, and RMPS for dipole-allowed transitions.



And for non-dipole spin-conserving transitions.

Figure 4. Cross sections as a function of collision energy for selected nondipole transitions in beryllium. The present BSR-660 and CCC-409 results are compared with those from an earlier RMPS-280 [6] calculation.

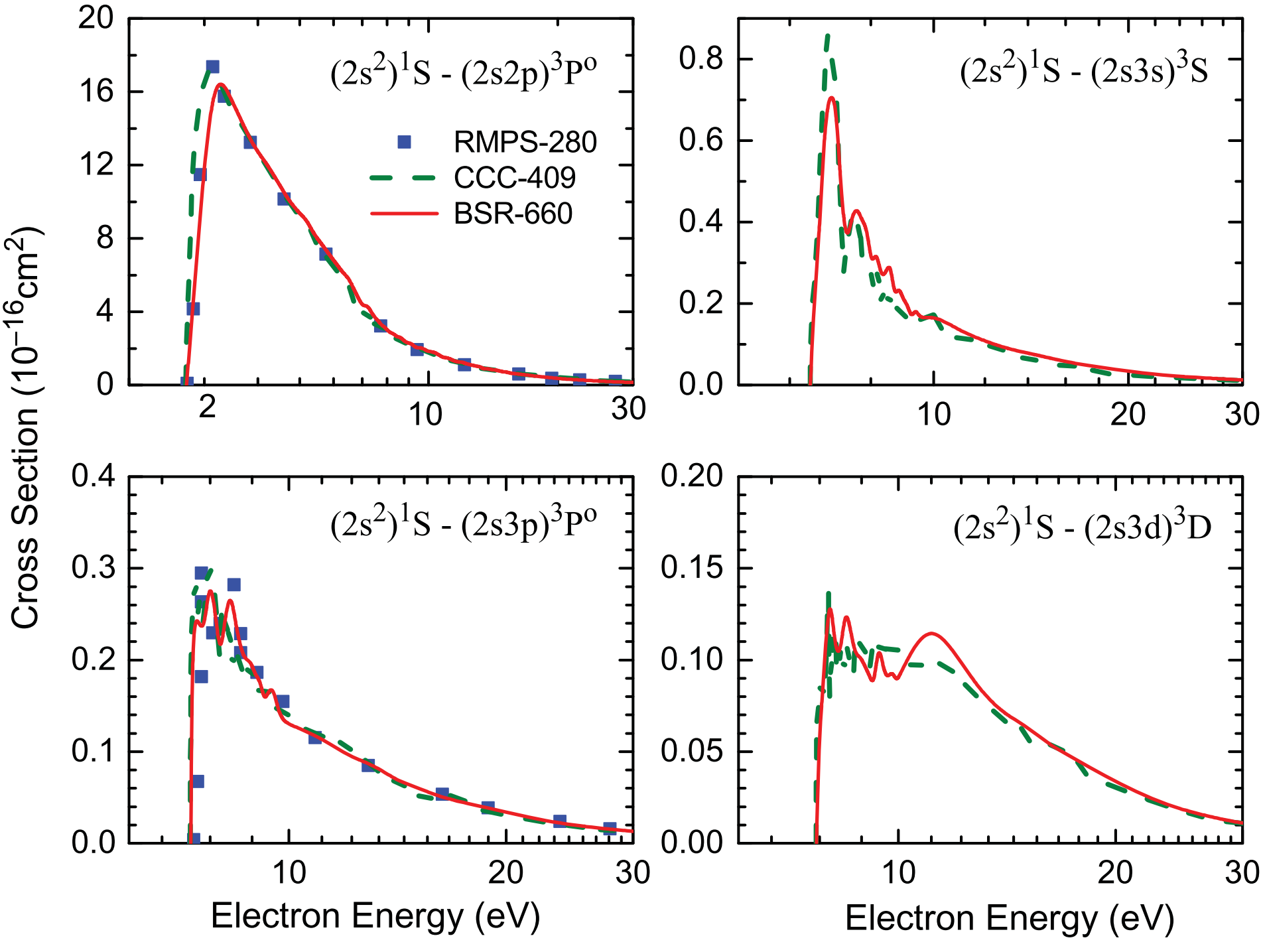


Figure 5. Cross sections as a function of collision energy for selected exchange tr nd CCC-409 results are compared with those from an earlier RMPS-280 [6] calculation.

