Electron Collisions with Atoms and Ions --- A Solved Problem?

GEC Don Madison Workshop, Oct. 9, 2023

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Extreme Science and Engineering Discovery Environment

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NSF support: PHY-1803844, OAC-1834740, PHY-2110023, OAC-2311928

Overview

- A few personal remarks about Don Madison
- The need for atomic and molecular data (again!)
- An (incomplete) overview of experimental methods
- An (incomplete) overview of theoretical methods
- Examples
- Where can you find the data?
- Can you produce them yourself?
- Summary and Conclusions

I have a lot of slides, which I am happy to share.

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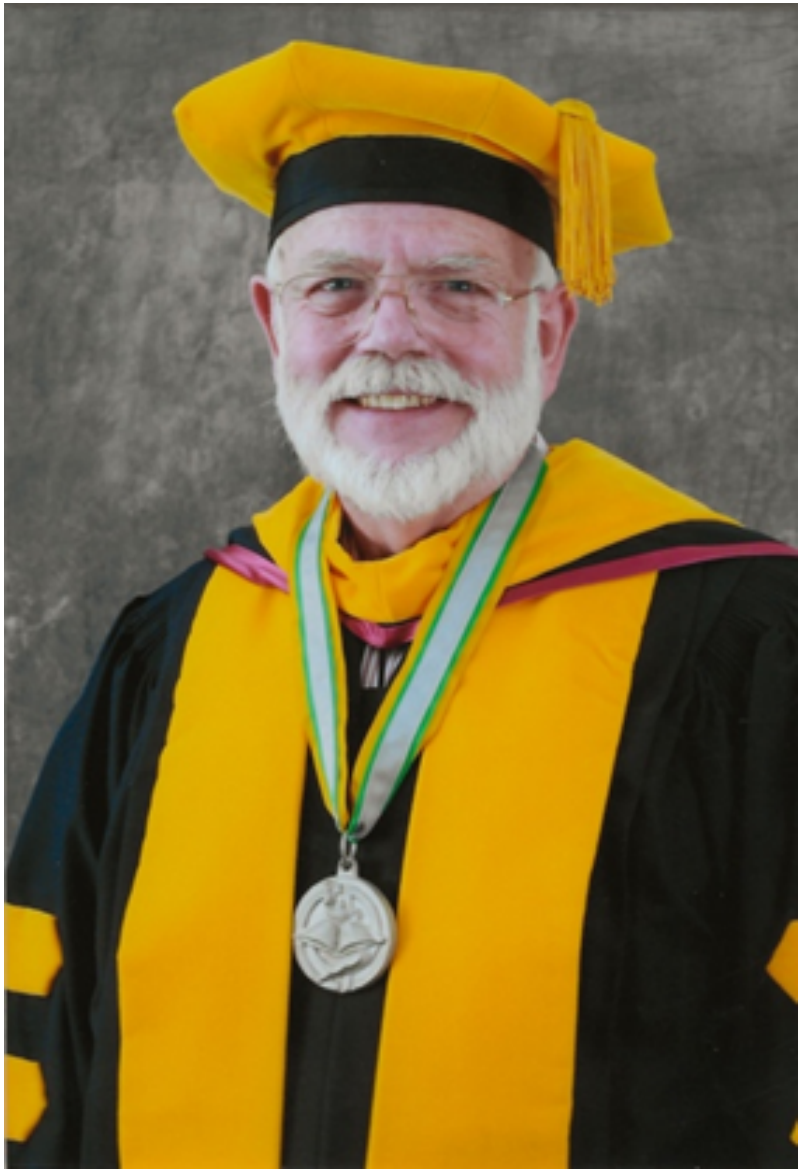
https://engage.aps.org/damop/blogs/charles-w-s-conover1/2022/05/26/tribute-to-prof-don-madison-from-klaus

Tribute to Prof. Don Madison from Klaus Bartschat and Timothy Gay



With deep sadness, we inform the scientific community that Don Madison, Curator's Professor at the Missouri University of Science and Technology, passed away on May 14, 2022.

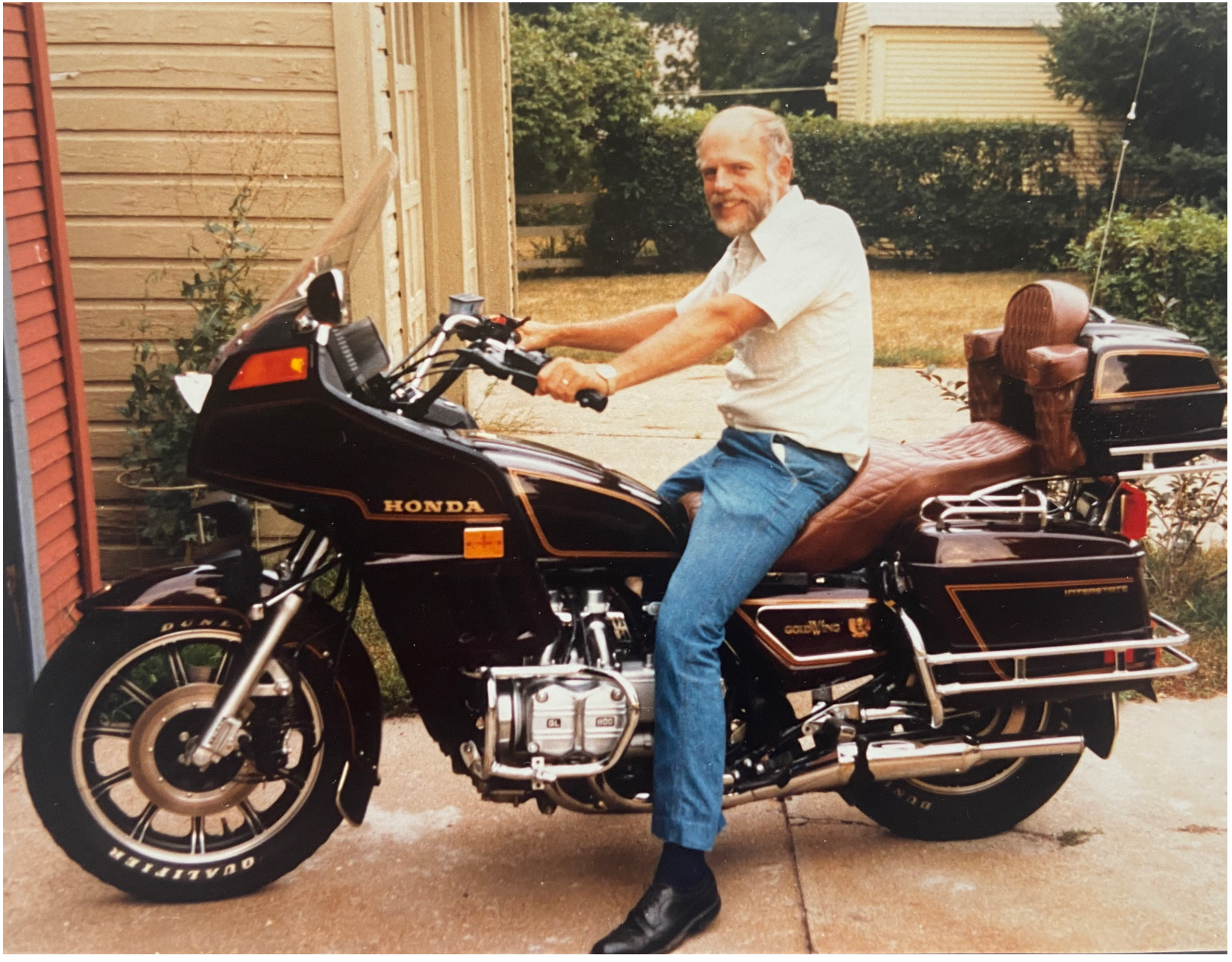
Don Harvey Madison was born in Pierre, South Dakota, on January 4, 1945 ....

Some career highlights:

287 papers
130 invited talks
APS Fellow
Levitt Professor at Drake University
Curator's Professor at Missouri University
Recipient of many teaching awards
Initiator of DAMOP Session on Undergraduate Research
Director of LAMOR
TAMOC Chair 1994 – 1998
Organizer of ICPEAC Satellite in 2001
GEC Treasurer 2002 – 2006

Some pictures from the past:

Don and his beloved motorcycle



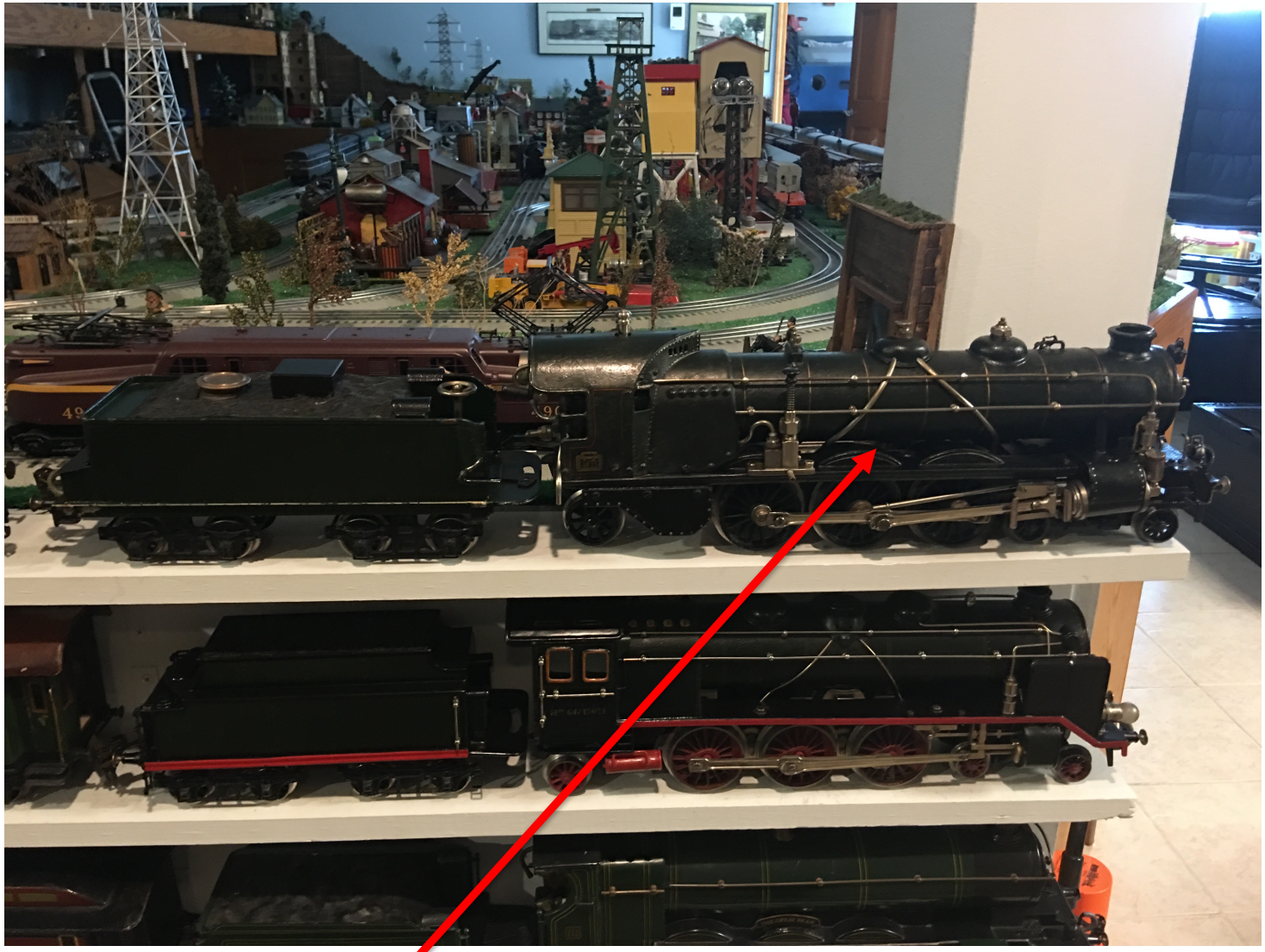
Don, Lina, Lisa, Kristi in 1985

The Madisons were incredibly generous hosts

4101 Ovid Avenue in Des Moines

I stayed there (**for free!**) for 2 months (!!!) in 1986 as part of the Madison family.

One more thing about the “other side” of Don:
In addition to family, friends, and physics, he loved his trains.



I believe this one is very precious, but I am not sure … 🤔

He had an entire (big) room in the house for them.

From now on it's mostly physics

FYI: Don did not just do First-Order DWBA – here is a (nearly random) selection of topics
More (not complete): https://academictree.org/physics/publications.php?pid=552188

Madison DH, Stewart ME, McCarthy IE, Stelbovics A. Third-order effects of electron-hydrogen scattering *Journal of Physics B: Atomic and Molecular Physics*. 16: 1063-1075 (**1983**). DOI: 10.1088/0022-3700/16/6/020

Tiwary SN, Macek J, **Madison DH**. Electron excitation of Auger transitions in atoms *Physical Review A*. 32: 2541-2543 (**1985**). DOI: 10.1103/Physreva.32.2541

Rudd ME, Kim YK, **Madison DH**, Gallagher JW. Electron production in proton collisions: Total cross sections *Reviews of Modern Physics*. 57: 965-994 (**1985**). DOI: 10.1103/RevModPhys.57.965

Madison DH, Csanak G, Cartwright DC. The sign of the orientation parameter in electron-photon coincidence experiments *Journal of Physics B: Atomic and Molecular Physics*. 19: 3361-3366 (1986). DOI: 10.1088/0022-3700/19/20/019

Bottcher C, Schultz DR, **Madison DH**. Correlated two-electron wave functions of any symmetry *Physical Review A*. 49: 1714-1723 (**1994**). DOI:

Jones S, **Madison DH**, Hanne GF. Spin-resolved (e,2e) coincidences for heavy rare-gas targets *Physical Review Letters*. 72: 2554-2556 (**1994**). DOI: 10.1103/Physrevlett.72.2554

Streun M, Baum G, Blask W, Rasch J, Bray I, Fursa DV, Jones S, **Madison DH**, Walters HRJ, Whelan CT. Spin dependence of (e,2e) collisions on lithium at 54.4 eV *Journal of Physics B: Atomic, Molecular and Optical Physics*. 31: 4401-4411 (**1998**). DOI: 10.1088/0953-4075/31/19/022

Buffington GD, **Madison DH**, Peacher JL, Schultz DR. Lattice, time-dependent approach for electron-hydrogen scattering *Journal of Physics B: Atomic, Molecular and Optical Physics*. 32: 2991-3001 (**1999**). DOI: 10.1088/0953-4075/32/12/316

DuBois RD, Doudna C, Lloyd C, Kahveci M, Khayyat K, Zhou Y, **Madison DH**. Energy-loss measurements for single and multiple ionization of argon by positron impact *Journal of Physics B: Atomic, Molecular and Optical Physics*. 34 (**2001**). DOI: 10.1088/0953-4075/34/24/105

Tabanli MM, Peacher JL, **Madison DH**. A convenient formalism for Auger and autoionization of overlapping resonances *Journal of Physics B: Atomic, Molecular and Optical Physics*. 36: 217-233 (**2003**). DOI: 10.1088/0953-4075/36/2/304

Jones S, Macek JH, **Madison DH**. Three-Coulomb-wave Pluvinage model for Compton double ionization of helium in the region of the cross-section maximum *Physical Review a - Atomic, Molecular, and Optical Physics*. 72 (**2005**). DOI: 10.1103/Physreva.72.012718

Milne-Brownlie DS, Foster M, Gao J, Lohmann B, **Madison DH**. Young-type interference in (e, 2e) ionization of H_2. *Physical Review Letters*. 96: 233201 (**2006**). DOI: 10.1103/Physrevlett.96.233201

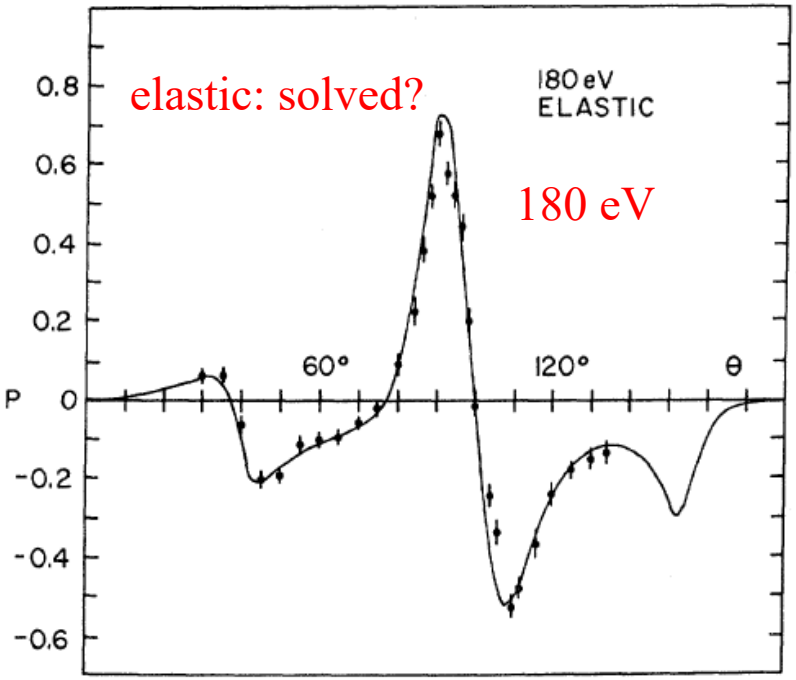
Colgan J, Al-Hagan O, **Madison DH**, Murray AJ, Pindzola MS. Deep interference minima in non-coplanar triple differential cross sections for the electron-impact ionization of small atoms and molecules *Journal of Physics B: Atomic, Molecular and Optical Physics*. 42 (**2009**). DOI: 10.1088/0953-4075/42/17/171001

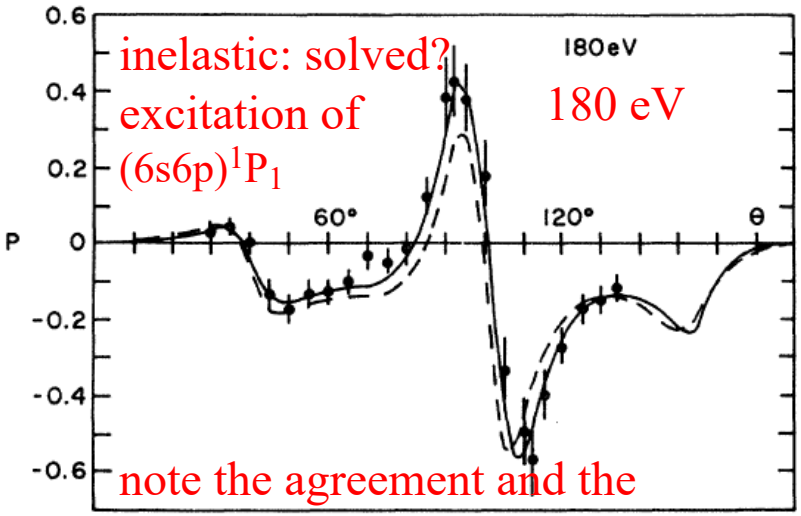
Armstrong GSJ, Colgan J, Pindzola MS, Amami S, **Madison DH**, Pursehouse J, Nixon KL, Murray AJ. Evidence for unnatural-parity contributions to electron-impact ionization of laser-aligned atoms *Physical Review a - Atomic, Molecular, and Optical Physics*. 92 (**2015**). DOI: 10.1103/Physreva.92.032706

Ali E, **Madison D**. Multicenter distorted-wave approach for electron-impact ionization of molecules *Physical Review A*. 100 (**2019**). DOI: 10.1103/PHYSREVA.100.012712

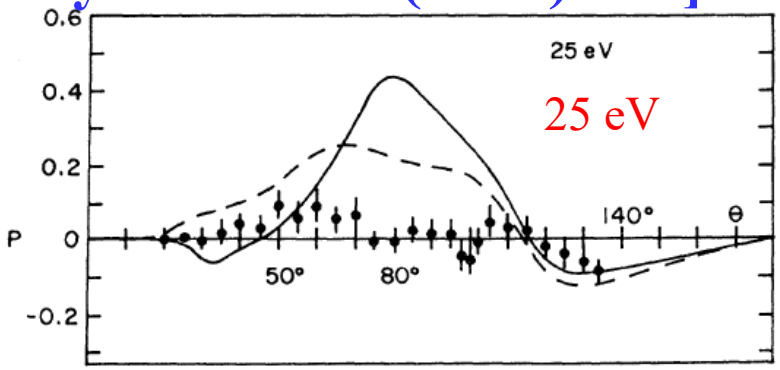
Ali E, Chakraborty HS, **Madison DH**. Improved theoretical calculations for electron-impact ionization of DNA analogue molecules. *The Journal of Chemical Physics*. 152: 124303 (**2020**). DOI: 10.1063/1.5143148

Spin Polarization in e-Hg Collisions
[Work from Don's PhD thesis; Phys. Rev. A 7 (1973) 514]





note the agreement and the similarity to elastic scattering



inelastic at lower energies: unsolved!

