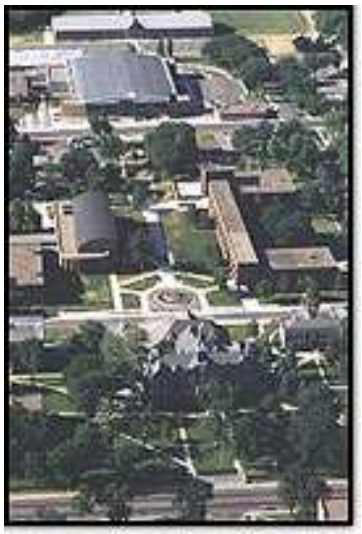
Atomic and Molecular Collision Data for Plasma Science

Klaus Bartschat

Drake University, Des Moines, Iowa 50311, USA

Gaseous Electronics Conference; Oct. 9, 2020



OVERVIEW:

Acknowledgements:

Oleg Zatsarinny
has been a close collaborator at Drake University since 2003.
Oleg produced a lot of high-quality data with his B-spline R-matrix (BSR) code.

Kathryn Hamilton
Post-doctoral researcher at Drake University
Kathryn performs calculations on many projects and maintains the BSR code on the AMP Gateway.

Phil Burke
(18.10.1932 – 3.6.2019)

Phil developed the R-matrix method in atomic physics, and he taught me a lot.

PHY-1803844; OAC-1834740; XSEDE-090031

Some relevant points of this talk are summarized here.

PERSPECTIVE

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)

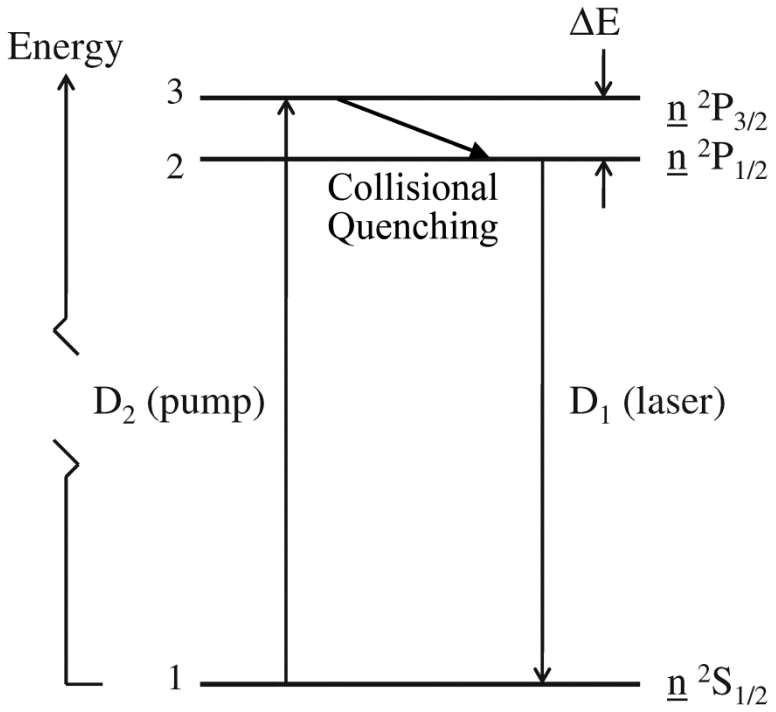
Electron collisions with atoms, ions, molecules, and surfaces are critically important to the understanding and modeling of low-temperature plasmas (LTPs), and so in the development of technologies based on LTPs. Recent progress in obtaining experimental benchmark data and the development of highly sophisticated 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

Motivation: The Need for Electron Collision Data

DIODE-PUMPED ALKALI LASERS (DPALs)

- **DPAL is a class of optically pumped lasers that leverage inexpensive semiconductor diode lasers to pump alkali vapor.**
- **Poor optical quality, wide bandwidth of diode laser (DL) is converted into high optical quality, narrow bandwidth from alkali laser.**



- **DL pumps the $D_2(^2S_{1/2} \rightarrow {}^2P_{3/2})$**
- **Collisional quenching: $^2P_{3/2} \rightarrow {}^2P_{1/2}$**
- **Lasing on $D_1(^2P_{1/2} \rightarrow {}^2S_{1/2})$**
- **Requires inversion of ground state.**
- **Collisional quenching agent N_2**

(slide adapted from a presentation by M. J. Kushner, University of Michigan, Institute for Plasma Science & Engineering.)

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**

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    - valuable but expensive **($$$)** benchmarks (often differential in energy, angle, spin, ...)
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  - **calculations** (Opacity Project, Iron Project, ...)
    - relatively cheap
    - almost any transition of interest is possible
    - often restricted to particular energy ranges:
      - high ($\rightarrow$ Born-type methods)
      - low ($\rightarrow$ close-coupling-type methods)
    - cross sections may peak at "intermediate energies" ($\rightarrow$ **???**)

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

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

Theoretical/Computational Methods

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)**

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  - How much input from experiment?
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  - 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?**

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**
  - CC$_n$, CCO, CCC, RM$_n$, IERM, RMPS, DARC, BSR, ...
  - Standard method of treating low-energy scattering; based upon the expansion

$$\Psi_\beta^{(e)^N}(\mathbf{r}_1,\ldots,\mathbf{r}_{N+1}) = \mathcal{A}\sum_\alpha \psi_\alpha^{(e)^N}(\mathbf{r}_1,\ldots,\mathbf{r}_N,\sigma)\frac{1}{r_{N+1}}f_{\alpha,\beta}(r_{N+1})$$

  - 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

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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, ...)**

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Inclusion of Relativistic Effects

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

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Now come a few examples ...

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

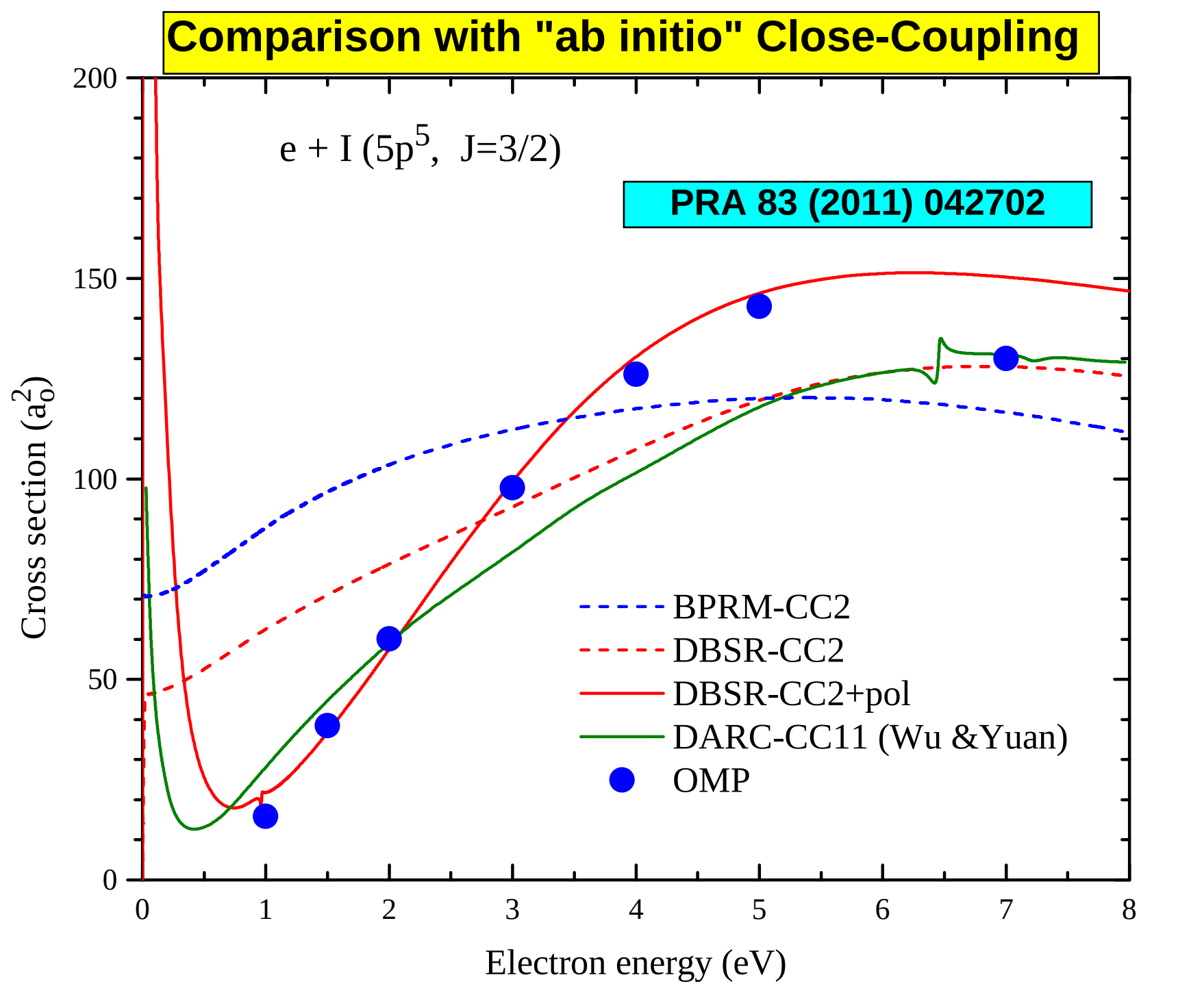
$$V_{\rm mp}(k,r) = V_{\rm static}(r) + V_{\rm exchange}(k,r) + V_{\rm polarization}(r) + iV_{\rm absorption}(k,r)$$

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's 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

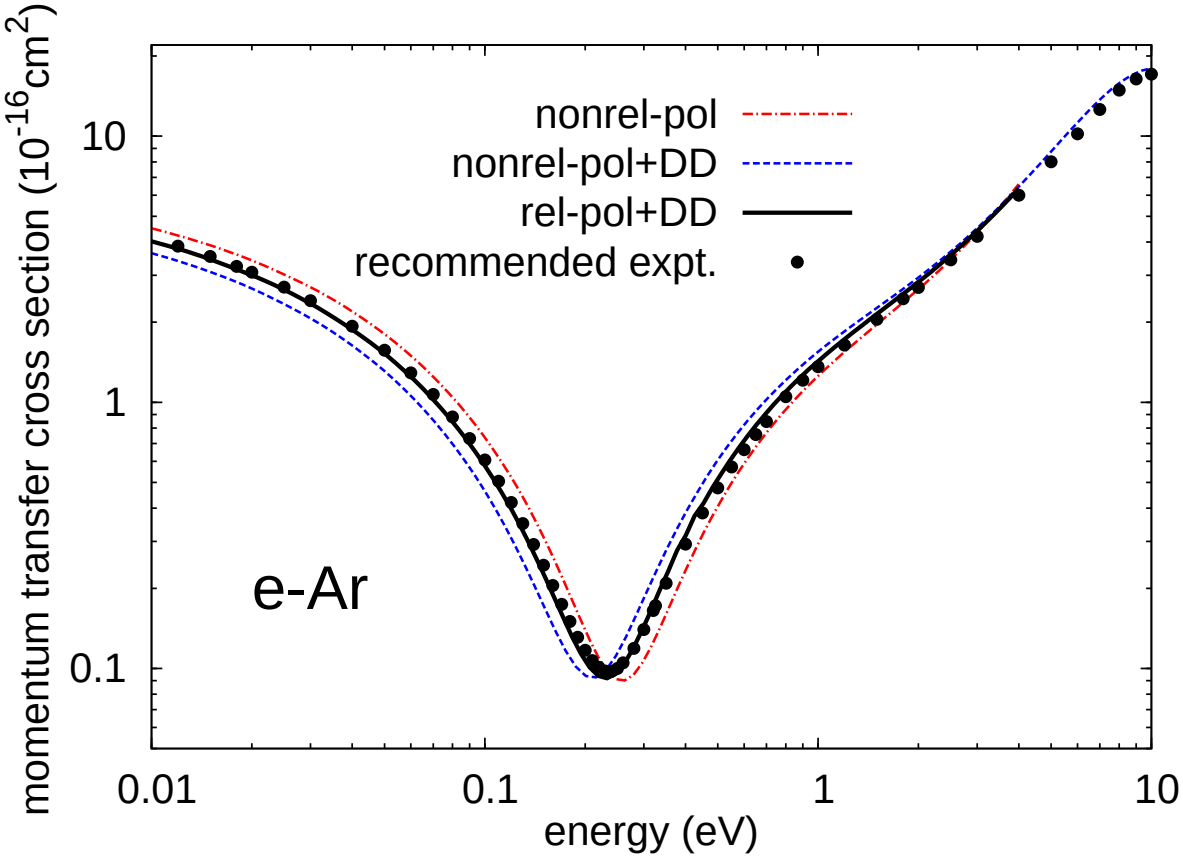
Polarized Orbital – an "Ab Initio Special Purpose" Approach

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

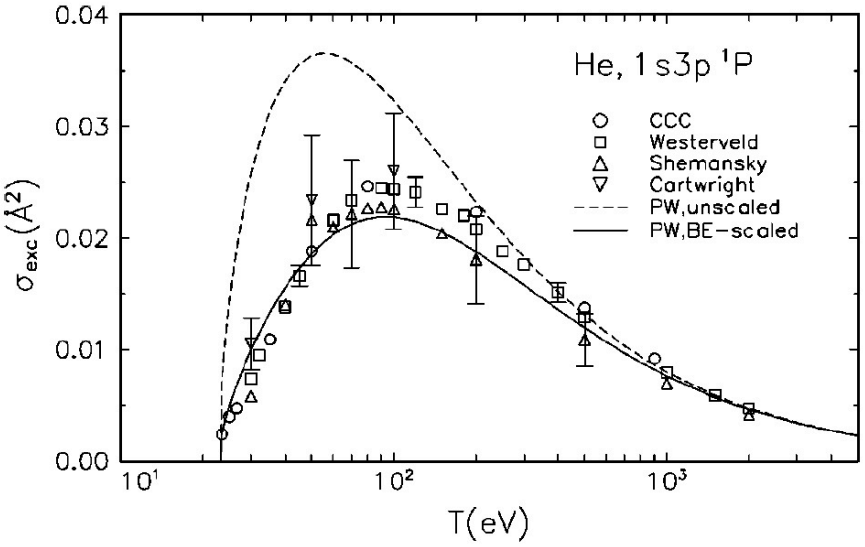
BEf-scaling; Plane-Wave Born with Experimental Optical Oscillator Strength and Empirical Energy Shift

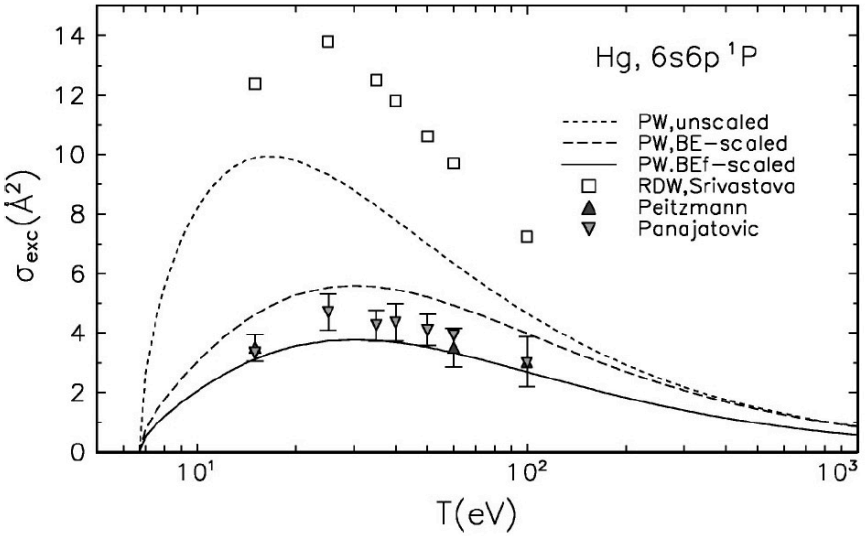
PHYSICAL REVIEW A, VOLUME 64, 032713

Scaling of plane-wave Born cross sections for electron-impact excitation of neutral atoms

Yong-Ki Kim
National Institute of Standards and Technology, Gaithersburg, Maryland 20899-8421
(Received 12 March 2001; published 20 August 2001)

Two methods to scale plane-wave Born cross sections for electron-impact excitations of neutral atoms are shown to produce excitation cross sections comparable in accuracy to those obtained by more sophisticated collision theories such as the convergent close-coupling method. These scaling methods are applicable to integrated cross sections for electric dipole-allowed transitions. Scaled cross sections are in excellent agreement with available theoretical and experimental data for excitations in H, He, Li, Be, Na, Mg, K, Ca, Rb, Sr, Cs, Ba, Hg, and Tl, indicating the possibility of rapid and reliable calculations of excitation cross sections for many other neutral atoms.





works well, but is limited to optically allowed transitions

Similar idea works even better for ionization of complex targets :=)

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., Dasgupta's NRL code)

MALONEY, PEACHER, BARTSCHAT, AND MADISON

Phys. Rev. A 61 (2000) 022701

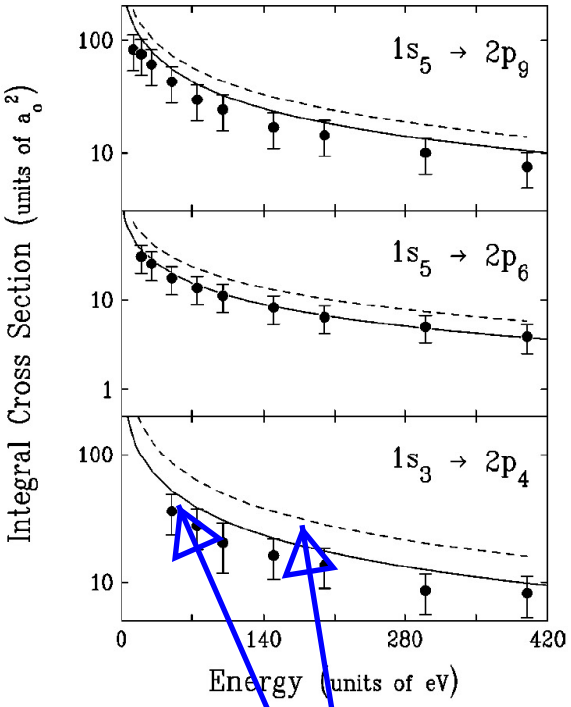


FIG. 1. Integral cross sections for electron-impact excitation of three states in the $2p$ manifold of argon from the metastable states in the $1s$ manifold as a function of incident electron energy. The experimental data are those of Boffard *et al.* [7]. The theoretical SRDW results are SS wave functions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

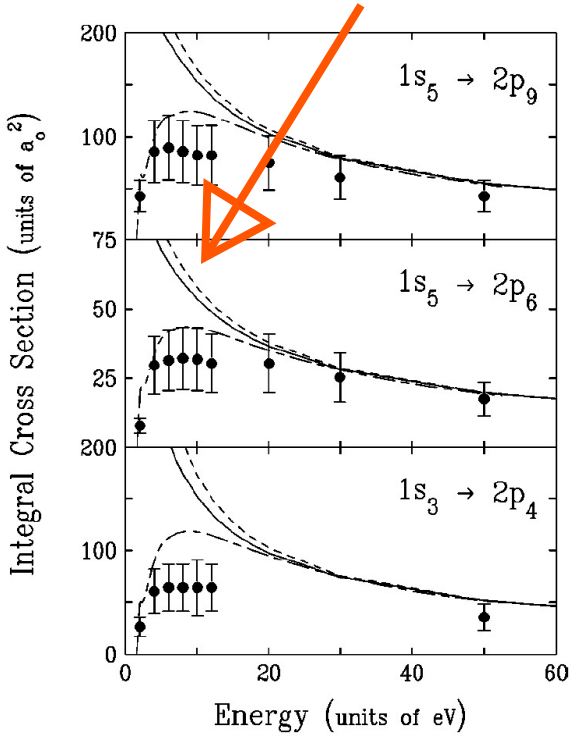


FIG. 2. Integral cross sections for electron-impact excitation of three states in the $2p$ manifold of argon from the metastable states in the $1s$ manifold as a function of incident electron energy. The experimental data are those of Boffard *et al.* [7]. The theoretical results are PWBA (dashed curve);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

Theoretical results depend on wavefunctions and potentials

If you want to try doing your own calculations, check out
https://www-amdis.iaea.org/FAC/ or the
Los Alamos Atomic Collision Codes (if the site is accessible)

Los Alamos National Laboratory Atomic Data Sets

Interface to Los Alamos Atomic Physics Codes

An interface is available to run several Los Alamos atomic physics codes for calculation of atomic structure, electron impact excitation, as well as ionization processes.

The well known Hartree-Fock method of R.D. Cowan, developed at Group T-4 of the Los Alamos National Laboratory, is used for the atomic structure calculations.

Electron impact excitation cross sections are calculated using either the distorted wave approximation (DWA) or the first order many body theory (FOMBT).

Electron impact ionization cross sections can be calculated using the scaled hydrogenic method developed by Sampson and co-workers, the binary encounter method or the distorted wave method. Photoionization cross sections and, where appropriate, autoionizations are also calculated.

Link to Los Alamos atomic physics code center

Completed Atomic Data Sets by LANL codes

A group at LANL participated at the CRP for "Atomic Data For Heavy Element Impurities in Fusion Reactors" and produced atomic data sets for argon, chlorine and silicon atoms for users.

The data sets are available for level energies and statistical weights of fine-structure levels of the ground and excited configurations, oscillator strengths and electron-impact excitation cross-sections, photo-ionization and electron-impact ionization cross-sections among the levels.

- Argon Atomic Data Sets
- Chlorine Atomic Data Sets
- Silicon Atomic Data Sets

Service Unavailable

Unavailable Service

This service is unavailable.

Service is unavailable

Online Computing

Below are some links to online computing resources for calculating plasma properties.

HEAVY: Cross sections for excitation and charge transfer for collisions between hydrogenic targets and bare ions.

AAEXCITE: An interface to average approximation cross sections for calculating electron impact cross sections for atomic ions.

RATES: Results from collisional radiative calculations of plasmas carried out with the Los Alamos modeling codes are available. Interpolations allow the user to obtain total radiated power, average ion charge, and relative ionization populations in a steady state plasma.

(This resource is currently unavailable.)
LANL: An interface is available to run several Los Alamos atomic physics codes for calculation of atomic structure, electron impact excitation, as well as ionization processes. Since 2010, atomic data sets of argon, chlorine and silicon produced by a group at LANL can be downloaded for all ionization stages.

FLYCHK: An interface to the FLYCHK code available at NIST, which generates atomic level populations and charge state distributions for low-Z to mid-Z elements under NLTE(Non-Local Thermodynamic Equilibrium) conditions.

FAC (Flexible Atomic Code): A complete set of collisional and radiative data of atoms from Z=2 (Helium) to Z=14(Silicon).

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About Flexible Atomic Code (FAC)

It is an integrated software package by M. F. Gu to calculate various atomic radiative and collisional processes, including energy levels, radiative transition rates, collisional excitation and ionization by electron impact, photoionization, autoionization, radiative recombination and dielectronic capture. The package also includes a collisional radiative model to construct synthetic spectra for plasmas under different physical conditions. Physics and code descriptions can be found in the reference [Can. J. Phys. 86: 675-689 (2008)].

cFAC was started around 2010 (based on FAC-1.1.1, released in 2006), initially focusing on providing large volumes of data as required, e.g., for collisional-radiative (CR) plasma modeling, and eliminating reliance upon third-party Fortran numerical libraries with their C equivalents (hence the change in the package name). Databases and source codes for CR modeling will be available shortly.

Source Codes

FAC and cFAC codes are currently available at GitHub repositories of FAC and cFAC and managed by M. F. Gu and E. Stambulchik.

I didn't get a chance to test it out completely, but the download and installation worked.

FAC Input Files

General guidelines to write input files for FAC calculations are available.

FAC_input_guidelines.pdf

Examples of input files to run FAC codes are provided below.

Atomic data for K-shell and L-shell charge states
Si1.py Si2.py Si3.py Si4.py Si5.py Si6.py Si7.py Si8.py Si9.py Si10.py Si11.py Si12.py
This is an example of calculating atomic data for K-shell and L-shell ions of silicon atoms.

Atomic data for M-shell ions by UTA levels
uta_data.py: For Au ion with 31 electrons, please type "python uta_data.py 31"
The input files create a set of atomic data to be used for M-shell ions.

Atomic data for Zeeman split levels
ebfield.py: For Fe, please type "python ebfield.py Fe"
This is an example of computing zemmann splitted levels and transition rates for He-like ions.

Atomic data for polarized atoms
pol_data.py pol_spec.py
This is an example of calculating poplarizations under unidirectional excitation of an electron beam. pol_data.py calculates the atomic data and pol_spec.py calculates the spectral model and produce the linear polarization of the spectral lines.