And for spin-forbidden transitions.

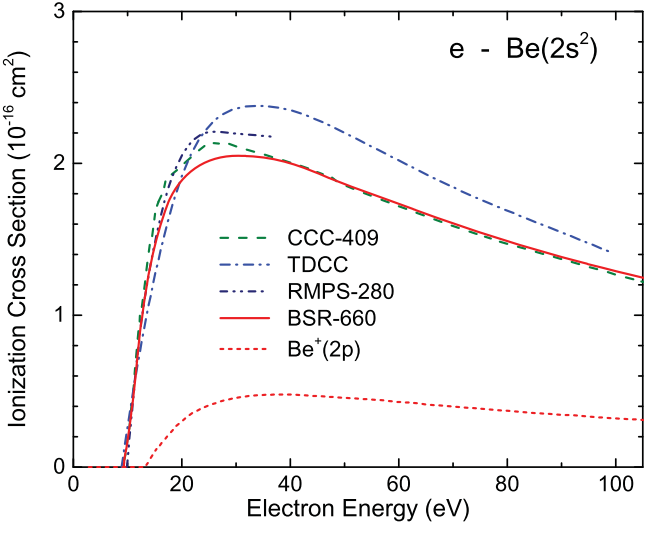


Figure 6. Cross section for electron-impact ionization of beryllium from the $(2s^2)^1S$ ground state. The pr… results are compared with those from earlier RMPS-280 [6] and TDCC [8] calculations. Also shown is the partial cross section for producing the excited $1s^22p$ state of Be^+ (obtained with BSR-660).

And for ionization, total, momentum transfer.

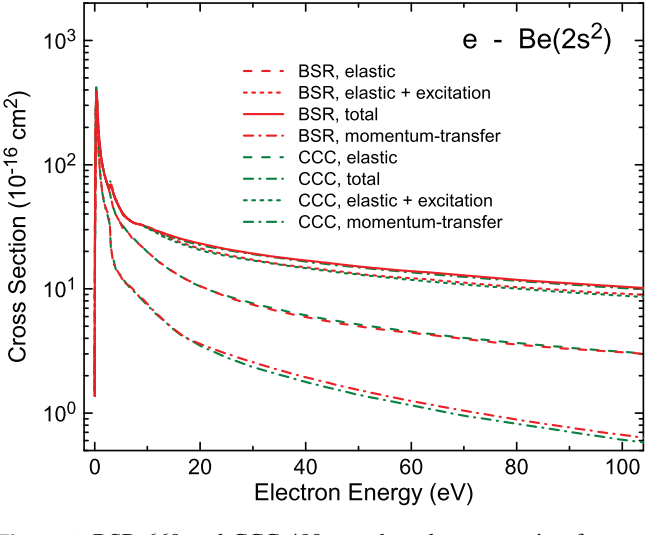
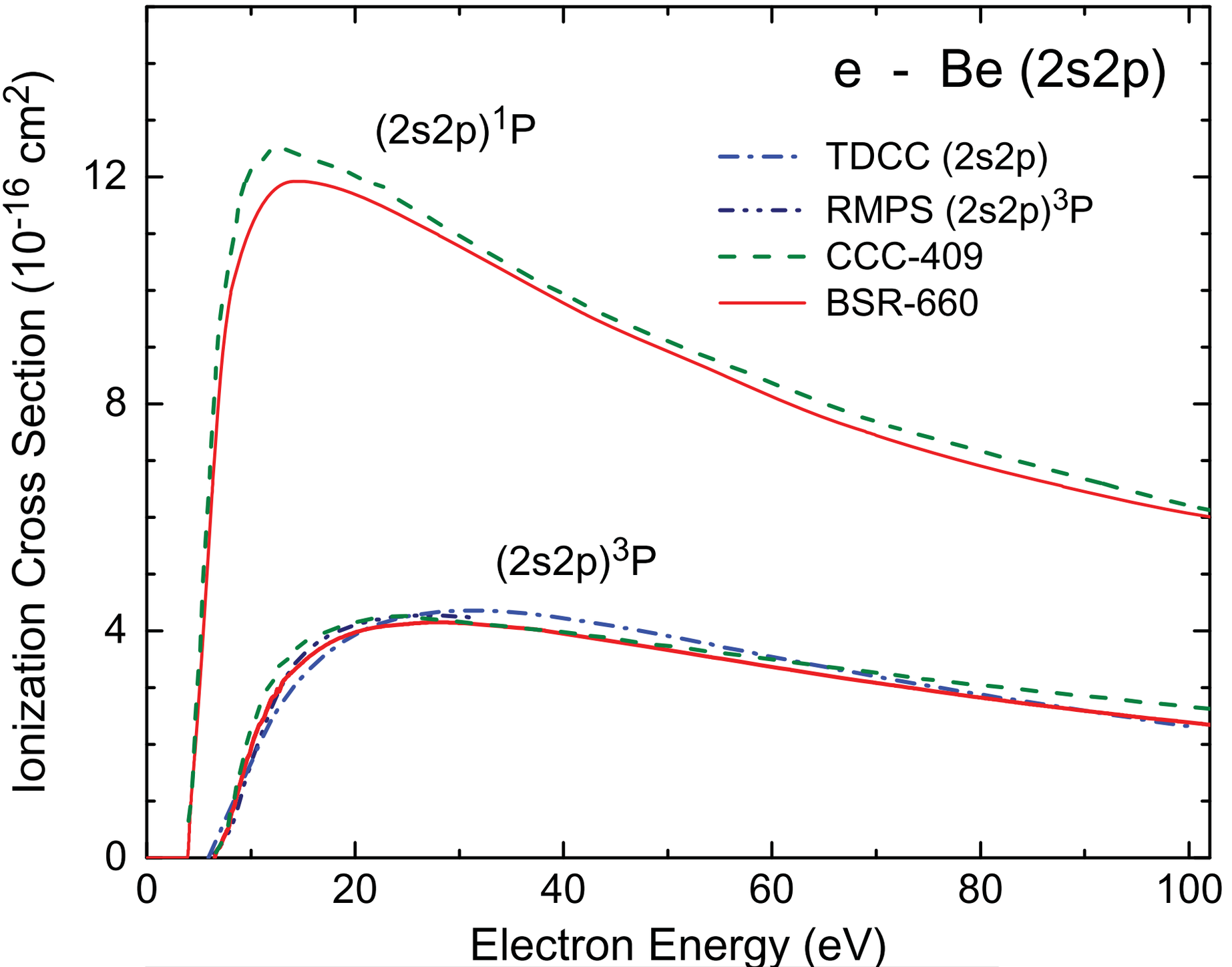