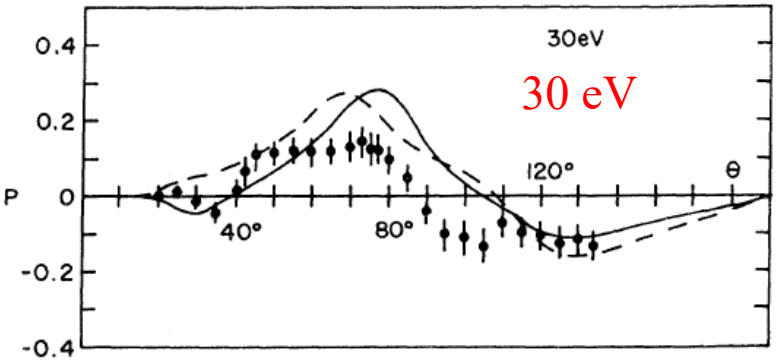


FIG. 1. Theoretical and experimental spin polarizations of scattered electrons following excitation of the $6s6p\ ^1P_1$ state of mercury at incident-electron energies of 25 and 30 eV. The theoretical curves are DW calculations performed using Mayer's potential (solid line) and Coulthard's potential (dashed line). The experimental data are those of Eitel and Kessler.

This topic was studied experimentally in great detail in Münster by J. Keßler, G.F. Hanne, and their students (including me!)

This paper might have given me the position at Drake after Don left for Missouri-Rolla in 1987 😊

J. Phys. B: At. Mol. Phys. **20** (1987) 5839–5863. Printed in the UK

Electron impact excitation of rare gases: differential cross sections and angular correlation parameters for neon, argon, krypton and xenon

K Bartschat† and D H Madison

Physics Department, Drake University, Des Moines, Iowa 50311, USA

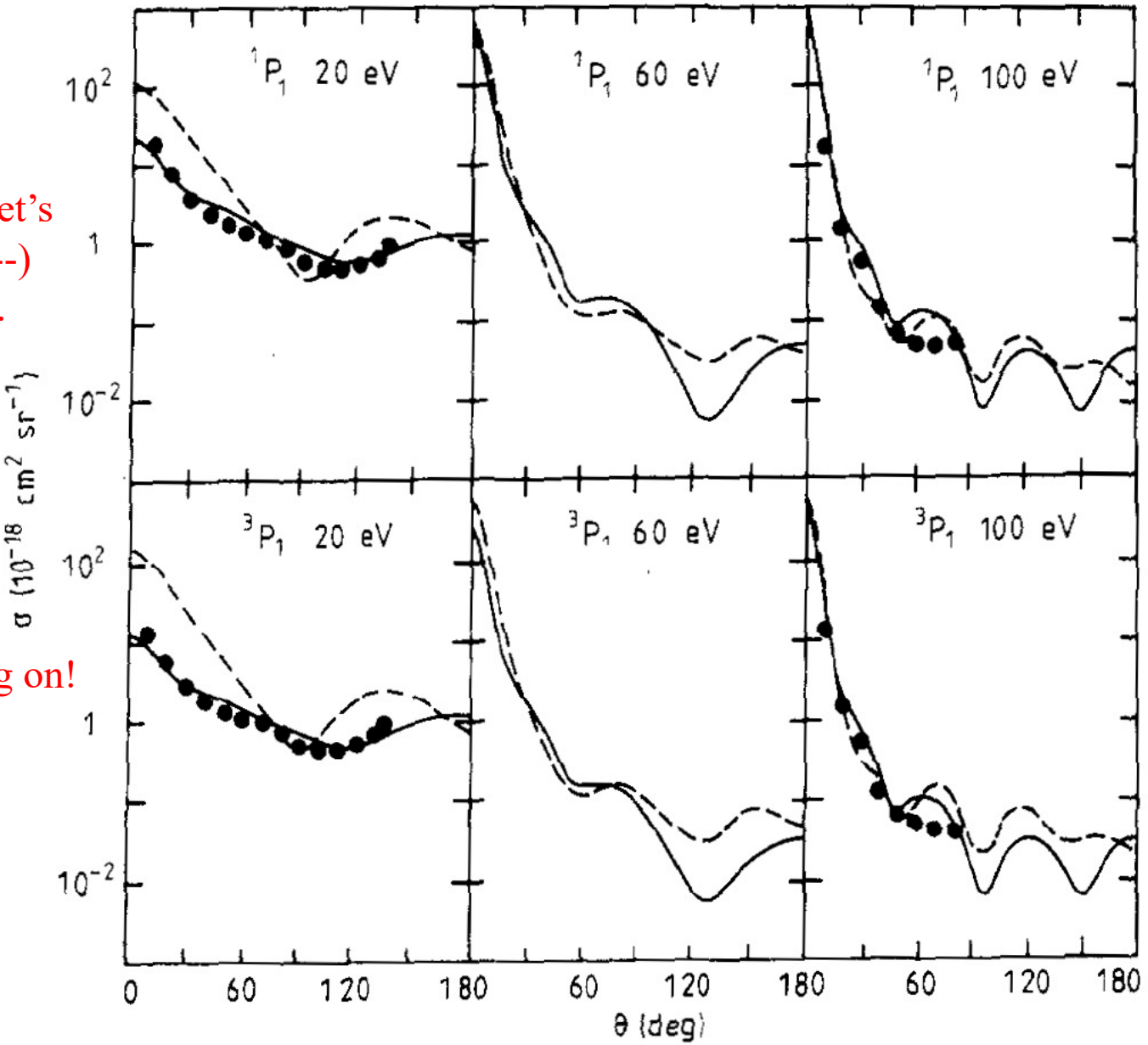
Received 13 May 1987

Abstract. Distorted-wave Born approximation results for the differential cross sections and various angular correlation parameters for electron impact excitation of the rare gases Ne, Ar, Kr and Xe are presented and compared with recent experimental data and other theoretical calculations. The sensitivity of the results to different static and optical potentials in the calculation of the distorted waves is analysed and the importance of relativistic effects both in the description of the target states (intermediate coupling) as well as in the wavefunction for the continuum electron is investigated. The overall agreement with the available experimental data is very satisfactory over a wide range of incident-electron energies.

Electron-impact excitation of Kr ($4p^5 5s$) J=1 angle-differential cross section

Without giving names, let's just say that the other (---) calculation looks wrong.

Solved?
Not so fast – please hang on!



More Acknowledgements:

Oleg Zatsarinny

(4.11.1953 – 2.3.2021)

was a close collaborator at Drake University since 2003.

Oleg produced a lot of high-quality data with his B-spline R-matrix (BSR) code.

Phil Burke

(18.10.1932 – 3.6.2019)

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

Kathryn Hamilton

Former post-doctoral researcher at Drake University; now Asst. Prof. at CU-Denver

Kathryn performs calculations on many projects and maintains the BSR code on the AMOS Gateway.

PHY-1803844; PHY-2110023; OAC-1834740; OAC-2311928

PERSPECTIVE

This describes the connection between data producers and data users, as well as fundamental research and applications.

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

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

Proc. Nat. Acad. of Sciences 113 (2016) 7026

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

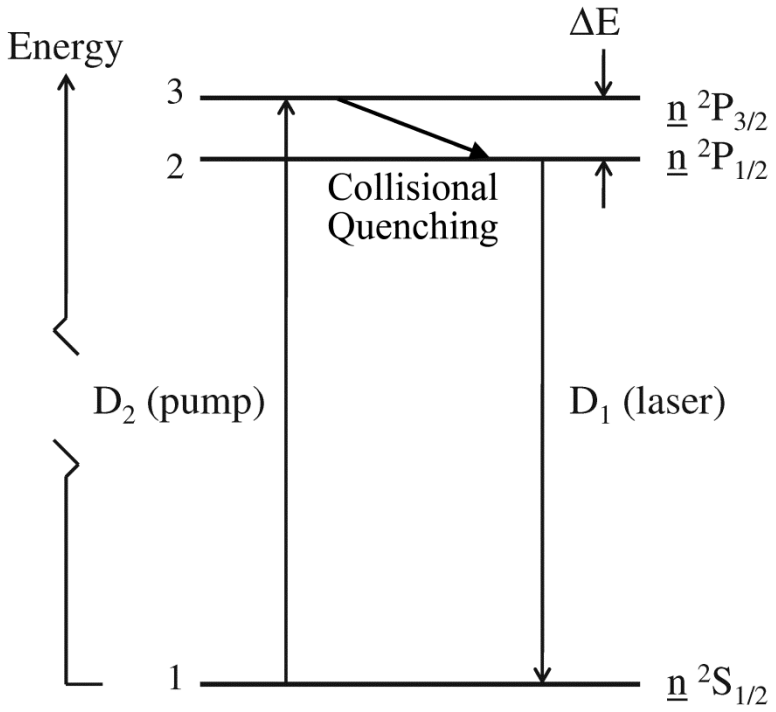
Electron collisions with atoms, ions, molecules, and surfaces are critically important to the understanding and modeling of low-temperature plasmas (LTPs), and so in the development of technologies based on LTPs. Recent progress in obtaining experimental benchmark data and the development of highly sophisticated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

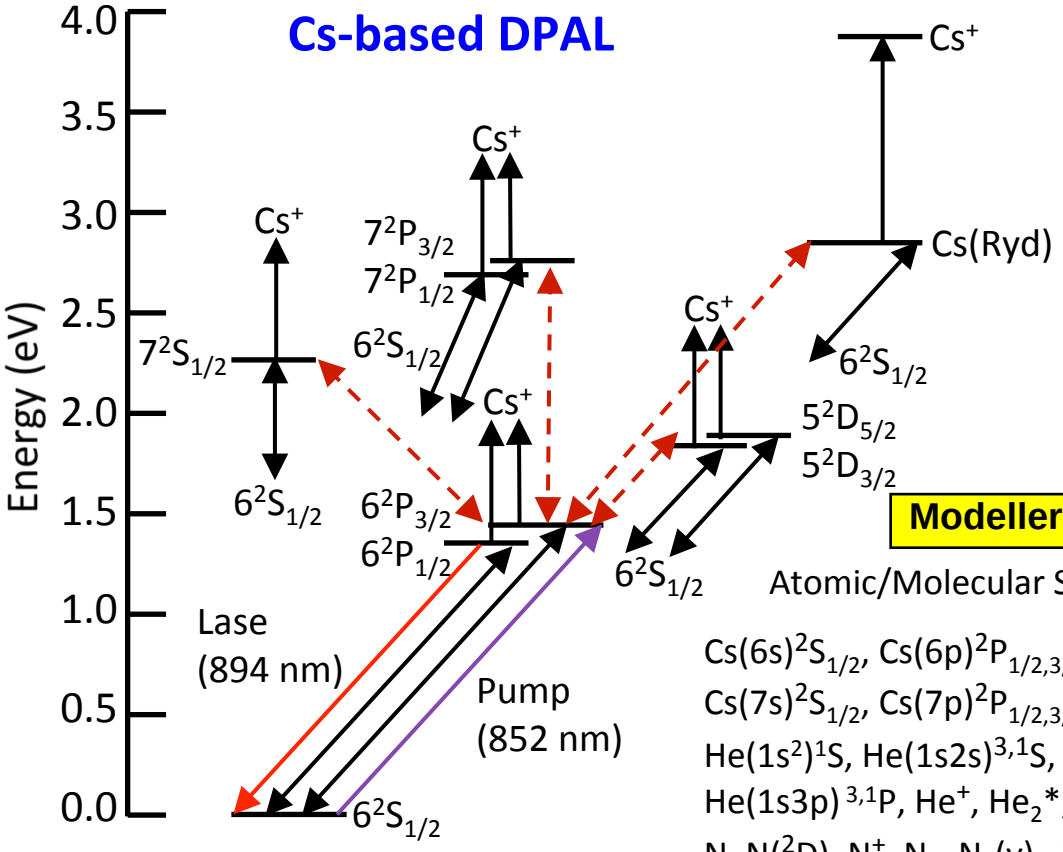
DIODE-PUMPED ALKALI LASERS (DPALs)

- **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.)



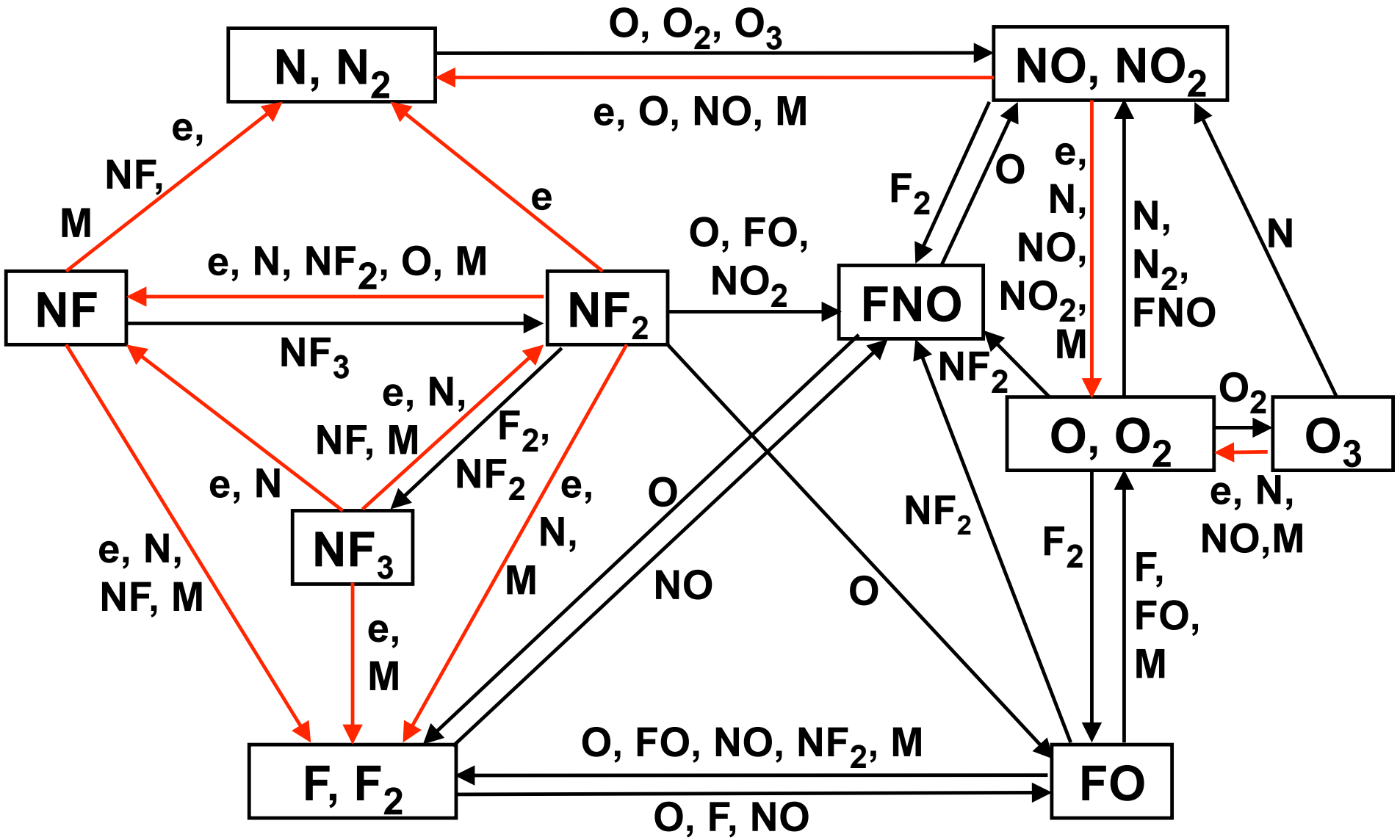
Modellers need a lot of data!

Atomic/Molecular Species in the Model

$Cs(6s)^2S_{1/2}$, $Cs(6p)^2P_{1/2,3/2}$, $Cs(5d)^2D_{5/2,3/2}$,
$Cs(7s)^2S_{1/2}$, $Cs(7p)^2P_{1/2,3/2}$, Cs(Ryd), Cs^+, Cs_2, Cs_2^+
$He(1s^2)^1S$, $He(1s2s)^{3,1}S$, $He(1s2p)^{3,1}P$, $He(1s3s)^{3,1}S$,
$He(1s3p)^{3,1}P$, He^+, He_2*, He_2^+
N, $N(^2D)$, N^+, N_2, $N_2(v)$, $N_2(A)$, $N_2(B,C)$, N_2^+,N_4^+

WOW! Modelers need a lot of data ...

