BENCHMARK CALCULATIONS OF ATOMIC DATA FOR PLASMA AND DISCHARGE APPLICATIONS

Klaus Bartschat, Drake University

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Moscow, June 29, 2011

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Phil Burke, Charlotte Froese Fischer, Oleg Zatsarinny

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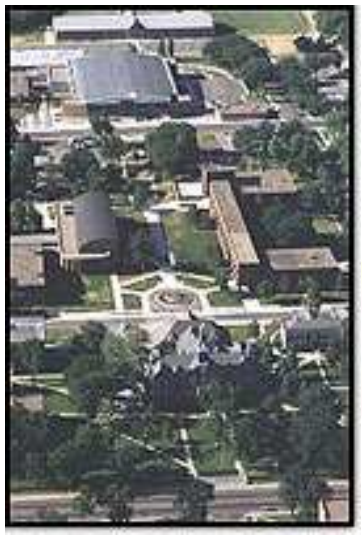

BENCHMARK CALCULATIONS OF ATOMIC DATA FOR PLASMA AND DISCHARGE APPLICATIONS

OVERVIEW:

I. Introduction:

- **Who cares, and why ?**
- Data **Wanted** vs. Data **Available**
- Production and Assessment of Atomic Collision Data

II. Numerical Methods

- **Distorted-Wave Methods**
- The **Close-Coupling Method**: Recent Developments
  CCC, RMPS, IERM, TDCC, ECS, ..., **BSR**

III. Selected Results

- Energy Levels
- Oscillator Strengths
- Cross Sections for Electron−Impact Excitation and Ionization (H, He, ..., Au, Hg)

IV. Applications

- Modelling of a Molybdenum-Oxide Lamp
- Modelling of a Ne Discharge

V. Summary and Outlook

Motivation (Theoretical investigations)

Why Study Excitation of Neutral Complex Atoms?

Basic research on electron collision with heavy atomic species:

- Theoretical investigation is challenging due to difficult target description; channel coupling is also difficult.

- Accurate cross sections are needed for a wide range of electron energies; need for different theoretical approaches valid for low and high energy regions.

- Large disparities between recent calculations and measurements; available experimental datasets are limited but can be used as benchmark checks.

Motivation (Applications)

Rare gases in plasma applications

plasma display panels	plasma processing	z-pinches
	laser amplifiers	lighting

Ar-Xe laser at NRL; high-pressure Xe lamp (Greifswald)

Develop a thorough understanding of the Ar-Xe atomic and molecular processes, kinetics, and reaction channels that affect the gain of the Ar-Xe laser.

As a first step, calculate accurate cross sections for all electron-induced transitions between the ground state $5p^6$ and the excited $5p^5 6s$, $5p^5 6p$, and $5p^5 5d$ states in Xenon.

Major Challenge: Lasing is between highly excited levels

Motivation (Applications)

Spectroscopic analysis of Plasma discharges

Molybdenum-oxide lamp

To predict the most important kinetic pathways leading to emission of visible and ultraviolet radiation.

Challenge: The Mo atom has extremely complicated atomic structure. The visible radiation is a result of a sequence of transitions between the excited states of Mo with electrons.

TR 24 complex plasmas

IPP

Neon

Reconstruction of Electron Energy Distribution Functions from Optical Emission Spectroscopy

Dirk Dodt[1], Andreas Dinklage[1], Rainer Fischer[1], Klaus Bartschat[2],Oleg Zatsarinny[2]

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[1]Max-Planck-Institut für Plasmaphysik (IPP)

[2]Drake University, Des Moines

Motivation: Somebody wants to know about Xe ...

IOP PUBLISHING JOURNAL OF PHYSICS D: APPLIED PHYSICS

J. Phys. D: Appl. Phys. **40** (2007) 4532–4543 doi:10.1088/0022-3727/40/15/025

Electron kinetics of the e-beam pumped Ar–Xe laser

G M Petrov[1], J L Giuliani[1], J P Apruzese[1], A Dasgupta[1], Tz Petrova[2], K Bartschat[3] and D Rose[4]

IOP PUBLISHING JOURNAL OF PHYSICS D: APPLIED PHYSICS

J. Phys. D: Appl. Phys. **42** (2009) 185203 (8pp) doi:10.1088/0022-3727/42/18/185203

Near-infrared collisional radiative model for Xe plasma electrostatic thrusters: the role of metastable atoms

Rainer A Dressler[1], Yu-hui Chiu[2], Oleg Zatsarinny[3], Klaus Bartschat[3], Rajesh Srivastava[4] and Lalita Sharma[4,5]

... for a variety of reasons

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Dielectric barrier discharge lamp comprising an uv-b phosphor