Figure 8. BSR-660 and CCC-409 grand total cross section for electron collisions with beryllium atoms in their $(2s^2)^1S$ ground state, … from elastic scattering alone as well as elastic scattering plus excitation processes. Also shown is the momentum-transfer cross section.



And for ionization (and excitation) from excited states

Figure 7 neutral beryllium from the first excited $2s2p$ configuration. The present BSR-660 and CCC-409 results are compared with those from earlier RMPS-280 [6] and TDCC [8] calculations.

Ionization in the Close-Coupling Formalism

- **Recall: We are interested in the ionization process**

$$e_0(\boldsymbol{k}_0, \mu_0) + A(L_0, M_0; S_0, M_{S_0}) \rightarrow e_1(\boldsymbol{k}_1, \mu_1) + e_2(\boldsymbol{k}_2, \mu_2) + A^+(L_f, M_f; S_f, M_{S_f})$$

- **We need the ionization amplitude**

$$f(L_0, M_0, S_0; \boldsymbol{k}_0 \rightarrow L_f, M_f, S_f; \boldsymbol{k}_1, \boldsymbol{k}_2)$$

- **We employ the *B*-spline *R*-matrix method of Zatsarinny (CPC 174 (2006) 273) with a large number of pseudo-states:**
  - **These pseudo-states simulate the effect of the continuum.**
  - **The scattering amplitudes for excitation of these pseudo-states are used to form the ionization amplitude:**