Collisional-Radiatve model calculations
d.py: type "phtyon d.py 10 3 5"
s.py: type "phtyon s.py 10 3"
sel.py: type "phtyon sel.py 10 3"
This is an example of running the process, starting from generating the atomic data, solving rate equation and postprocessing. d.py generates atomic data for Z=10, number of electrons =3, maximum n=5 for excitation. s.py runs the collisional radiative module. sel.py prints the line intensities in ascii format. Due to matrix size limitation, the CR module in FAC code is best suited for a single charge state calculation. For charge balance calculations which involve numerous autoionizing states (dielectronic recombination channels), it is recommended to use a different code to solve the rate matrix equations.

Atomic Data Sets generated by FAC codes

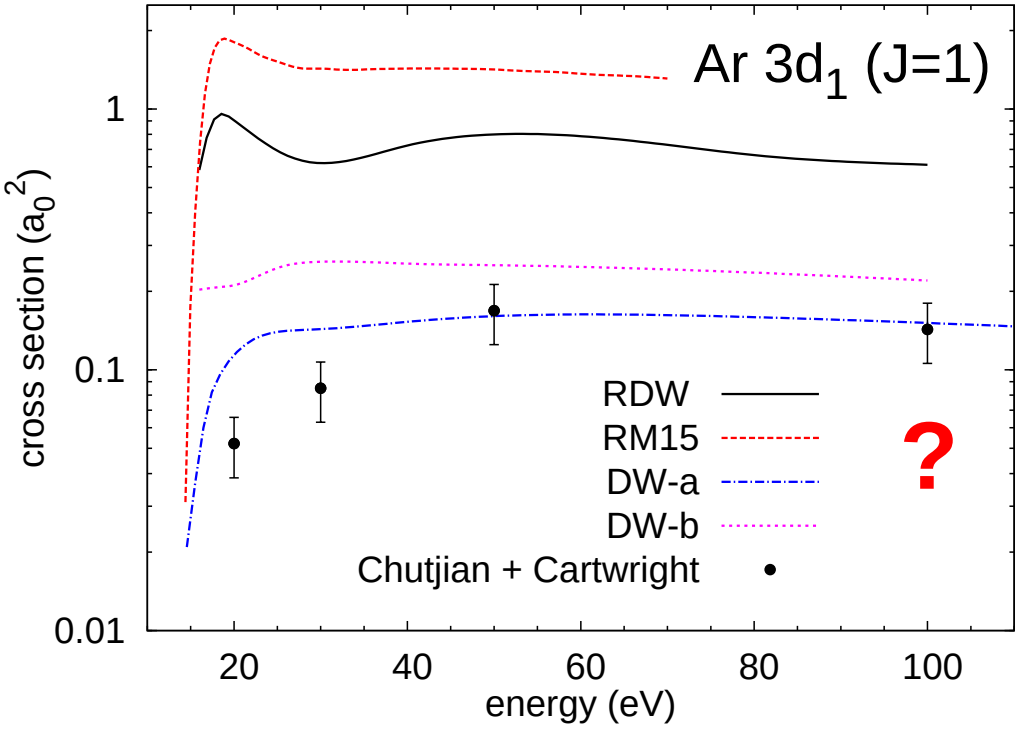
- Helium Atomic Data Sets
- Lithium Atomic Data Sets
- Beryllium Data Sets
- Boron Data Sets
- Carbon Data Sets
- Nitrogen Data Sets
- Oxygen Data Sets
- Fluorine Data Sets
- Neon Data Sets
- Sodium Data Sets
- Magnesium Data Sets
- Aliminium Data Sets
- Silicon Data Sets

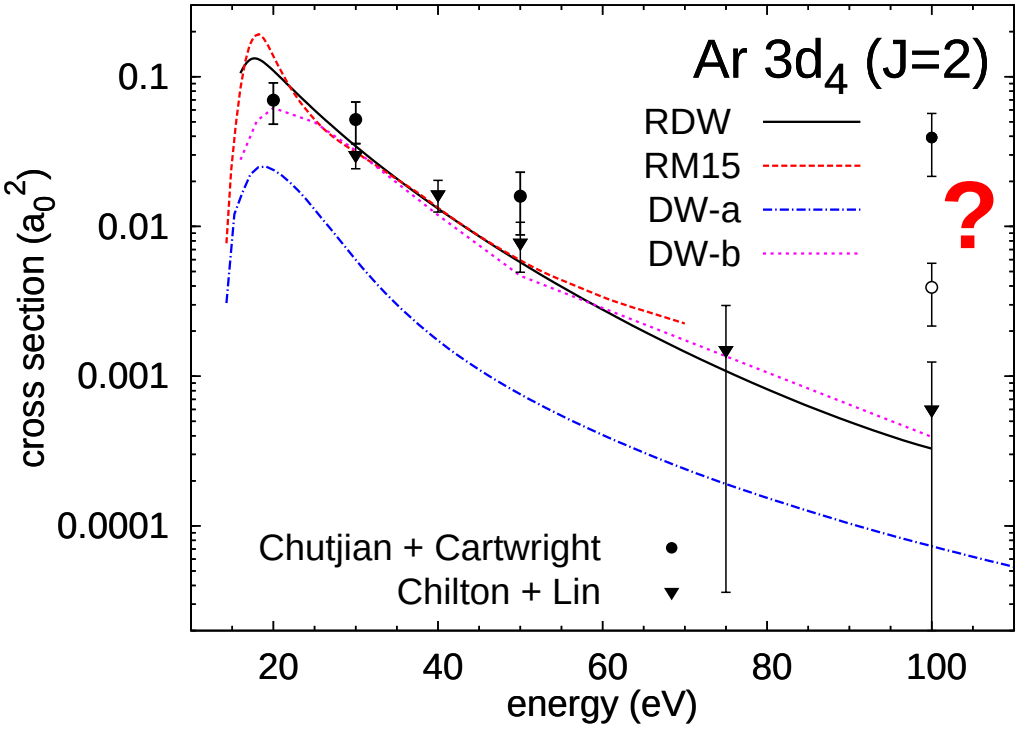
Relativistic DWBA; Semi-Relativistic DWBA; R-Matrix; Experiment

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?

One more ... **poster LT1.00009**

Electron-impact excitation of the $(5s^2 5p)\ ^2P_{1/2} \rightarrow (5s^2 6s)\ ^2S_{1/2}$ transition in indium: Theory and experiment

K. R. Hamilton, O. Zatsarinny, and K. Bartschat
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Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

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R. P. McEachran
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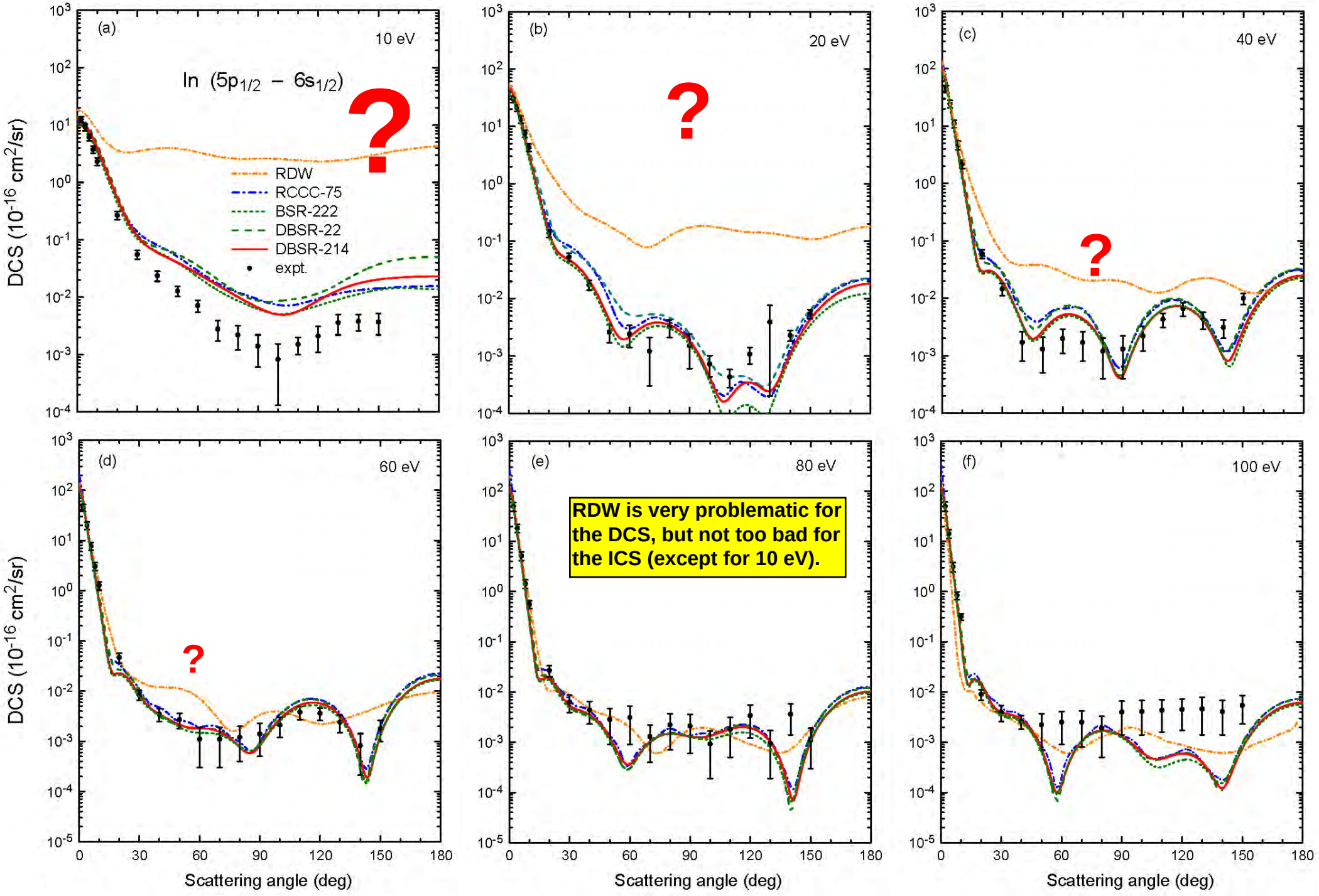
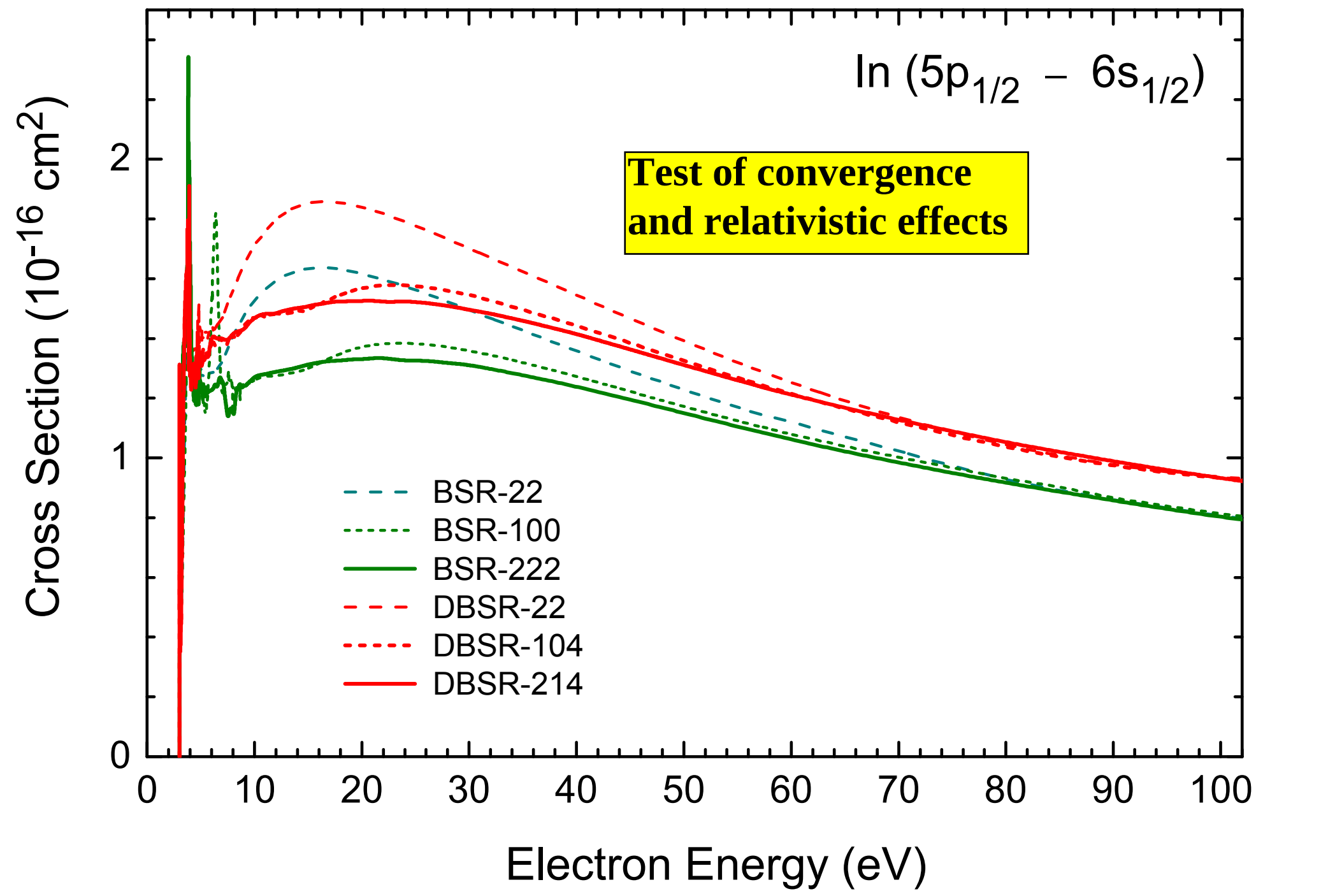
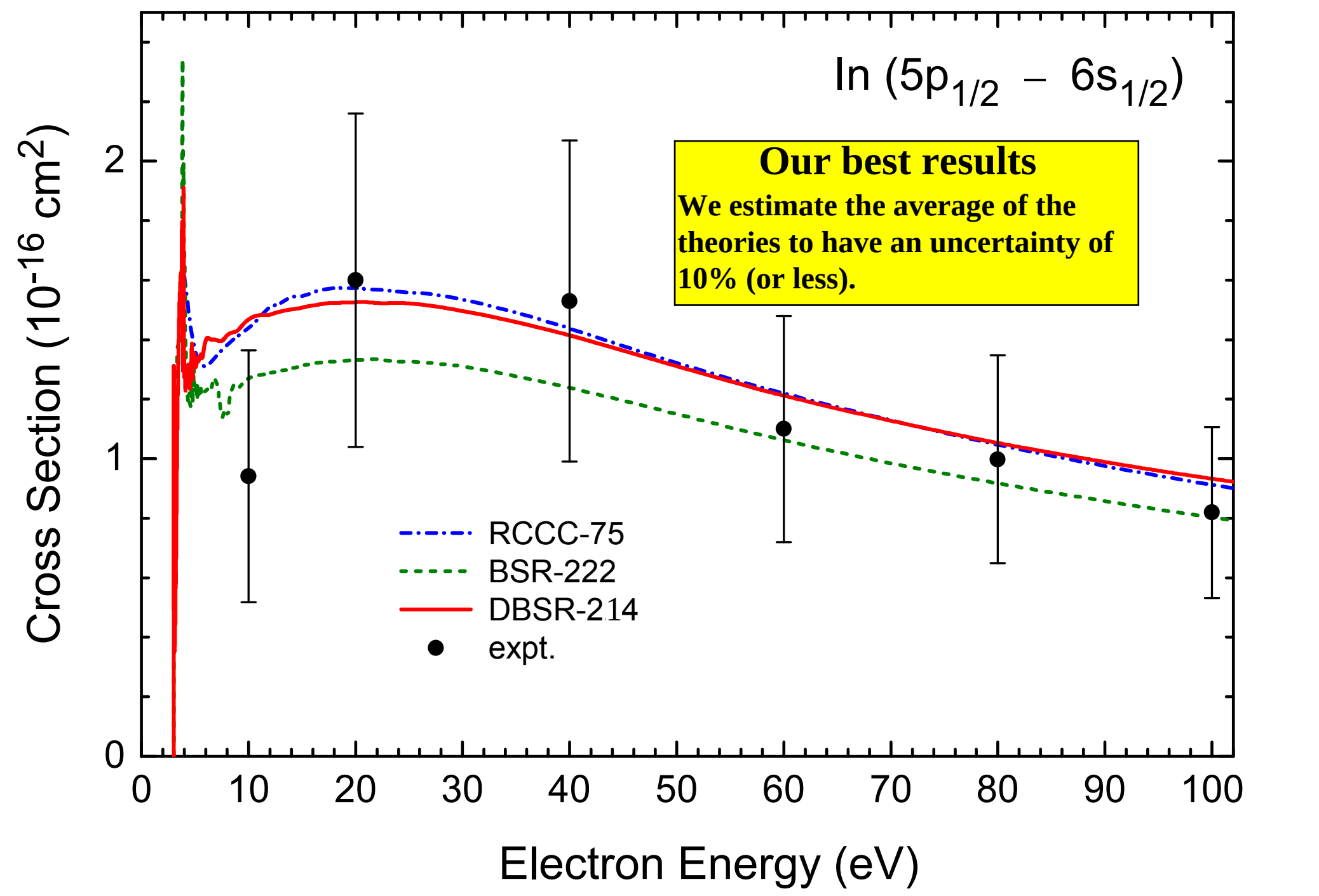
(Received 17 May 2020; accepted 6 July 2020; published 3 August 2020)

We present angle-integrated and angle-differential cross sections for electron-impact excitation of the $(5s^2 5p)\ ^2P_{1/2} \rightarrow (5s^2 6s)\ ^2S_{1/2}$ transition in atomic indium. Experimental data for six incident electron energies between 10 and 100 eV are compared with predictions from semirelativistic and fully relativistic *B*-spline *R*-matrix calculations, as well as a fully relativistic convergent close-coupling model. Agreement between our measured and calculated data is, with a few exceptions, found to be typically very good. Additionally, the agreement between the present theoretical predictions is generally excellent, with the remaining small deviations being associated with the slightly different, although still very accurate, descriptions of the target structure. Agreement between the present results and an earlier relativistic distorted-wave computation [T. Das, R. Srivastava, and A. D. Stauffer, Phys. Lett. A **375**, 568 (2011)] was, however, found to be marginal, particularly at 10 and 20 eV.

DOI: 10.1103/PhysRevA.102.022801


(a)
10 eV
In (5p1/2 – 6s1/2)
?
RDW
RCCC-75
BSR-222
DBSR-22
DBSR-214
expt.
(b)
20 eV
?
(c)
40 eV
?
(d)
60 eV
?
(e)
80 eV
RDW is very problematic for the DCS, but not too bad for the ICS (except for 10 eV).
(f)
100 eV
DCS (10-16 cm2/sr)
Scattering angle (deg)


In ($5p_{1/2}$ – $6s_{1/2}$)
Test of convergence and relativistic effects
BSR-22
BSR-100
BSR-222
DBSR-22
DBSR-104
DBSR-214
Cross Section (10^{-16} cm^2)
Electron Energy (eV)
0
1
2
0
10
20
30
40
50
60
70
80
90
100


In ($5p_{1/2}$ – $6s_{1/2}$)
Our best results
We estimate the average of the theories to have an uncertainty of 10% (or less).
RCCC-75
BSR-222
DBSR-214
expt.
Cross Section (10^{-16} cm^2)
Electron Energy (eV)
0
1
2
0
10
20
30
40
50
60
70
80
90
100

Time-Independent Close-Coupling

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

$\mathbf{H\,\Psi = E\,\Psi}$

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

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

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

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

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

with the direct coupling potentials

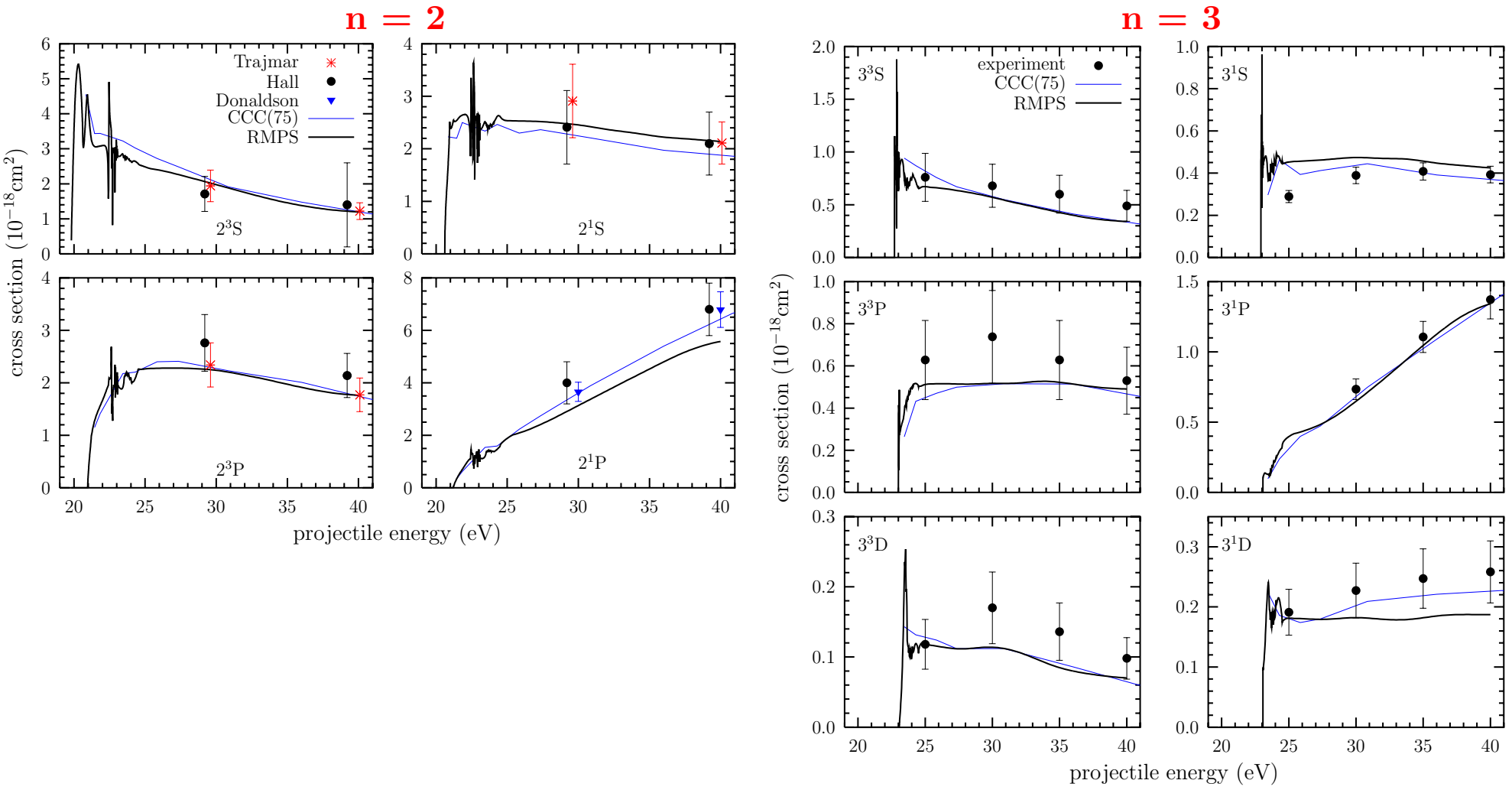
$$V_{ij}(r) = -\frac{Z}{r}\,\delta_{ij} + \sum_{k=1}^{N}\langle \Phi_i \mid \frac{1}{|\mathbf{r}_k - \mathbf{r}|} \mid \Phi_j \rangle$$

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

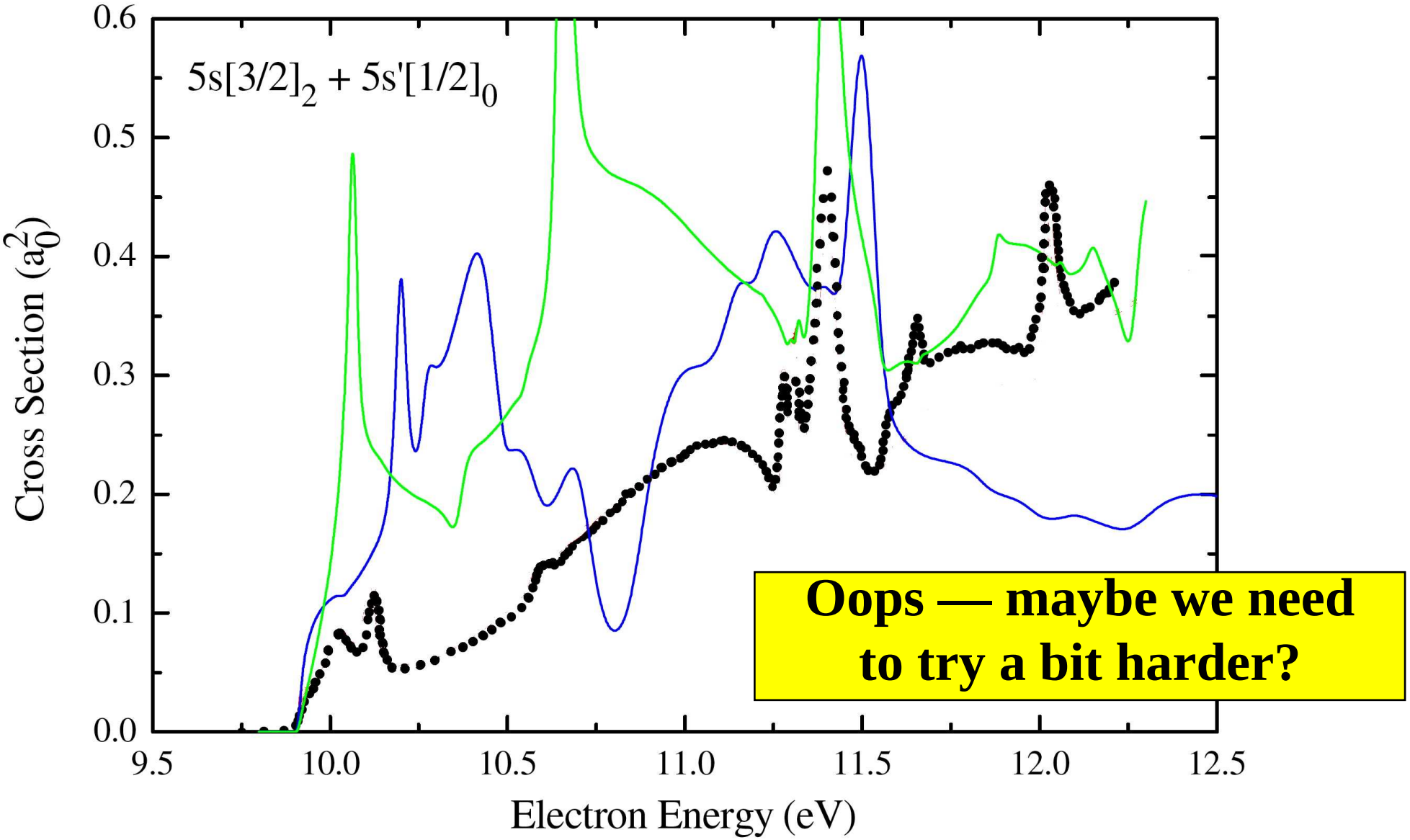


Already in 1998, de Heer recommends 0.5 x (CCC+RMPS) for uncertainty of 10% — independent of experiment!