[This is for a diode-pumped alkali laser (PSST 23 (2014) 035011]



Modeling EUV light source plasmas for nanolithography

Another example [Invited Talk at ICPEAC 2023 in Ottawa Canada]

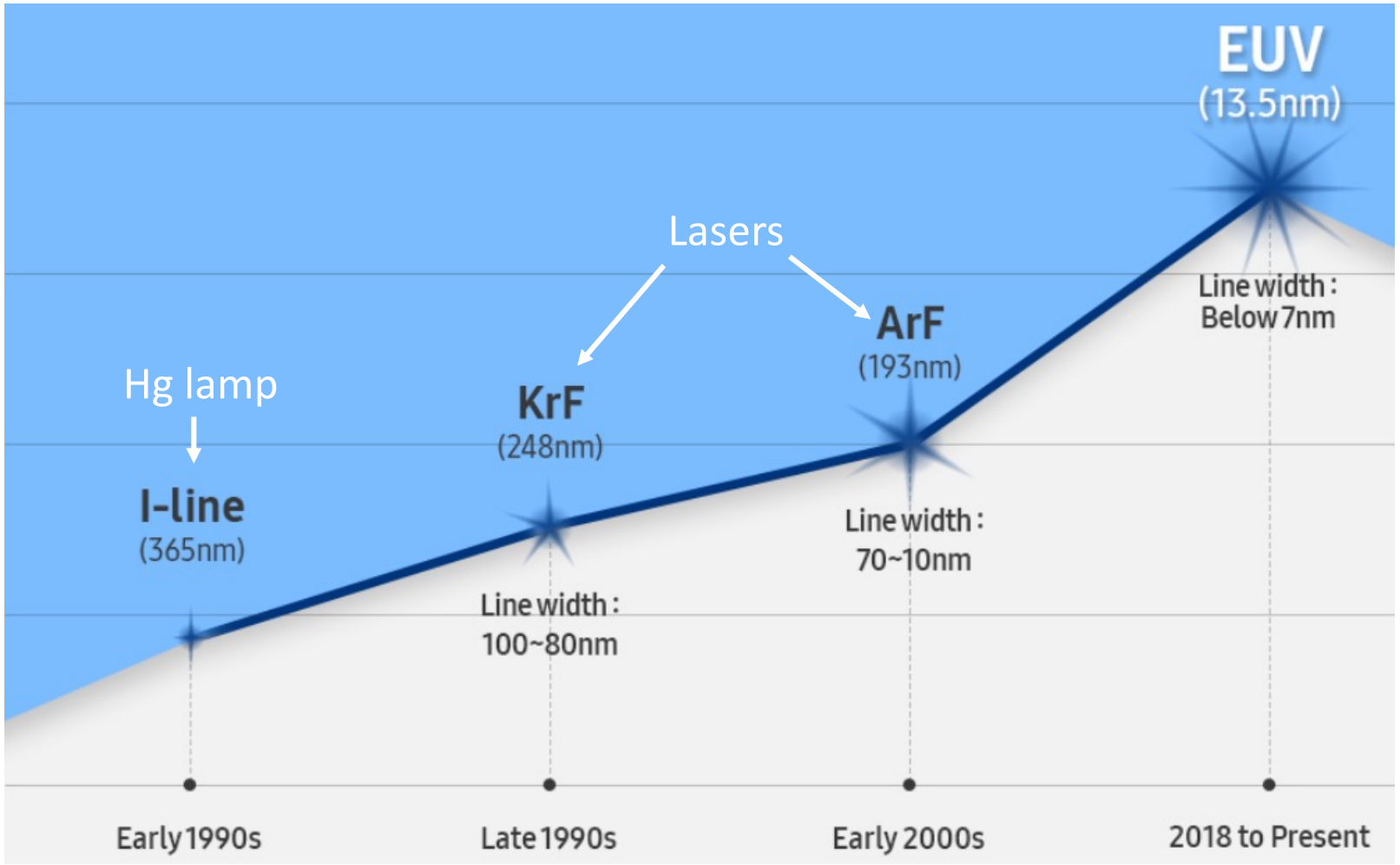
John Sheil

Advanced Research Center for Nanolithography, Amsterdam, The Netherlands

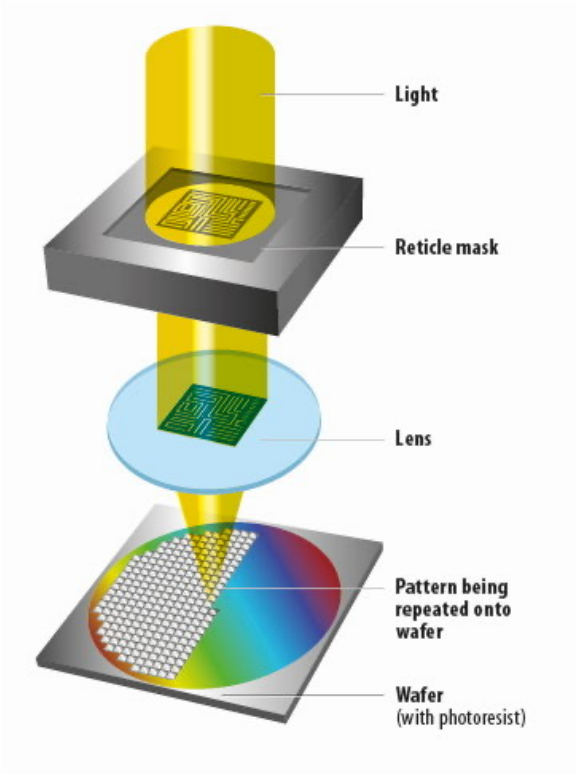
Department of Physics and Astronomy, and LaserLab, Vrije Universiteit Amsterdam, Amsterdam, The Netherlands

Light sources for lithography

Industrial light sources



Lithography

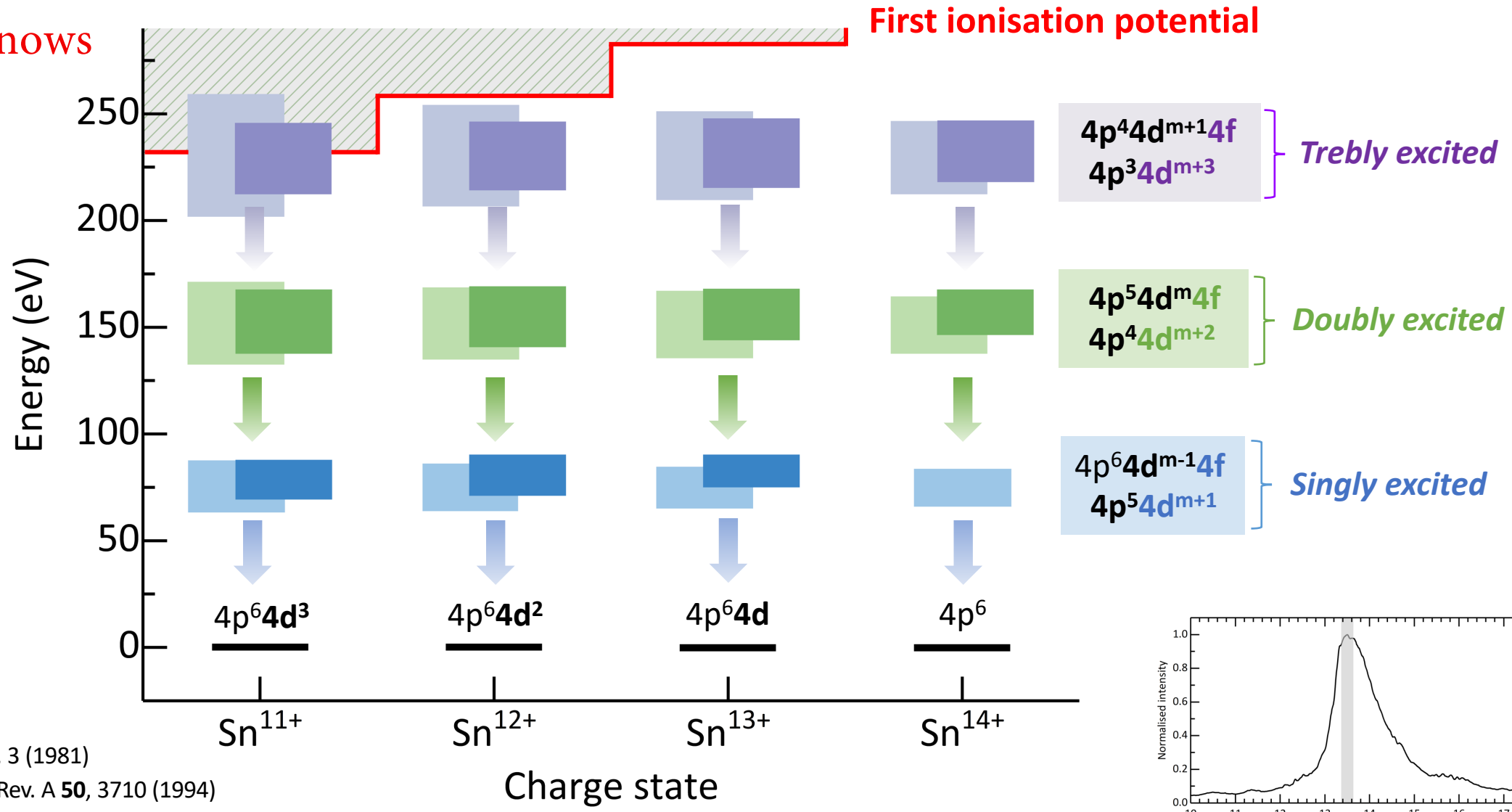


$$Critical\ dimension \propto \frac{\lambda}{NA}$$

Origin of EUV light

James Colgan knows a lot about this.

Tin (Sn) charge states are bred in the plasma



O'Sullivan and Carroll, JOSA **71**, 3 (1981)

Svendsen and O'Sullivan, Phys Rev. A **50**, 3710 (1994)

Churilov and Ryabtsev, Phys. Scr. **73**, 614 (2006), Sasaki *et al.,* J. Appl. Phys. **107**, 113303 (2010)

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"!

Let's start with experiment: Total Cross Sections

PHYSICAL REVIEW A VOLUME 19, NUMBER 2 FEBRUARY 1979

Absolute total cross sections for electron-mercury scattering

K. Jost and B. Ohnemus
Physikalisches Institut, Westfälische Wilhelms Universität, Münster, Germany
(Received 25 April 1978)

The total cross section for e^--Hg scattering has been measured in the energy range between 0.1 and 500 eV. Absolute data taken at a few energies by means of a static target were used to normalize the relative cross sections, which were measured in the whole energy range by scattering from an atomic beam. This technique was used to help meet the high-angular-resolution requirements. The cross sections obtained are considerably larger than those obtained in most of the other measurements performed around 1930. Satisfactory agreement is found, however, with semiempirical cross sections (mainly based on recent measurements) and with a recent theoretical calculation. The most pronounced structure is a cross section maximum at 0.4 eV, which probably can be ascribed to a $(6s\,^2 6p_{1/2})^2P_{1/2}$ shape resonance.

Nevertheless, there are surprisingly few measurements of the total cross section,[3-6] and moreover these are not very recent. These old data are now considered to be rather unreliable.[7]

Transmission Setup: $I = I_0 \exp(-nlQ)$

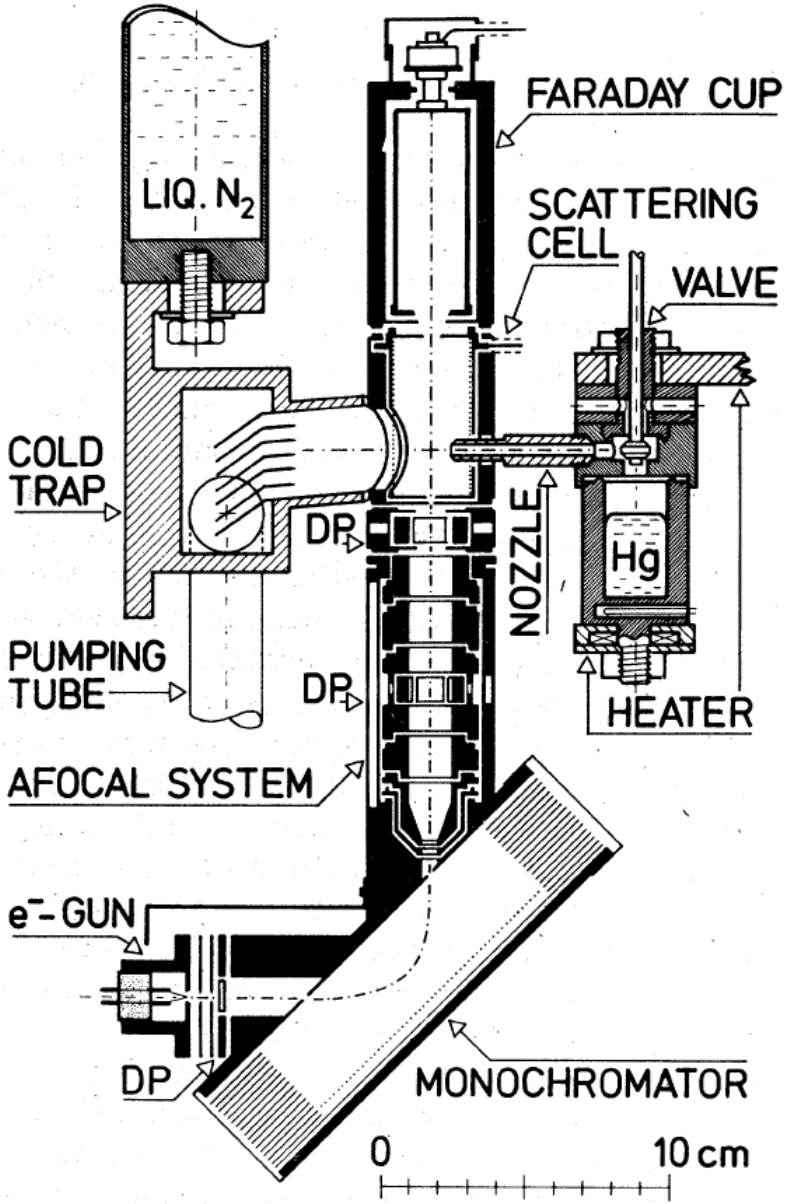


FIG. 1. Electron optical arrangement for low energie (0.1–70 eV) with atomic beam target. Deflector plates are denoted by DP.

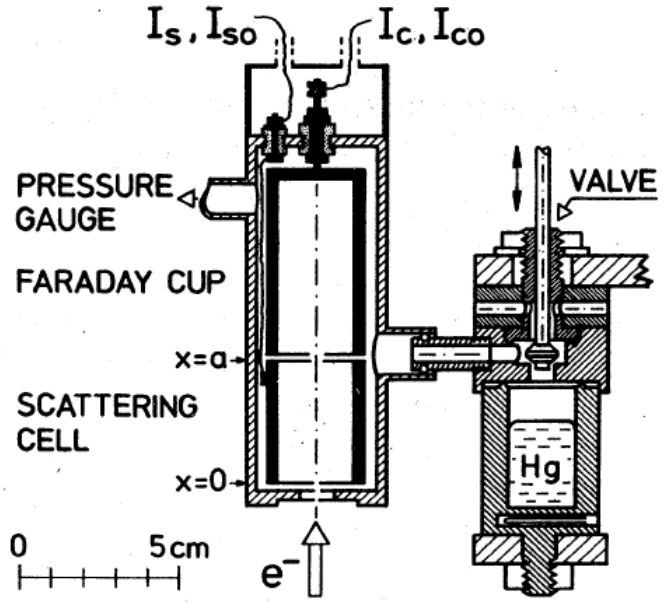


FIG. 3. Target cell for absolute measurements. This arrangement is used together with the electron optics of Fig. 1.

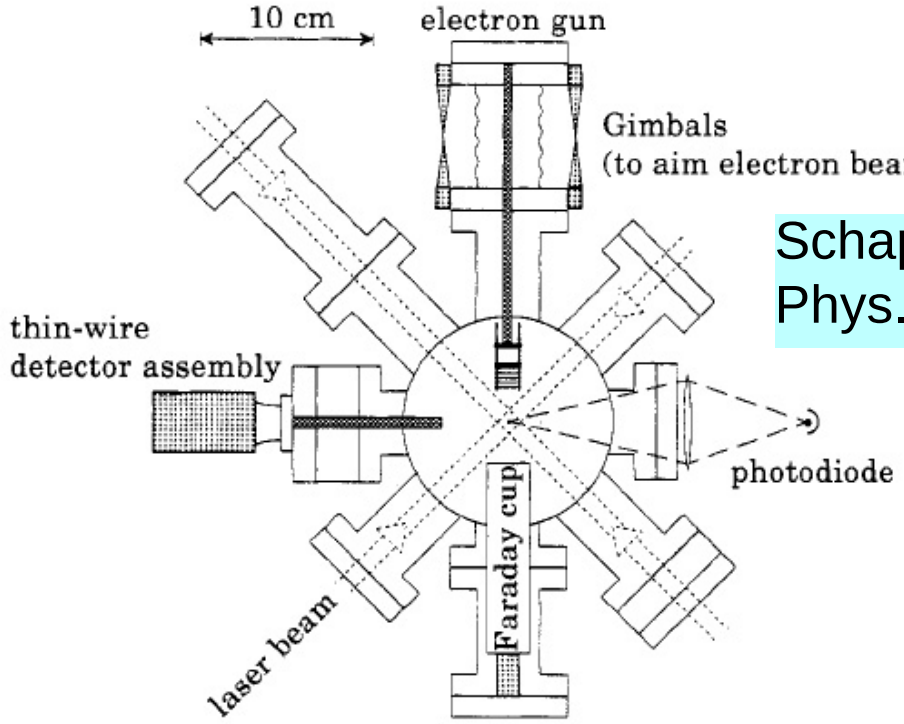
$$I = I_0 \exp(-nlQ)\,, \tag{1}$$

where

$$Q = (nl)^{-1} \ln(I_0/I) \sim \ln(I_0/I) \tag{2}$$

is the total cross section. An absolute measurement of Q requires knowledge of n and l, whereas the relative shape of the cross-section curve versus energy E can be obtained even in an inhomogeneous target such as an atomic beam, if care is taken to keep the product of mean path length l and mean target density n constant during the measurement. In order to check the constancy

Trap Setup: Loss Rate $\Gamma_e = \sigma J/e$



Schappe, Walker, Anderson, Lin;
Phys. Rev. Lett. **76** (1996) 4328

further developed by
J.F. McConkey
and collaborators

Fig. 1. – Schematic diagram of the vacuum chamber. Not shown are two of the laser beams, the magnetic-field coils, and the diode laser with its stabilization and modulation equipment.

When the electron beam is turned on, atoms are ejected from the trap due to the electron-atom collisions at a rate

$$\Gamma_e = \sigma J/e\,, \qquad (1)$$

where σ is the cross-section for ejecting the atoms from the trap, J is the electron current density, and e the electron charge.
By measuring Γ_e and J, we determine σ directly from eq. (1).

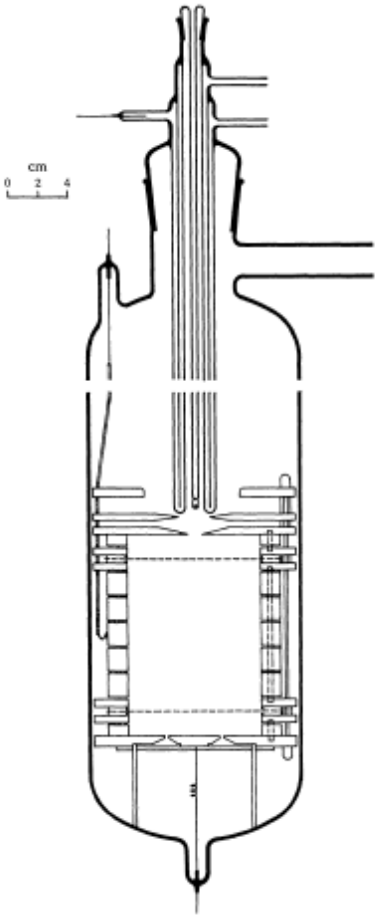
Note: The cross section is measured directly!

Swarm Experiments (Phelps, Crompton, ...)

THE MOMENTUM TRANSFER CROSS SECTION FOR ELECTRONS IN HELIUM

By R. W. Crompton,* M. T. Elford,* and R. L. Jory*†

Measurements of the drift velocity, the ratio of diffusion coefficient to mobility, and the "magnetic drift velocity" for electrons in helium have been made at 293°K in the range $1{\cdot}8\times10^{-19} < E/N < 3\times10^{-17}$ V cm². From an analysis of the drift velocity data, an energy-dependent momentum transfer cross section has been derived for which an error of less than ±2% is claimed over the central portion of the energy range. The cross section agrees with the theoretical cross section of ...



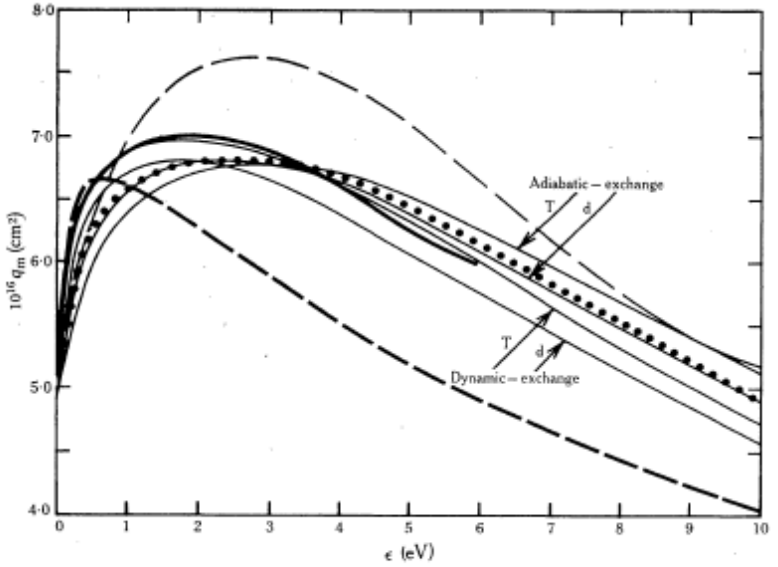


Fig. 7.—A comparison between theoretical and experimental momentum transfer cross sections. —— Crompton, Elford, and Jory; — — Frost and Phelps; — — Bauer and Browne; ——— La Bahn and Callaway; ••• Williamson and McDowell.