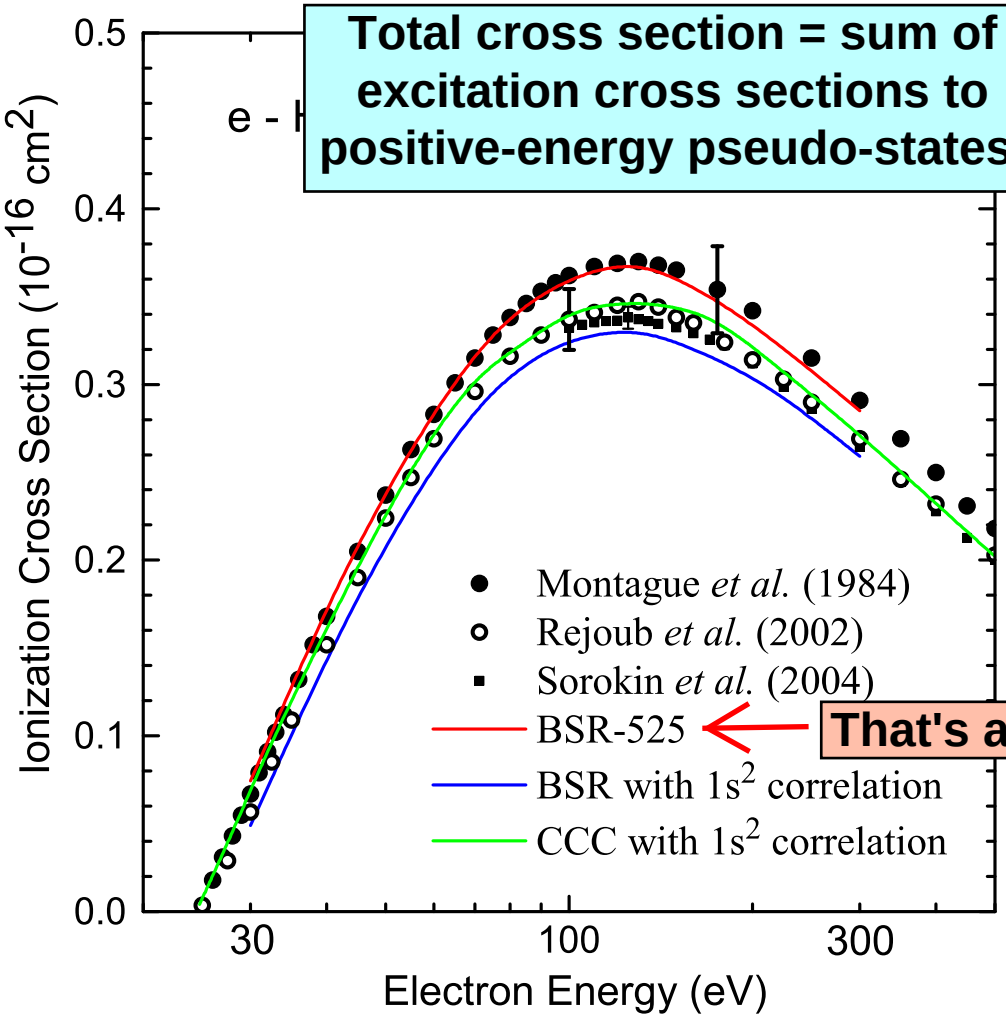
$$f(L_0, M_0, S_0; \boldsymbol{k}_0 \rightarrow L_f, M_f, S_f; \boldsymbol{k}_1, \boldsymbol{k}_2) = \sum_p \langle \Psi_f^{\boldsymbol{k}_2 -} | \Phi(L_p S_p) \rangle \; f(L_0, M_0, S_0; \boldsymbol{k}_0 \rightarrow L_p, M_p, S_p; \boldsymbol{k}_{1p}).$$

This direct projection is the essential idea. It's not based on first principles, but we'll see if it works.