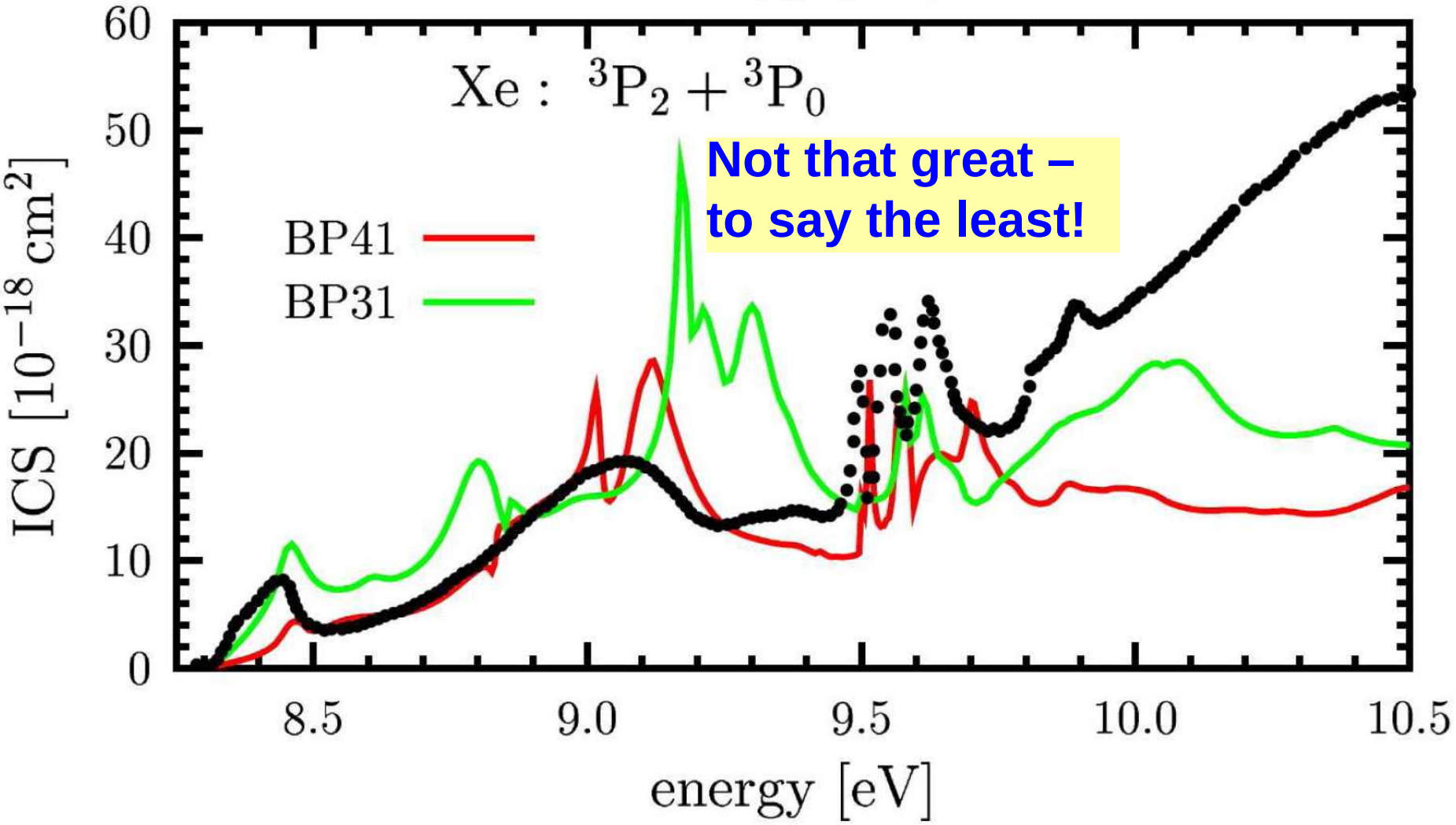
Xe or Xe/Ne mix

USPTO Application #: 20090223901
Title: Dielectric barrier discharge lamp comprising an uv-b phosphor
Abstract: This invention relates to a dielectric barrier Xe discharge lamp comprising an UV-B phosphor. The lamp consists of a gas-tight, discharge vessel with a gas filling containing Xe or a Xe/Ne mixture and is provided with a luminescent layer, which comprises at least one luminescent material emitting in the UV-B range (280 to 320 nm). The luminescent layer comprises a Gd3+ activated phosphor according to the formulas McPO4:Gd, Lal1—XAl3(BO3)4:Gdx, and La1—xB3O6:Gdx which is eventually sensitised by Bi3+, Pr3+ or Nd3+ The advantages of such an UV-B emitting discharge lamp over fluorescent lamps based on a Hg low-pressure discharge are a high power density, 10 instant light, long lifetime, a spectral power distribution which is only determined by the phosphor blend, and an arbitrary burner design. (end of abstract)

Agent: Philips Intellectual Property & Standards - Briarcliff Manor, NY, US
Inventors: Thomas Juestel, Petra Huppertz, Detlef Uwe Wiechert, Walter Mayr, Heinrich Von Busch
USPTO Applicaton #: 20090223901 - **Class:** 210748 (USPTO)

Calculations are extremely difficult!

- **Experiment: Buckman *et al.* (1983) – not absolute**
- **Theory: Semi-relativistic Breit-Pauli *R*-matrix (close-coupling) models**

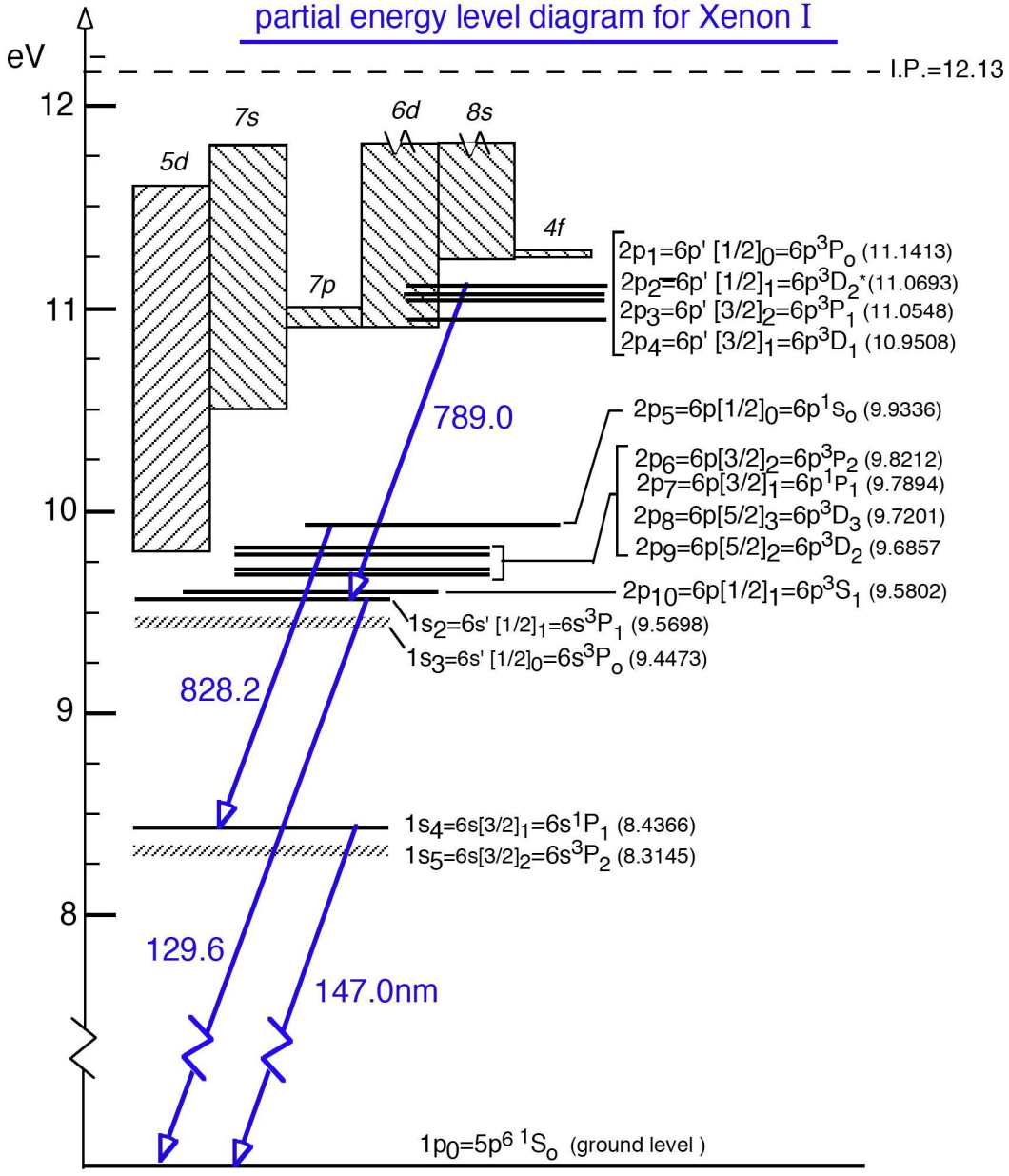


Data Wanted vs. Data Available ...