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)



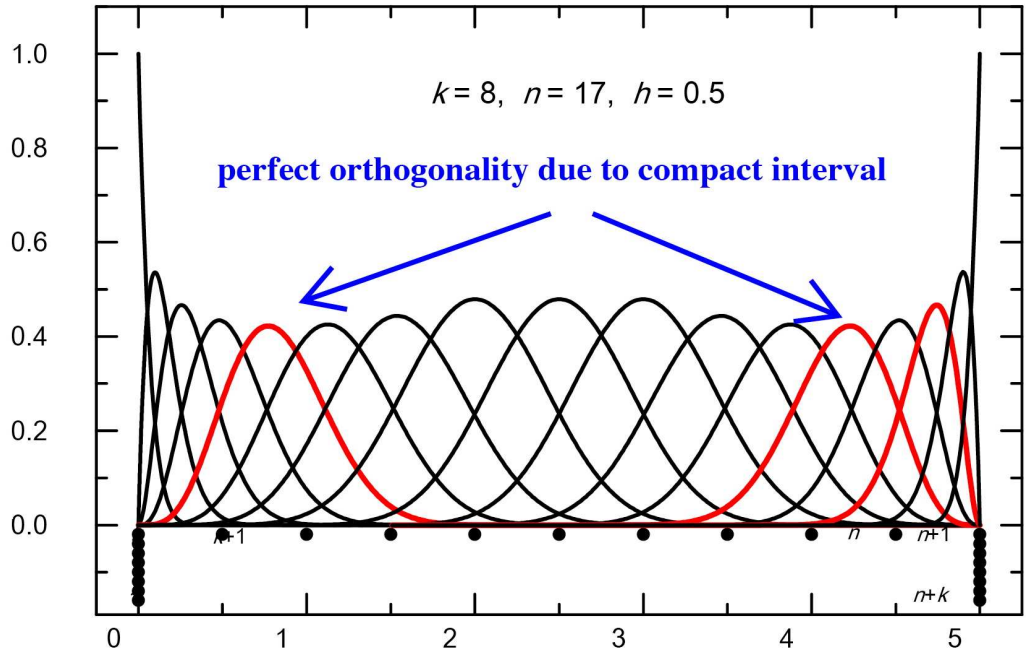
Oops — maybe we need to try a bit harder?

We have a great program now :):):)

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: 400,000 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)

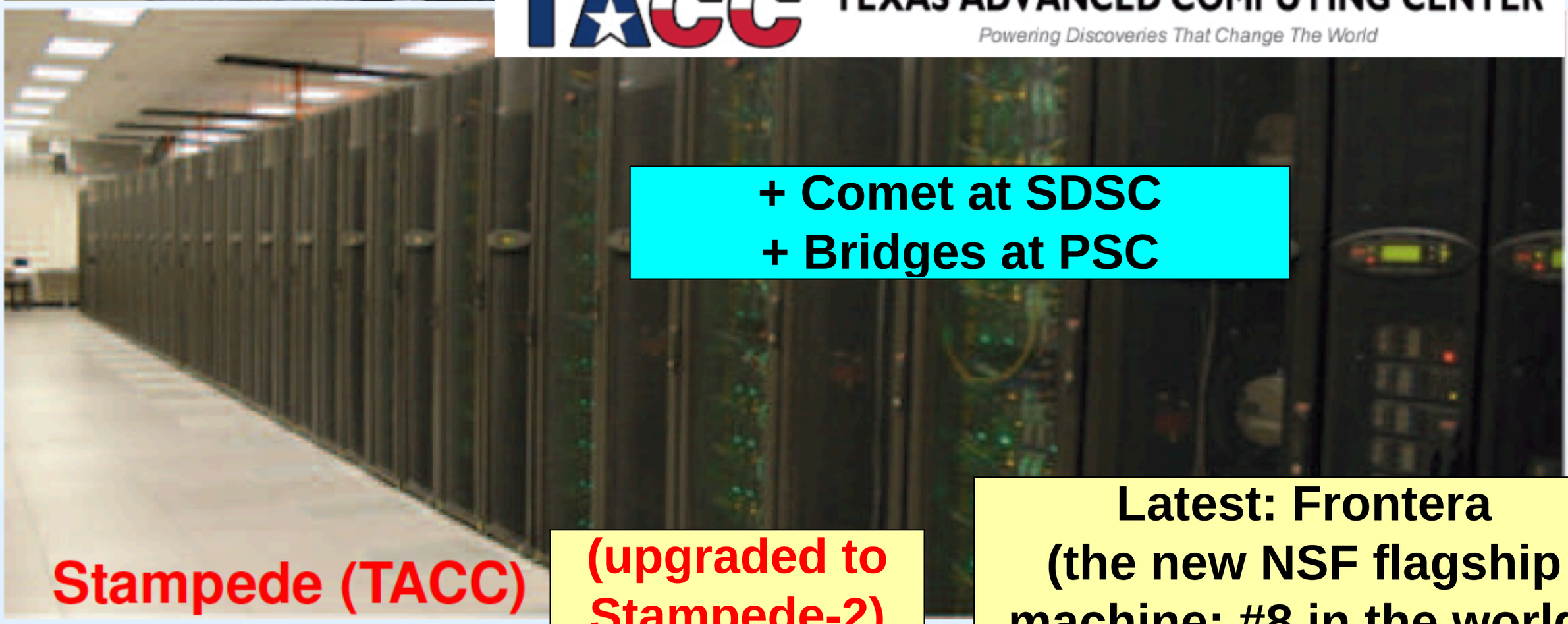
at least 100 more since 2013

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

Our Apparatus — Supercomputers

Kraken (NICS)

TACC TEXAS ADVANCED COMPUTING CENTER
Powering Discoveries That Change The World



+ Comet at SDSC
+ Bridges at PSC

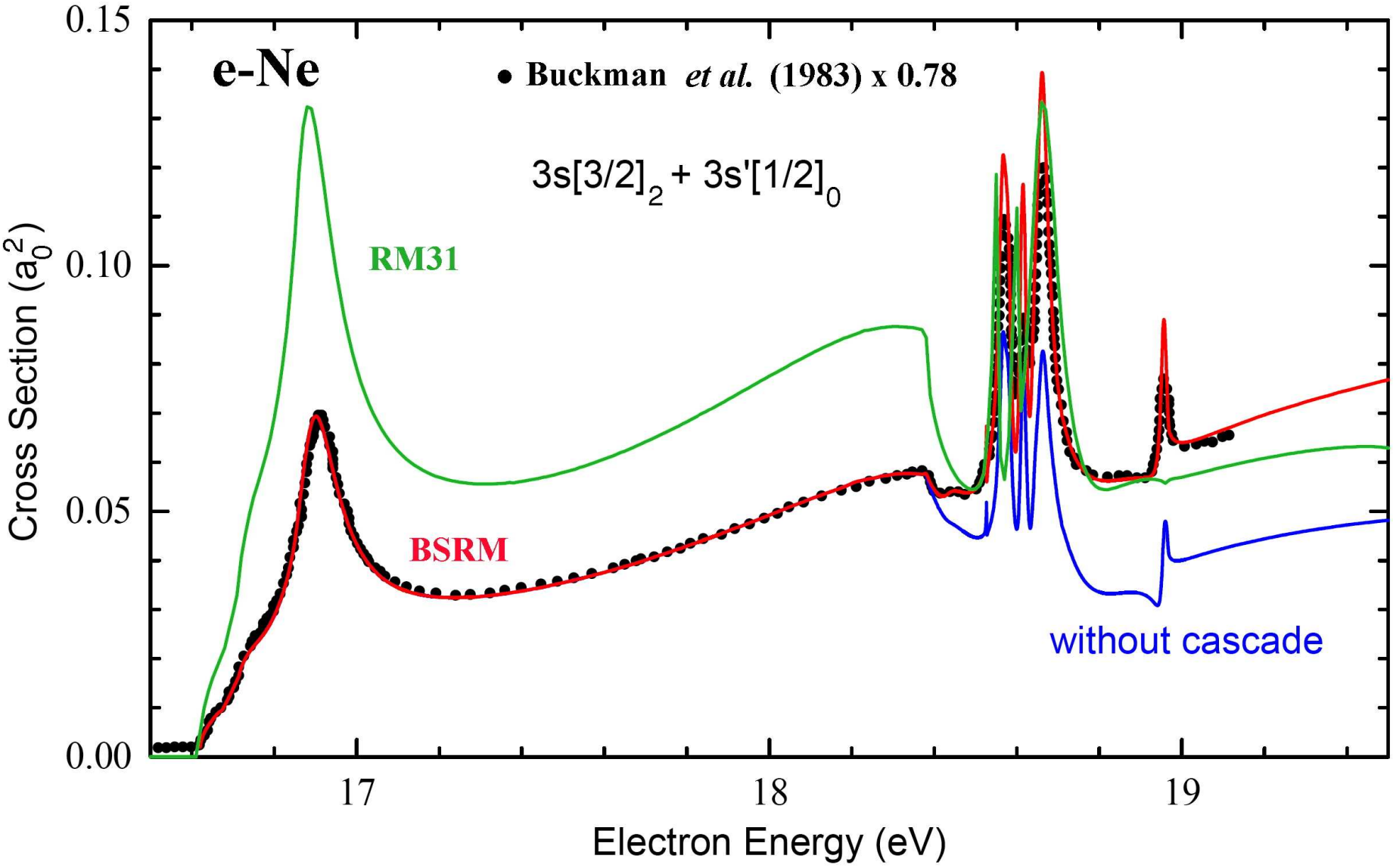
(upgraded to Stampede-2)

Latest: Frontera (the new NSF flagship machine; #8 in the world)

A few examples of (mostly) BSR calculations ...

Metastable yield in e-Ne collisions

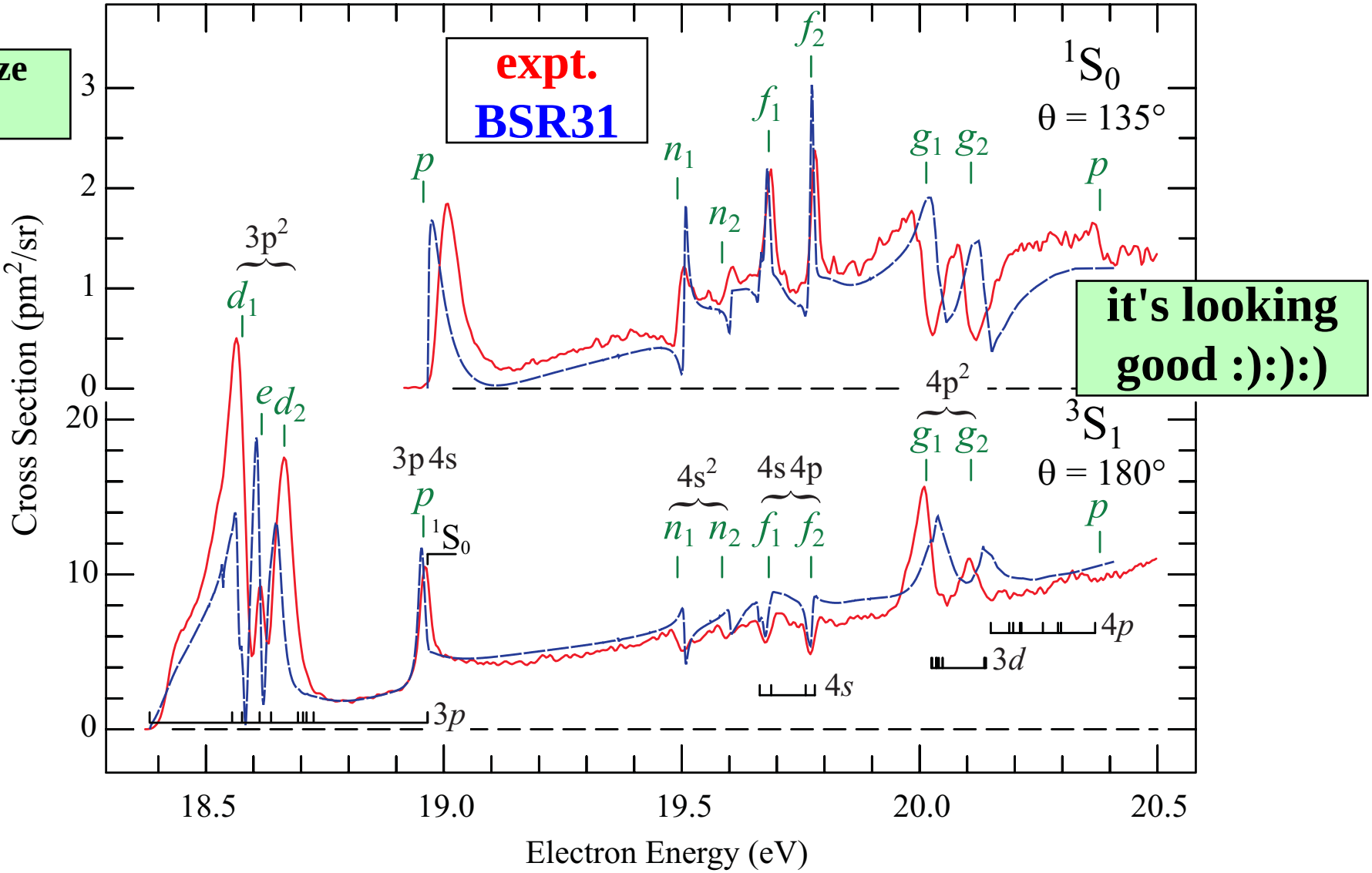
- Using our semi-relativistic B-spline R-matrix (BSR) method [Zatsarinny and Bartschat, J. Phys. B 37, 2173 (2004)], we achieved unprecendented agreement with experiment for angle-integrated cross sections in e−Ne collisions.



Resonances in the excitation of the Ne ($2p^5 3p$) states

Allan, Franz, Hotop, Zatsarinny, Bartschat (2009), J. Phys. B 42, 044009

Allis-Prize 2020



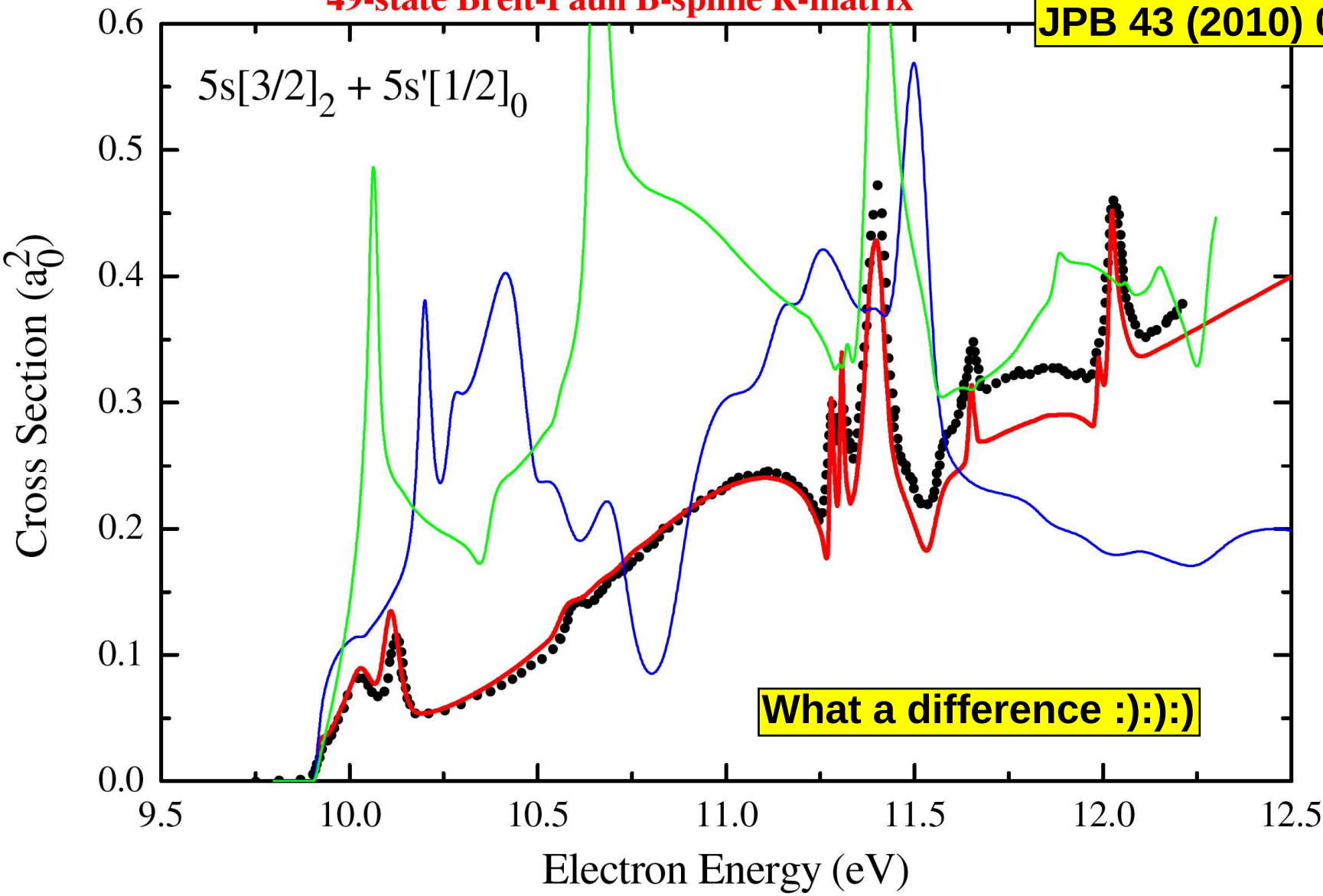
it's looking good :):):)

Expanded view of the resonant features in selected cross sections for the excitation of the 3p states. Experiment is shown by the more ragged red line, theory by the smooth blue line. The present experimental energies, labels (using the notation of Buckman *et al*. (1983), and configurations of the resonances are given above the spectra. Threshold energies are indicated below the lower spectrum.

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

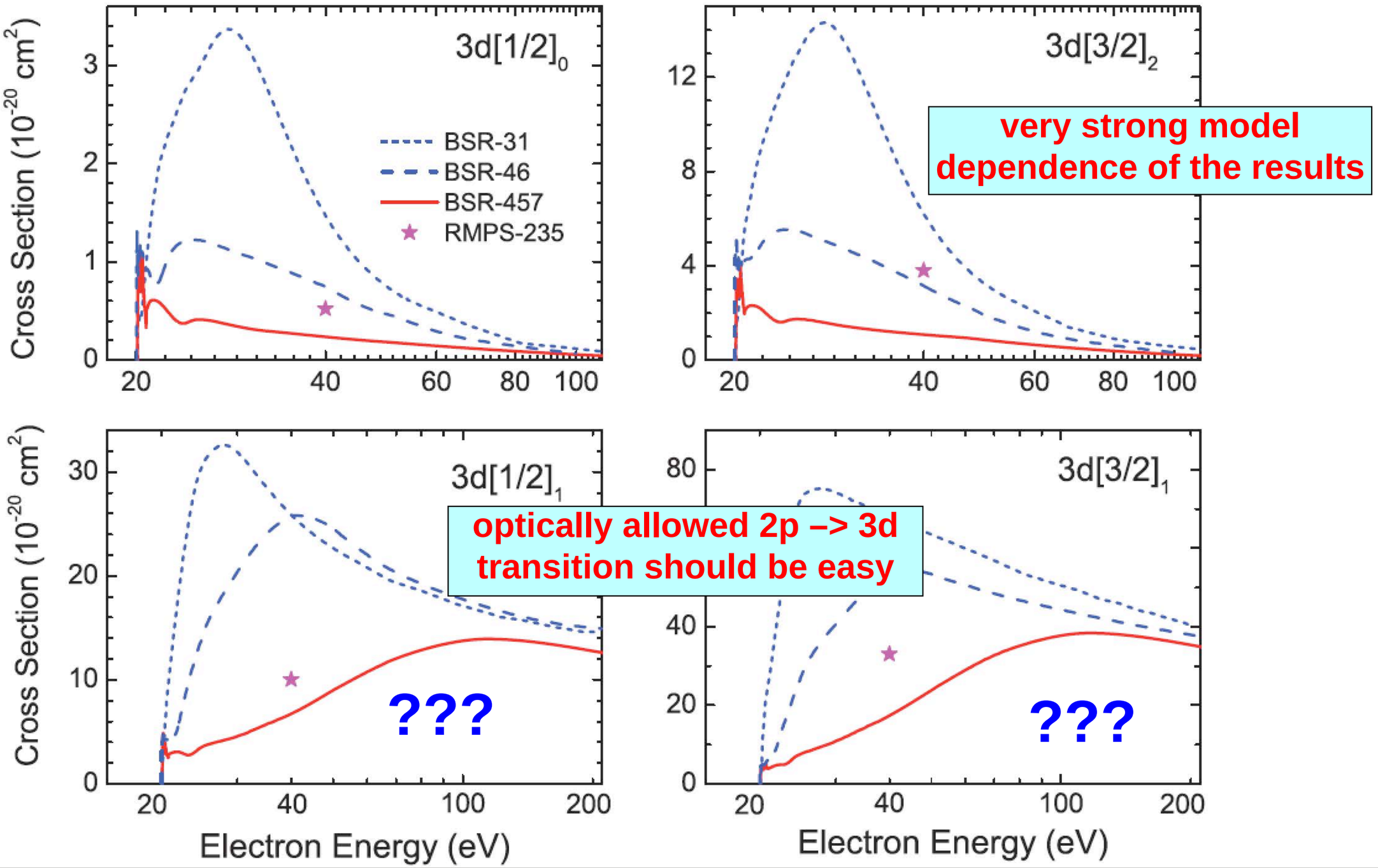


PHYSICAL REVIEW A **86**, 022717 (2012)

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.