Since the first extensive calculations of the total scattering cross section by Morse and Allis (1933)...

Will Allis did calculations for this in 1933!

Swarm Experiments and Their Interpretation

- **Pioneered by "GEC Giants" such as Art Phelps and Bob Crompton.**
- **General Idea (thanks to Leanne Pitchford for enlightening me):**
  - Pull electrons through a gas and measure macroscopic parameters such as:
    - transition times ($\rightarrow$ **drift velocity, mobility**)
    - radial or axial spreading ($\rightarrow$ **diffusion coefficients**)
    - current growth ($\rightarrow$ **ionization rates**)
  - In "equilibrium conditions", these parameters depend on the **"reduced electric field"** $\boldsymbol{E/N}$, the **gas (composition)**, and the **relevant cross sections**. In low-energy elastic scattering, the **momentum transfer cross section** dominates.
- **Absolute** (momentum transfer) **cross sections** are determined **indirectly** as follows:

  indirect measurement

  (1) Assume an initial set of cross sections.
  (2) Calculate the macroscopic parameters.
  (3) Assume that any deviations are due to errors in the assumed cross sections.
  (4) Adjust the cross section(s) until things fit.
  (5) Hope for:
    - convergence of the procedure;
    - uniqueness of the results in multi-parameter fits.

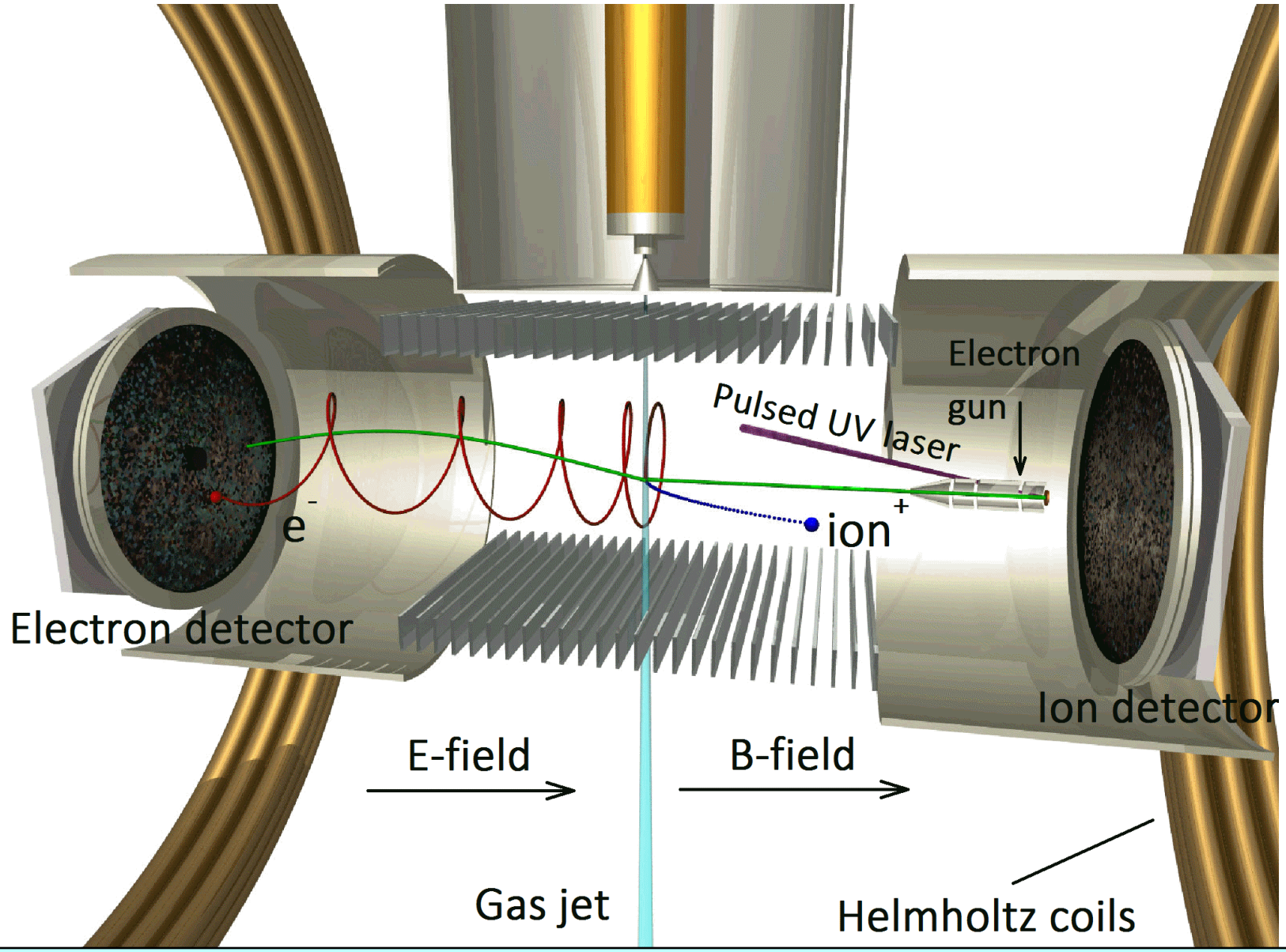
Other Techniques (Incomplete List)

- **Optical Emission**:
  - **State-Selective**
  - **Relative**
  - **Cascade Effects**
- **Time-of-Flight Setups (Metastables)**
- **Storage Rings (e-Ion Collisions)**
- **Integrate Angle-Differential Cross Sections from Crossed-Beam Setups**
  - **State-Selective** (measure energy loss/gain)
  - **Often Relative** – **Absolute Normalization Attempts** include
    - **Mixed-Flow Technique with a Reference Gas**
    - **Generalized Oscillator Strength**
    - **Help from Theory** (**Yes, we are good for something!**)

Sorry, but this talk is NOT a comprehensive review!

The Reaction Microscope

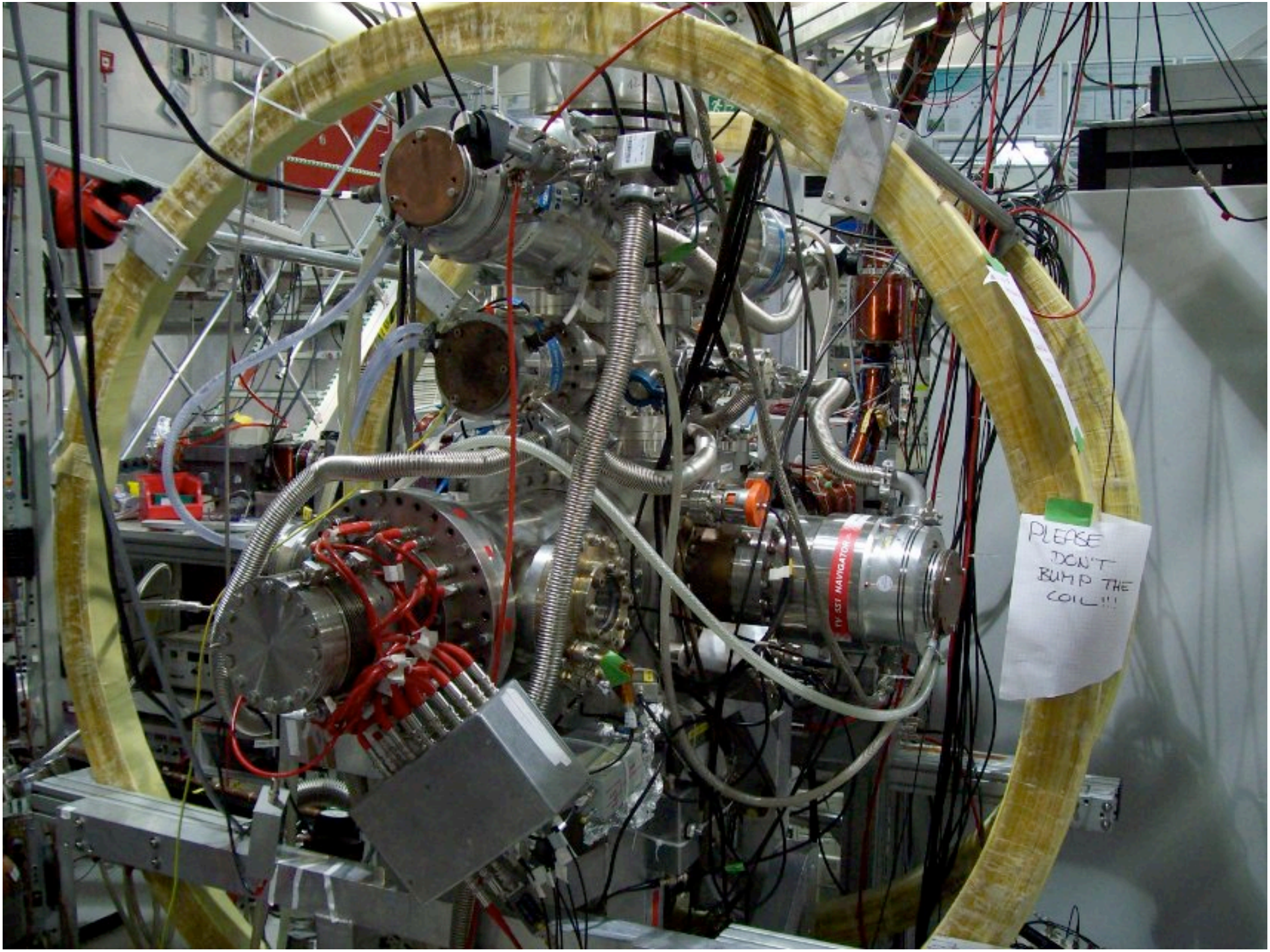
Ullrich, Moshammer, Dorn, *et al.*, Rep. Prog. Phys. 66 (2003) 1463



Used in A. Dorn's group for (e,2e) and even (e,2eγ)

They can get the full 3D-picture in a single shot!

This is how it really looks like!



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)**
- **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**
  - CCn, CCO, CCC, RMn, IERM, RMPS, DARC, BSR, ...
  - Standard method of treating low-energy scattering; based upon the expansion

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

  - 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 calculated between **non-relativistic wavefunctions**
- **Dirac-based approach**

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

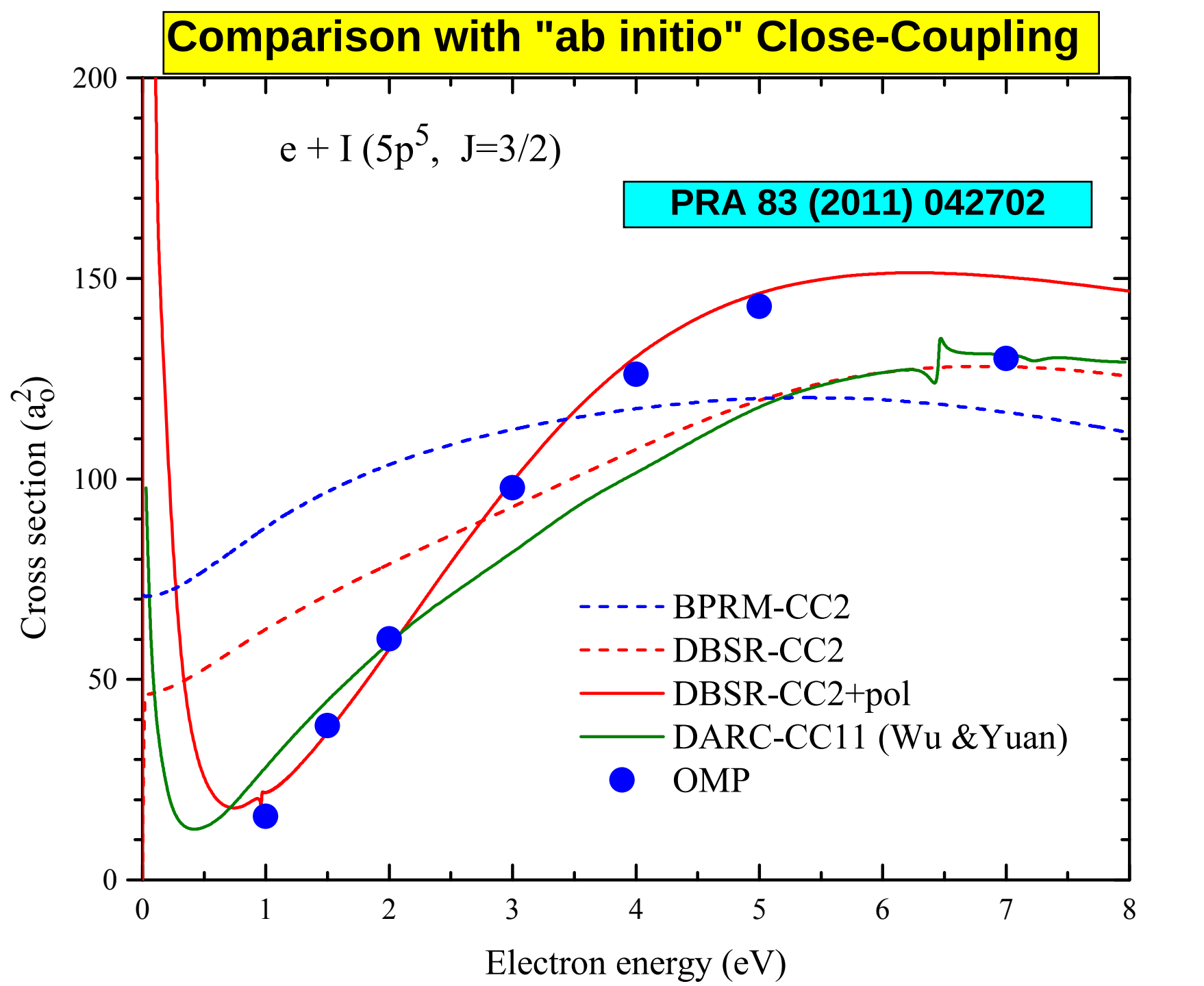
$$V_{\rm mp}(k,r) = V_{\rm static}(r) + V_{\rm exchange}(k,r) + V_{\rm polarization}(r) + iV_{\rm absorption}(k,r)$$

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

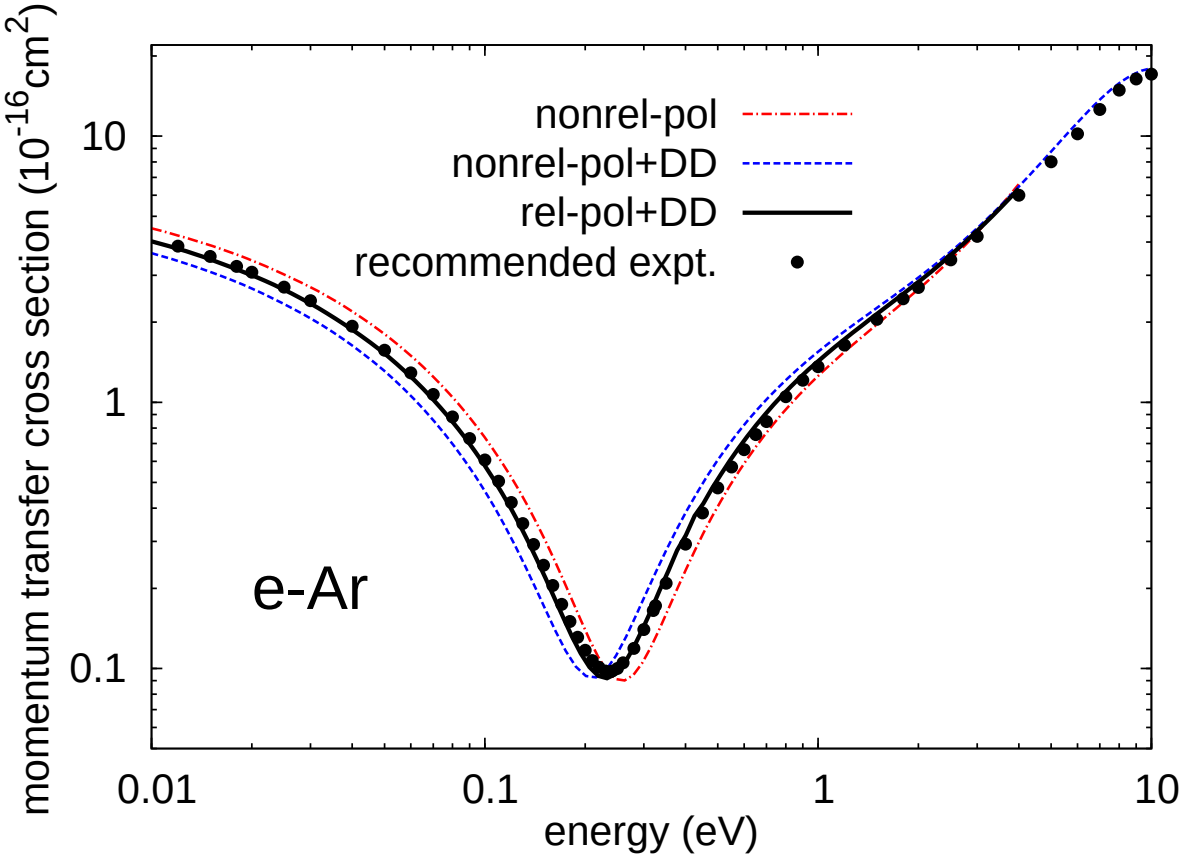
Polarized Orbital – an "Ab Initio Special Purpose" Approach

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

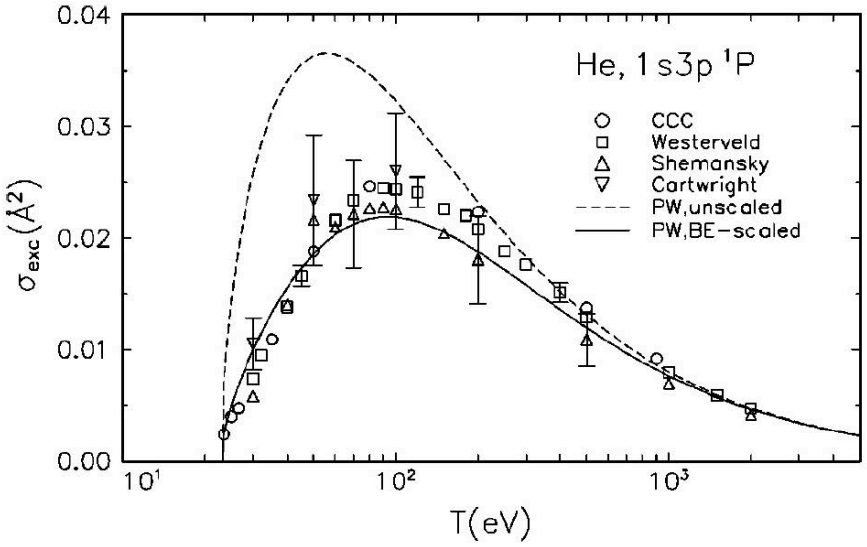
BEf-scaling; Plane-Wave Born with Experimental Optical Oscillator Strength and Empirical Energy Shift