Spectrum of Xenon (→ Ar-Xe laser at NRL; high-pressure Xe-lamp (Greifswald))

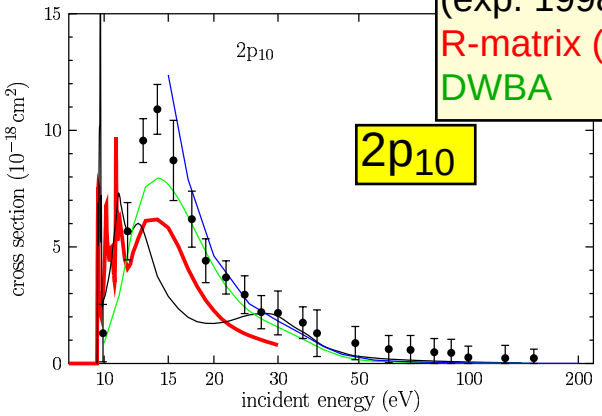
Wanted: Level-to-Level + Ionization

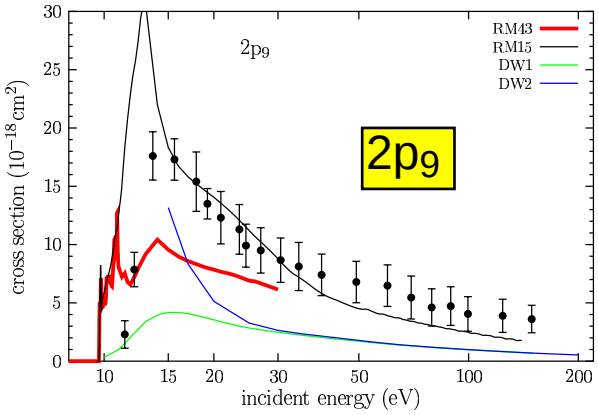
partial energy level diagram for Xenon I

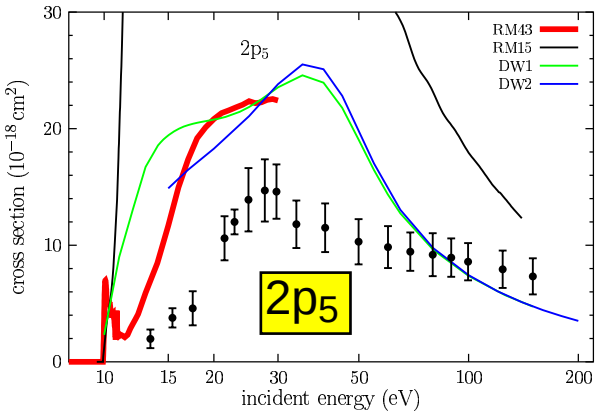


Available

Fons and Lin (exp. 1998)
R-matrix (CC)
DWBA







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"!

Numerical Approaches

- **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.

Numerical Methods

- **Born-type methods**
- **Close-coupling-type methods** (time-independent)
- **Time-dependent and other direct methods**

The (First-Order) Distorted-Wave Approximation

- Standard method of treating high-energy scattering
- Based upon the "two-potential approach"

$$V = V_1 + (V - V_1) = V_1 + V_2$$

and the solution of differential equation

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - 2\{U_E(r) + V_{E,\mathrm{rel}}(r) - E\}\right] \chi_{E,l}(r) = 0.$$

- The potential

$$\begin{aligned} V_1 &\equiv U_E(r) + V_{\mathrm{E,rel}}(r) \\ &= U_{\mathrm{static}}(r) + U_{E,\mathrm{exch}}(r) + U_{E,\mathrm{pol}}(r) + i\,U_{E,\mathrm{abs}}(r) + V_{E,\mathrm{rel}}(r) \end{aligned}$$

is "easy" to handle, while the rest (V_2) is only accounted for to first order.

- **Advantages:**
  - fast
  - relatively easy to implement
  - flexible target description possible
  - easy to test assumptions about the physics involved
- **Disadvantages:**
  - channel coupling is neglected (no Feshbach resonances)
  - problems for low energies and optically forbidden transitions
  - results depend on the choice of V_1
  - lack of unitarization can be a problem

The (Time-Independent) Close-Coupling Expansion

- 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

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

- For each "i", one needs several sets of independent solutions subject to the boundary conditions

$$
\begin{aligned}
&F_{E,ij}(r=0) = 0 \\
&\lim_{r\to\infty} F_{E,ij} = \delta_{ij}\,\sin\left(k_i r - \tfrac{1}{2}\ell_i\pi\right) + \mathcal{K}_{ij}\,\cos\left(k_i r - \tfrac{1}{2}\ell_i\pi\right);\ i = 1, n_{open} \\
&\lim_{r\to\infty} F_{E,ij} = \mathcal{C}_{ij}\,\exp(-|k_i|r);\ i > n_{open}
\end{aligned}
$$

- Collision problem consists of finding the solution for each total energy.
- **Possible simplifications:**
  - No exchange outside a sphere of radius a (**→ *R*-matrix method**)
  - "Effective range formula" and simpler Born-type approximations
- **Advantages:**
  - based on an "exact" expansion
  - simultaneous results for transitions between **all states** in the expansion
  - sophisticated, publicly available codes exist
- **Disadvantages:**
  - expansion must be cut off
  - **usually, a single set of mutually orthogonal one-electron orbitals is used for all states in the expansion**
  - pseudo-orbitals may increase the flexibility but bring new problems with them

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

Big Problem:
Treatment of the Target Continuum States ?

- "Convergent Close-Coupling" **CCC**
- "$\mathcal{R}$-Matrix with Pseudo-States" **RMPS** Method
- "Intermediate Energy $\mathcal{R}$-Matrix" **IERM** Method

- Idea: Represent both the discrete and the continuum target states by diagonalizing the target Hamiltonian in a large square-integrable basis:
  - lower eigenvalues and eigenvectors represent physical bound states;
  - discrete negative-energy pseudo-states approximate the effect of the infinite number of physical discrete states;
  - discrete positive-energy pseudo-states approximate the effect of the target continuum.

All three methods can handle IONIZATION
via excitation of pseudo-states with positive energy!

Inclusion of Relativistic Effects

- **Re-coupling** of non-relativistic results (**CCC**; problematic near threshold) **listen for updates !**
- **Perturbative approach** (matrix elements calculated between non-relativistic wavefunctions; **Breit-Pauli R-matrix**)
- **Dirac**-based approach (**DARC** = **D**irac **A**tomic **R**-Matrix **C**ode; needs further development)

2008: CCC and BSR now fully relativistic! (applied to outer-shell e-Cs and e-Au)

2009: DBSR fully operational: e-Kr, Xe, Au, Hg with opening of core ===> e-W, W^+ may be within reach :):):)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS B: ATOMIC, MOLECULAR AND OPTICAL PHYSICS

J. Phys. B: At. Mol. Opt. Phys. **38** (2005) 1667–1678 doi:10.1088/0953-4075/38/11/008

The agreement of Breit–Pauli and Dirac *R*-matrix collision strengths for iron peak elements: an Fe^{14+} case study

K A Berrington[1], C P Ballance[2], D C Griffin[2] and N R Badnell[3]

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Abstract

In calculating collision strengths and excitation rates for electron impact on moderately ionized iron peak elements, one might question whether the Breit–Pauli *R*-matrix method is sufficiently accurate as compared with the Dirac *R*-matrix method. We test this for Fe^{14+} by removing as far as possible any variation in algorithmic features, such as the energy mesh and target state expansion, as opposed to genuine differences between the two approaches. We find the average difference between the Breit–Pauli and Dirac *R*-matrix effective collision strengths is only 6%, which confirms the hypothesis that if one gets the Dirac and Breit–Pauli target states close, and resolves the resonances adequately (we use up to 384 101 points), then the Dirac and Breit–Pauli collision strengths are in good agreement. We finally tabulate the best converged effective collision strengths for $T = 10^5$–10^7 K for all transitions involving the lowest 10 levels of Fe^{14+}.