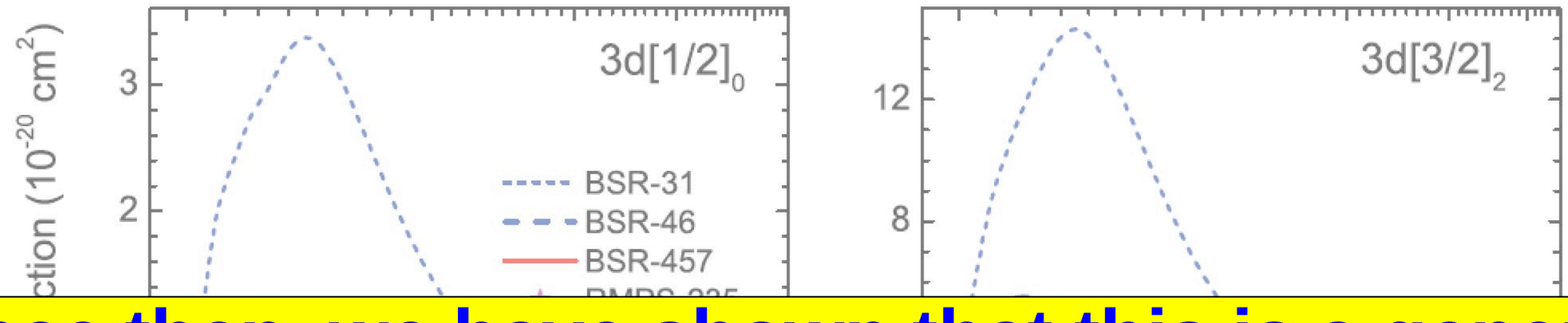
PHYSICAL REVIEW A **86**, 022717 (2012)

Electron-impact excitation of neon at intermediate energies

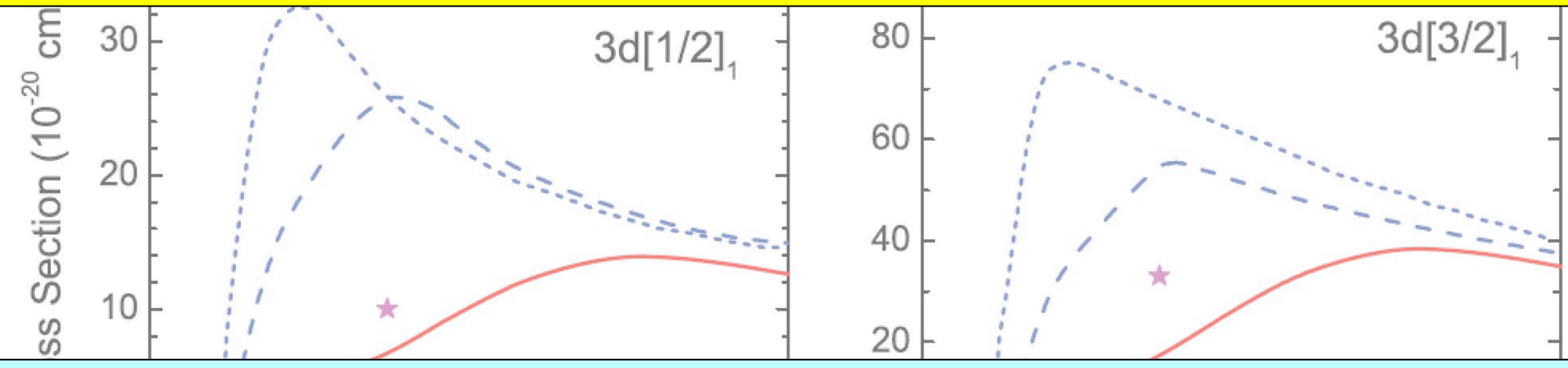
Oleg Zatsarinny and Klaus Bartschat

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, ...)

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:**

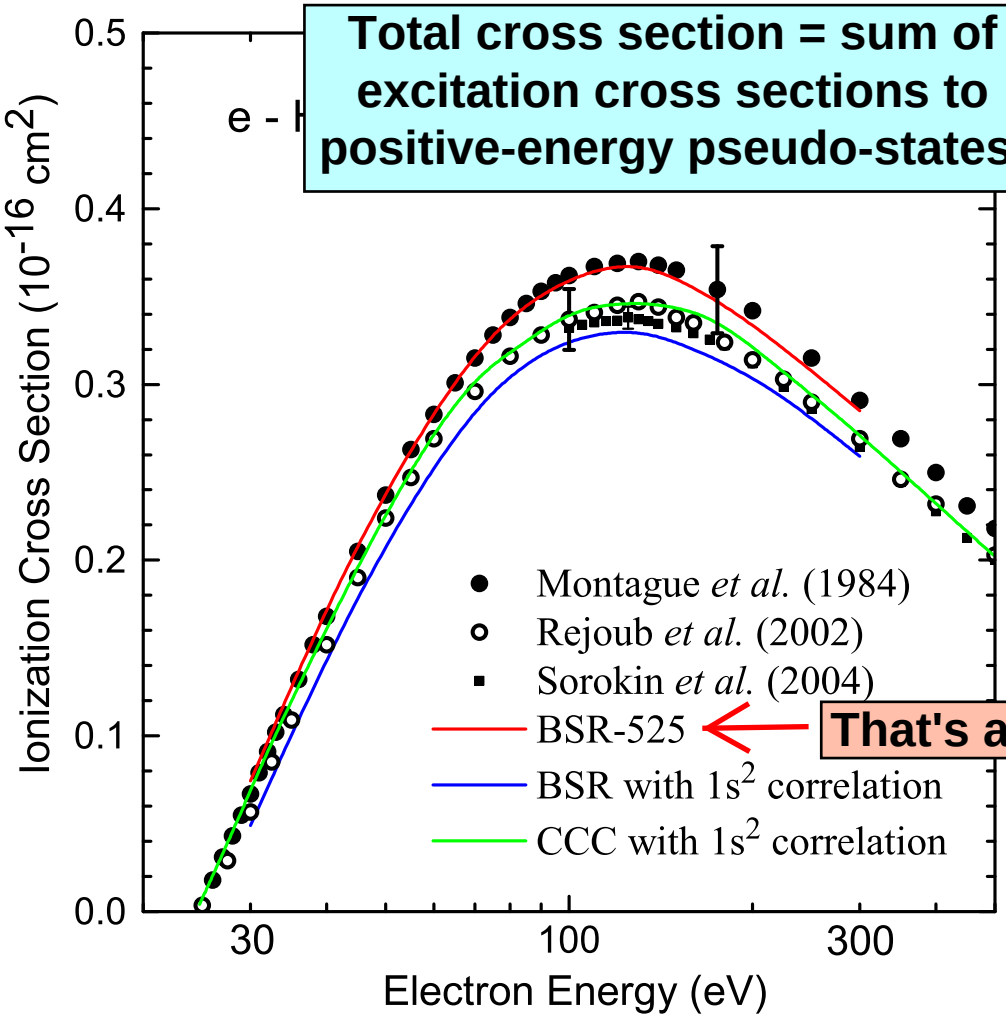
This direct projection is the essential idea – we'll see if it works.

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

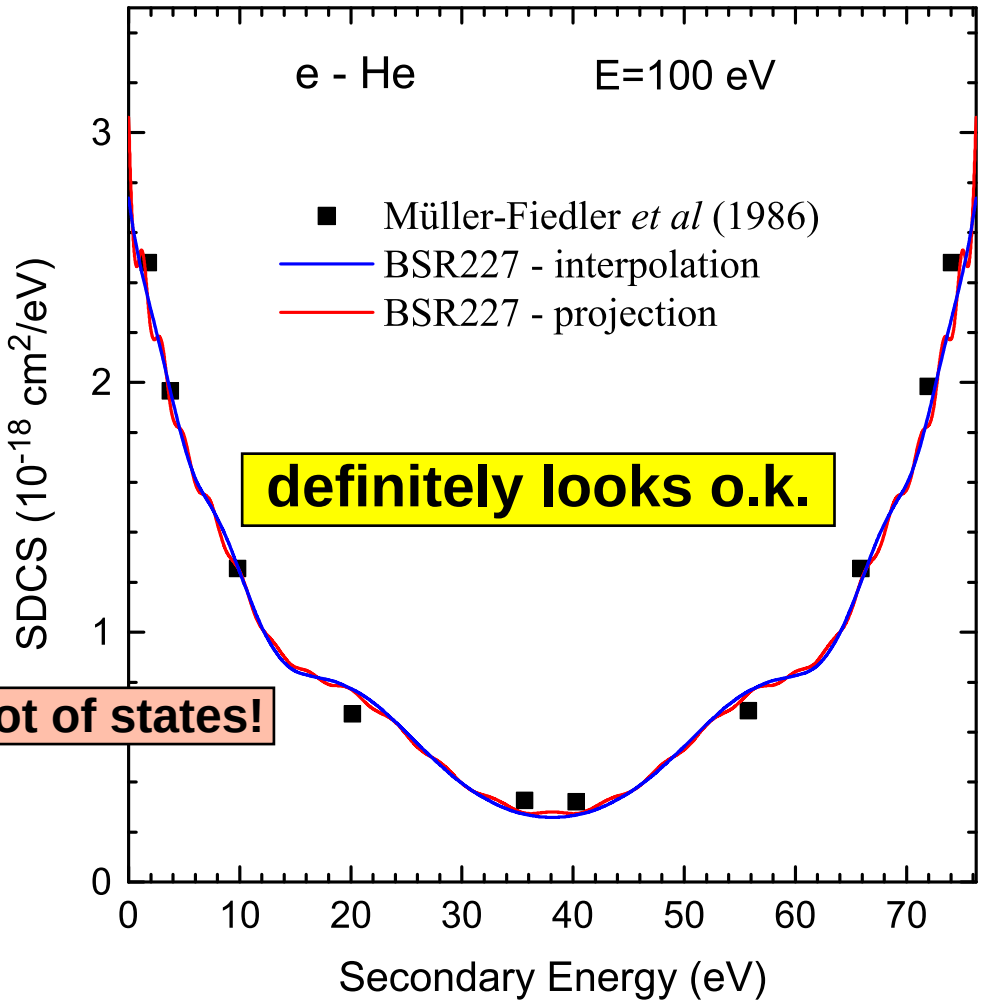
Some Checks: Ionization without Excitation (compare to CCC and TDCC)

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.

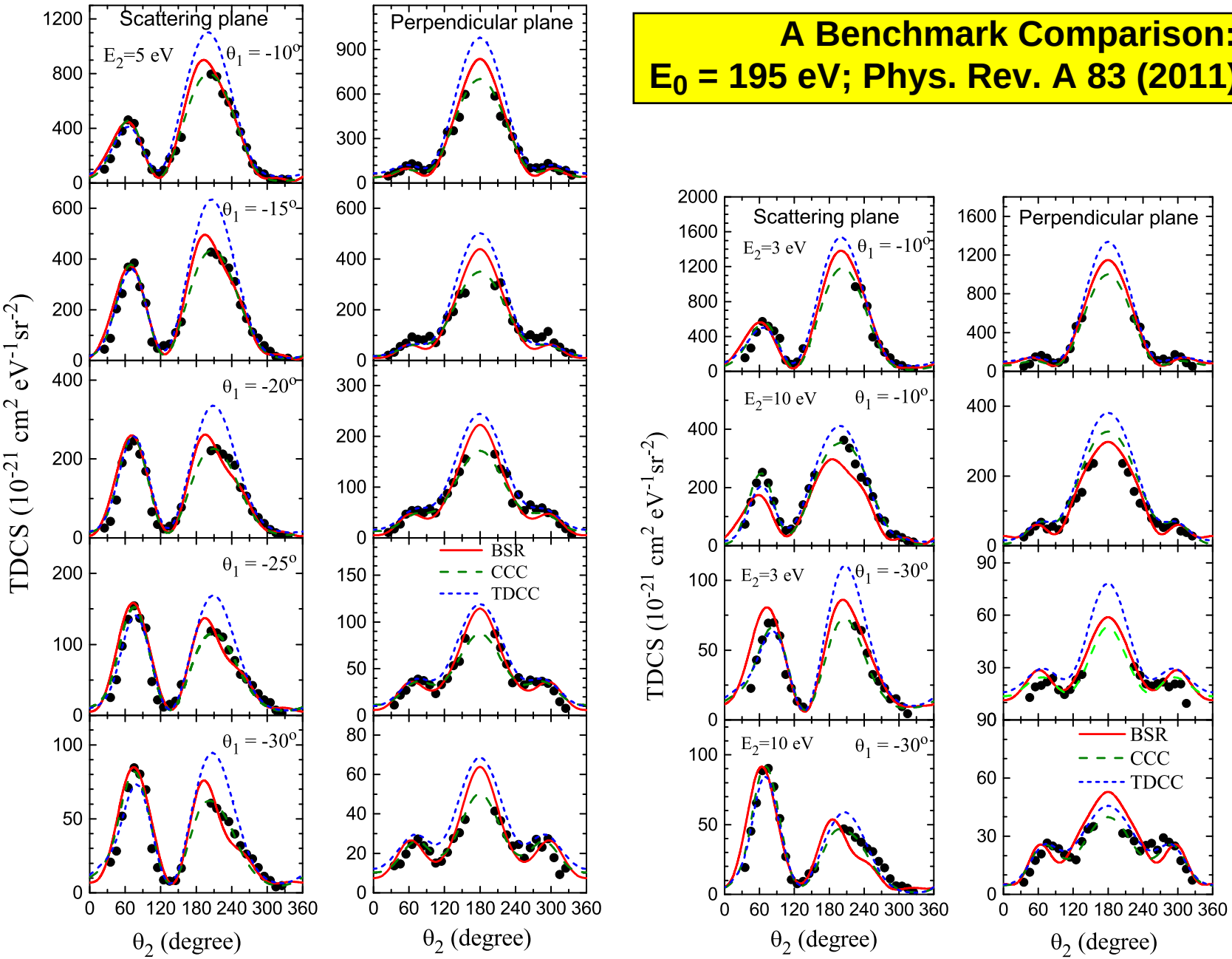
- **Including correlation in the ground state reduces the theoretical result.**
- **Interpolation yields smoother result, but direct projection is acceptable.**
- **DIRECT PROJECTION is NECESSARY for MULTI-CHANNEL cases!**

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

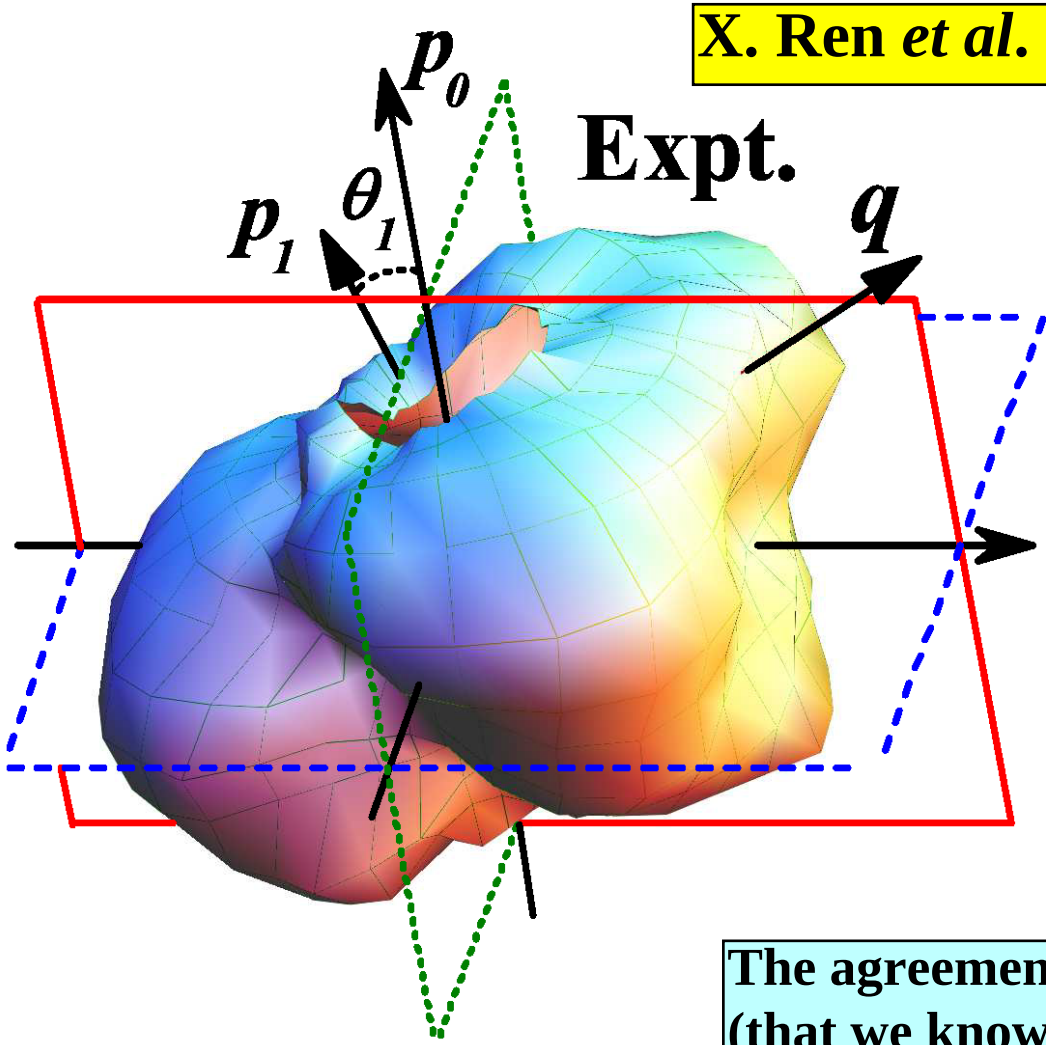


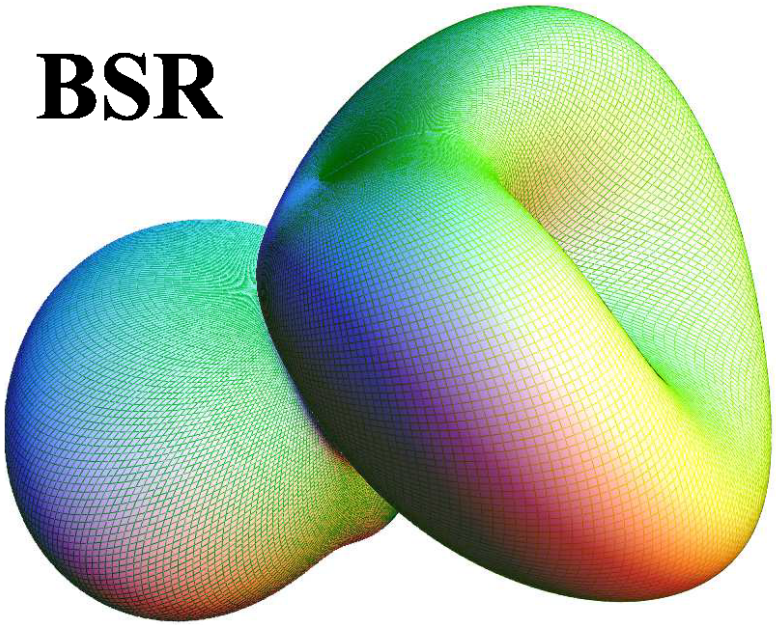
(e,2e) on Ar is a very l .. o .... n ..... g story. It includes the discovery of an error in the processing of the raw experimental data, which was found by the confidence gained in BSR predictions ...

(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.

About the project

Where do the results go?
One (of many) databases: LXCat
https://fr.lxcat.net/home/

The **Plasma Data Exchange Project** is a community-based p
Electronics Conference (GEC), a leading international meetin
part, the well-recognized needs for the community to organize the means of collecting, evaluating and sharing data both for modeling and for interpretation of experiments.

open-access website for collecting, displaying, and downloading electron and ion scattering cross sections, swarm parameters (*mobility*, *diffusion coefficients*, *etc.*), reaction rates, energy distribution functions, etc. and other data required for modeling low temperature plasmas.

This is a dynamic website, evolving as contributors add or upgrade data. Check back again frequently.

Supporting organizations

Laplace · CNRS · Plasmas Froids · Chatham University · Colorado Kinema · UNAM · Curtin University of Technology · CERN · Instituto Superior Técnico Lisboa · Drake University · Uppsala University · Quantemol · LPP · Institute of Space and Astronautical Science · York University · ABB · TU/e · STAE Toulouse · Australian National University · Plasma Matters.

LATEST NAVIGATION

PREV | NEXT »

NEWS AND EVENTS

2019-07-10 I New links to software
Links have been added to a multi-term Boltzmann solver, and to three tools by Mikhail Benilov and co-workers. Visit the recommended software page.

RECENT PUBLICATIONS

2019-03-05 I NEW UNPUBLISHED NOTES
Data needed for modeling low-temperature plasmas by LC Pitchford … read more »

PROJECT STATISTICS

Scattering cross sections: 24 databases I 94 x 415 species I 21.1k records I updated: 30 April 2019
Differential scattering cross sections: 4 databases I 29 species I 517 records I updated: 12 March 2019
Interaction potentials: 1 database I 78 x 8 species I 646 records I updated: 30 April 2019
Oscillator strengths: 1 database I 65 species I 150 records I updated: 25 November 2013
Swarm / transport data: 15 databases I 362 x 108 species I 169.4k records I updated: 30 April 2019
Publications, notes and reports: 5 databases I 30 records I updated: 5 March 2019

BSR (Quantum-mechanical calculations by O. Zatsarinny and K. Bartschat)

PERMLINK: www.lxcat.net/BSR

DESCRIPTION: The results in this database are from a semirelativistic Breit-Pauli B-spline R-matrix (close coupling) treatment of e-Ar collisions. An individually optimized, term-dependent set of non-orthogonal valence orbitals was used to account for the strong term dependence in the one-electron orbitals. The predictions have been validated against a number of benchmark experimental data measured in crossed-beam setups. Particularly good agreement was achieved in the near-threshold resonance regime, where the excitation process is dominated by negative-ion resonances.

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HOW TO REFERENCE: O. Zatsarinny and K. Bartschat 2004 J. Phys. B: At. Mol. Opt. Phys. 37 4693 and
M. Allan, O. Zatsarinny, and K. Bartschat 2006 Phys. Rev. A 74 030701 (R).

SCATTERING CROSS SECTIONS

Species: e + **Ar {30}** , **Be {19}** , **C {83}** , **F {8}** , Kr [70], **N {27}** , Ne [34], Xe [76]

Updates: 2011-06-28 .. 2017-09-09

Downloads: 5020 times from 2010-11-21

grown to **9339** by Sept. 27, 2020

Data **collections** by Phelps, Morgan, Hayashi, Biagi, ..., have about 30,000 downloads each; BSR (for only a few atoms and ions) is fully *ab initio* based on quantum mechanics.

DIFFERENTIAL SCATTERING CROSS SECTIONS

Species: e + Ar [62]

Updates: 2013-11-06 .. 2016-05-29

Downloads: 1219 times from 2013-11-07

grown to **1355** by Sept. 27, 2020

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

How good are the data?
[This question is not just for theory!]

Uncertainty estimates for theoretical atomic and molecular data

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

H-K Chung[1], B J Braams[1], K Bartschat[2], A G Császár[3], G W F Drake[4], T Kirchner[5], V Kokoouline[6] and J Tennyson[7]

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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.

IOP PUBLISHING PHYSICA SCRIPTA

Phys. Scr. **T134** (2009) 014020 (9pp) doi:10.1088/0031-8949/2009/T134/014020

B-spline calculations of oscillator strengths in noble gases

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Abstract

B-spline box-based multi-channel calculations of transition probabilities in noble gases are reported for energy levels up to $n = 12$. Energy levels and oscillator strengths for transitions from the p^6 ground-state configuration, as well as for transitions between excited states, have been computed in the Breit–Pauli approximation. Individually optimized, term-dependent sets of non-orthogonal valence orbitals are used to account for the strong term dependence in the one-electron orbitals. The agreement in the length and velocity gauges of the transition data and the accuracy of the binding energies are used to estimate the accuracy of our results, which are also compared with experimental and other theoretical data. It is shown that the present method can be used for accurate calculations of oscillator strengths for states with intermediate to high n-values, for which it is difficult to apply standard multi-configuration Hartree–Fock (MCHF) methods. Recent developments based on the extension of our computer codes from the semi-relativistic Breit–Pauli Hamiltonian to the full relativistic Dirac–Breit Hamiltonian are also reported.

Energy Levels in Heavy Noble Gases

Phys. Scr. **T134** (2009) 014020 O Zatsarinny and K Bartschat

Table 1. Binding energies (NIST [1]) and energy differences (computed–observed) in eV for some low-lying levels in Ne, Ar, Kr and Xe. The values in bold are average differences for the states in the respective configuration obtained when the core–valence correlation is omitted.