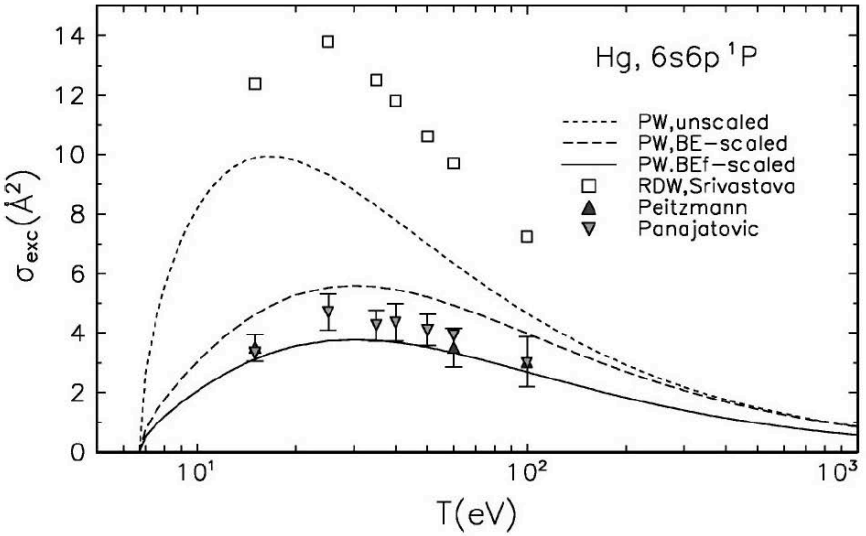
PHYSICAL REVIEW A, VOLUME 64, 032713

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

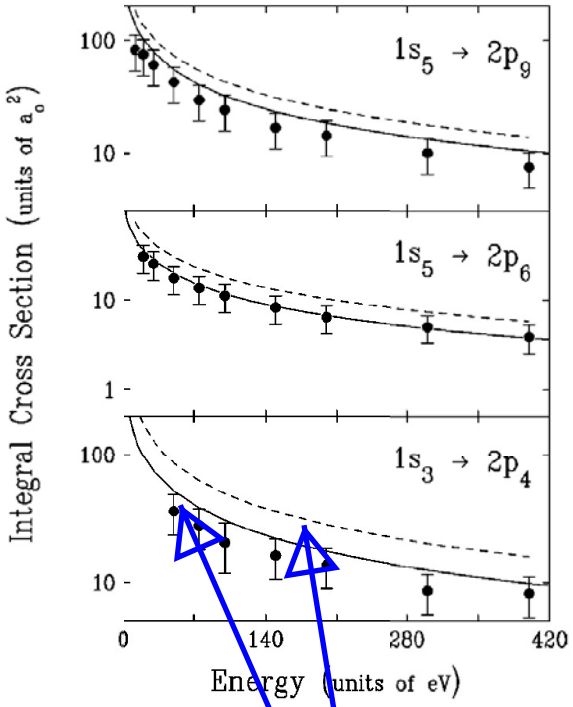


FIG. 1. Integral cross sections for electron-impact excitation of three states in the $2p$ manifold of argon from the metastable states in the $1s$ manifold as a function of incident electron energy. The experimental data are those of Boffard *et al.* [7]. The theoretical SRDW results are ss wave functions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

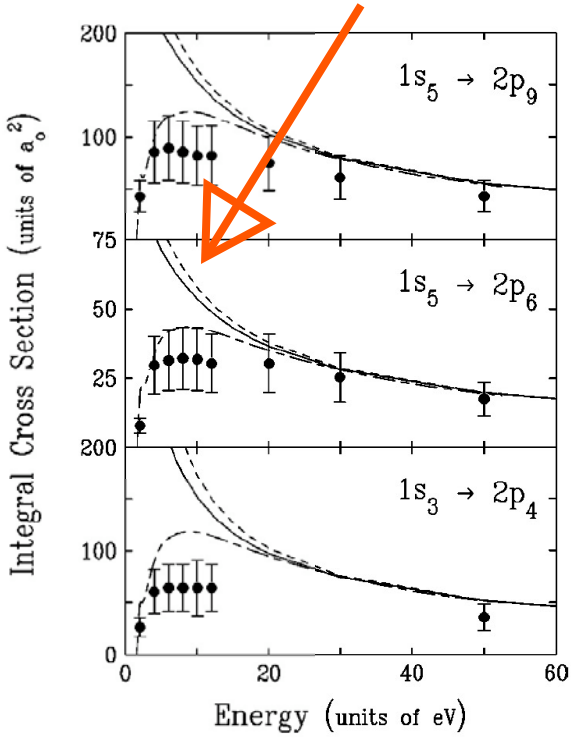


FIG. 2. Integral cross sections for electron-impact excitation of three states in the $2p$ manifold of argon from the metastable states in the $1s$ manifold as a function of incident electron energy. The experimental data are those of Boffard *et al.* [7]. The theoretical results are PWBA (dashed curve);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

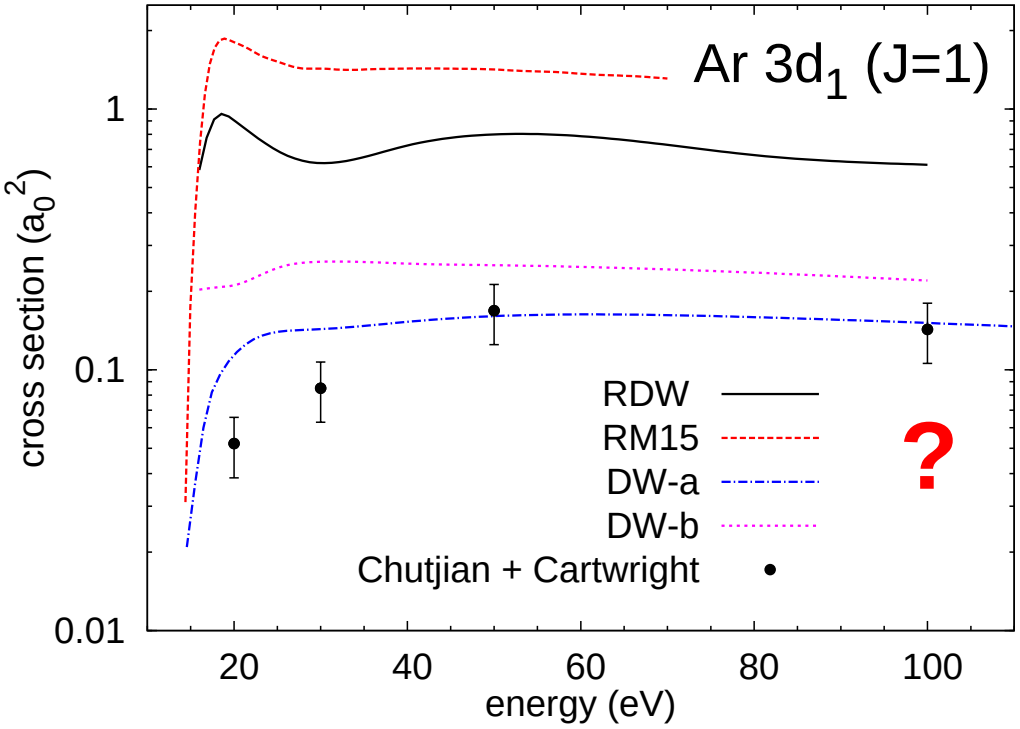
Theoretical results depend on wavefunctions and potentials

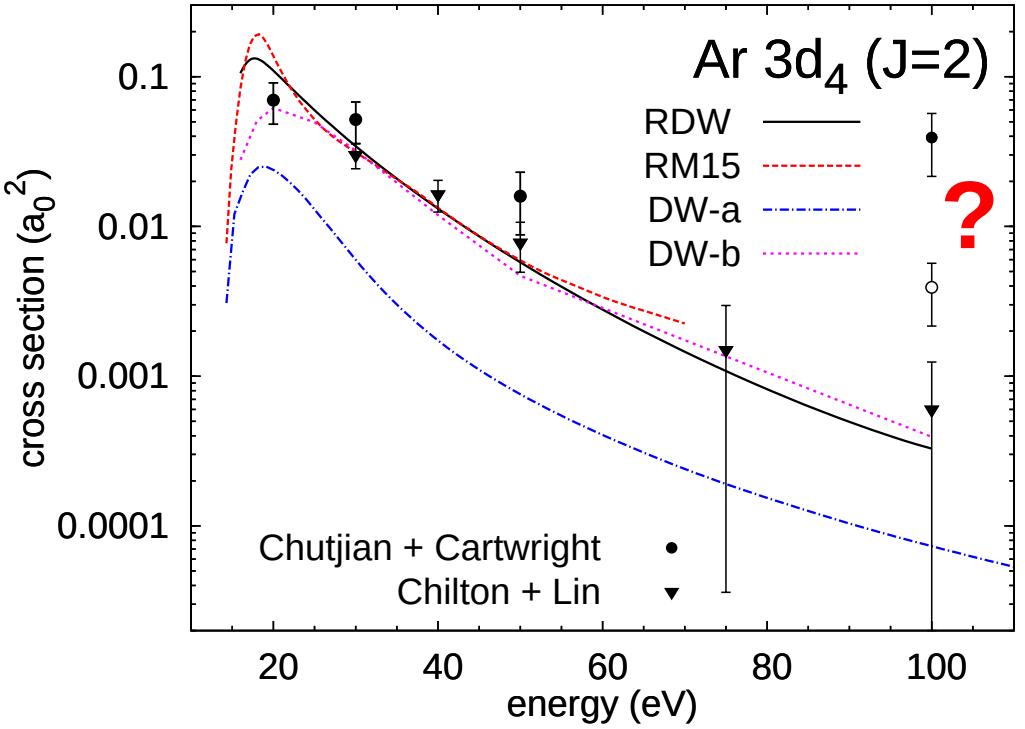
Relativistic DWBA; Semi-Relativistic DWBA; R-Matrix; Experiment

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?

Time-Independent Close-Coupling

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

H Ψ = E Ψ

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

- 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

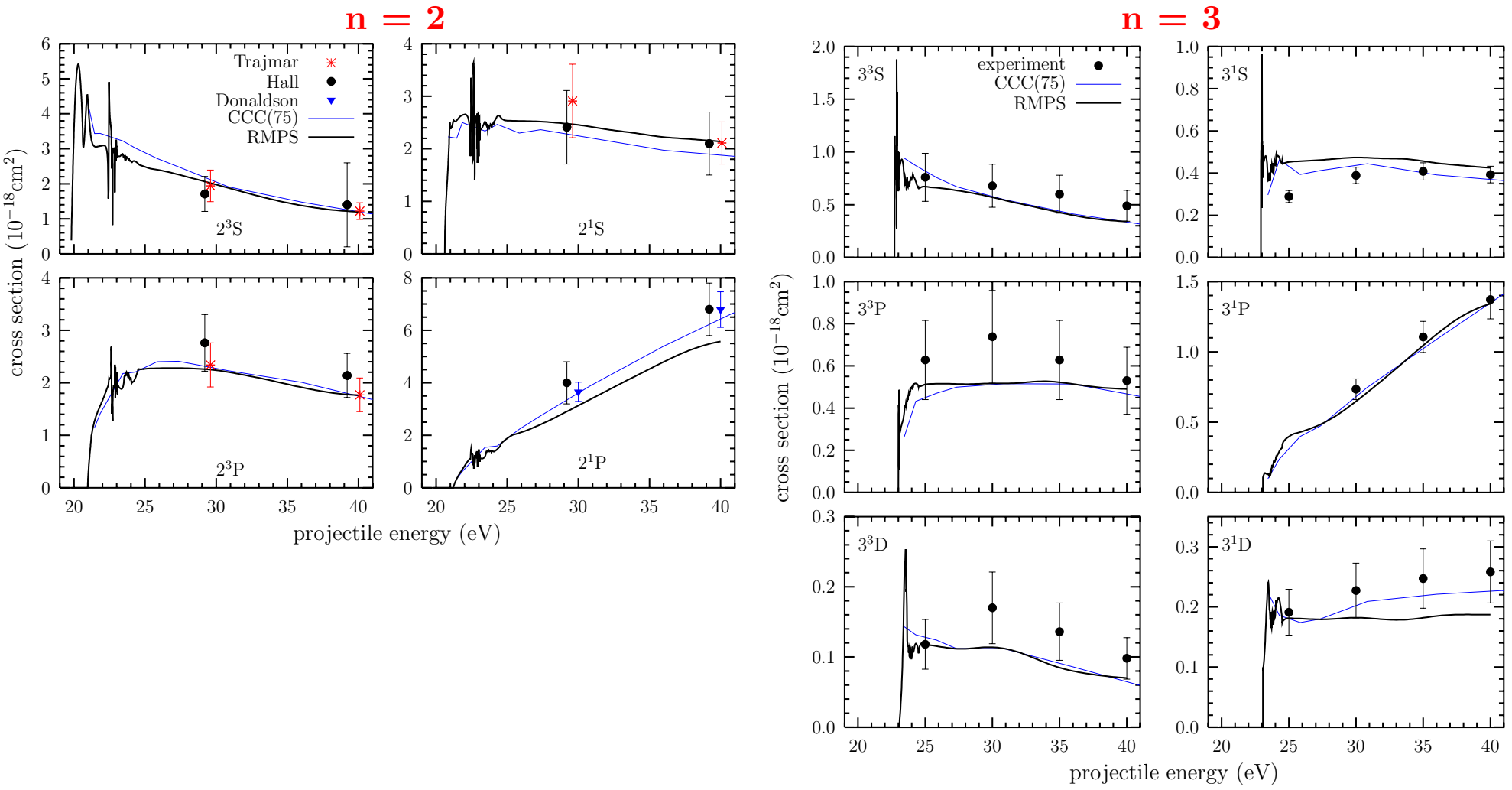
$$V_{ij}(r) = -\frac{Z}{r}\,\delta_{ij} + \sum_{k=1}^{N}\langle \Phi_i \mid \frac{1}{|\mathbf{r}_k - \mathbf{r}|} \mid \Phi_j \rangle$$

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

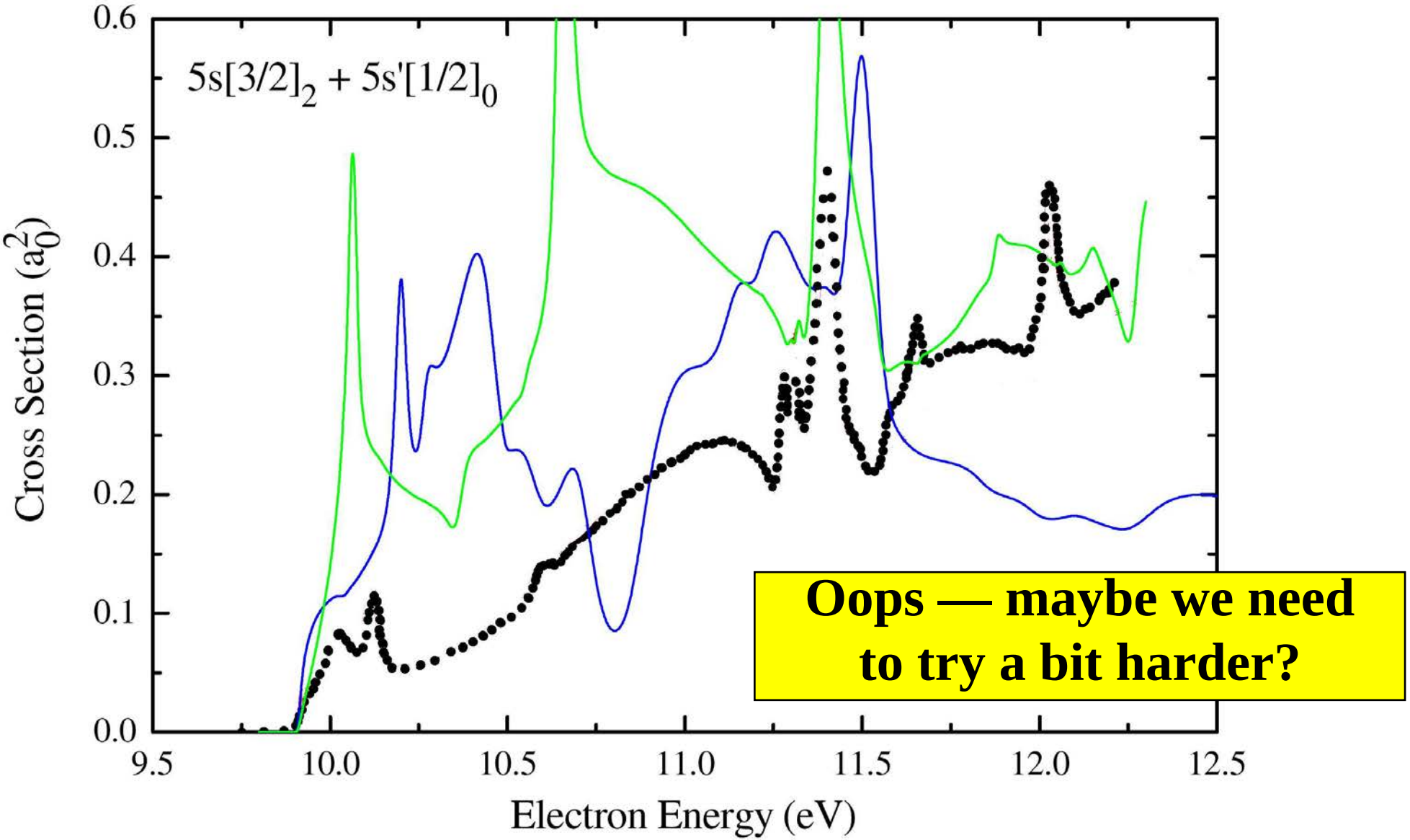


Already in 1998, de Heer recommends 0.5 x (CCC+RMPS) for uncertainty of 10% — independent of experiment!

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)



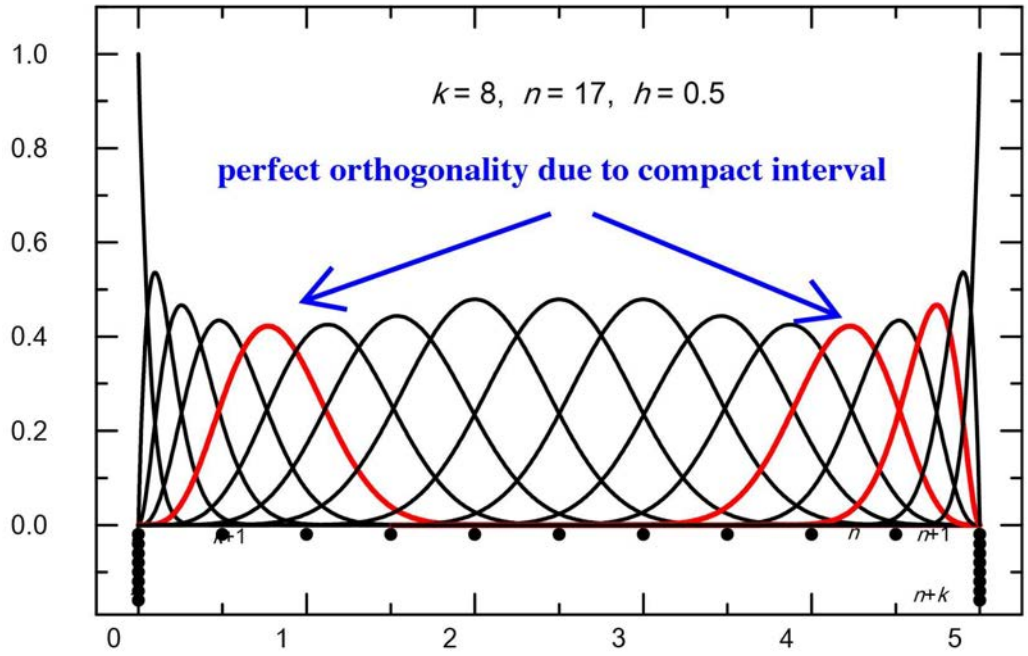
Oops — maybe we need to try a bit harder?