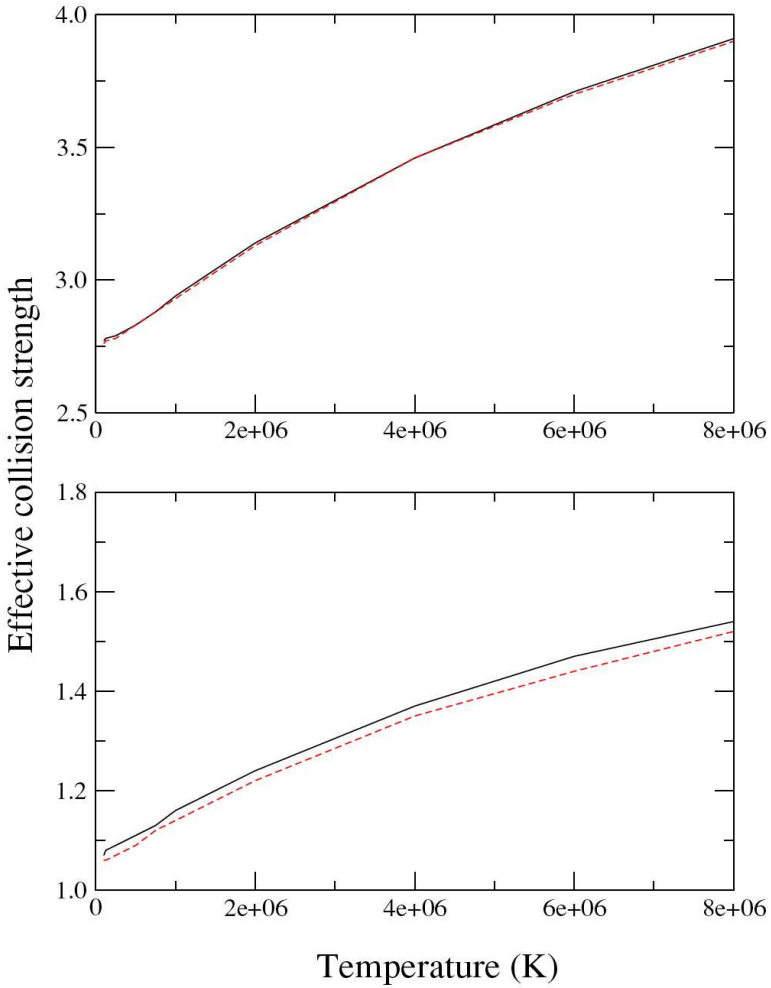


Figure 1. Effective collision strengths for two strong dipole-allowed transitions; results from the Breit–Pauli *R*-matrix calculation are represented by the solid lines and those from the Dirac *R*-matrix calculation by the dashed lines. The upper graph is for the $3s^2\ ^1S_0$–$3s3p\ ^1P_1$ transition and the bottom graph is for the $3s3p\ ^3P_1$–$3p^2\ ^3P_2$ transition.

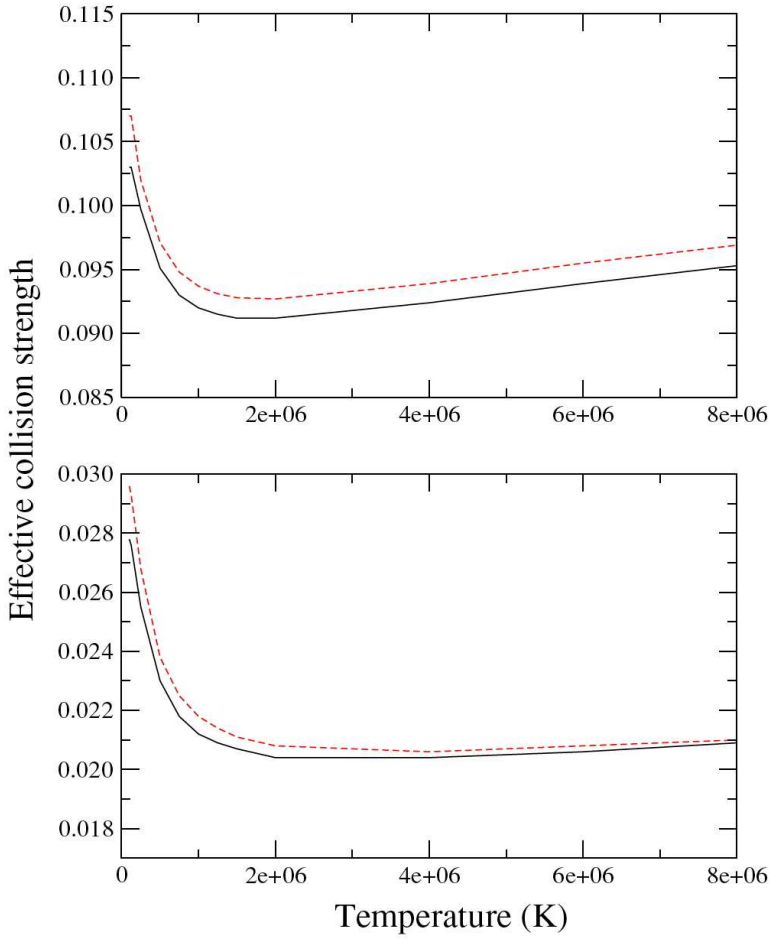


Figure 2. Effective collision strengths for two double-electron transitions; results from the Breit–Pauli *R*-matrix calculation are represented by the solid lines and those from the Dirac *R*-matrix calculation by the dashed lines. The upper graph is for the $3s^2\ ^1S_0$–$3p^2\ ^1D_2$ transition and the lower graph is for the $3s^2\ ^1S_0$–$3p^2\ ^3P_2$ transition.

Breit-Pauli seems o.k. for this case (and many others!)