Ne	NIST	Diff.	**Ar**	NIST	Diff.	**Kr**	NIST	Diff.	**Xe**	NIST	Diff.
$2p^6$	21.565	0.061	$3p^6$	15.760	0.044	$4p^6$	14.000	0.024	$5p^6$	12.565	0.020
$3s[3/2]_2$	4.945	0.012	$4s[3/2]_2$	4.211	0.102	$5s[3/2]_2$	4.084	0.128	$6s[3/2]_2$	4.250	0.100
$3s[3/2]_1$	4.894	0.015	$4s[3/2]_1$	4.136	0.100	$5s[3/2]_1$	3.967	0.115	$6s[3/2]_1$	4.129	0.094
		0.200			**0.310**			**0.350**			**0.300**
$3p[1/2]_1$	3.183	0.007	$4p[1/2]_1$	2.853	0.033	$5p[1/2]_1$	2.696	0.033	$6p[1/2]_1$	2.985	0.071
$3p[5/2]_3$	3.009	0.009	$4p[5/2]_3$	2.684	0.024	$5p[5/2]_3$	2.557	0.036	$6p[5/2]_2$	2.880	0.068
$3p[5/2]_2$	2.989	0.007	$4p[5/2]_2$	2.665	0.028	$5p[5/2]_2$	2.555	0.046	$6p[5/2]_3$	2.845	0.055
$3p[3/2]_1$	2.952	0.009	$4p[3/2]_1$	2.606	0.022	$5p[3/2]_1$	2.473	0.031	$6p[3/2]_1$	2.776	0.043
$3p[3/2]_2$	2.928	0.008	$4p[3/2]_2$	2.588	0.029	$5p[3/2]_2$	2.454	0.036	$6p[3/2]_2$	2.744	0.057
$3p[1/2]_0$	2.853	0.008	$4p[1/2]_0$	2.487	0.024	$5p[1/2]_0$	2.334	0.052	$6p[1/2]_0$	2.632	0.064
		0.070			**0.130**			**0.140**			**0.130**
$3d[1/2]_0$	1.540	0.004	$3d[1/2]_0$	1.915	0.116	$4d[1/2]_0$	2.001	0.116	$5d[1/2]_0$	2.675	0.014
$3d[1/2]_1$	1.538	0.004	$3d[1/2]_1$	1.896	0.113	$4d[1/2]_1$	1.963	0.112	$5d[1/2]_1$	2.648	0.066
$3d[7/2]_4$	1.530	0.001	$3d[3/2]_2$	1.856	0.105	$4d[3/2]_2$	1.888	0.101	$5d[7/2]_4$	2.622	0.168
$3d[7/2]_3$	1.530	0.006	$3d[7/2]_4$	1.780	0.081	$4d[7/2]_4$	1.874	0.094	$5d[3/2]_4$	2.607	0.042
$3d[3/2]_2$	1.528	0.005	$3d[7/2]_3$	1.747	0.072	$4d[7/2]_3$	1.821	0.083	$5d[7/2]_3$	2.526	0.144
$3d[3/2]_1$	1.524	0.005	$3d[5/2]_2$	1.697	0.064	$4d[5/2]_2$	1.742	0.072	$5d[5/2]_2$	2.408	0.109
$3d[5/2]_2$	1.516	0.007	$3d[5/2]_3$	1.661	0.048	$4d[5/2]_3$	1.715	0.068	$5d[5/2]_3$	2.345	0.122
$3d[5/2]_3$	1.516	0.006	$3d[3/2]_1$	1.607	0.047	$4d[3/2]_1$	1.645	0.058	$5d[3/2]_1$	2.164	0.011
		0.015			**0.180**			**0.200**			**0.250**

effect of core-valence correlations

Oscillator Strengths in Neon

Table 2. Oscillator strengths for excitation from the ground state in Ne, as obtained in the length (f_L) and velocity (f_V) forms of the electric dipole operator.

Upper level	f_L	f_V	Other theory			Experiment	
			[10]	[13]	[29]	[2]	[28]
$3s[3/2]_1$	0.0118	0.0116	0.0109	0.0102	0.0126	0.0118(6)	0.0124(38)
	0.0163[a]	0.0156[a]					
	0.0130[b]	0.0135[b]					
$3s'[1/2]_1$	0.159	0.156	0.151	0.146	0.168	0.159(8)	0.0156(9)
	0.161[a]	0.147[a]					
	0.144[b]	0.148[b]					
$4s[3/2]_1$	0.0126	0.0129	0.0132	0.0131	0.0152	0.0129(6)	0.0126(6)
$4s'[1/2]_1$	0.0174	0.0179	0.0152	0.0181	0.0193	0.0165(8)	0.0167(7)
$3d[1/2]_1$	0.00479	0.00487	0.00396	0.0066	0.00558		
$3d[3/2]_1$	0.0146	0.0149	0.0129	0.0130	0.0167		
$3d[1/2]_1 + 3d[3/2]_1$	0.0194	0.0198	0.0169	0.0199	0.0223	0.0186(9)	0.0183(8)
$3d'[3/2]_1$	0.00718	0.00731	0.00631	0.0069	0.00859	0.00665(33)	0.00687(32)
$5s[3/2]_1$	0.00628	0.00640		0.0068	0.00727	0.00637(32)	0.00645(18)
$5s'[1/2]_1$	0.00481	0.00490		0.0053	0.00502	0.00461(23)	0.00407(29)
$4d[1/2]_1 + 4d[3/2]_1$	0.00906	0.00895			0.0101	0.00944(32)	0.00937(37)
$4d'[3/2]_1$	0.00432	0.00427			0.00481	0.00439(22)	0.00447(13)
$6s[3/2]_1$	0.00325	0.00331			0.00371	0.00330(30)	0.00324(19)
$6s'[1/2]_1$	0.00168	0.00172			0.00203	0.00156(16)	0.00220(45)
$5d[1/2]_1 + 5d[3/2]_1$	0.00520	0.00510			0.00538	0.00543(54)	0.00449(52)
$5d'[3/2]_1$	0.00255	0.00249			0.00273	0.00229(23)	

[a] Avgoustoglou and Beck [12]—relativistic MBPT.

[b] Dong *et al* [15]—MCDF calculations.

Oscillator Strengths in Xenon

Table 5. Oscillator strengths for excitation from the ground state in Xe, as obtained in the length (f_L) and velocity (f_V) forms of the electric dipole operator.

Upper level	Breit–Pauli		Dirac		Experiment
	f_L	f_V	f_L	f_V	[3]
$6s[3/2]_1$	0.278	0.224	0.260	0.258	0.273(14)
	0.249[a]	0.256[a]	0.271[b]	0.263[b]	
$6s'[1/2]_1$	0.186	0.157	0.188	0.189	0.186(9)
			0.158[b]	0.154[b]	
$5d[1/2]_1$	0.0399	0.0345	0.0083	0.0071	0.0105(5)
$5d[3/2]_1$	0.380	0.303	0.303	0.327	0.379(19)
$7s[3/2]_1$	0.0785	0.0633	0.0791	0.0783	0.0859(43)
$6d[1/2]_1$	< 0.0001		0.0003	0.0005	< 0.001
$6d[3/2]_1$	0.0939	0.0758	0.0987	0.0873	0.0835(84)
$8s[3/2]_1$	0.0262	0.0211	0.0201	0.0192	0.0222(22)
$7d[1/2]_1$	0.0146	0.0105	0.0395	0.0441	0.0227(23)
$7d[3/2]_1$	0.0001	0.0002	0.0064	0.0081	< 0.001
$9s[3/2]_1$	0.0088	0.0072	0.0002	0.0003	< 0.001
$5d'[3/2]_1$	0.151	0.114	0.167	0.170	0.191(19)
$8d[1/2]_1$	0.0123	0.0091	0.0068	0.0071	0.0088(9)
$8d[3/2]_1$	0.119	0.091	0.0846	0.0835	0.0967(97)
$10s[3/2]_1$	0.0139	0.0110	0.0139	0.0134	0.0288(29)

Summary of structure work

- The non-orthogonal orbital technique allows us account for **term-dependence** and **relaxation** effects practically to full extent. At the same time, this reduce the size of the configuration expansions, because we use **specific non-orthogonal sets of correlation orbitals** for different kinds of correlation effects.
- ***B***-spline multi-channel models allow us to treat entire Rydberg series and can be used for accurate calculations of oscillator strengths for states with **intermediate and high *n*-values**. For such states, it is difficult to apply standard CI or MCHF methods.
- The accuracy obtained for the low-lying states is close to that reached in large-scale MCHF calculations.
- **Good agreement with experiment** was obtained for the transitions from the ground states and also for transitions between excited states.
- **Calculations performed in this work**: s-, p-, d-, and f-levels up to ***n* = 12**.

```
Ne - 299 states  -  11300 transitions
Ar - 359 states  -  19000 transitions
Kr - 212 states  -   6450 transitions
Xe - 125 states  -   2550 transitions
```

- **All calculations are fully *ab initio*.**
- The **computer code BSR** used in the present calculations and the results for Ar were ~~recently~~ published:

BSR: O. Zatsarinny, Comp. Phys. Commun. **174** (2006) 273
Ar: O. Zatsarinny and K. Bartschat, J. Phys. B **39** (2006) 2145

A "simple"(?) collision problem. e-Be^+: coupling to continuum most important for i) optically forbidden transitions and/or ii) small cross sections

good agreement between CCC, RMPS, TDCC — no experiment !

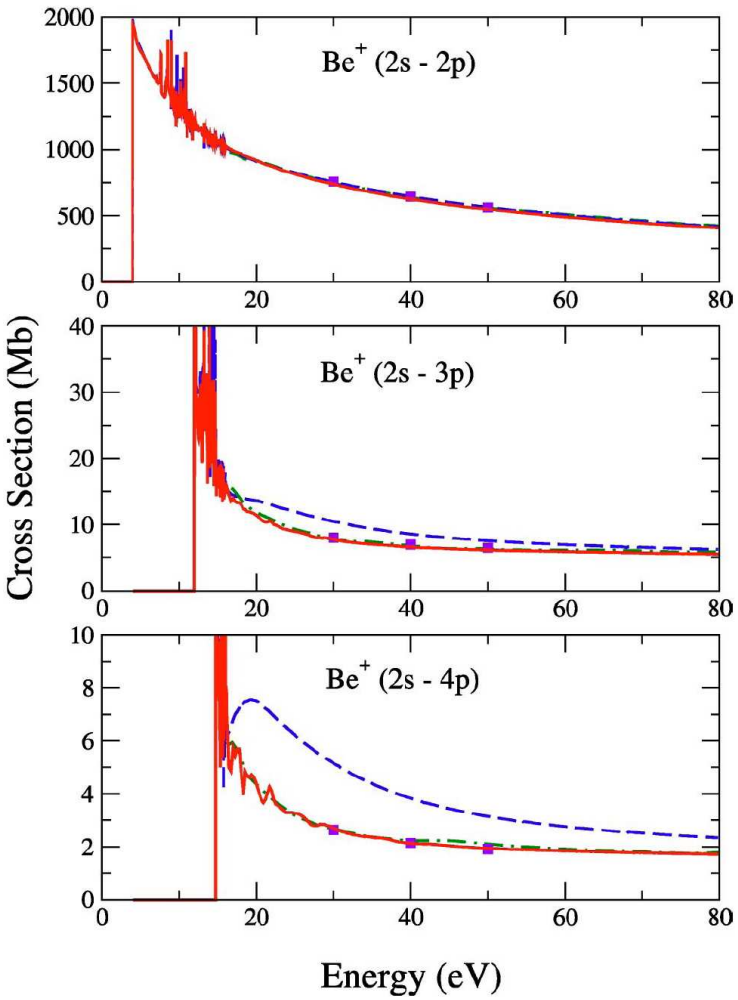

FIG. 4. Electron-impact excitation cross sections from the 2*s* ground term of Be^+ to the *np* excited terms. Dashed curves are from the present 14-term *R*-matrix calculation; solid curves are from the present 49-term RMPS calculation; solid squares are from the present TDCC calculation; dot-dashed curves from the CCC calculation by Bartschat and Bray [14].

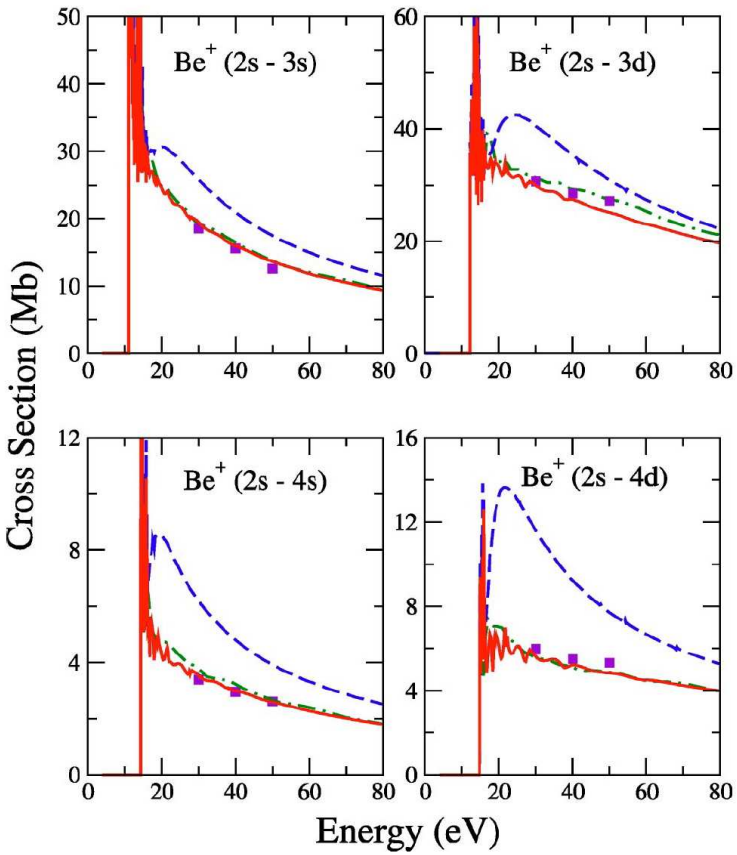

FIG. 5. Electron-impact excitation cross sections from the 2*s* ground term of Be^+ to the *ns* and *nd* excited terms. Dashed curves are from the present 14-term *R*-matrix calculation; solid curves are from the present 49-term RMPS calculation; solid squares are from the present TDCC calculation; dot-dashed curves from the CCC calculation by Bartschat and Bray [14].

This is a light quasi-one electron system. Essentially solved 15 years ago.

Phys. Rev. A 68 (2003) 062705

Another simple one. **e-Be: coupling to continuum most important for i) optically forbidden transitions and/or ii) small cross sections**

good agreement between CCC, RMPS, TDCC — no experiment !

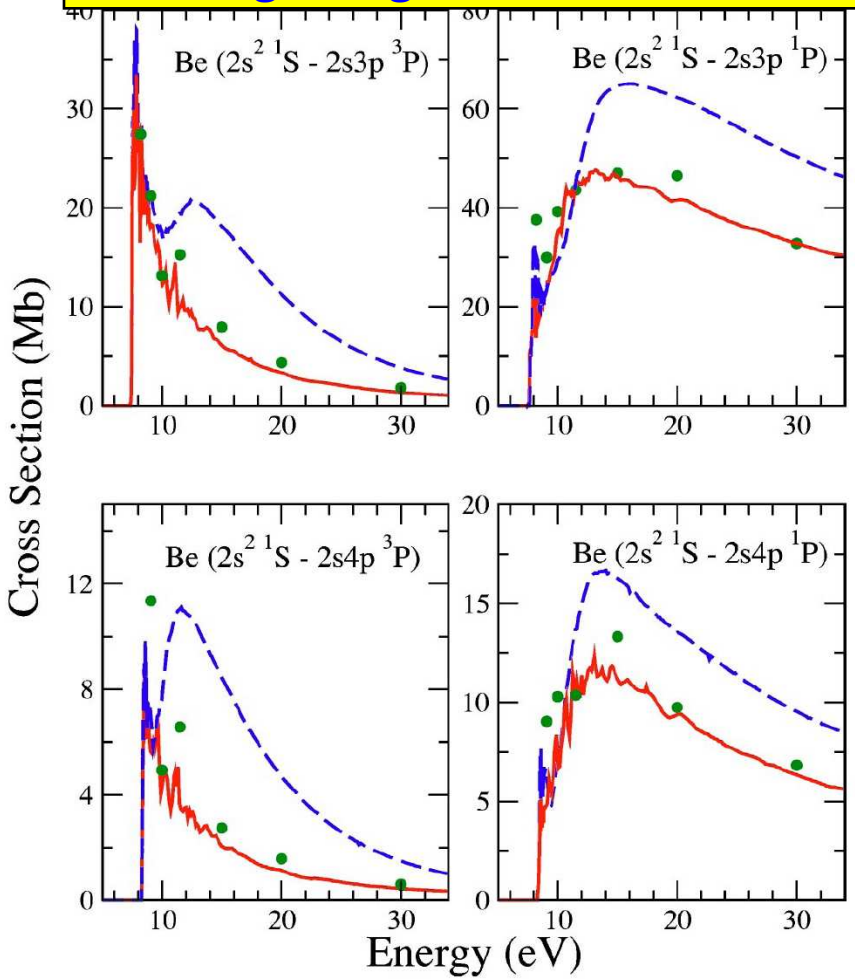

FIG. 2. Electron-impact excitation cross sections from the $2s^2\,{}^1S$ ground term of Be to the $2snp\,{}^3P$ and $2snp\,{}^1P$ excited terms for $n=3$ and 4. Dashed curves are from the present 29-term R-matrix calculation; solid curves are from the present 280-term RMPS calculation; solid circles are from CCC calculations as described in Fursa and Bray [10] and provided at the CCC database web site [11].

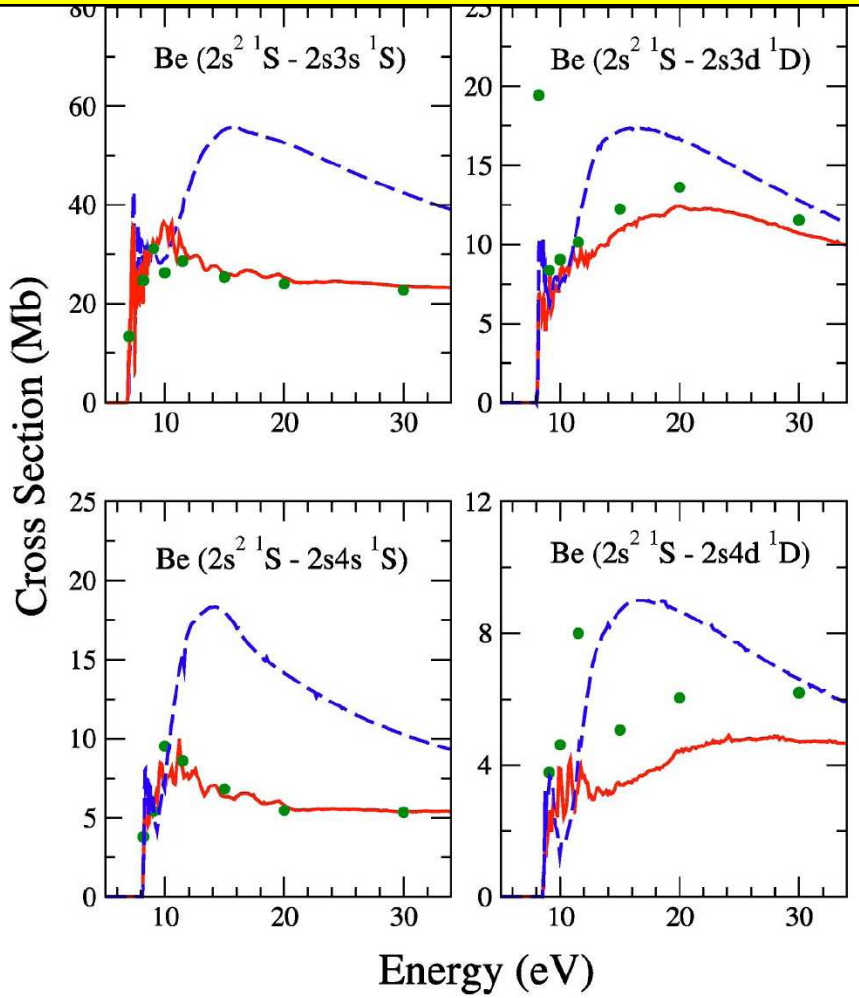

FIG. 3. Electron-impact excitation cross sections from the $2s^2\,{}^1S$ ground term of Be to the $2sns\,{}^1S$ and $2snd\,{}^1D$ excited terms. Dashed curves are from the present 29-term R-matrix calculation; solid curves are from the present 280-term RMPS calculation; solid circles are from CCC calculations as described in Fursa and Bray [10] and provided at the CCC database web site [11].

This is a light quasi-two electron system. Essentially solved 15 years ago.

Phys. Rev. A 68 (2003) 032712

Atomic Data and Nuclear Data Tables 127–128 (2019) 1–21

Contents lists available at ScienceDirect

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journal homepage: www.elsevier.com/locate/adt

One can now safely recommend extensive datasets for this system.

Recommended electron-impact excitation and ionization cross sections for Be I

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ABSTRACT

Analytic fits to the recommended electron-impact excitation and ionization cross sections for Be I are presented. The lowest 19 terms of configurations $2snl$ ($n \leq 4$) and $2p^2$ terms below the first ionization limit are considered. The fits are based on the accurate calculations with the convergent close coupling (CCC) method as well as the B-spline R-matrix (BSR) approach. The fitted cross sections provide rate coefficients that are believed to approximate the original data within 10% with very few exceptions. The oscillator strengths for the dipole-allowed transitions between all the considered states are calculated with the relativistic multi-configuration Dirac–Hartree–Fock (MCDHF) approach and compared with the CCC and BSR results. This comparison shows a very good agreement except for a handful of cases with likely strong cancellations.

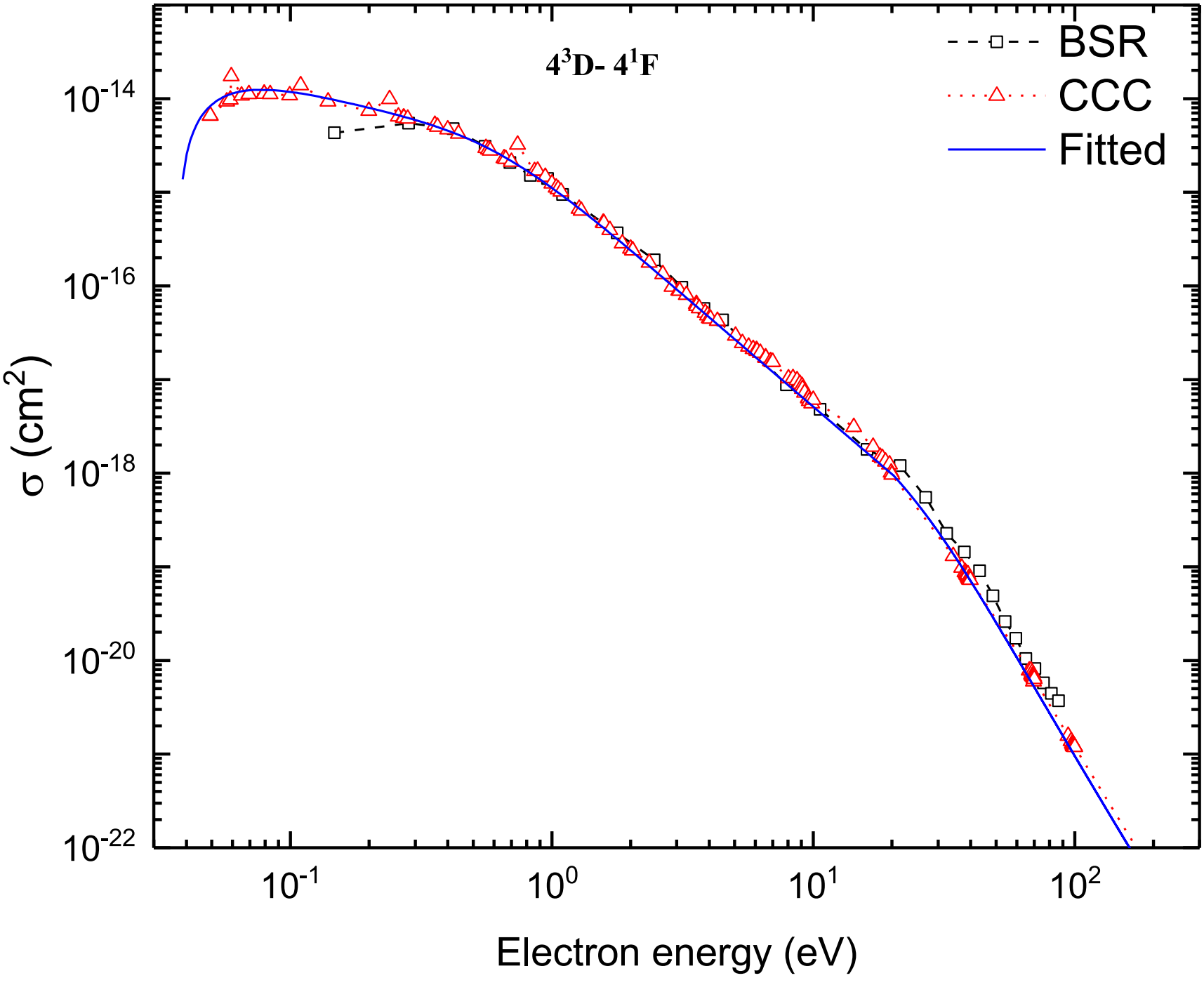


Fig. 4. Electron-impact excitation cross sections for the spin-forbidden ($4^3D \rightarrow 4^1F$) transition.