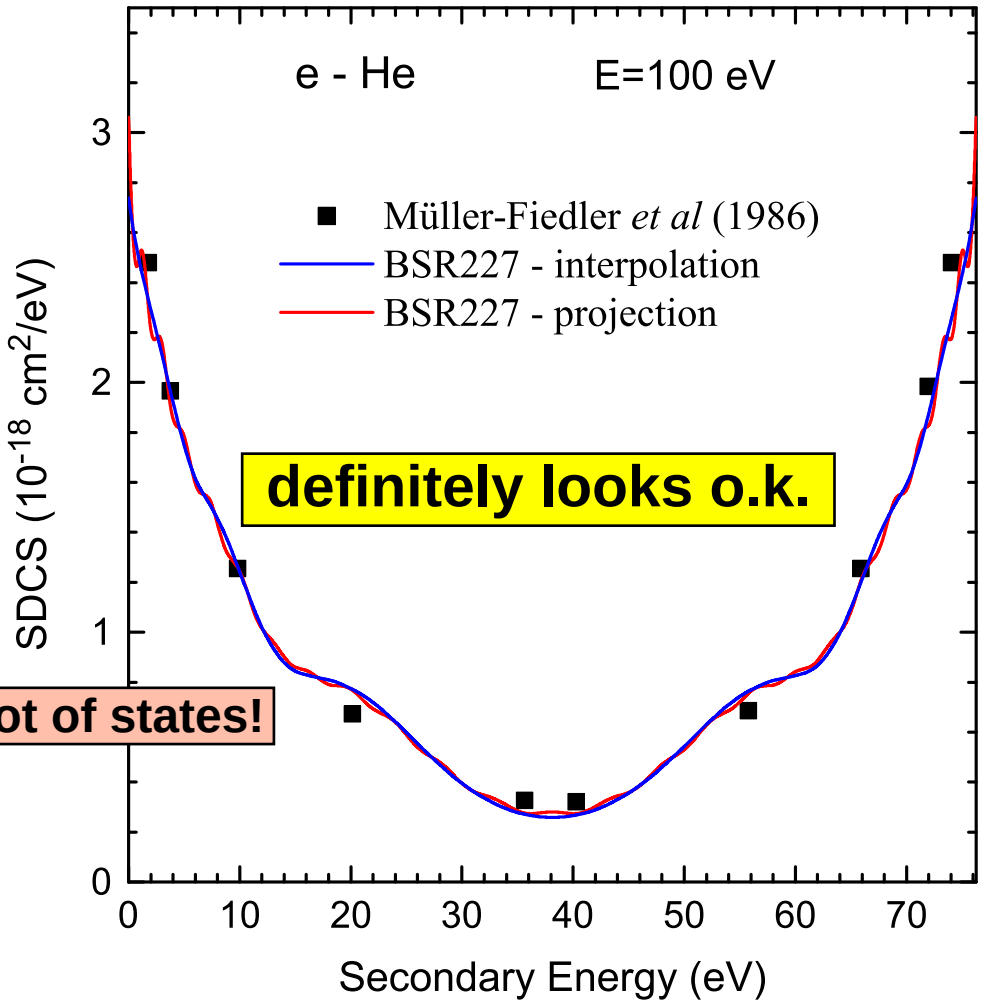
Some Checks: Ionization without Excitation (compare to CCC and TDCC)

Total and Single-Differential Cross Section

Total cross section = sum of excitation cross sections to positive-energy pseudo-states.



That's a lot of states!



definitely looks o.k.