Time-dependent and time-independent close-coupling methods for the electron-impact ionization of Be^+

M. S. Pindzola and F. Robicheaux
Department of Physics, Auburn University, Auburn, Alabama 36849

H Ψ = *i* δ/δt Ψ

N. R. Badnell
Department of Physics and Applied Physics, University of Strathclyde, Glasgow G4 0NG, United Kingdom

T. W. Gorczyca
Department of Physics, Western Michigan University, Kalamazoo, Michigan 49008

$$i\,\frac{\partial P^{LS}_{\ell_1\ell_2}(r_1,r_2,t)}{\partial t}=T_{l_1l_2}(r_1,r_2)P^{LS}_{l_1l_2}(r_1,r_2,t)+\sum_{l_1',l_2'}V^{L}_{l_1l_2,l_1'l_2'}(r_1,r_2)P^{LS}_{l_1'l_2'}(r_1,r_2,t), \tag{1}$$

$$T_{l_1l_2}(r_1,r_2)=-\frac{1}{2}\frac{\partial^2}{\partial r_1^2}-\frac{1}{2}\frac{\partial^2}{\partial r_2^2}+V^{l_1}_{PP}(r_1)+V^{l_2}_{PP}(r_2), \tag{2}$$

$$V^{L}_{l_1l_2,l_1'l_2'}(r_1,r_2)=(-1)^{L+l_2+l_2'}\sqrt{(2l_1+1)(2l_1'+1)(2l_2+1)(2l_2'+1)}\sum_{\lambda}\frac{r_<^{\lambda}}{r_>^{\lambda+1}}\begin{pmatrix}l_1&\lambda&l_1'\\0&0&0\end{pmatrix}\begin{pmatrix}l_2&\lambda&l_2'\\0&0&0\end{pmatrix}\begin{Bmatrix}L&l_2'&l_1'\\\lambda&l_1&l_2\end{Bmatrix}. \tag{3}$$

The coupled partial differential equations are solved on a two-dimensional lattice using an explicit time propagator. At time $t=0$ the wave function $P^{LS}_{l_1l_2}(r_1,r_2,0)$ is constructed as a symmetric product of an incoming radial wave packet for the scattering electron and a bound radial orbital $P_{nl}(r)$ for the valence electron. Following the collision at time $t=T$, the spin-averaged electron-impact ionization cross section is given by

Time-development of a wavepacket for e-Be$^+$

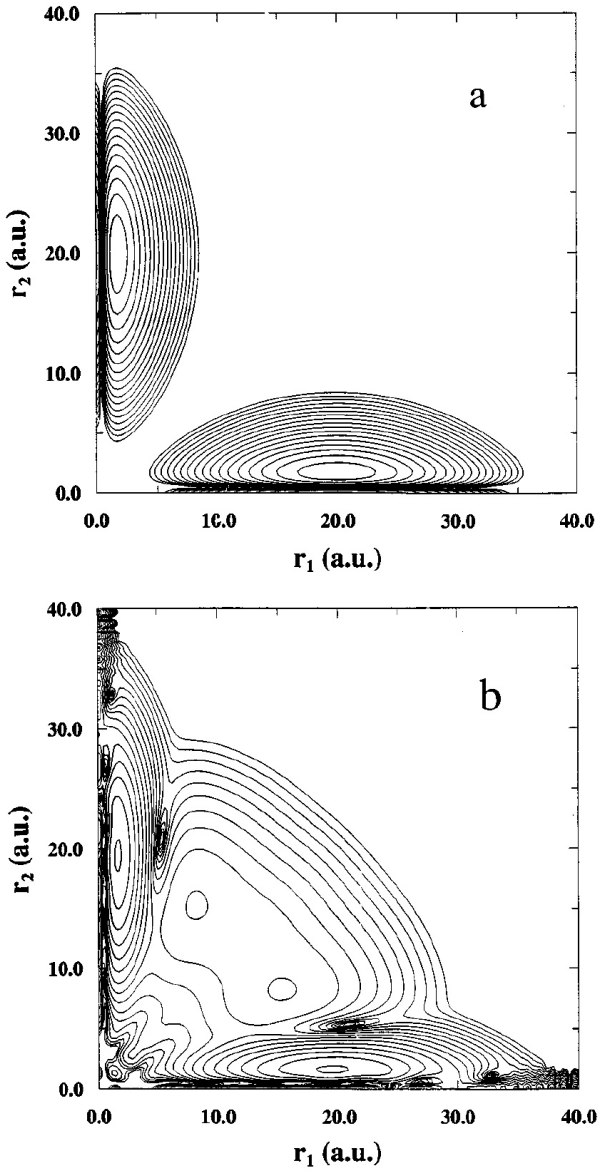


FIG. 1. ^1S partial-wave probability densities for electron-impact ionization of Be^+ at 50.0 eV using a model potential: (a) contour plot for $|P^{00}_{ss}(r_1,r_2,t=0)|^2$ and (b) contour plot for $|P^{00}_{ss}(r_1,r_2,t=20)|^2$.