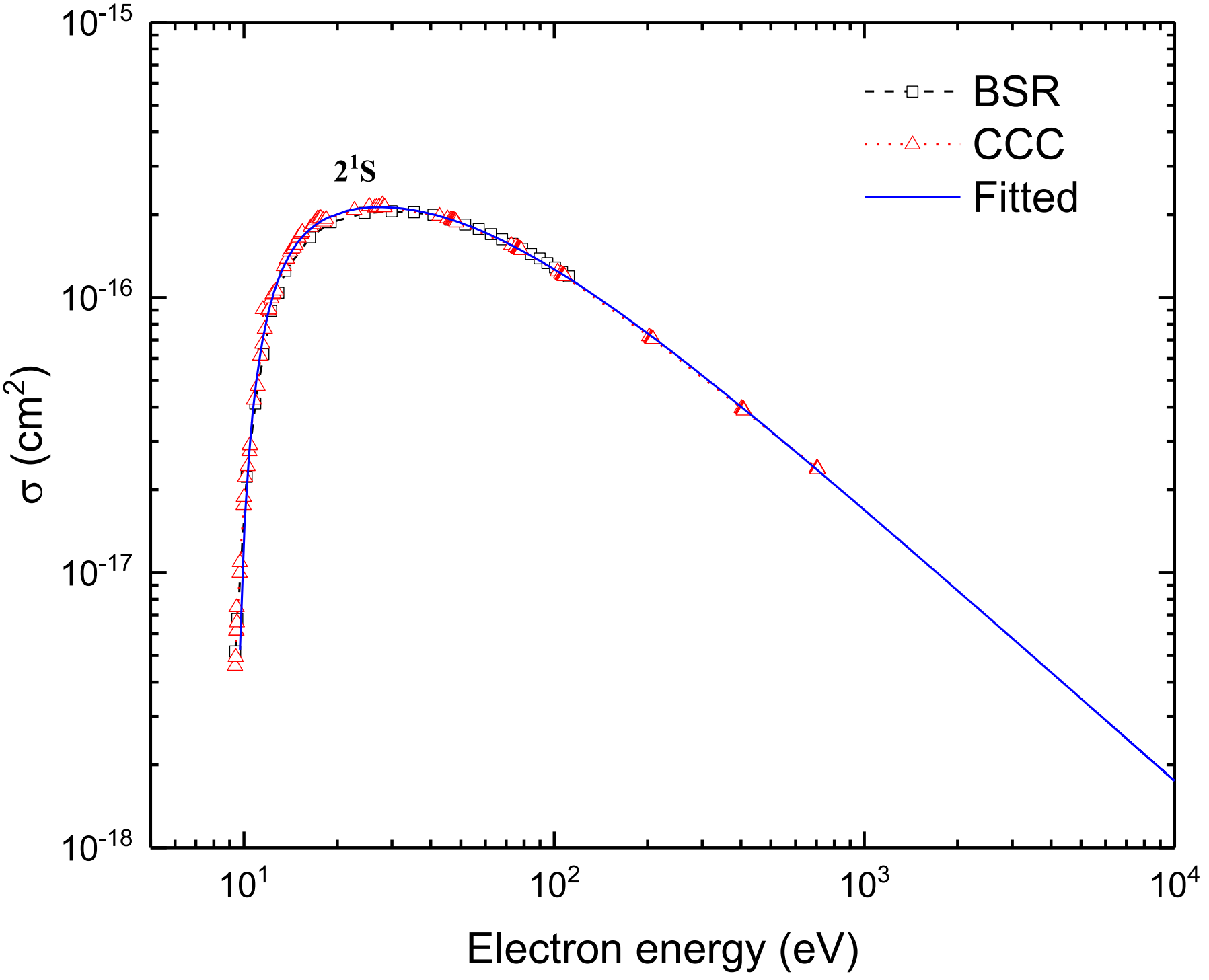


Fig. 6. Electron-impact ionization cross sections from the 2^1S state.

TABLE II. Excitation energies (in eV) of the Fe II final target levels included in the present photoionization calculations.

Index	Configuration	Term	Present	NIST [17]	Diff.	Index	Configuration	Term	Present	NIST [17]	Diff.
1	$3d^6(^5D)4s$	$a\ ^6D$	0.00000	0.00000	0.000	51	$3d^6(^3P)4p$	$y\ ^4D^o$	7.68767	7.67642	0.012
2	$3d^7$	$a\ ^4F$	0.22873	0.23746	−0.008	52	$3d^6(^3H)4p$	$z\ ^2I^o$	7.75384	7.68254	0.071
3	$3d^6(^5D)4s$	$a\ ^4D$	1.00085	0.98236	0.019	53	$3d^6(^3F)4p$	$x\ ^4D^o$	7.79919	7.78729	0.012
4	$3d^7$	$a\ ^4P$	1.61611	1.64122	−0.025	54	$3d^6(^3F)4p$	$z\ ^2F^o$	7.93216	7.92629	0.006
5	$3d^7$	$a\ ^2G$	1.97335	1.93060	0.042	55	$3d^6(^3F)4p$	$y\ ^4G^o$	7.96447	7.87869	0.086
6	$3d^7$	$a\ ^2P$	2.15249	2.25549	−0.102	56	$3d^6(^3P)4p$	$z\ ^2P^o$	7.98689	7.98813	−0.001
7	$3d^7$	$a\ ^2H$	2.45967	2.48451	−0.025	57	$3d^6(^3F)4p$	$y\ ^2G^o$	8.02078	7.99718	0.024
8	$3d^7$	$a\ ^2D$	2.52821	2.52757	0.000	58	$3d^6(^3H)4p$	$z\ ^2H^o$	8.05252	8.05993	−0.007
9	$3d^6(^3H)4s$	$a\ ^4H$	2.59340	2.60163	−0.009	59	$3d^6(^3G)4p$	$x\ ^4G^o$	8.14564	8.09909	0.047
10	$3d^6(^3P)4s$	$b\ ^4P$	2.62235	2.61313	0.009	60	$3d^54s^2$	^2I	8.16405		
11	$3d^6(^3F)4s$	$b\ ^4F$	2.78328	2.77477	0.008	61	$3d^6(^3G)4p$	$x\ ^4F^o$	8.16627	8.16450	0.002
12	$3d^54s^2$	$a\ ^6S$	2.94341	2.84212	0.101	62	$3d^6(^3P)4p$	$z\ ^2S^o$	8.18361	8.16489	0.019
13	$3d^6(^3G)4s$	$a\ ^4G$	3.12934	3.13143	−0.002	63	$3d^6(^3G)4p$	$y\ ^4H^o$	8.19170	8.19302	−0.001
14	$3d^6(^3P)4s$	$b\ ^2P$	3.13657	3.20920	−0.072	64	$3d^6(^3F)4p$	$y\ ^2D^o$	8.27347	8.26940	0.005
15	$3d^6(^3H)4s$	$b\ ^2H$	3.16495	3.20032	−0.035	65	$3d^6(^3G)4p$	$y\ ^2H^o$	8.35303	8.33407	0.019
16	$3d^6(^3F)4s$	$a\ ^2F$	3.33076	3.34805	−0.017	66	$3d^5(^6S)4s4p$	$x\ ^4P^o$	8.53341	8.53496	−0.001
17	$3d^6(^3G)4s$	$b\ ^2G$	3.77259	3.72956	0.043	67	$3d^6(^3G)4p$	$y\ ^2F^o$	8.58723	8.58270	0.004
18	$3d^6(^3D)4s$	$b\ ^4D$	3.84077	3.84398	−0.003	68	$3d^6(^3G)4p$	$x\ ^2G^o$	8.70428	8.67498	0.029
19	$3d^7$	$b\ ^2F$	3.88267	3.90300	−0.020	69	$3d^6(^1I)4p$	$z\ ^2K^o$	8.76101	8.76208	−0.001
20	$3d^6(^1I)4s$	$a\ ^2I$	3.97082	4.02791	−0.057	70	$3d^6(^3D)4p$	$w\ ^4P^o$	8.84826	8.88371	−0.036
21	$3d^6(^1G)4s$	$c\ ^2G$	4.08447	4.10141	−0.016	71	$3d^6(^1G)4p$	$x\ ^2H^o$	8.85140	8.89788	−0.047
22	$3d^6(^3D)4s$	$b\ ^2D$	4.43813	4.43693	0.001	72	$3d^6(^3D)4p$	$w\ ^4F^o$	8.90035	8.91993	−0.020
23	$3d^6(^1S)4s$	$a\ ^2S$	4.58154	4.56669	0.015	73	$3d^54s^2$	^2D	8.92103		
24	$3d^6(^1D)4s$	$c\ ^2D$	4.69523	4.68494	0.010	74	$3d^6(^3D)4p$	$y\ ^2P^o$	8.97058	9.02530	−0.054
25	$3d^6(^5D)4p$	$z\ ^6D^o$	4.75973	4.74993	0.010	75	$3d^6(^3D)4p$	$w\ ^4D^o$	8.99030	8.94838	0.042
26	$3d^6(^5D)4p$	$z\ ^6F^o$	5.16594	5.17773	−0.012	76	$3d^6(^1G)4p$	$x\ ^2F^o$	9.01599	9.00526	0.011

We need the structure of Fe II (collision) and Fe I (initial bound states)

TABLE I. Excitation energies (in eV) of the Fe I target levels included in the present photoionization calculations.

Index	Configuration	Term	Present	NIST [17]	Diff.	Index	Configuration	Term	Present	NIST [17]	Diff.
1	$3d^64s^2$	$a\ ^5D$	0.00000	0.00000	0.000	23	$3d^7(^2H)4s$	$a\ ^1H$	3.52020	3.52326	−0.003
2	$3d^7(^4F)4s$	$a\ ^5F$	0.86082	0.87493	−0.014	24	$3d^64s^2$	$a\ ^1I$	3.48480	3.58439	−0.003
3	$3d^7(^4F)4s$	$a\ ^3F$	1.48145	1.48836	−0.007	25	$3d^6(^5D)4s4p$	$z\ ^5P^o$	3.54575	3.58639	0.005
4	$3d^7(^4P)4s$	$a\ ^5P$	2.16087	2.14265	0.018	26	$3d^64s^2$	$b\ ^3D$	3.56252	3.58977	−0.003
5	$3d^64s^2$	$a\ ^3P$	2.28122	2.30004	−0.019	27	$3d^64s^2$	$b\ ^1G$	3.60328	3.64464	−0.004
6	$3d^64s^2$	$a\ ^3H$	2.36601	2.37711	−0.011	28	$3d^6(^5D)4s4p$	$z\ ^3D^o$	3.77607	3.86382	−0.003
7	$3d^6(^5D)4s4p$	$z\ ^7D^o$	2.40412	2.38311	0.021	29	$3d^6(^5D)4s4p$	$z\ ^3F^o$	3.82394	3.87662	0.030
8	$3d^64s^2$	$b\ ^3F$	2.54367	2.53060	0.013	30	$3d^8$	$c\ ^3F$	4.05592	4.07445	0.015
9	$3d^64s^2$	$a\ ^3G$	2.67804	2.67132	0.007	31	$3d^7(^4F)4p$	$y\ ^5D^o$	4.13847	4.10398	−0.006
10	$3d^7(^4P)4s$	$b\ ^3P$	2.77262	2.78906	−0.016	32	$3d^7(^4F)4p$	$y\ ^5F^o$	4.16598	4.18009	−0.018
11	$3d^6(^5D)4s4p$	$z\ ^7F^o$	2.77755	2.79275	−0.015	33	$3d^6(^5D)4s4p$	$z\ ^3P^o$	4.16824	4.18450	−0.064
12	$3d^64s^2$	$a\ ^1S$	2.80530			34	$3d^7(^2D)4s$	$b\ ^1D$	4.23998	4.24445	0.005
13	$3d^7(^2G)4s$	$b\ ^3G$	2.93034	2.93053	−0.000	35	$3d^7(^4F)4p$	$z\ ^5G^o$	4.32527	4.30728	−0.017
14	$3d^6(^5D)4s4p$	$z\ ^7P^o$	2.93705	2.93277	0.004	36	$3d^7(^4F)4p$	$z\ ^3G^o$	4.37188	4.37506	−0.019
15	$3d^7(^2P)4s$	$c\ ^3P$	2.98683	2.99573	−0.009	37	$3d^7(^2F)4s$	$d\ ^3F$	4.51238	4.53713	−0.000
16	$3d^7(^2G)4s$	$a\ ^1G$	3.00166	2.99691	0.005	38	$3d^6(^5D)4s4p$	$y\ ^5P^o$	4.57776	4.54064	−0.014
17	$3d^6(^5D)4s4p$	$z\ ^5D^o$	3.17777	3.19232	−0.015	39	$3d^7(^4F)4p$	$y\ ^3F^o$	4.49736	4.54289	−0.062
18	$3d^7(^2H4s$	$b\ ^3H$	3.20414	3.21453	−0.010	40	$3d^7(^2F)4s$	^1F	4.53208		
19	$3d^7(^2D)4s$	$a\ ^3D$	3.21687	3.22250	−0.006	41	$3d^7(^4F)4p$	$y\ ^3D^o$	4.76043	4.72430	0.024
20	$3d^6(^5D)4s4p$	$z\ ^5F^o$	3.30659	3.32482	−0.018	42	$3d^8$	^1D	4.73248		
21	$3d^7(^2P)4s$	$a\ ^1P$	3.35960	3.36494	−0.005	43	$3d^6(^5D)4s4p$	$x\ ^5D^o$	4.86200	4.90585	−0.006
22	$3d^64s^2$	$a\ ^1D$	3.49993	3.49656	0.003	44	$3d^6(^5D)4s4p$	$x\ ^5F^o$	4.97766	4.98932	−0.012

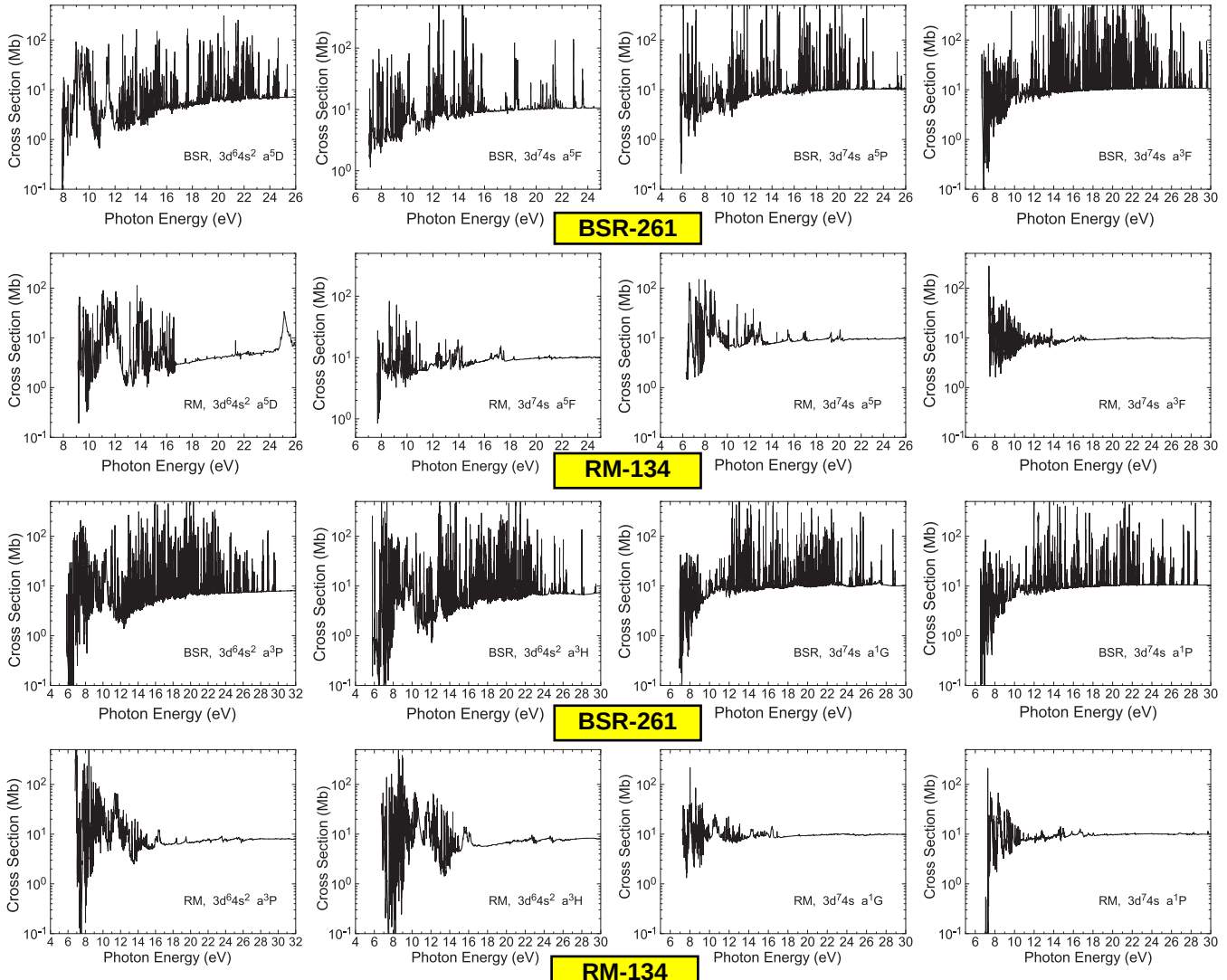


FIG. 1. Photoionization cross sections as a function of photon energy for a sample of low-lying even-parity states of Fe I. The present BSR-261 (BSR in the legend, first and third row) predictions are compared with the RM-134 (RM in the legend, second and fourth row) results of Bautista *et al.* [3].

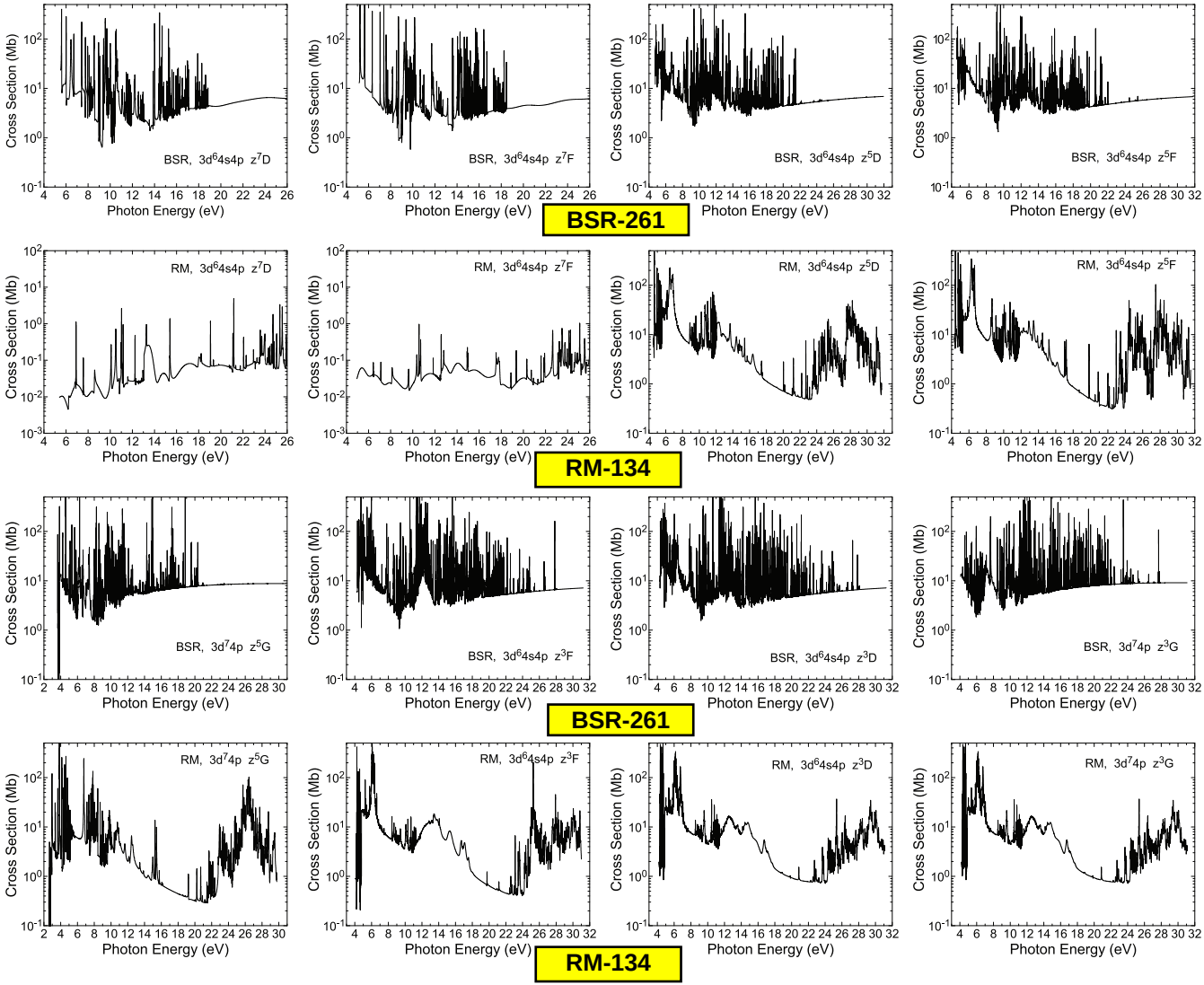


FIG. 4. Photoionization cross section for transitions from the first few odd-parity excited terms of Fe I. The present BSR-261 (BSR in the legend, first and third row) predictions are compared with the RM-134 (RM in the legend, second and fourth row) results of Bautista *et al.* [3].

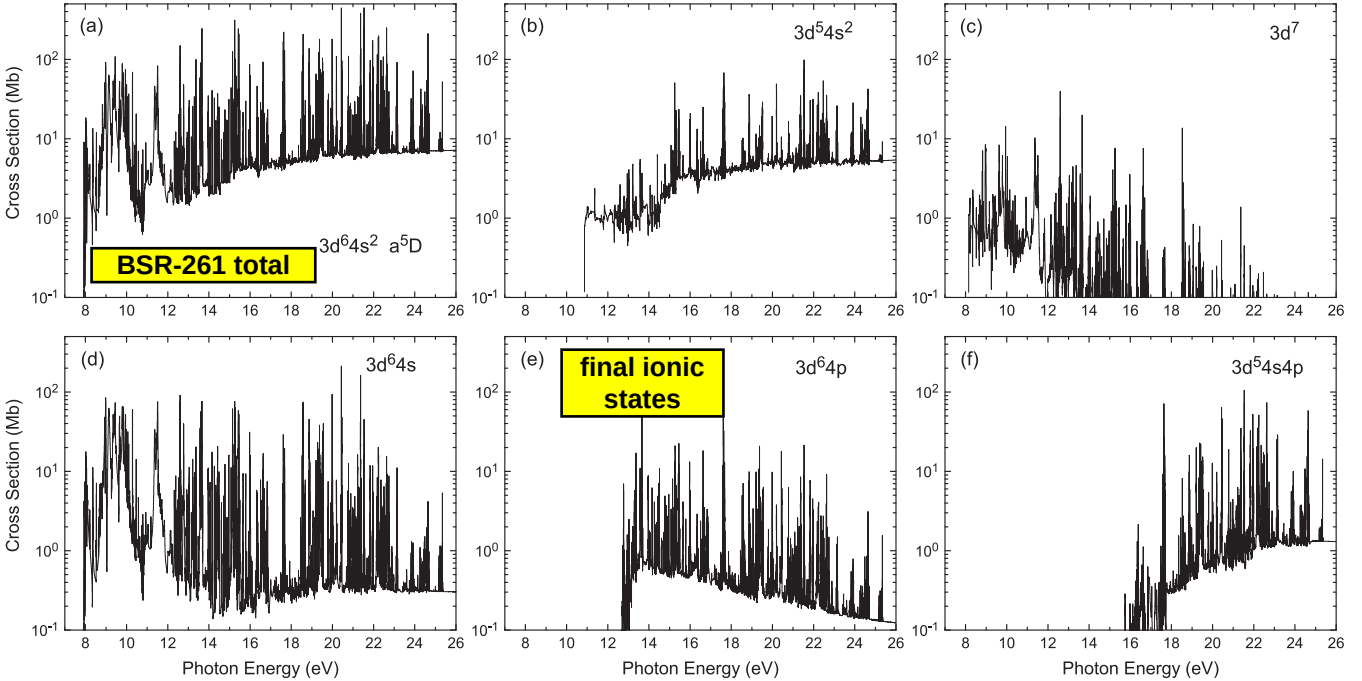
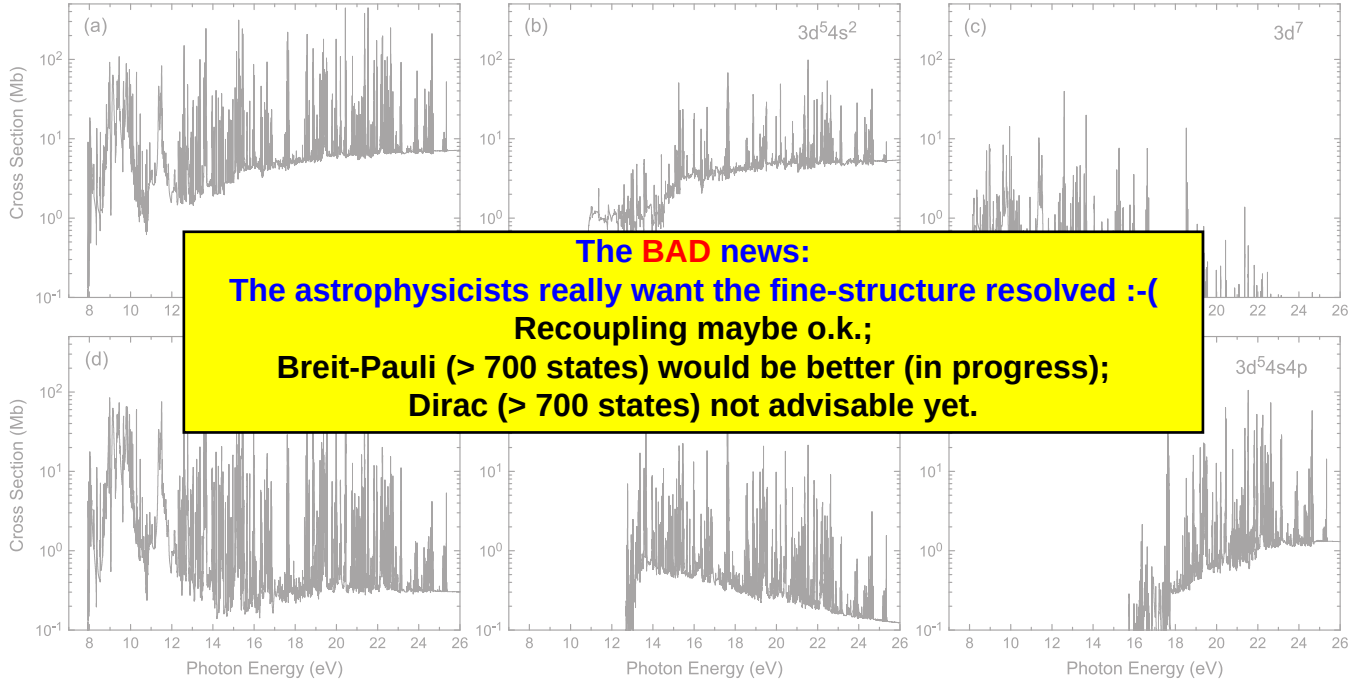


FIG. 2. Photoionization cross section of the $3d^6 4s^2\ ^5D$ ground state of Fe I (a), along with the contributions from different subsets (b)–(f) of final ionic configurations indicated in the legend.