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)

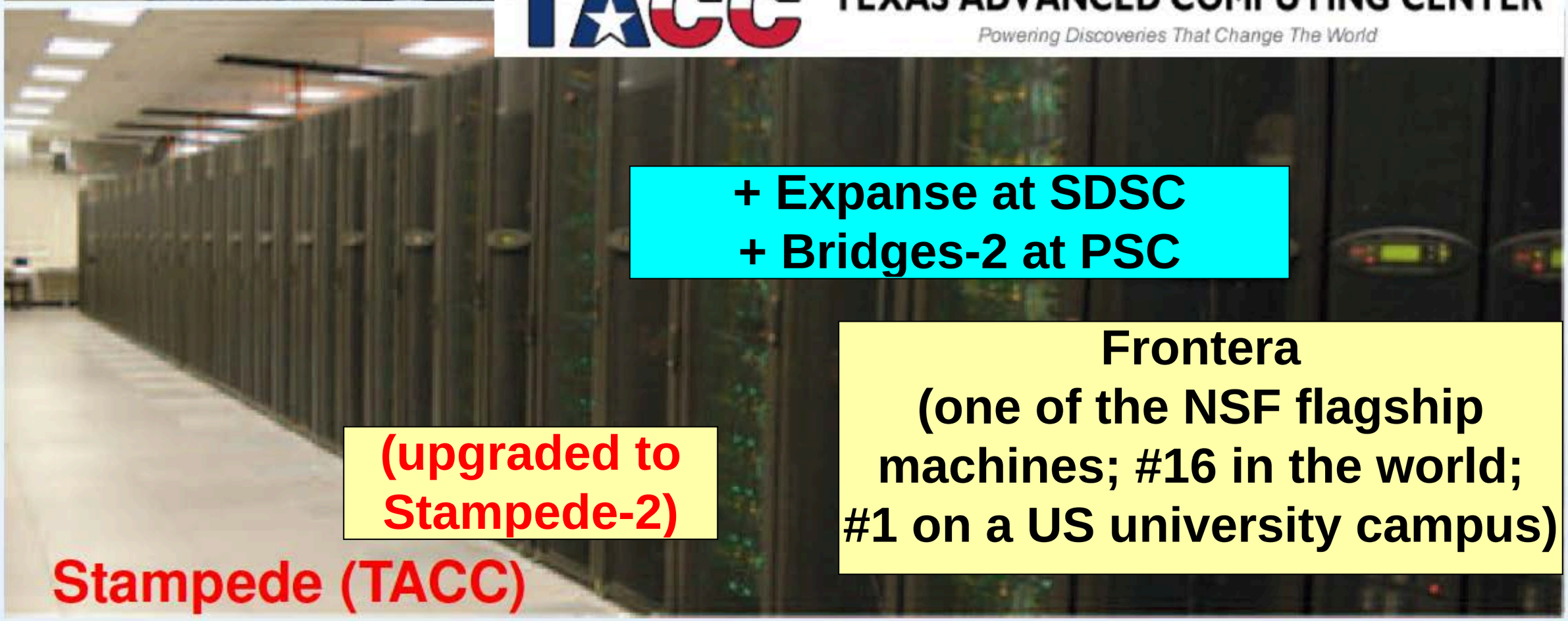
at least 100 more since 2013

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

Our Apparatus — Supercomputers

Kraken (NICS)

TACC
TEXAS ADVANCED COMPUTING CENTER
Powering Discoveries That Change The World



+ Expanse at SDSC
+ Bridges-2 at PSC

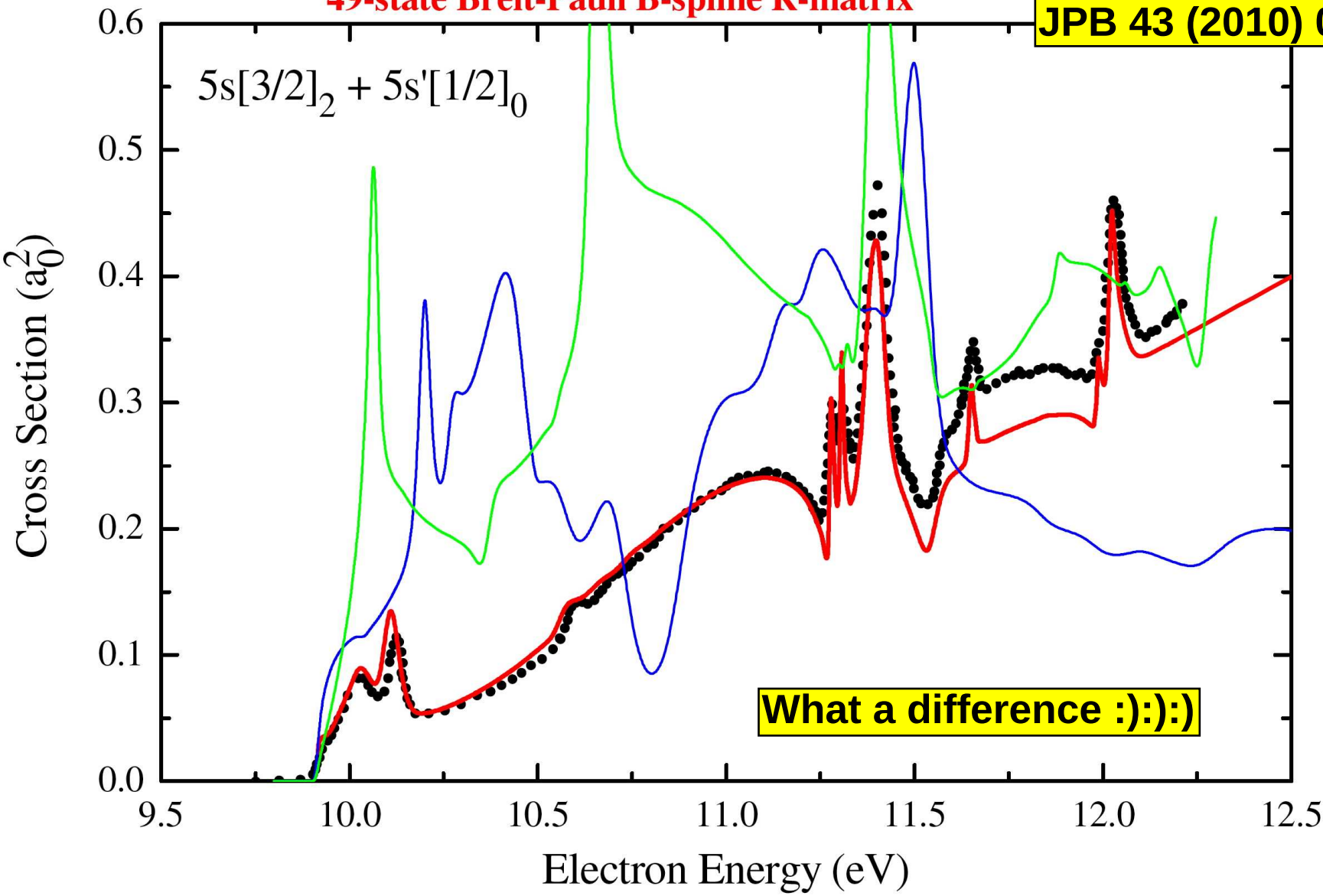
(upgraded to Stampede-2)

Frontera
(one of the NSF flagship machines; #16 in the world; #1 on a US university campus)

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



One more ...

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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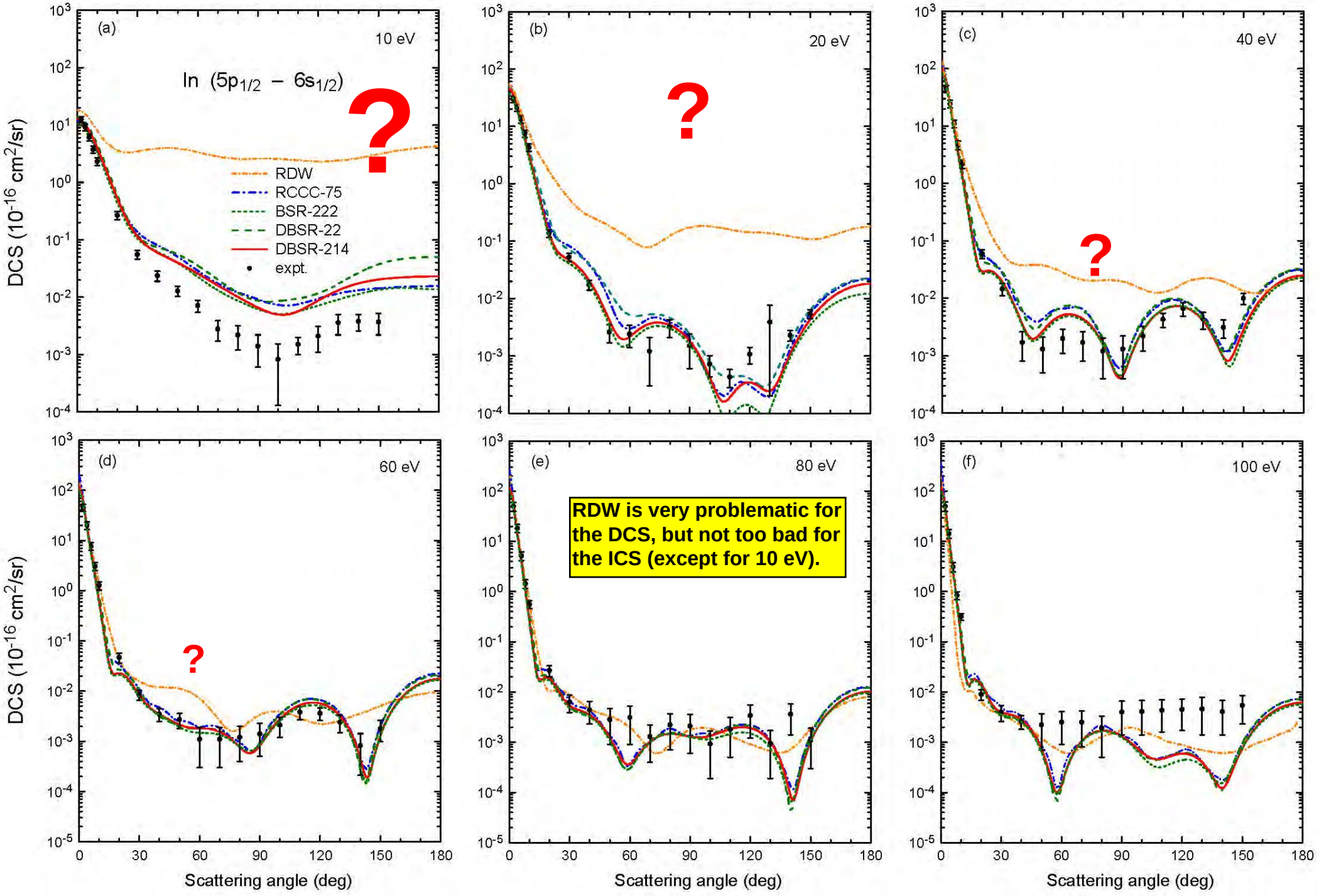
(Received 17 May 2020; accepted 6 July 2020; published 3 August 2020)

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)

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:**

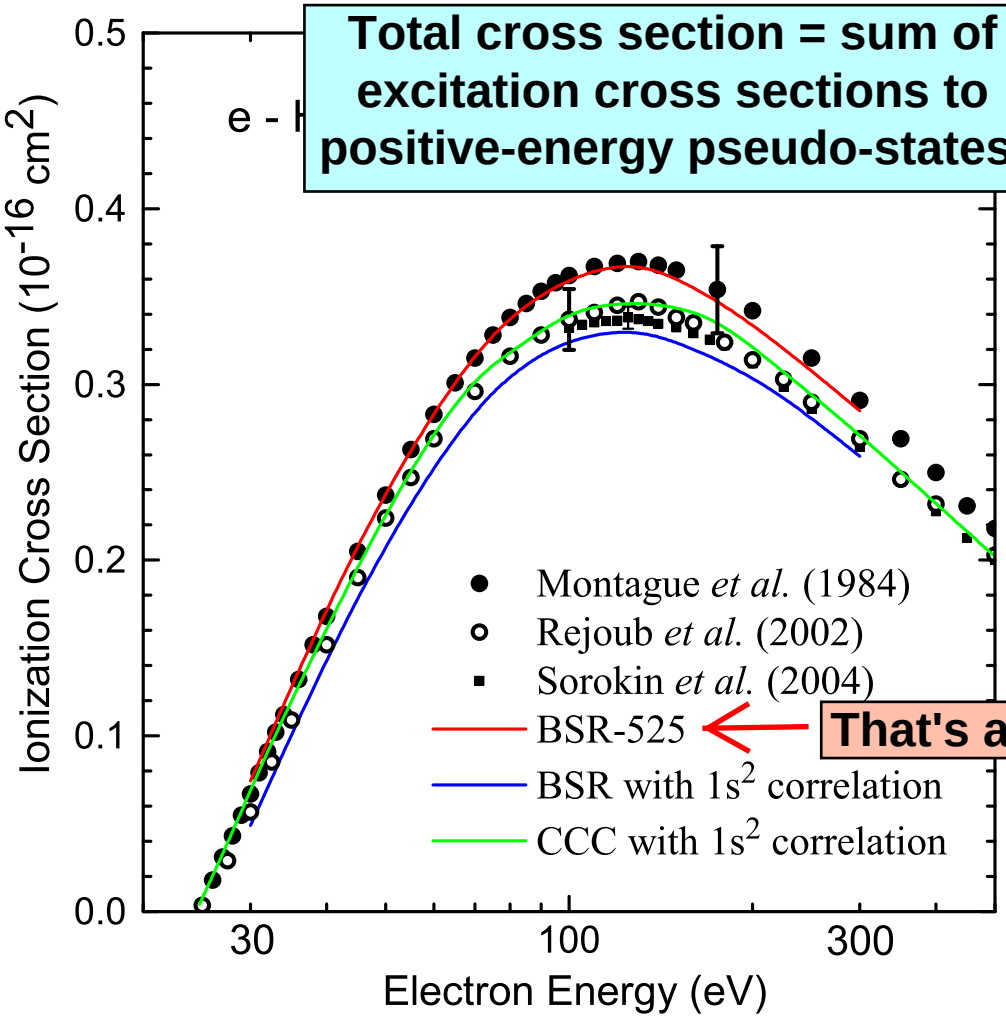
$$f(L_0, M_0, S_0; \boldsymbol{k}_0 \rightarrow L_f, M_f, S_f; \boldsymbol{k}_1, \boldsymbol{k}_2) = \sum_p \langle \Psi_f^{\boldsymbol{k}_2 -} | \Phi(L_p S_p) \rangle \, f(L_0, M_0, S_0; \boldsymbol{k}_0 \rightarrow L_p, M_p, S_p; \boldsymbol{k}_{1p}).$$

James Colgan may say more about this. We'll see if it works.

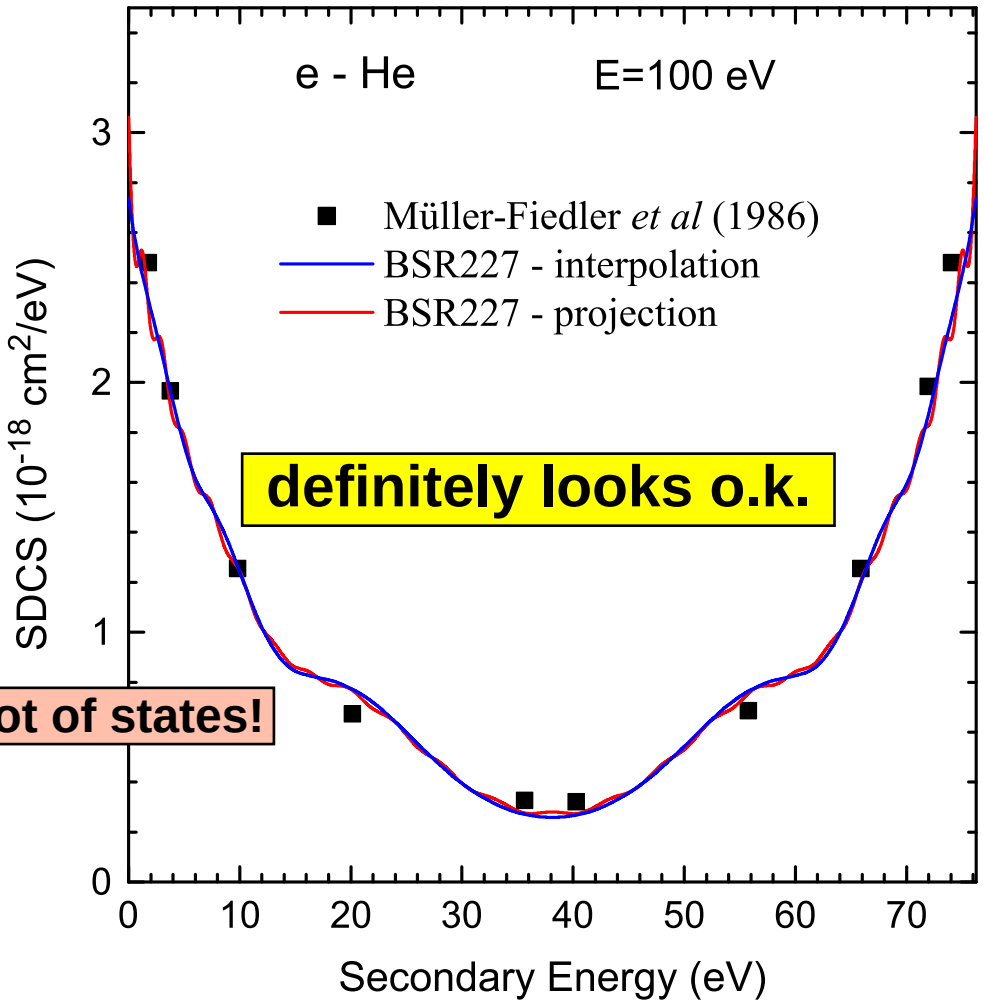
Some Checks: Ionization without Excitation (compare to CCC and TDCC)

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!**

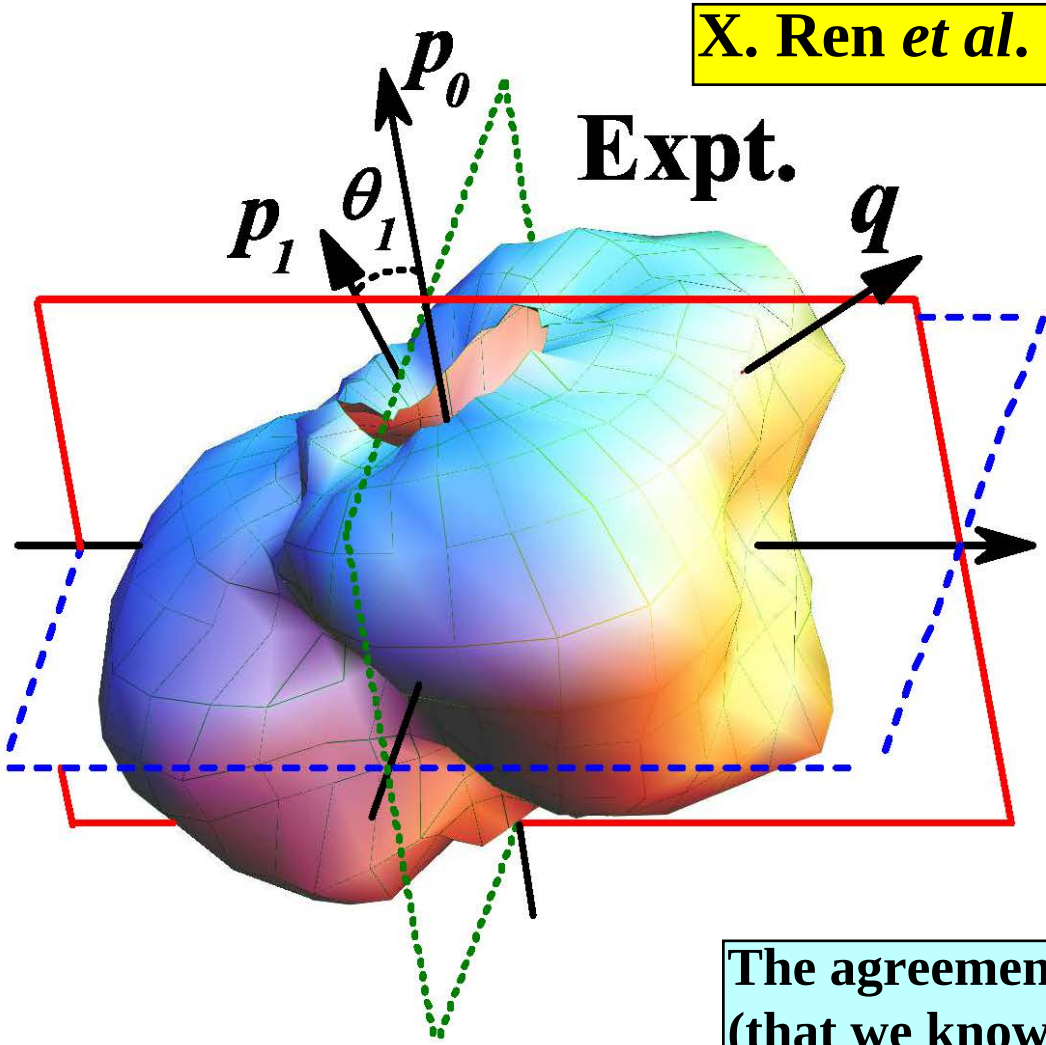
So far, so good ... Let's go for more detail!