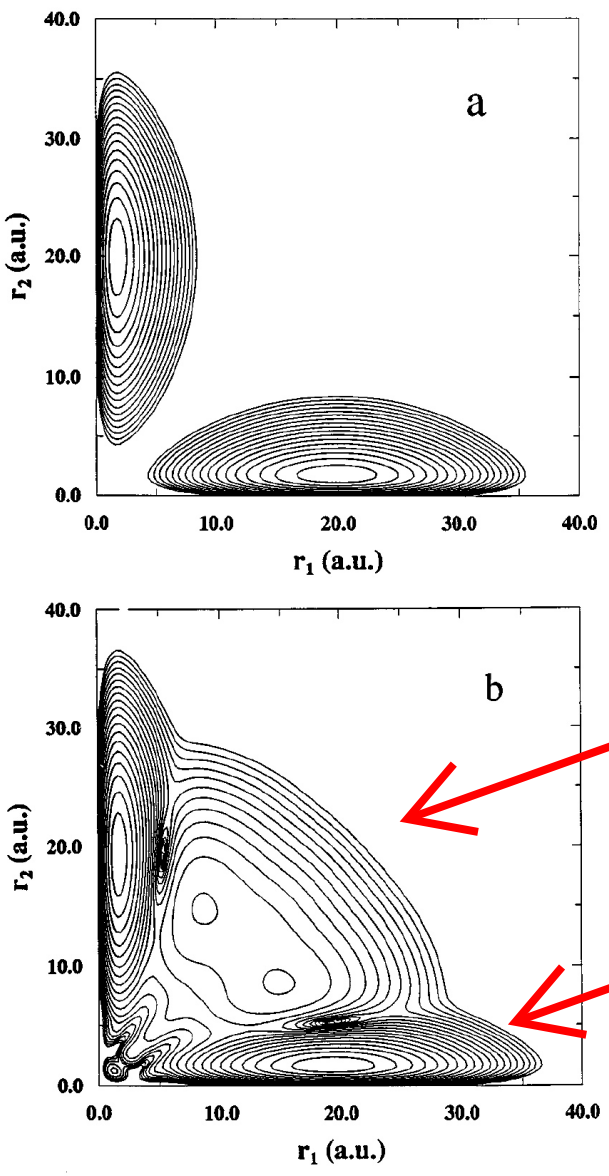
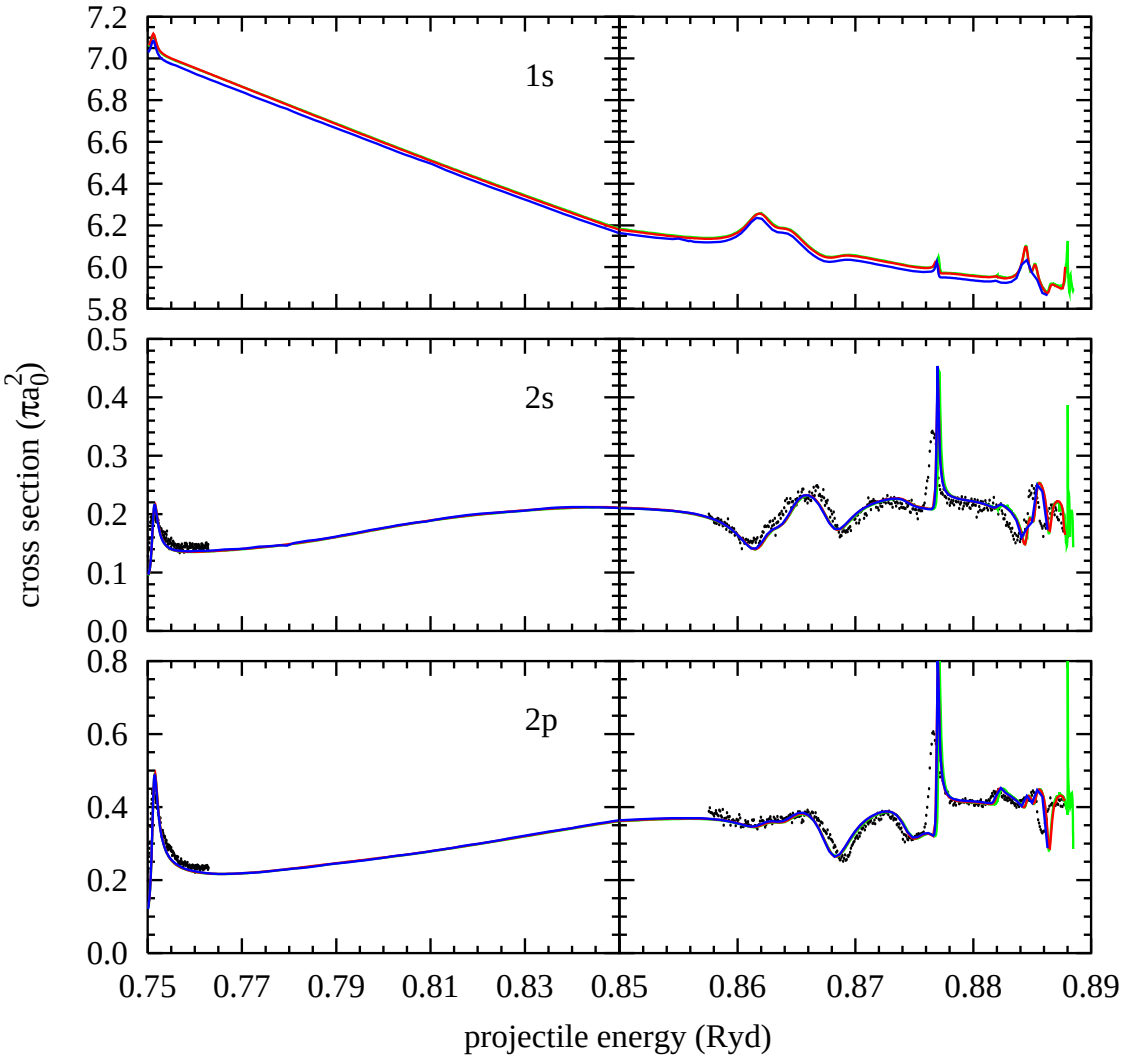


FIG. 2. ^1S partial-wave probability densities for electron-impact ionization of Be^+ at 50.0 eV using a model pseudopotential: (a) contour plot for $|P^{00}_{ss}(r_1,r_2,t=0)|^2$ and (b) contour plot for $|P^{00}_{ss}(r_1,r_2,t=20)|^2$.

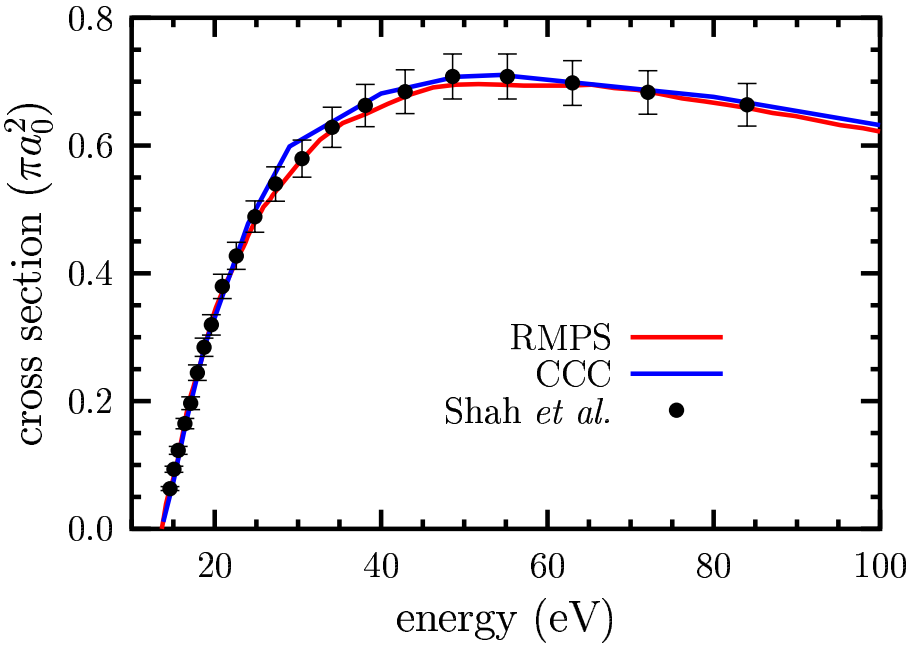
Benchmark Results for e-H Excitation
Bartschat, Bray, Burke, and Scott, J. Phys. B 29 (1996) 5493