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And astrophysicists are not alone ...

A xenon collisional-radiative model applicable to electric propulsion devices: I. Calculations of electron-impact cross sections for xenon ions by the Dirac B-spline R-matrix method

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Published 7 October 2019

Table 1. Comparison of selected oscillator strengths for excitation of Xe^+ from $5p^4 6s$ to $5p^4 6p$ in the velocity (V) and length (L) forms. λ denotes the wavelength of the optical transition.

Lower level	Upper level	λ (nm)	PAD[a] [17]	HCL[b] [18]	NIST [20]	This work	
						V	L
$5p^4(^3P_2)6s\ ^2[2]_{3/2}$	$5p^4(^3P_2)6p\ ^2[1]°_{3/2}$	460.3	0.239	–	0.26	0.238	0.323
$5p^4(^3P_2)6s\ ^2[2]_{5/2}$	$5p^4(^3P_2)6p\ ^2[3]°_{7/2}$	484.4	0.408	0.540	0.52	0.517	0.586
$5p^4(^3P_0)6s\ ^2[0]_{1/2}$	$5p^4(^3P_0)6p\ ^2[1]°_{3/2}$	488.4	0.480	–	–	0.569	0.641
$5p^4(^3P_2)6s\ ^2[2]_{5/2}$	$5p^4(^3P_2)6p\ ^2[2]°_{5/2}$	529.2	0.380	0.403	0.37	0.404	0.462
$5p^4(^3P_2)6s\ ^2[2]_{5/2}$	$5p^4(^3P_2)6p\ ^2[2]°_{3/2}$	533.9	0.191	0.187	–	0.193	0.216
$5p^4(^3P_2)6s\ ^2[2]_{3/2}$	$5p^4(^3P_2)6p\ ^2[3]°_{5/2}$	541.9	0.429	0.452	0.41	0.548	0.614
$5p^4(^3P_1)6s\ ^2[1]_{3/2}$	$5p^4(^3P_1)6p\ ^2[0]°_{1/2}$	543.9	0.153	–	0.16	0.191	0.222
$5p^4(^1D_2)6s\ ^2[2]_{3/2}$	$5p^4(^1D_2)6p\ ^2[3]°_{5/2}$	627.1	–	–	0.16	0.130	0.139

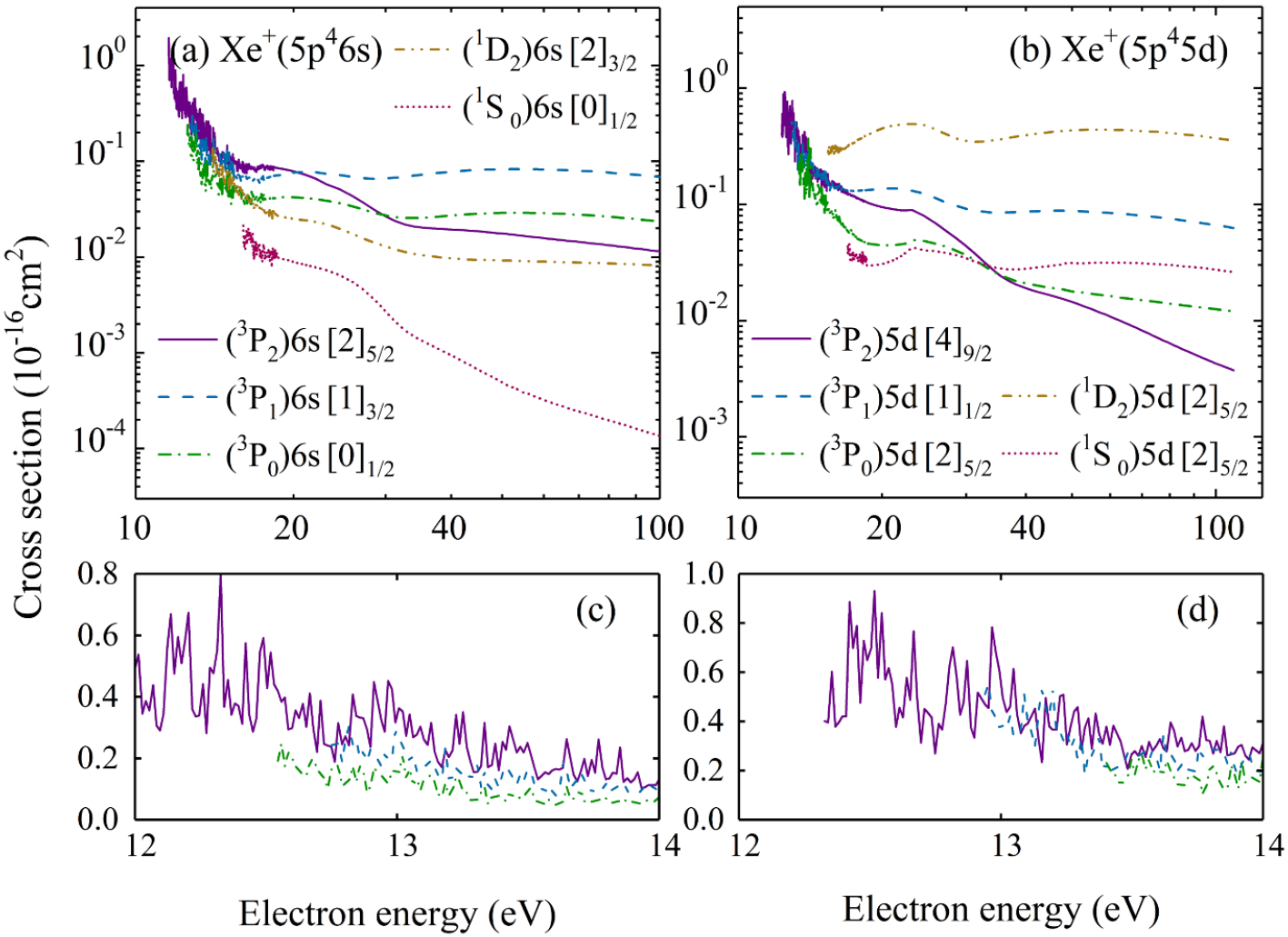

Figure 2. Electron-impact excitation cross sections for transitions from $5p^5\ ^2P^o_{3/2}$ to selected $5p^46s$ (a) and $5p^45d$ (b) states. For brevity the notation has been shortened in the legend, e.g., from $5p^4(^3P_2)6s\ ^2[2]_{5/2}$ to $(^3P_2)6s\,[2]_{5/2}$, etc. Panels (c) and (d) show the near-threshold results on a linear scale.

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A xenon collisional-radiative model applicable to electric propulsion devices: II. Kinetics of the 6*s*, 6*p*, and 5*d* states of atoms and ions in Hall thrusters

Xi-Ming Zhu[1,4], Yan-Fei Wang[1], Yang Wang[1,4], Da-Ren Yu[1], Oleg Zatsarinny[2], Klaus Bartschat[2], Tsanko Vaskov Tsankov[3] and Uwe Czarnetzki[3]

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What about really complex, heavy systems?

At a recent IAEA meeting, a scientist from the ITER project stated:
The three most important elements for us are …

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Here are our best results for e–W^{n+} collisions:

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Here are our best results for e–W^{n+} collisions:

NOTHING (yet)

A lot of work is still required before a reliable calculation can be carried out.
It seems advisable for people collaborate in code development and maintenance.

Two-Photon Double Ionization of H_2

X. Guan and K. Bartschat (Drake U.), L. Koesterke (TACC), B.I. Schneider (NSF)

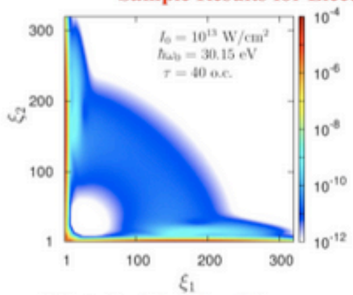
Goal: Resolve large discrepancies in previous calculations of this fundamental process.

Steps taken: 1) Optimized existing FEDVR code for Stampede
2) Sampled parameter space (photon energy, pulse duration) with about **100 runs (3000 cores and 10-20 hours of wallclock time each)**

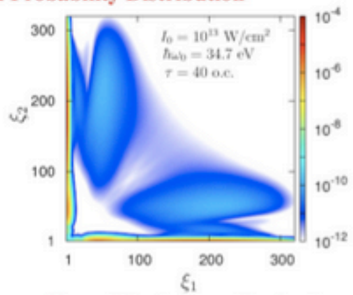
Findings: Discrepancies are due to surprisingly strong dependence of theoretical predictions on laser parameters and (previously unresolved) effect of autoionizing states.

Broad Impact: These calculations support/explain very expensive FEL experiments.

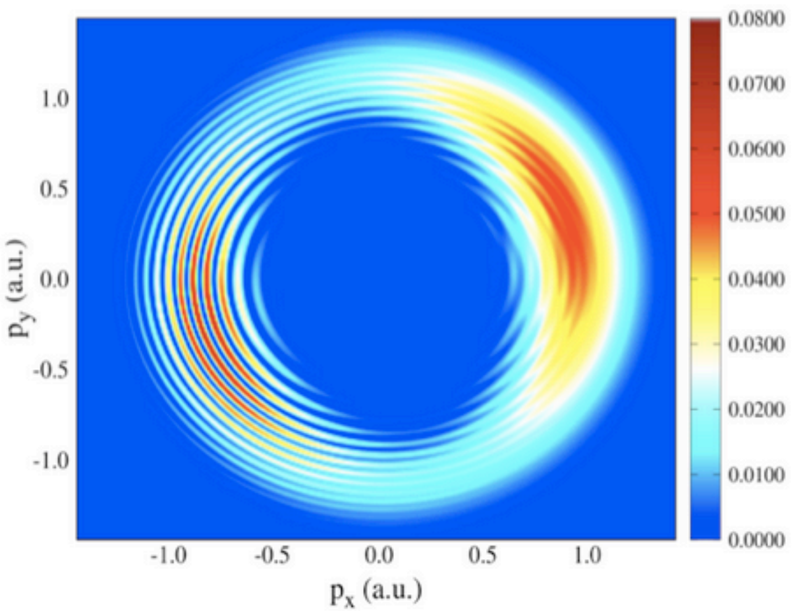
Sample Results for Electron Probability Distribution



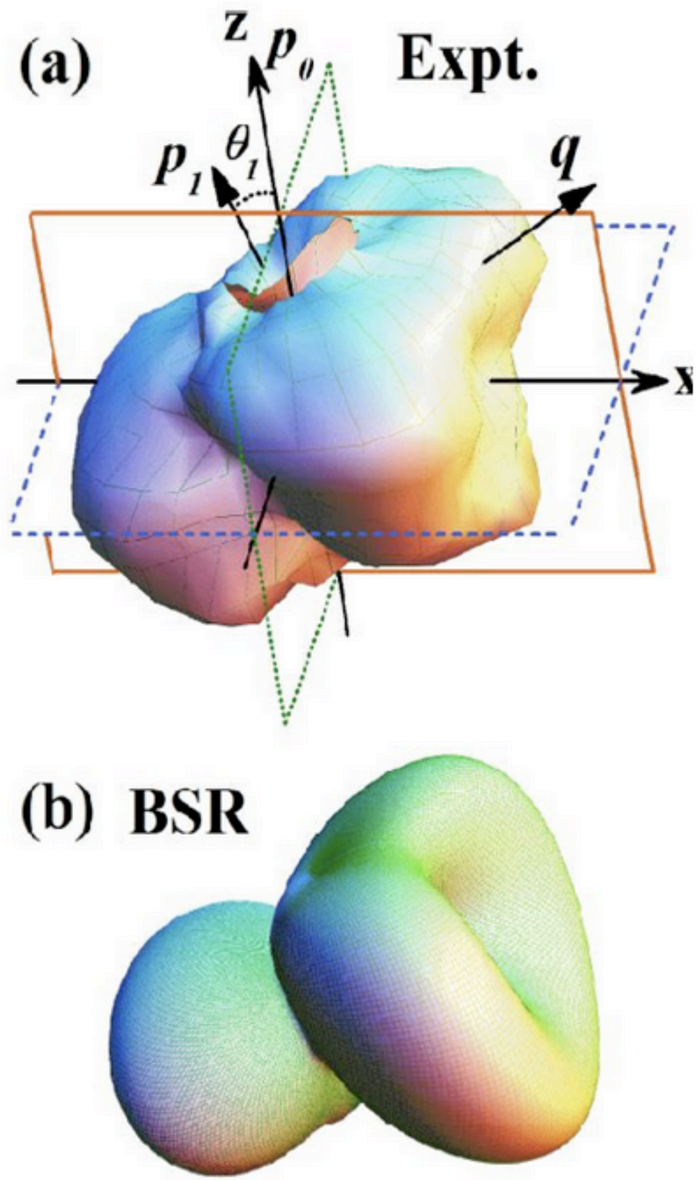
Effect of **autoionizing states** on non-sequential double ionization



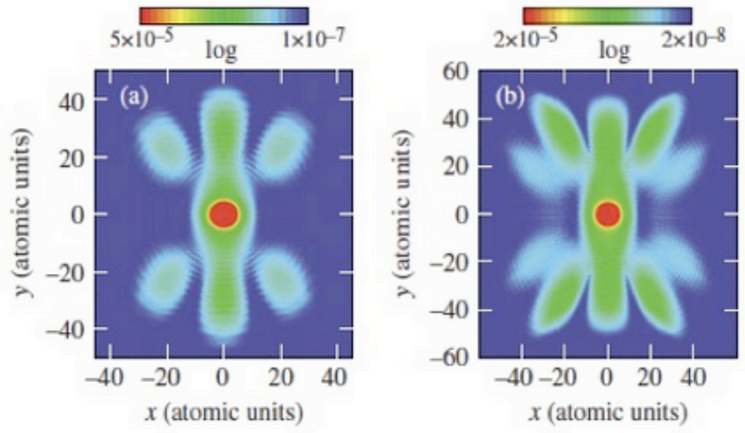
Competition between **direct** and **sequential** double ionization



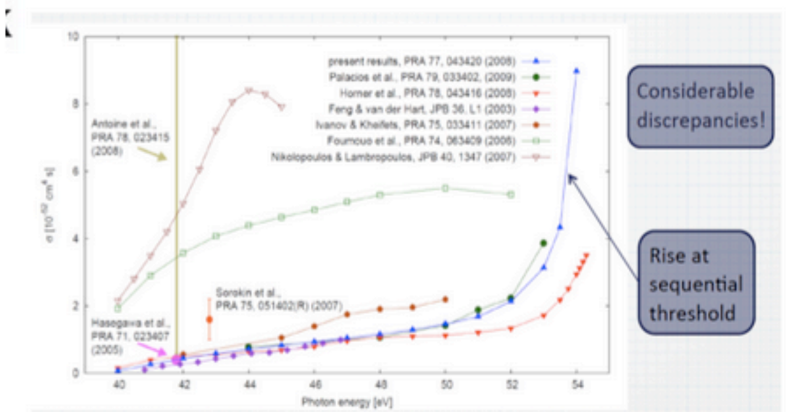
Photoelectron Momentum Distribution for Ar Ionization in Strong Electromagnetic Field



Ionization of Ar(3p) by electron Impact: Experiment(a) and Theory(b)



H^+_2 Ionization in strong, ultrafast electromagnetic field: Note the Patterns caused by wave interference from the nuclei



2-Photon Double Ionization in He: Approaching the Sequential Threshold

CSSI Element: A General and Effective B-Spline R-Matrix Package for Charged-Particle and Photon Collisions with Atoms, Ions, and Molecules

PI: Oleg Zatsarinny; Co-PI: Klaus Bartschat; Post-Doc: Kathryn Hamilton
Dept. of Physics & Astronomy, Drake Univ., Des Moines, IA 50311, USA

Award: OAC-1834740

Introduction

- BSR is a general program package to calculate high-quality atomic data for:
  - structure (energy levels, oscillator strengths)
  - photoionization (bound –> free transitions)
  - electron scattering from atoms and ions
- BSR can be run in non-relativistic (LS), semi-relativistic (Breit-Pauli), and full-relativistic (Dirac-Coulomb) mode.
- Data from BSR are used in:
  - fundamental research to support many experiments
  - data-intensive modelling applications, especially in plasma and astrophysics

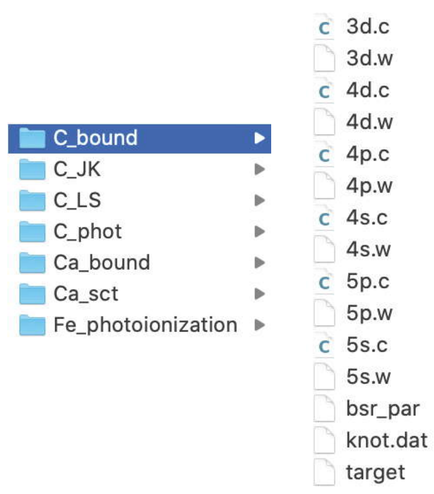
Goals

- Further development of the code (efficiency; parallelization; more physics: molecules and short-pulse, intense laser-atom interactions)
- Simplification of input and output to facilitate use by non-experts
- Creation of many sample inputs, run scripts, and extensive documentation
- Creation of a website with possibility for questions and feedback
- Wide and free distribution via CPC, github, AMP Gateway, etc.

B-spline atomic R-Matrix code (BSR)

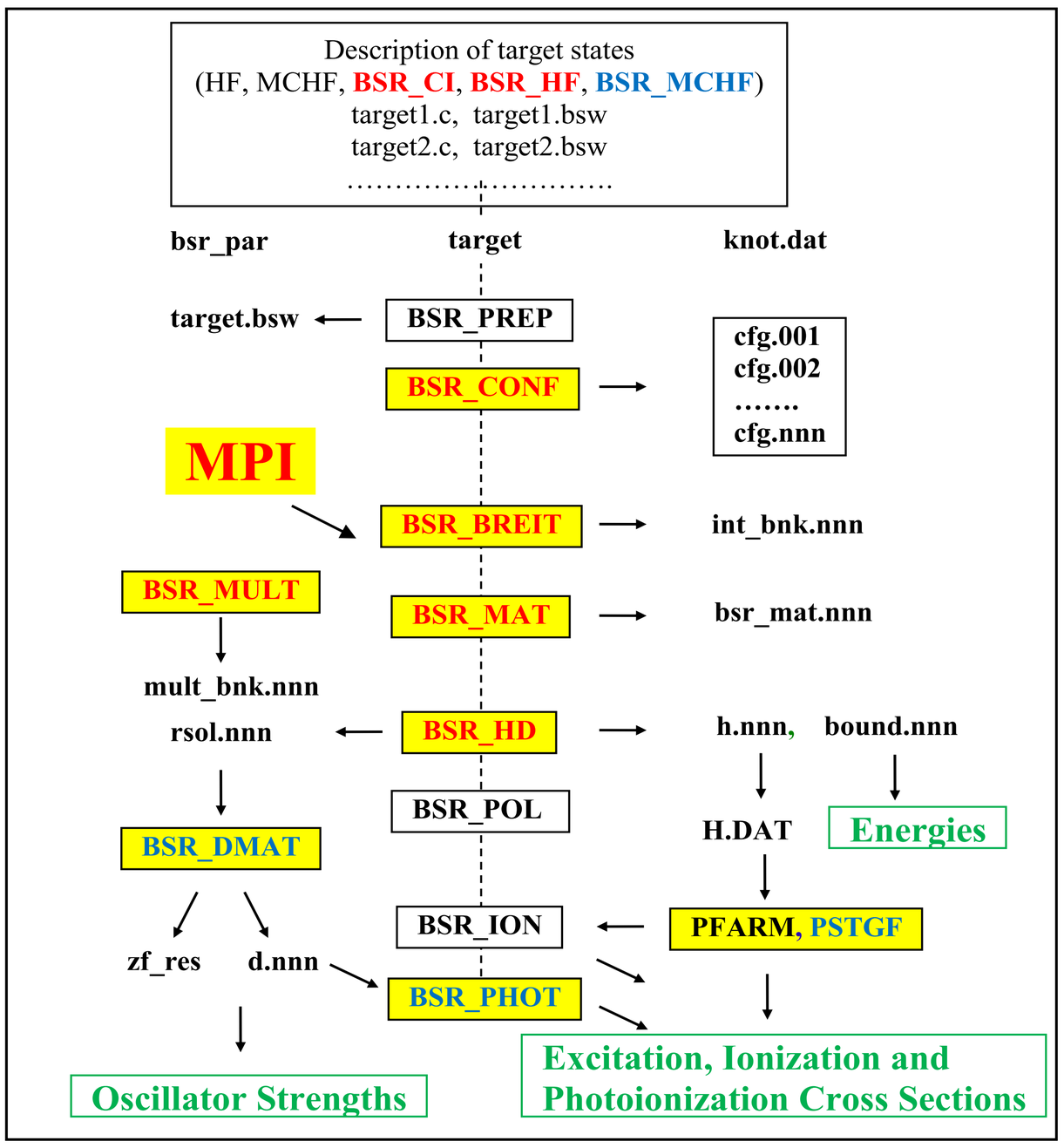
```
e + Ca+
-------------------------------------------------------------------------------
coupling = LS     !   coupling scheme
nz       =   20   !   nuclear charge
nelc     =   19   !   number of electrons
-------------------------------------------------------------------------------
ntarg  =    6     !   number of target states
-------------------------------------------------------------------------------
4s                targ_001      0   2   1     -676.59058592   10    9
4d                targ_002      2   2   1     -676.53378783    6    6
4p                targ_003      1   2  -1     -676.47473702   15    6
5s                targ_004      0   2   1     -676.35162078   10    0
3d                targ_005      2   2   1     -676.33047471    6    0
5p                targ_006      1   2  -1     -676.31379441   15    0
-------------------------------------------------------------------------------
nct    =   62     !   total number of target configurations
nwt    =   25     !   total number of target orbitals
nsub   =   11     !   number of substitution orbitals
-------------------------------------------------------------------------------
nlsp   =   14     !   number of partial waves
-------------------------------------------------------------------------------

       8 ==>  order  of splines (ks)
     140 ==>  number of splines (ns)
20.00000 ==>  nuclear charge (z)
 0.25000 ==>  step size from 0 to 1 (h for z*r, = (1/2)^n)
 0.70000 ==>  maximum step size (hmax for r)
80.00000 ==>  maximum r (rmax)
```

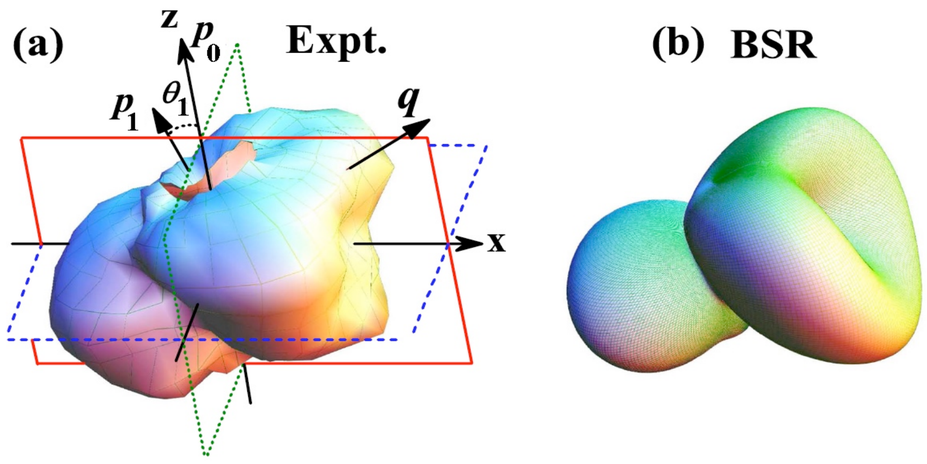


Preview of BSR test suite including sample target and knot.dat files.