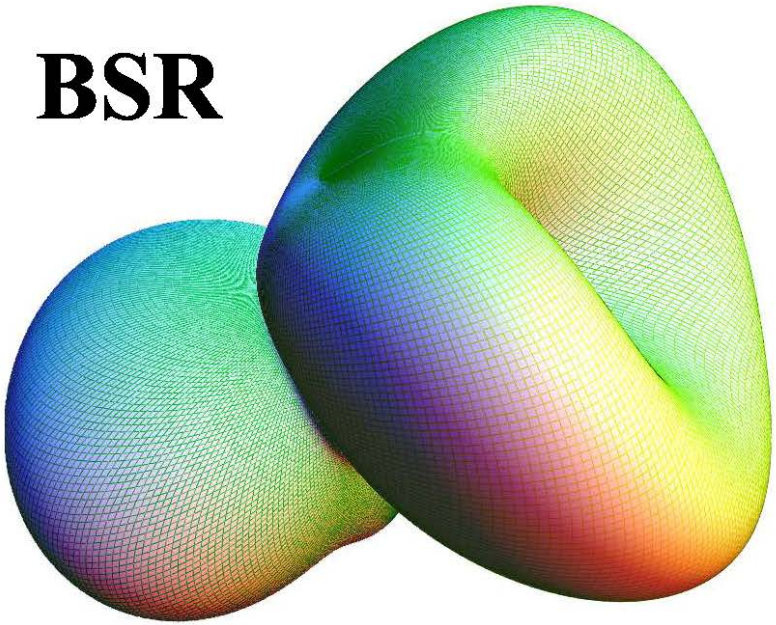
(e,2e) on Ar is a very l .. o .... n ..... g story. It includes the discovery of an error in the processing of the raw experimental data, which was found by the confidence gained in BSR predictions ...

(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.

L Cat is a non-profit project that relies on volunteer input, mostly from universities and research institutions.

Supporting organizations

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

EWS 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.

CONTACT: O. Zatsarinny and K. Bartschat
Drake University
Des Moines, Iowa 50311, USA
e-mails: oleg_zoi@@yahoo.com and klaus.bartschat@@drake.edu

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

grown to 20046 by Oct. 5, 2023

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

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

grown to 1874 by Oct. 5, 2023

Species: e + Ar [62]

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

Downloads: 1219 times from 2013-11-07

OPEN ACCESS
IOP Publishing
Plasma Sources Science and Technology
Plasma Sources Sci. Technol. **31** (2022) 095020 (28pp)
https://doi.org/10.1088/1361-6595/ac907e

The 2021 release of the Quantemol database (QDB) of plasma chemistries and reactions

Quantemol Ltd is a commercial business that originated from and still relies on fundamental collision physics.

Jonathan Tennyson[1,*], Sebastian Mohr[2], M Hanicinec[1], Anna Dzarasova[2], Carrick Smith[2], Sarah Waddington[2], Bingqing Liu[1], Luís L Alves[3], Klaus Bartschat[4], Annemie Bogaerts[5], Sebastian U Engelmann[6], Timo Gans[7,13], Andrew R Gibson[8,9], Satoshi Hamaguchi[10], Kathryn R Hamilton[4], Christian Hill[11], Deborah O'Connell[7,13], Shahid Rauf[12], Kevin van 't Veer[5] and Oleg Zatsarinny[4,†]

Table 2. Classification of processes considered in QDB.

Abbrev	Type of reaction	Description	Total
Electron processes			
EDX	Deexcitation	$e + A^* \rightarrow e + A$	2648
EEL	Elastic scattering	$e + A \rightarrow e + A$	554
EIN	Ionization	$e + A \rightarrow e + A^+ + e$	329
EIP	Ion pair creation	$e + AB \rightarrow A^+ + B^- + e$	3
EMT	Momentum transfer		20
ERR	Radiative recombination	$e + A^+ \rightarrow A + h\nu$	2
EDR	Dissociative recombination	$e + AB^+ \rightarrow A + B$	826
EDS	Dissociation	$e + AB \rightarrow e + A + B$	660
EDA	Dissociative attachment	$e + AB \rightarrow A + B^-$	153
EDE	Dissociative excitation	$e + AB \rightarrow A^* + B + e$	4
EDI	Dissociative ionization	$e + AB \rightarrow A^+ + B + 2e$	400
EEX	Electron-impact electronic excitation	$e + A \rightarrow e + A^*$	2228
ECX	Change of excitation	$e + A^* \rightarrow e + A^{**}$	9601
ERC	Recombination (general)	$e + A^{+z} \rightarrow A^{+(z-1)}$	41
EDT	Electron attachment	$e + A + B \rightarrow A + B^-$	50
EVX	Electron-impact vibrational excitation	$e + A \rightarrow e + A\ [v = *]$	615
EXR	Electron-impact rotational excitation	$e + A \rightarrow e + A\ [J = *]$	11
ETS	Electron total scattering	$e + A \rightarrow e + \Sigma A$	11
ETI	Electron total ionisation	$e + A \rightarrow e + e + \Sigma A^+$	15
ETA	Electron total attachment	$e + A \rightarrow \Sigma A^-$	8
ETD	Electron total dissociation	$e + A \rightarrow e + \Sigma A$	36
ETN	Electron total neutral dissociation	$e + A \rightarrow e + \Sigma A$	4

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.

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 !

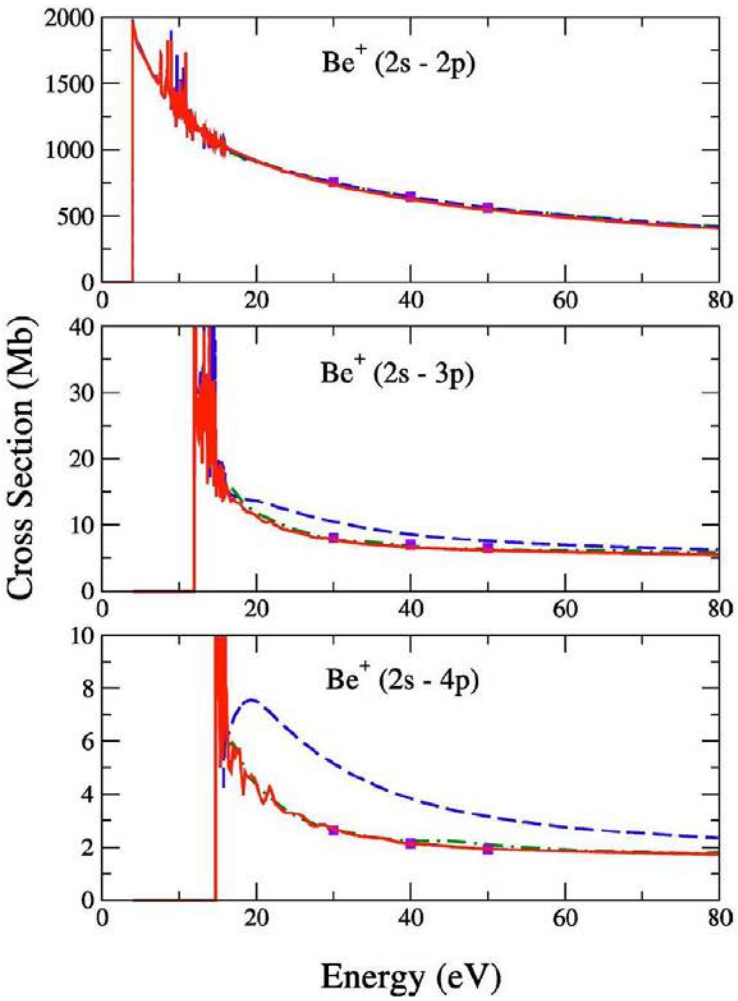

FIG. 4. Electron-impact excitation cross sections from the 2*s* ground term of Be^+ to the *np* excited terms. Dashed curves are from the present 14-term *R*-matrix calculation; solid curves are from the present 49-term RMPS calculation; solid squares are from the present TDCC calculation; dot-dashed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

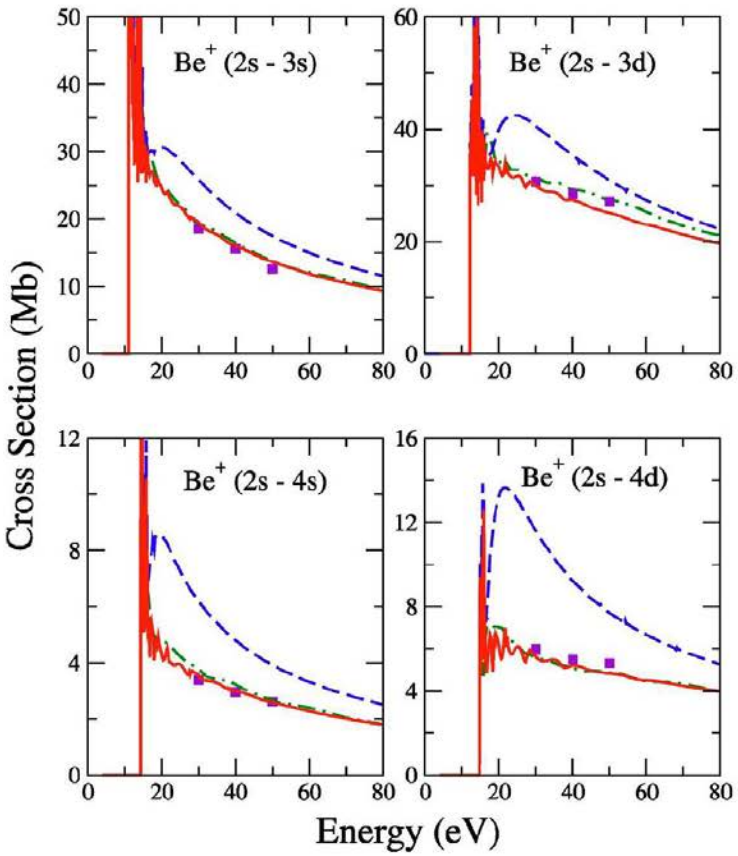

FIG. 5. Electron-impact excitation cross sections from the 2*s* ground term of Be^+ to the *ns* and *nd* excited terms. Dashed curves are from the present 14-term *R*-matrix calculation; solid curves are from the present 49-term RMPS calculation; solid squares are from the present TDCC calculation; dot-dashed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

This is a light quasi-one electron system. Essentially solved 20 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 !

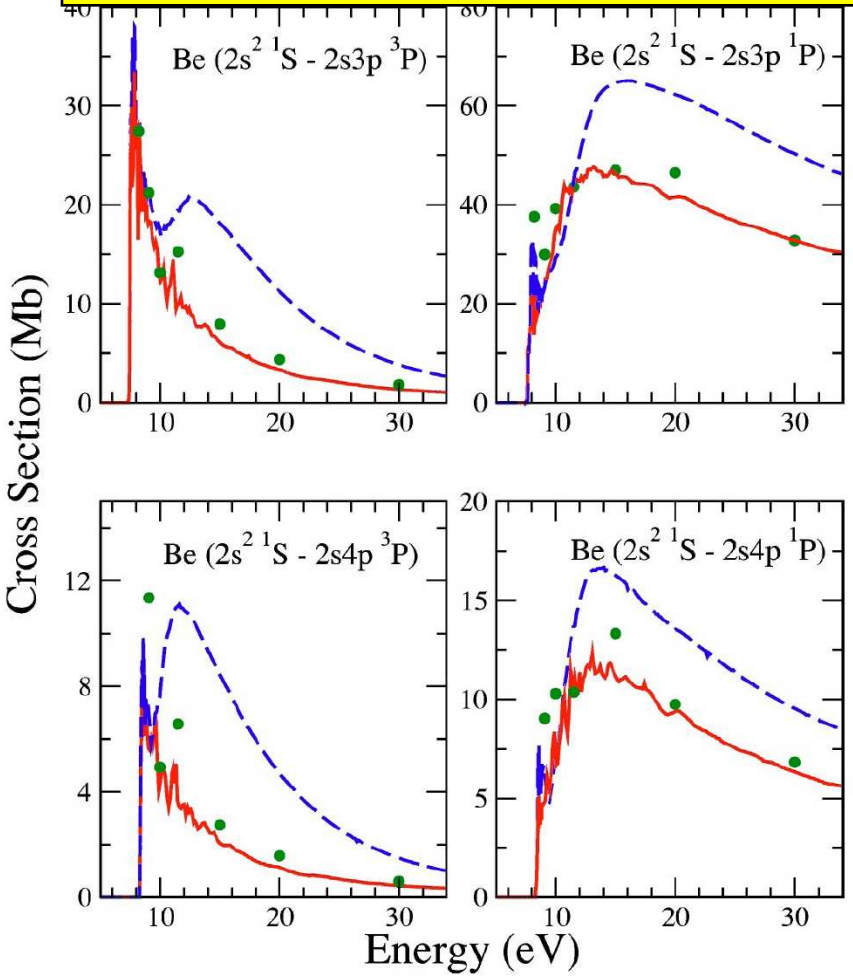

FIG. 2. Electron-impact excitation cross sections from the $2s^2\,{}^1S$ ground term of Be to the $2snp\,{}^3P$ and $2snp\,{}^1P$ excited terms for $n=3$ and 4. Dashed curves are from the present 29-term R-matrix calculation; solid curves are from the present 280-term RMPS calculation; solid circles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

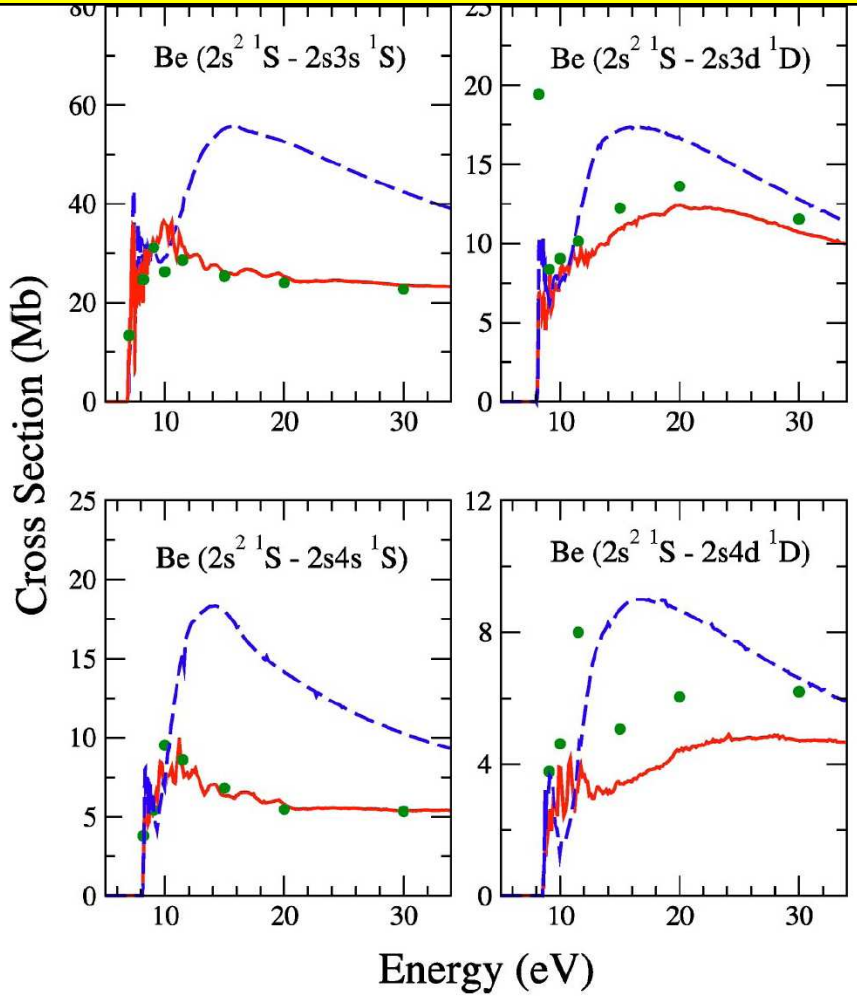

FIG. 3. Electron-impact excitation cross sections from the $2s^2\,{}^1S$ ground term of Be to the $2sns\,{}^1S$ and $2snd\,{}^1D$ excited terms. Dashed curves are from the present 29-term R-matrix calculation; solid curves are from the present 280-term RMPS calculation; solid circles are from CCC calculations 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 20 years ago.

Phys. Rev. A 68 (2003) 032712

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

Contents lists available at ScienceDirect

Atomic Data and Nuclear Data Tables

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

Dipti [a,*], T. Das [b,1], K. Bartschat [c], I. Bray [d], D.V. Fursa [d], O. Zatsarinny [c], C. Ballance [e], H.-K. Chung [b,2], Yu. Ralchenko [a,*]

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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.

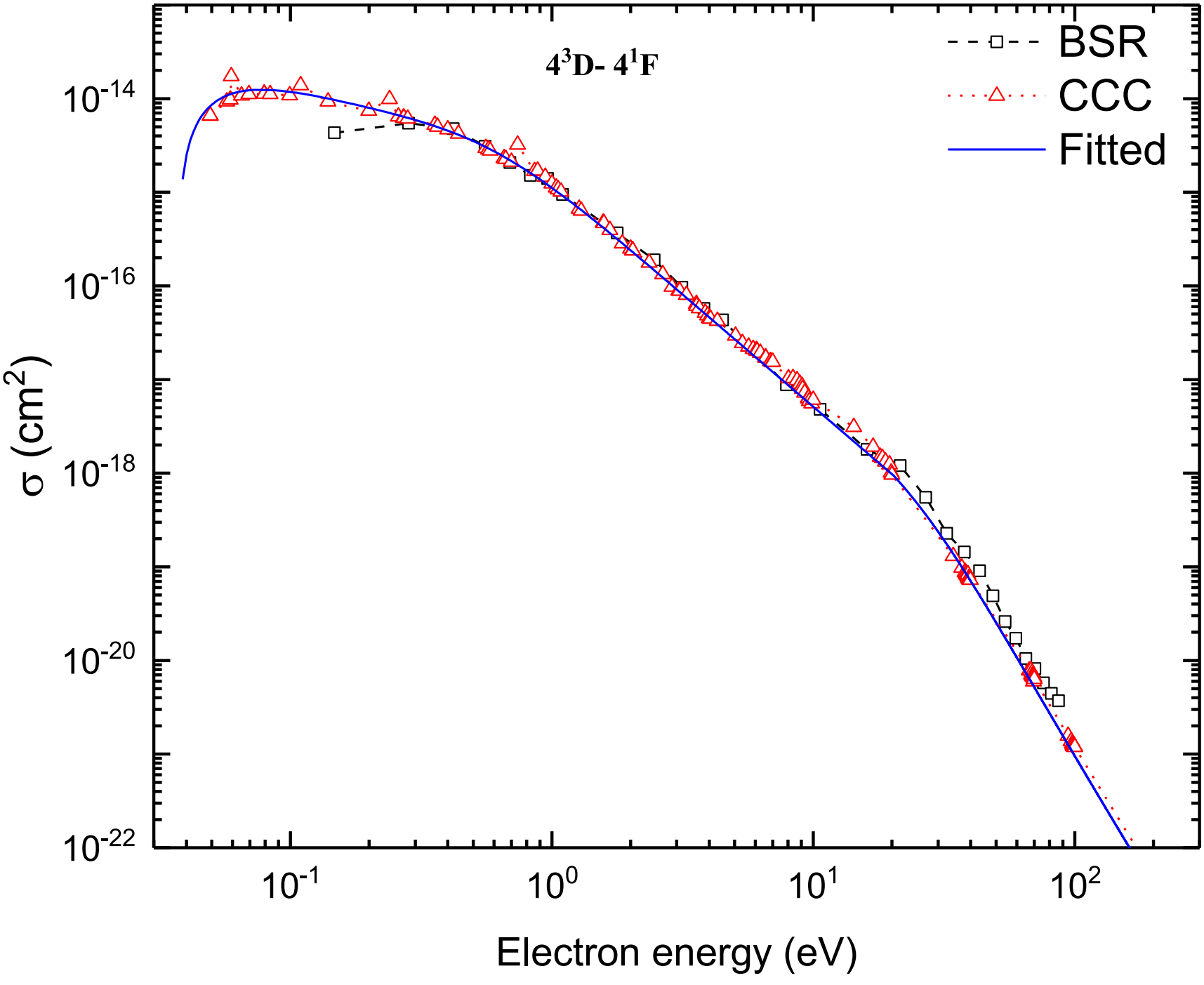

Fig. 4. Electron-impact excitation cross sections for the spin-forbidden ($4^3D \rightarrow 4^1F$) transition.