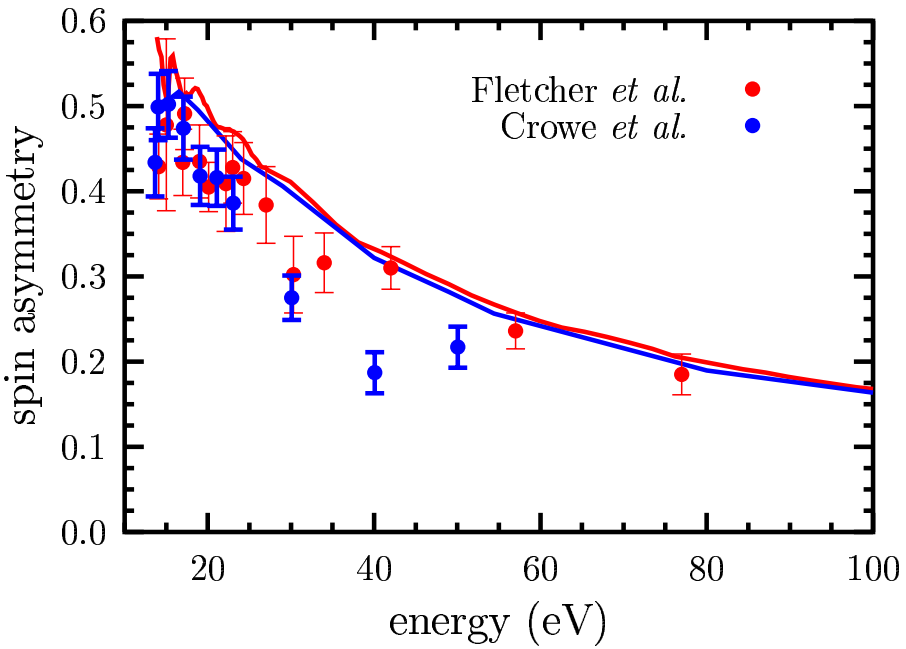
- Using a variational method, Schwartz solved the **low-energy elastic e−H scattering problem** with high accuracy in the early 1960's.
- As seen in further benchmark work in the inelastic regime, **CCC**, **RMPS**, and **IERM** predictions agree extremely well with each other, and also with the experimental data (dots on 2s, 2p) of Williams (1988). [From Bartschat, Bray, Burke, and Scott, J. Phys. B **29** (1996) 5493.]



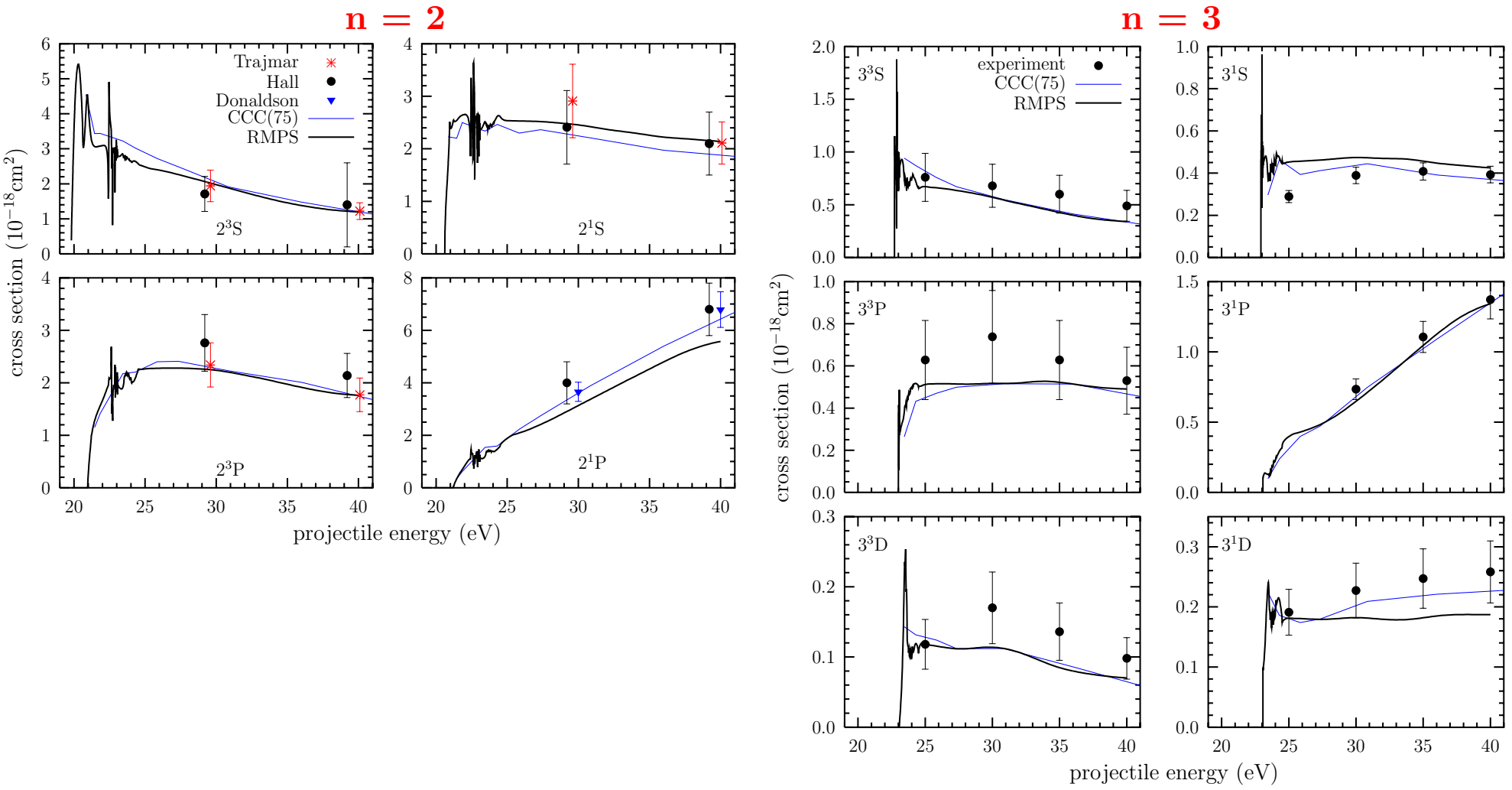
Total Cross Section and Spin Asymmetry in e-H Ionization