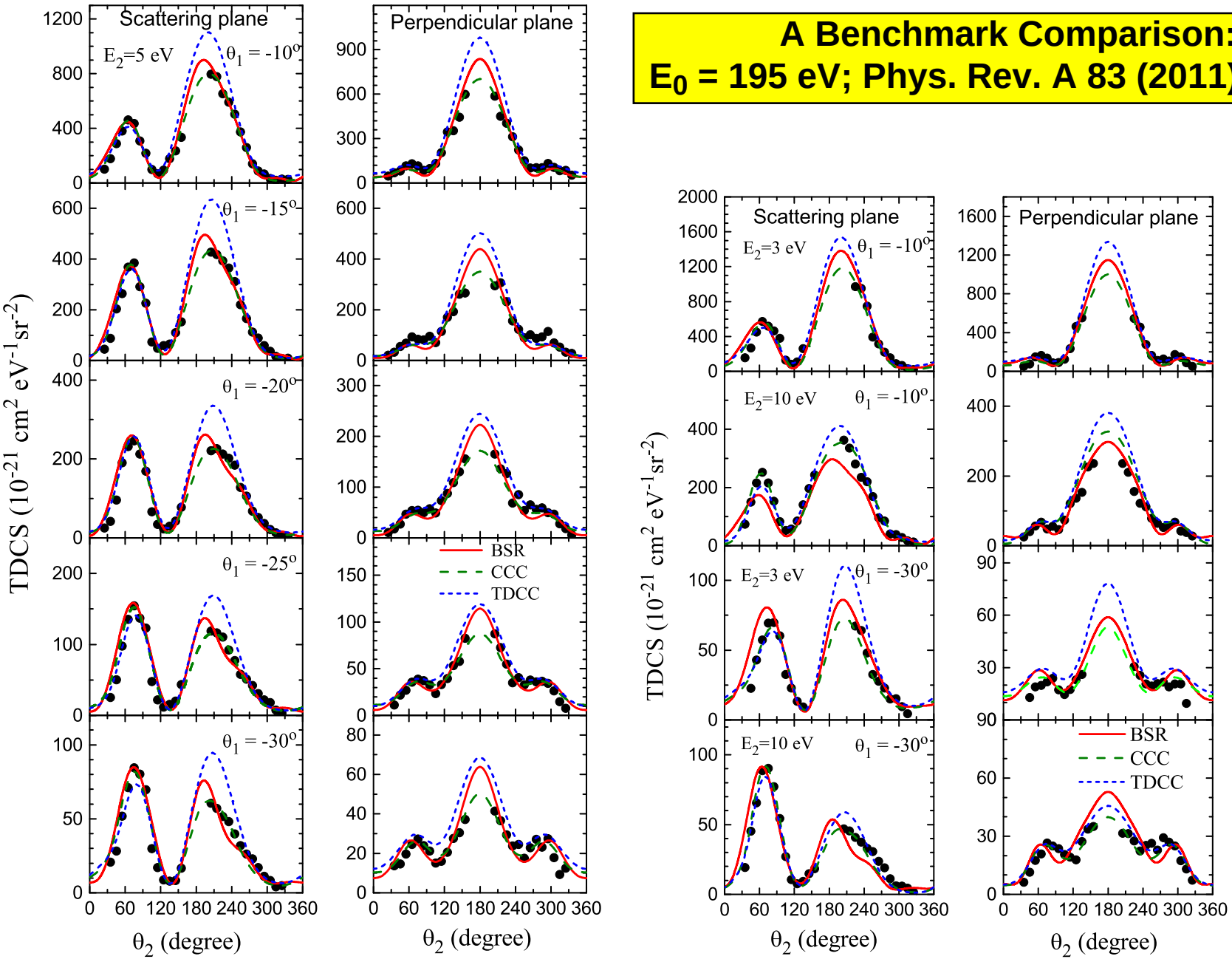
- **Including correlation in the ground state reduces the theoretical result.**
- **Interpolation yields smoother result, but direct projection is acceptable.**
- **DIRECT PROJECTION is NECESSARY for MULTI-CHANNEL cases!**

So far, so good ... Let's go for more detail!

Triple-Differential Cross Section for Direct Ionization

experiment: Ren et al. (2011)