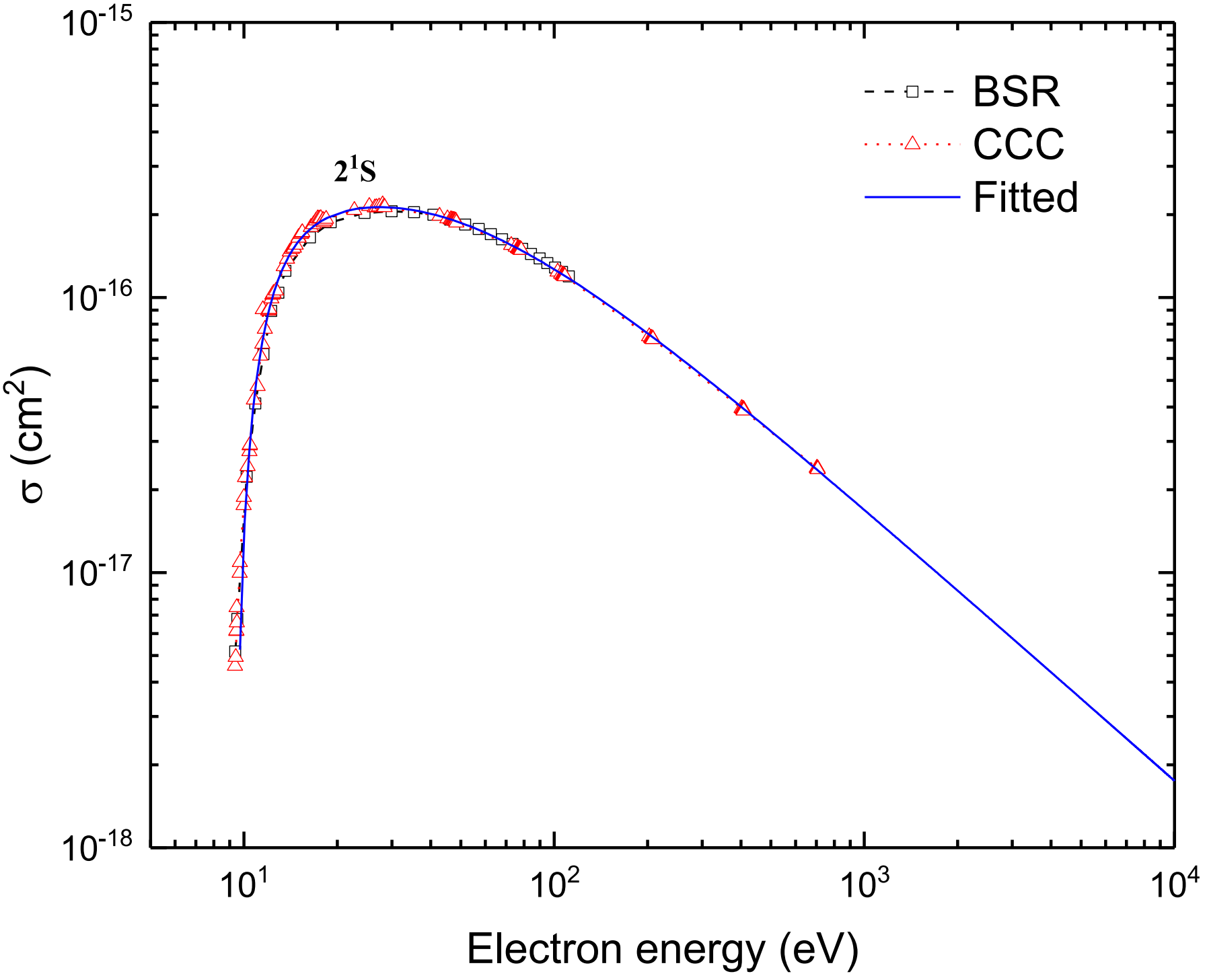

Fig. 6. Electron-impact ionization cross sections from the 2^1S state.

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

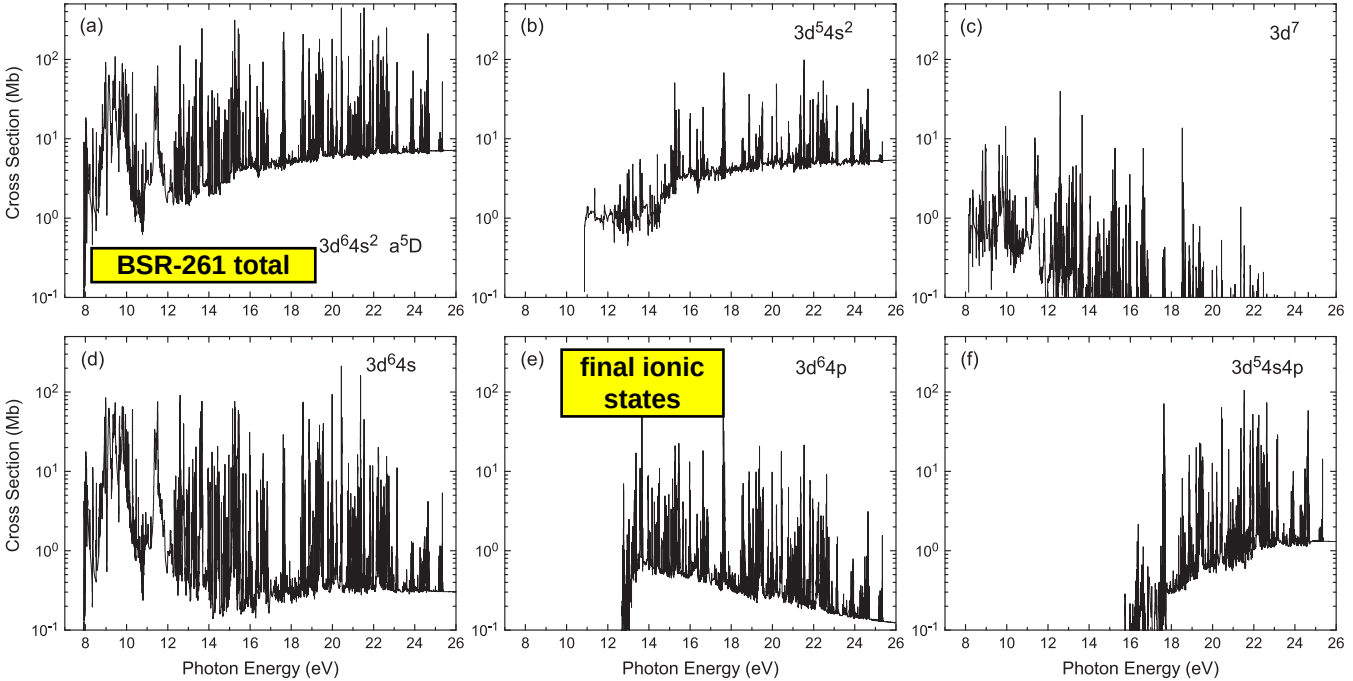

FIG. 2. Photoionization cross section of the $3d^6 4s^2\ ^5D$ ground state of Fe I (a), along with the contributions from different subsets (b)–(f) of final ionic configurations indicated in the legend.

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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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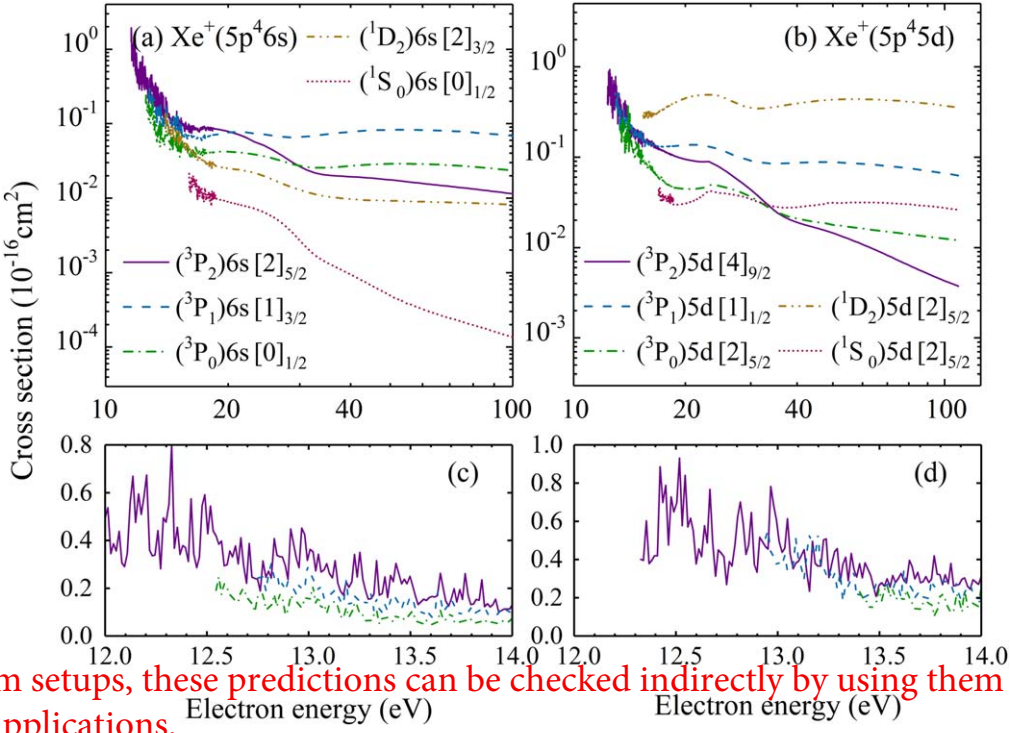

As in swarm setups, these predictions can be checked indirectly by using them in modeling applications.

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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A xenon collisional-radiative model applicable to electric propulsion devices: III. Determination of the ionization fraction in low-temperature xenon plasma by using ionic and atomic 6*p* lines

Xi-Ming Zhu[1,2,*], Yan-Fei Wang[1,*], Sheng-Feng Meng[1], Yang Wang[1], Zhong-Xi Ning[1,2,*], Da-Ren Yu[1,2] and Klaus Bartschat[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 …

tungsten, tungsten, and tungsten

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

NOTHING (yet)

A lot of work will be required before reliable calculations can be carried out for this problem. Collaborations in code development and maintenance seem highly advisable.

Can you just do it yourself ?

[Unless you want to just wait for ChatGPT ...]

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).

Two-Photon Double Ionization of H_2

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

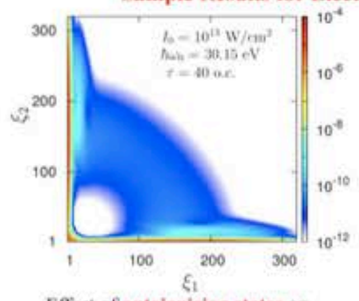
Goal: Resolve large discrepancies in previous calculations of this fundamental process.

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)**

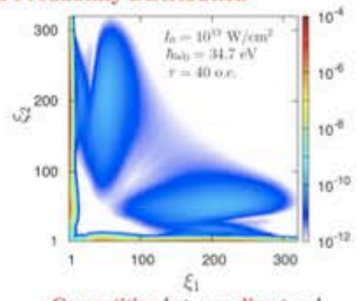
Findings: Discrepancies are due to surprisingly strong dependence of theoretical predictions on laser parameters and (previously unresolved) effect of autoionizing states.

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

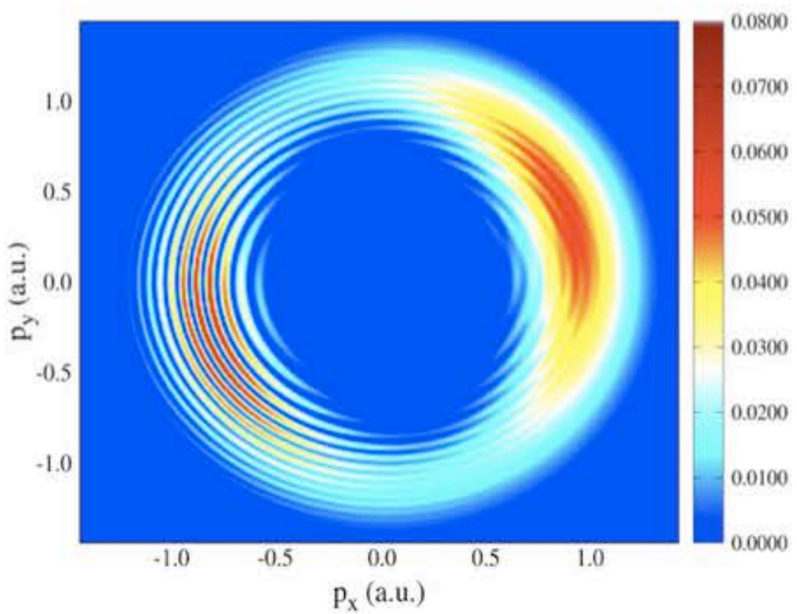
Sample Results for Electron Probability Distribution



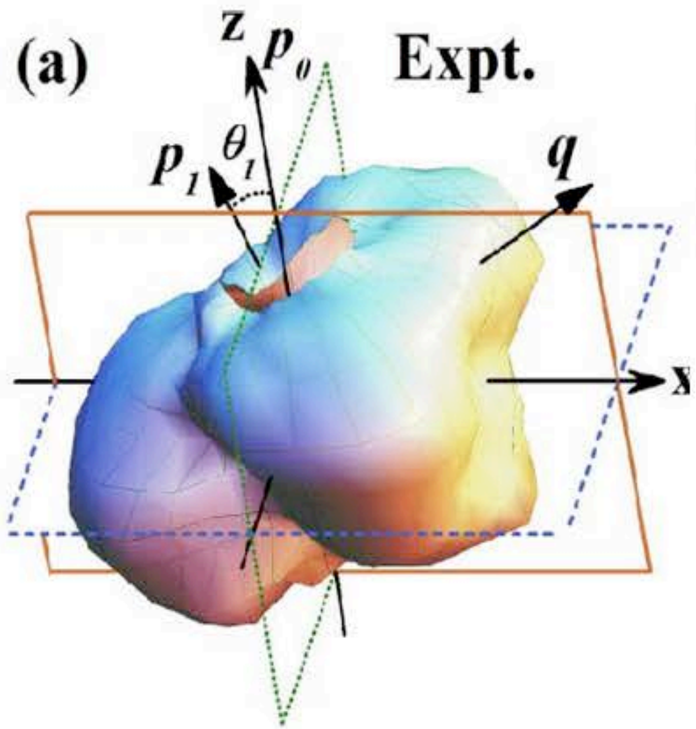
Effect of **autoionizing states** on non-sequential double ionization

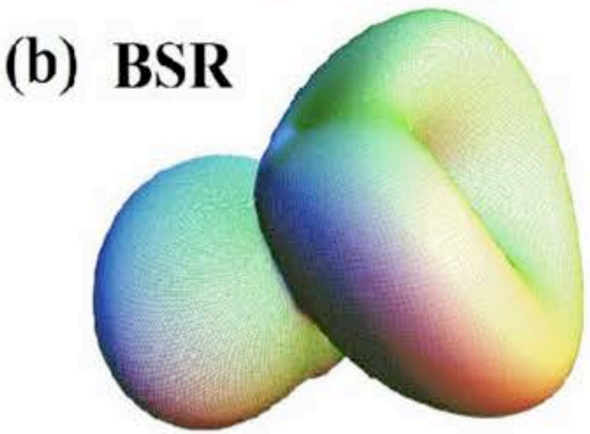


Competition between **direct** and **sequential** double ionization

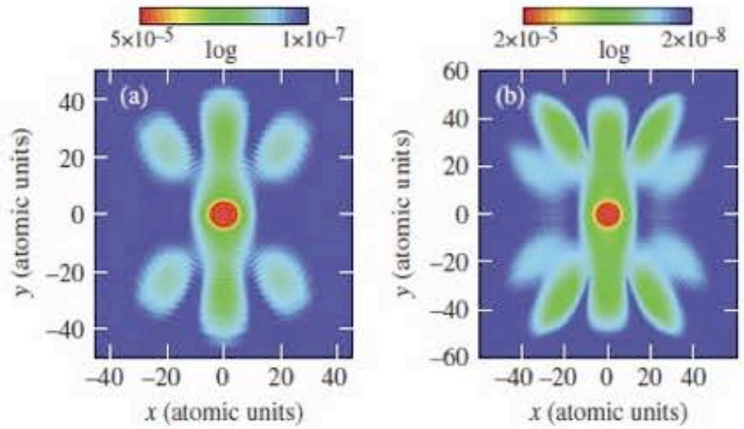


Photoelectron Momentum Distribution for Ar Ionization in Strong Electromagnetic Field

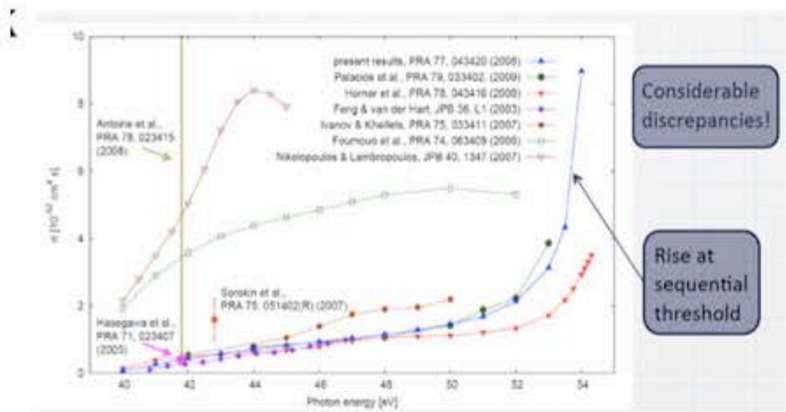




Ionization of Ar(3p) by electron Impact: Experiment(a) and Theory(b)



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

Details were just presented by Kathryn Hamilton.

Electron Collisions with Atoms and Ions --- A Solved Problem?

- Undoubtedly, a lot of progress has been made, both experimentally and theoretically.
- Advanced close-coupling and other non-perturbative methods can handle light quasi-one- and quasi-two-electron very well.
- Systems with more than one electron in more than one open shell (this includes excitation of heavy noble gases) are still problematic.
- Heavy complex atoms (Fe, W, transition elements) are far from being solved.
- Elastic scattering is easier than excitation, which is easier than ionization, where perturbative methods still have their place.
- Neutral systems are generally more difficult than ions, where the strong Coulomb force may dominate correlation effects.
- Molecules are much more difficult than atoms.

I hope this information will help you to come up with your own answer. 😉

The Legacy of Don Madison

- Don was a pioneer in the field of charged-particle collisions.
- He was an excellent teacher and mentor to many.
- He served the community with great distinction.
- I wouldn't be here without him.

Most importantly,
Don Madison was a good man!

Thank you, Don, and thank you all for your attention!