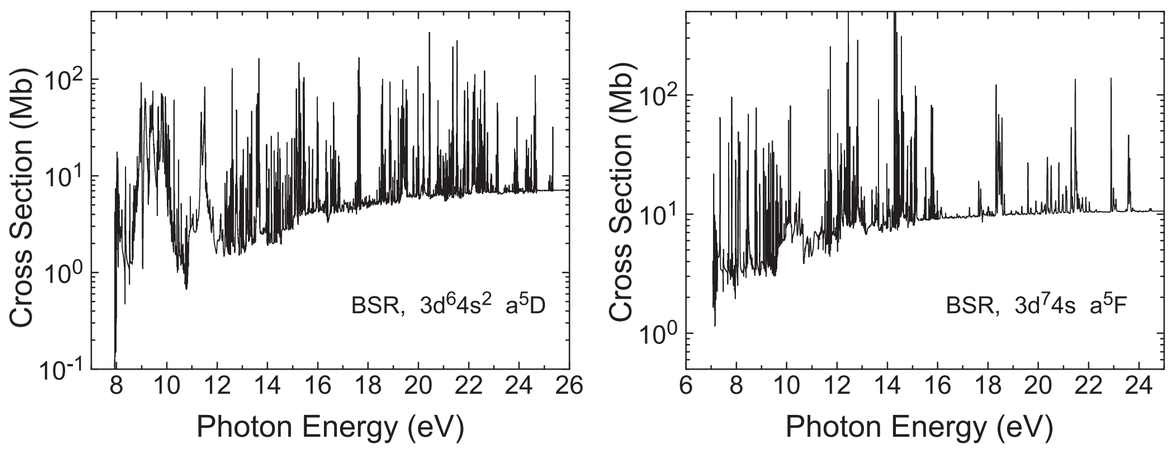
- 30,000-50,000 lines of FORTRAN 95 code organized in 10 modules
- Choice between serial and MPI parallelized versions of modules
- (SCA)LAPACK for diagonalization of large matrices
- Human-readable, descriptive BSR input files
- Target-state descriptions can be generated by widely-available non-BSR codes (HF, MCHF, DARC) with plans to include other packages (CIV3, FAC)
- Suite of utilities for processing BSR outputs
- Test suite with sample inputs, outputs, and run scripts for 7 different problems (more to come)
- Fully relativistic (Dirac-Coulomb) DBSR code with similar anatomy is undergoing development



Scientific Impact



Fully-differential cross section for **(e,2e) on Ar(3p)**; Ren *et al.*, Phys. Rev. A **93** (2016) 062704; no other theory comes even close to the data.



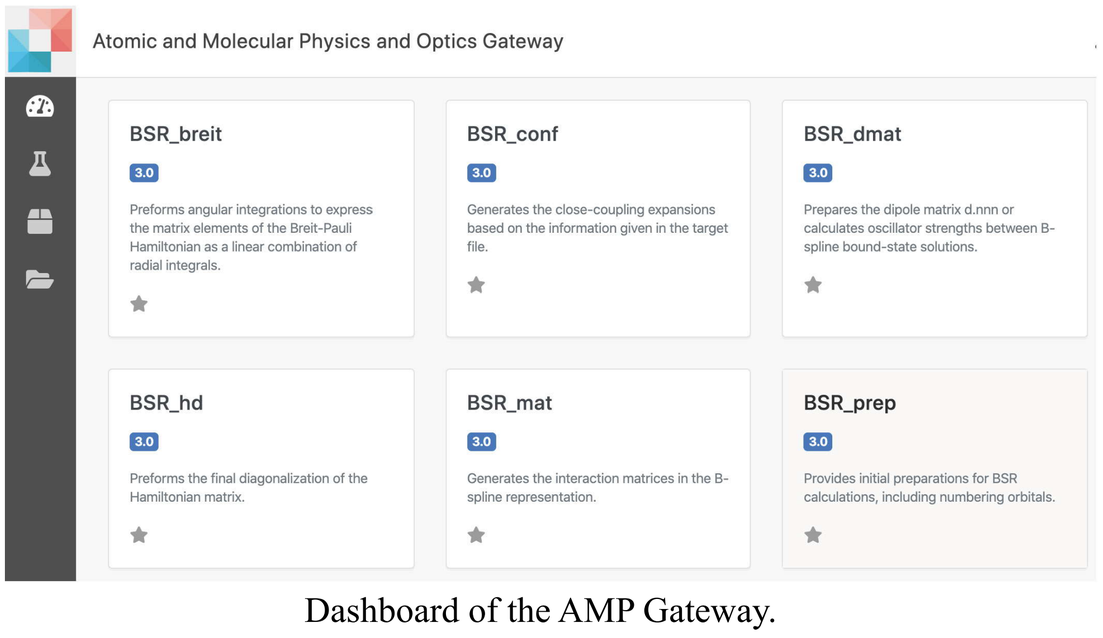
Photoionization of iron from ground and excited states; Zatsarinny *et al.*, Phys. Rev. A **99** (2019) 023430; very complex resonance structure.

Community Interaction

- First release of BSR downloadable from Computer Physics Communications
- BSR 3.0 available on the AMP Gateway:
  - Gateway is based on Apache Airavata
  - Institutional and individual (sign-up) logins allow access to BSR for researchers and students.
  - Access to XSEDE resources
  - Code documentation hosted on gateway
- Integration with existing open-source time-dependent R-matrix code is currently under development.

BSR CPC

AMP Gateway



Dashboard of the AMP Gateway.

Dashboard

BSR: B-spline atomic R-matrix codes

3.0

A general program to calculate continuum processes using the B-spline R-matrix method.

CCC

Convergent Close Coupling Code

CCC_GPU

1.0

GPU Version of Convergent Close-Coupling code

tRecX

1.0

tRecX-again for parallel execution on SKX nodes

tRecX-0.1

0.1

Time dependent recursive indexing Software
https://trecx.physik.lmu.de/home.html older version

ePolyScat

E3 version

ePolyScat is a suite of FORTRAN 90 programs and libraries that can be used to study electron-molecule scattering processes.

fds

6.7.4

Fire Dynamics Simulator (FDS) is a large-eddy simulation (LES) code for low-speed flows, with an emphasis on smoke and heat transport from fires.

xchem

2019.12-dev

XCHEM - The *ab initio* Solution for Multichannel Scattering Problems

OpenMolcas

OpenMolcas mod xchem-2019-12

OpenMolcas with XCHEM modifications

RMT: R-Matrix with Time- dependence

1.0

RMT is a program which solves the time-dependent Schrodinger equation for general, multielectron atoms, ions and molecules interacting with laser light.

UKRMol+

3.0

R matrix electron and positron scattering for molecules and photoionization.

Eur. Phys. J. D (2013) 67: 130
DOI: 10.1140/epjd/e2013-40111-9

THE EUROPEAN PHYSICAL JOURNAL D

Regular Article

Machine Learning
Disclaimer: I am not an expert on this!)

Applications of artificial neural networks to proton-impact ionization double differential cross sections

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Published online 27 June 2013 –

Abstract. We use artificial neural networks (ANNs) to study proton impact single ionization double differential cross sections of atoms and molecules. While widely used in other fields, to our knowledge, this is the first time that an ANN has been used to study differential cross sections for atomic collisions. ANNs are trained to learn patterns in data and make predictions for cases where no data exists. We test the validity of the ANN's predictions by comparing them to known measurements and find that the ANN does an excellent job of predicting the known data. We then use the ANN to make predictions of cross sections where no data currently exists.

6 Conclusions

We have used an Artificial Neural Network to predict proton impact double differential cross sections for single ionization of atoms and molecules, and have tested the accuracy of the ANN's predictions by comparing them to

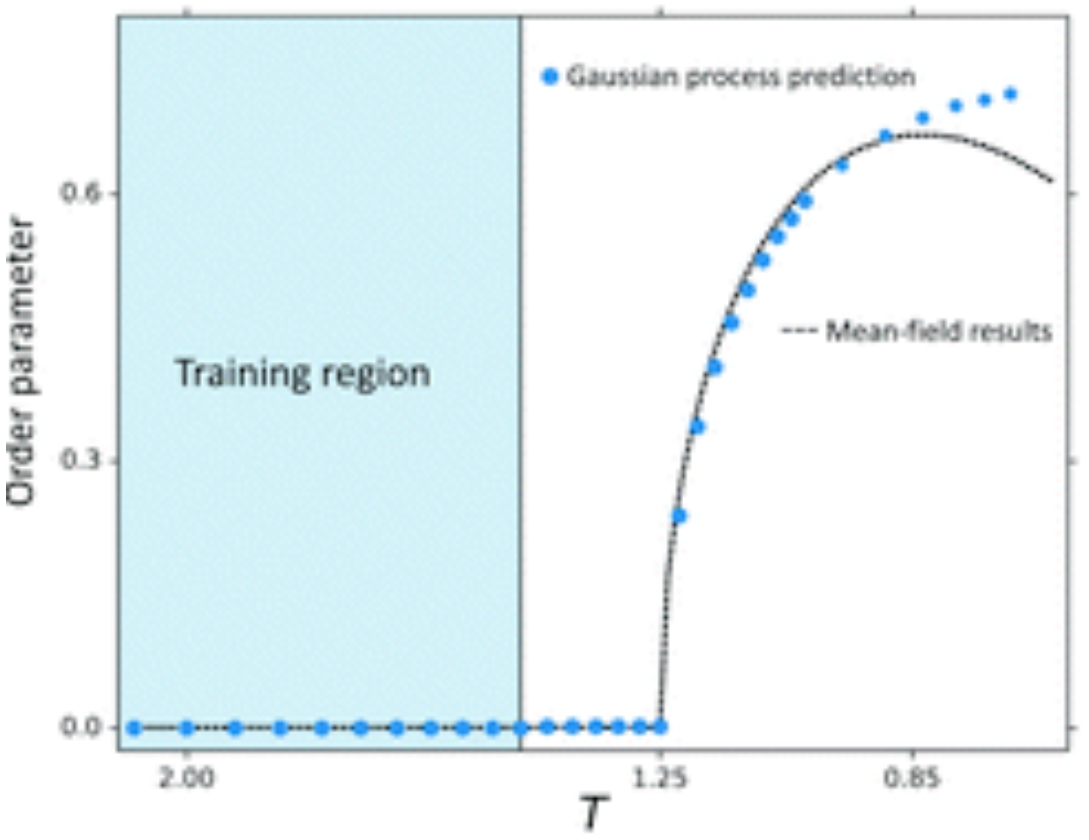
Overall, the results show that the ANN is able to give reasonable predictions for the shape and magnitude of DDCS for single ionization of atoms and molecules. We are currently exploring the application of ANNs to fully differential cross sections for both proton and electron impact ionization processes, and plan to use traditional theoretical models to test our predictions. Overall, we consider the use of ANNs to predict atomic collision data to be successful, and anticipate that they may be a useful tool to provide additional approximate data that can be used for modeling in other applications.

Roman V. Krems

Phys. Chem. Chem. Phys. 21 (2019) 13392–13410

Bayesian machine learning for quantum molecular dynamics

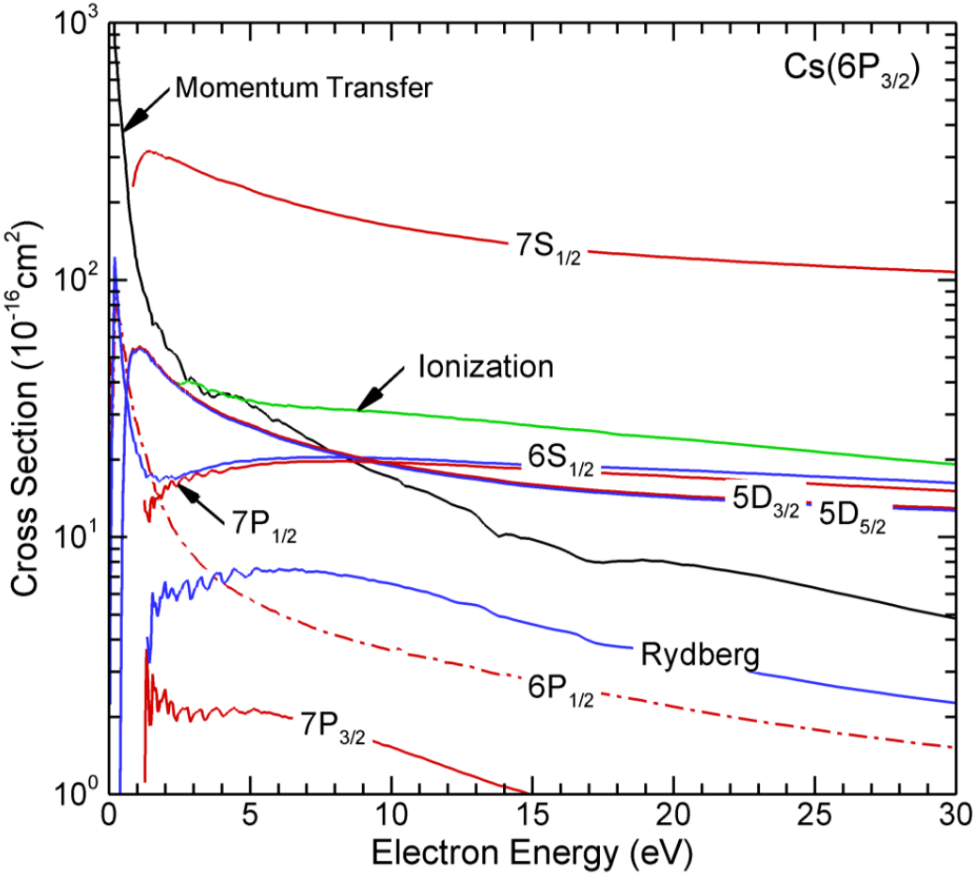
This article discusses applications of Bayesian machine learning for quantum molecular dynamics. One particular formulation of quantum dynamics advocated here is in the form of a machine learning simulator of the Schrödinger equation. If combined with the Bayesian statistics, such a simulator allows one to obtain not only the quantum predictions but also the error bars of the dynamical results associated with uncertainties of inputs (such as the potential energy surface or non-adiabatic couplings) into the nuclear Schrödinger equation. Instead of viewing atoms as undergoing dynamics on a given potential energy surface, Bayesian machine learning allows one to formulate the problem as the Schrödinger equation with a non-parametric distribution of potential energy surfaces that becomes conditioned by the desired dynamical properties (such as the experimental measurements). Machine learning models of the Schrödinger equation solutions can identify the sensitivity of the dynamical properties to different parts of the potential surface, the collision energy, angular momentum, external field parameters and basis sets used for the calculations. This can be used to inform the design of efficient quantum dynamics calculations. Machine learning models can also be used to correlate rigorous results with approximate calculations, providing accurate interpolation of exact results. Finally, there is evidence that it is possible to build Bayesian machine learning models capable of physically extrapolating the solutions of the Schrödinger equation. This is particularly valuable as such models could complement common discovery tools to explore physical properties at Hamiltonian parameters not accessible by rigorous quantum calculations or experiments, and potentially be used to accelerate the numerical integration of the nuclear Schrödinger equation.



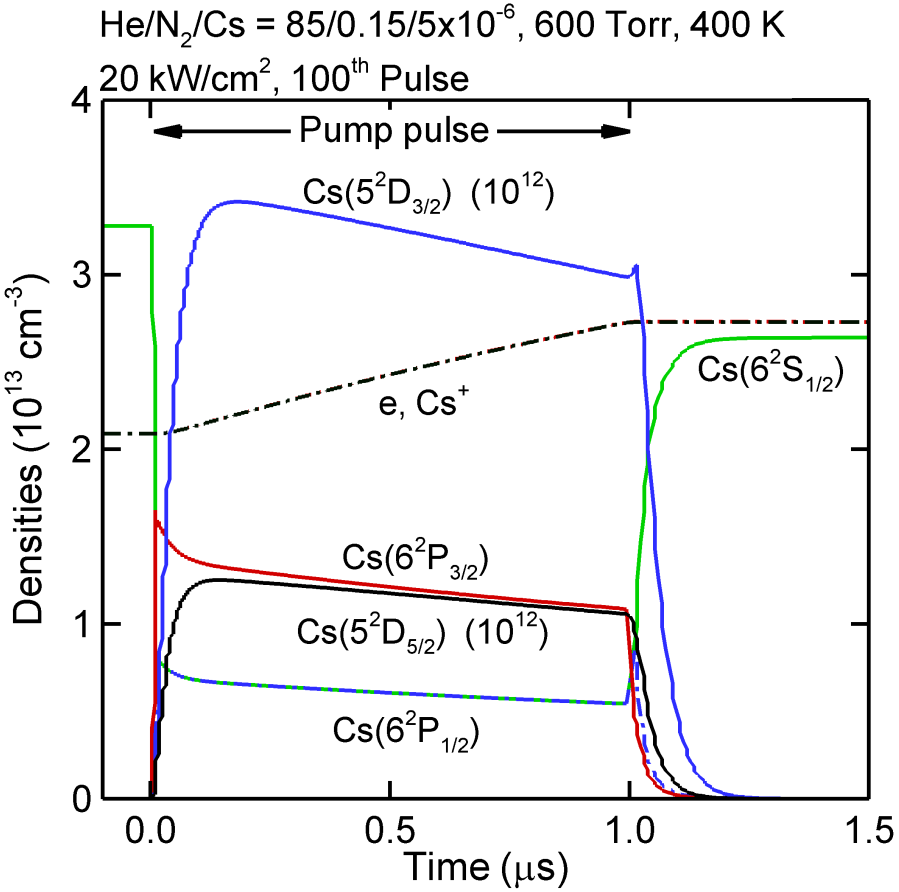
Closing the Loop:
Collision Input —> Modeling Output —> System Information

Modeling a Cs-based DPAL

Input: DBSR cross sections



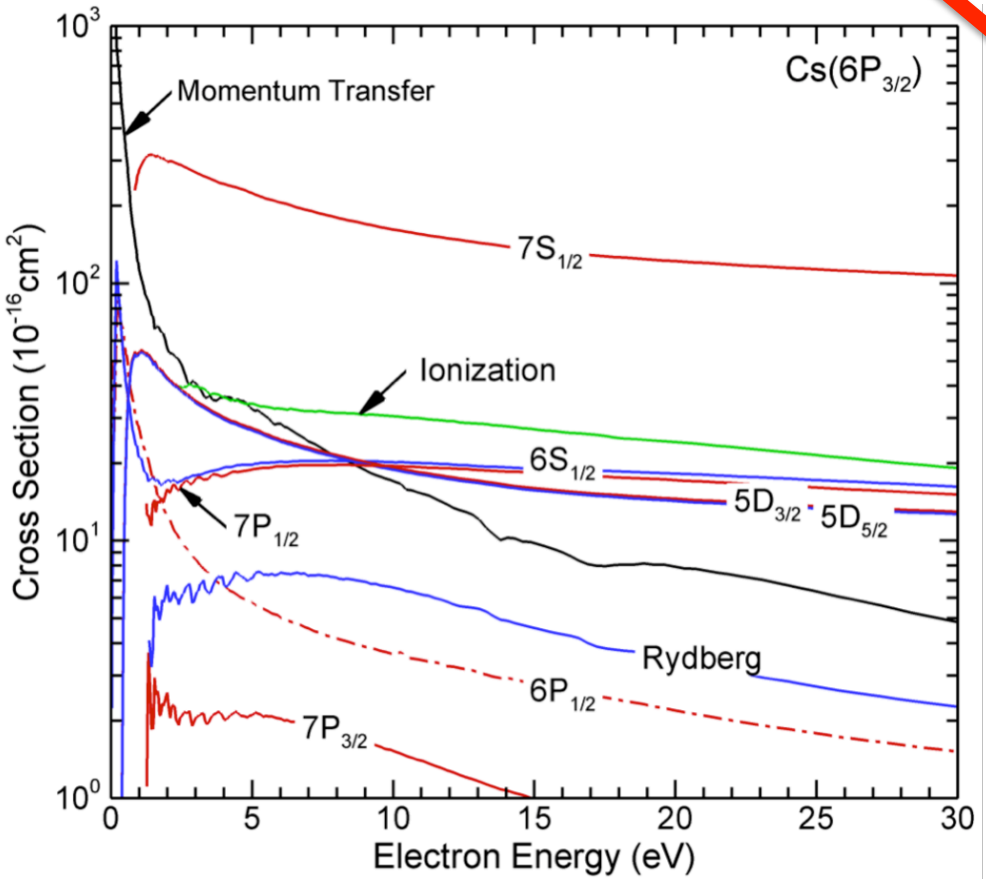
Output (M. J. Kushner's group): Densities of various species



Modeling a Cs-based DPAL

Information: There is significant plasma formation after a number of shots. This reduces the length of the pump pulse due to depletion of the neutral levels.

Input: DBSR cross sections



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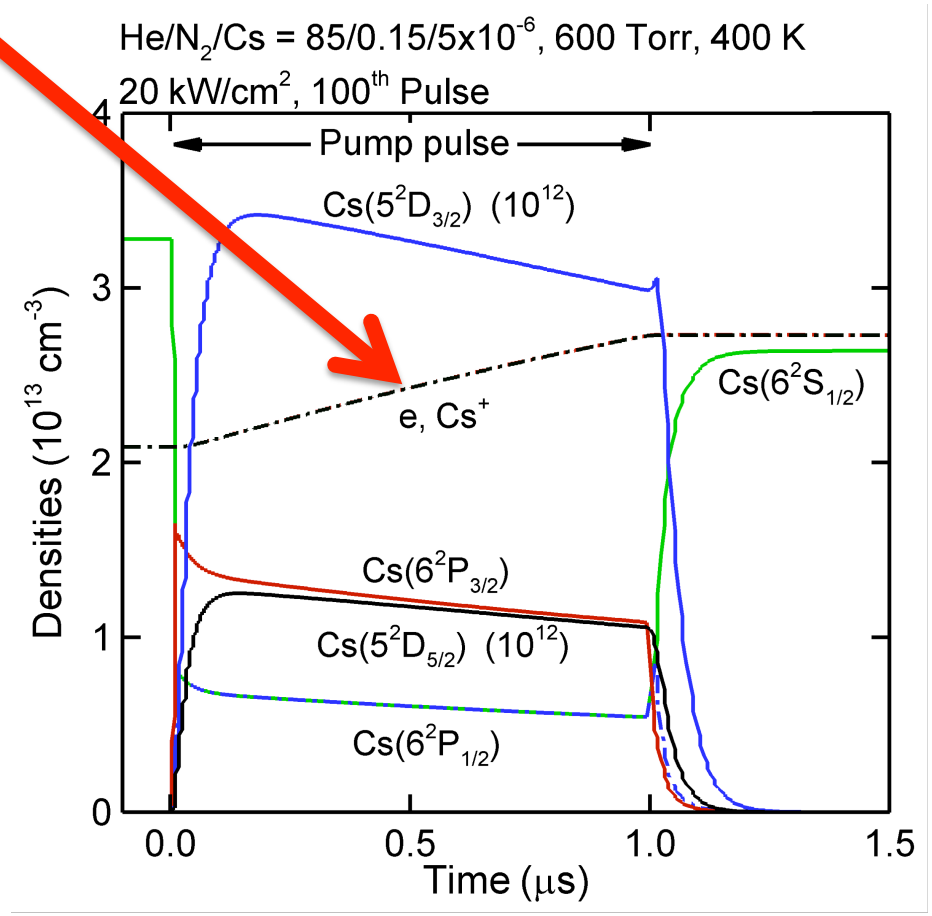

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- **Experimental benchmark data remain very important to test and push theory!**

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  - **The cross sections need to be combined with reliable plasma models. Maybe machine optimization can replace or even improve upon the work done by individuals whose datasets are available, for example, on LXCat.**
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