A Benchmark Comparison:
E_0 = 195 eV; Phys. Rev. A 83 (2011) 052711

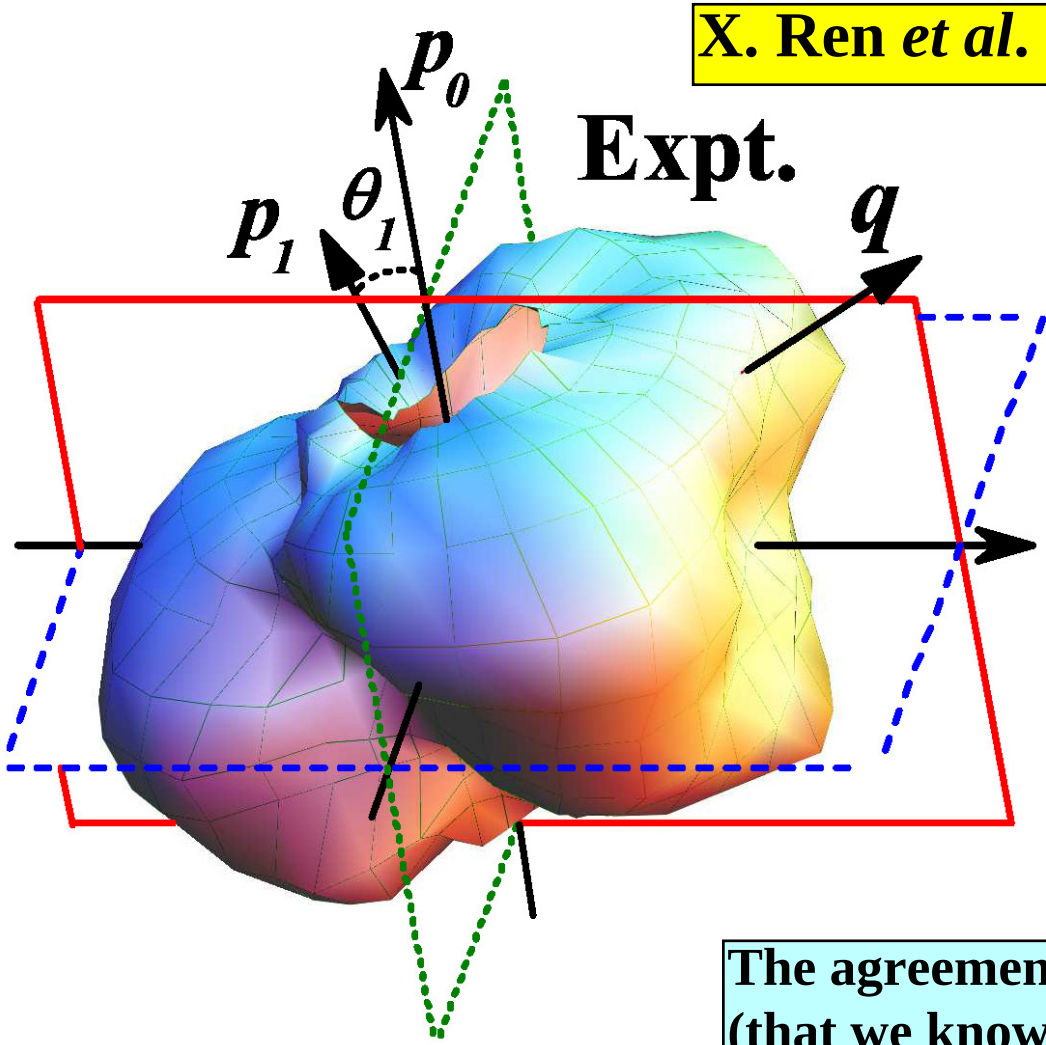


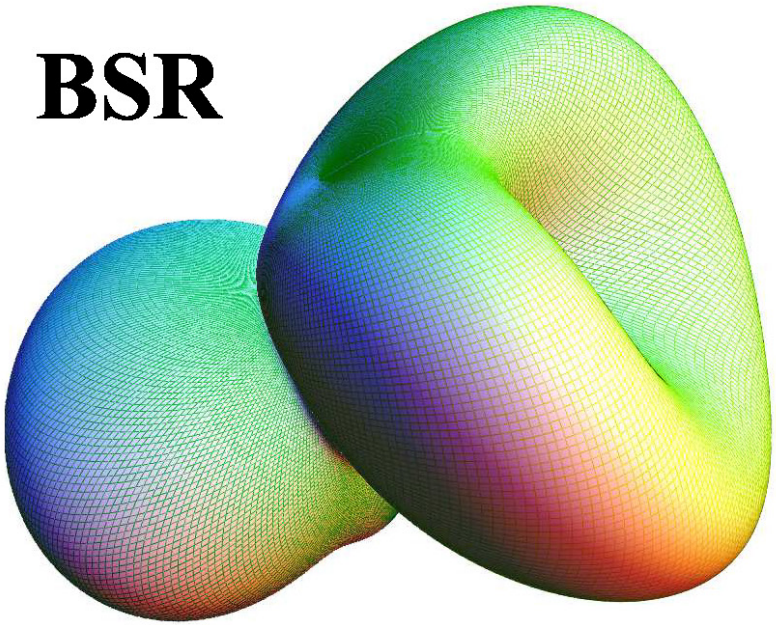
(e,2e) on Ar is a very l .. o .... n ..... g story. It includes the discovery of an error in the processing of the raw experimental data, which was found by the confidence gained in BSR predictions ...

The latest: (e,2e) on Ar ($3p^6$)

E_0 = 66 eV; E_1 = 47 eV; E_2 = 3 eV; $\theta_1 = 15^o$

X. Ren *et al*. (Phys. Rev. A 93 (2016) 062704)





The agreement is not perfect, but no other theory (that we know of) gets anywhere near experiment.

Conclusions

- **Despite the field's maturity, significant innovations are constantly being made to study electron collisions with atoms and molecules – and they are needed!**
- **There exist many fruitful collaborations between experimentalists, theorists, and users outside of AMO who need (and use) these data.**
- **Experimental benchmark data remain very important to test and push theory!**
- **With such benchmark data and comparisons between predictions from highly sophisticated methods in hand, we can finally estimate uncertainties of these predictions.**

Thank You for Your Attention!