K. Bartschat and I. Bray, J. Phys. B 29 (1996) L577





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

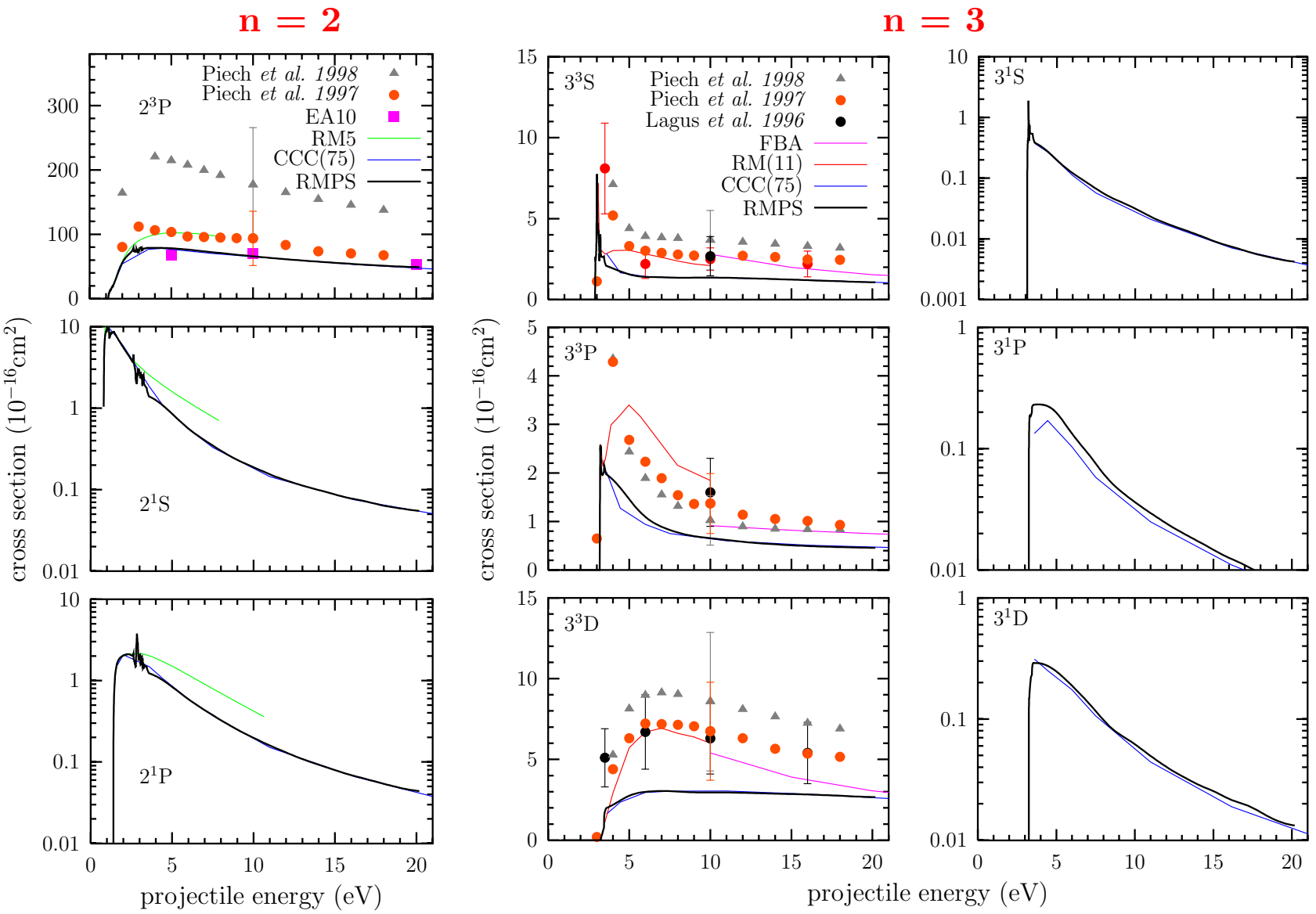


In 1998, de Heer recommends 0.5 x (CCC+RMPS) for uncertainty of 10% — independent of experiment!

So far, so good ...

Cross Section for Electron-Impact Excitation of He(1s2s)^{3}S

K. Bartschat, J. Phys. B 31 (1998) L469



There are BIG differences in excitation from the metastsable!

It looks like theory may be correct after all!

PRL **94,** 173201 (2005) PHYSICAL REVIEW LETTERS week ending 6 MAY 2005

Electron Collisions with Laser Cooled and Trapped Metastable Helium Atoms: Total Scattering Cross Sections

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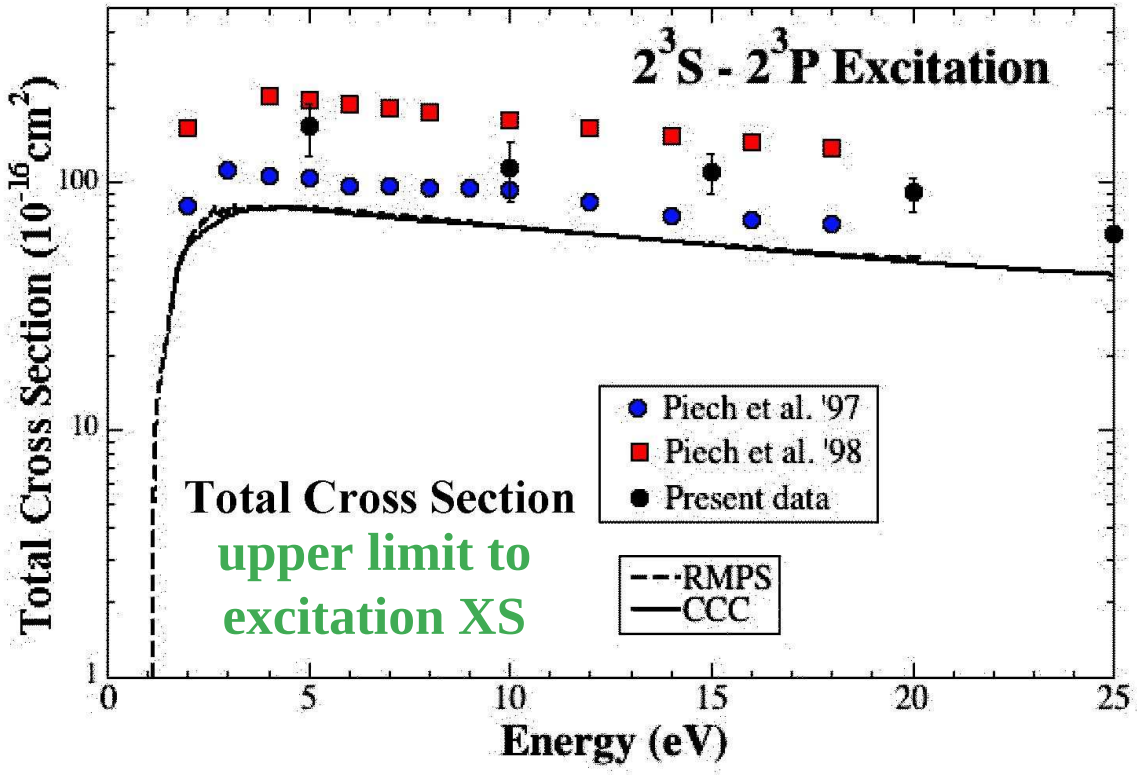

Bartschat [4] demonstrates that a total of four calculations, from an early eikonal approximation to several versions of the *R*-matrix approach, and the CCC technique all give essentially the same result, which favors the lower excitation cross section. The present total cross section result, also shown in Fig. 4, should, by definition, be larger than any partial cross section that contributes to it. Thus our measurements also strongly favor the earlier Wisconsin result [18], which is smaller than the present total cross section, over the later one [19].

PHYSICAL REVIEW A **68**, 062705 (2003)

Electron-impact excitation of beryllium and its ions

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(Received 24 August 2003; published 18 December 2003)

Inelastic electron scattering from light atomic species is of fundamental importance and has significant applications in fusion-plasma modeling. Therefore, it is of interest to apply advanced nonperturbative, close-coupling methods to the determination of electron-impact excitation for these atoms. Here we present the results of *R* matrix with pseudostate (RMPS) calculations of electron-impact excitation cross sections through the $n=4$ terms in Be, Be^{+}, Be^{2+}, and Be^{3+}. In order to determine the effects of coupling of the bound states to the target continuum in these species, we compare the RMPS results with those from standard *R*-matrix calculations. In addition, we have performed time-dependent close-coupling calculations for excitation from the ground and the metastable terms of Be^{+} and the metastable term of Be^{3+}. In general, these results are found to agree with those from our RMPS calculations. The full set of data resulting from this work is now available on the Oak Ridge National Laboratory Controlled Fusion Atomic Data Center web site, and will be employed for collisional-radiative modeling of Be in magnetically confined plasmas.

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 !

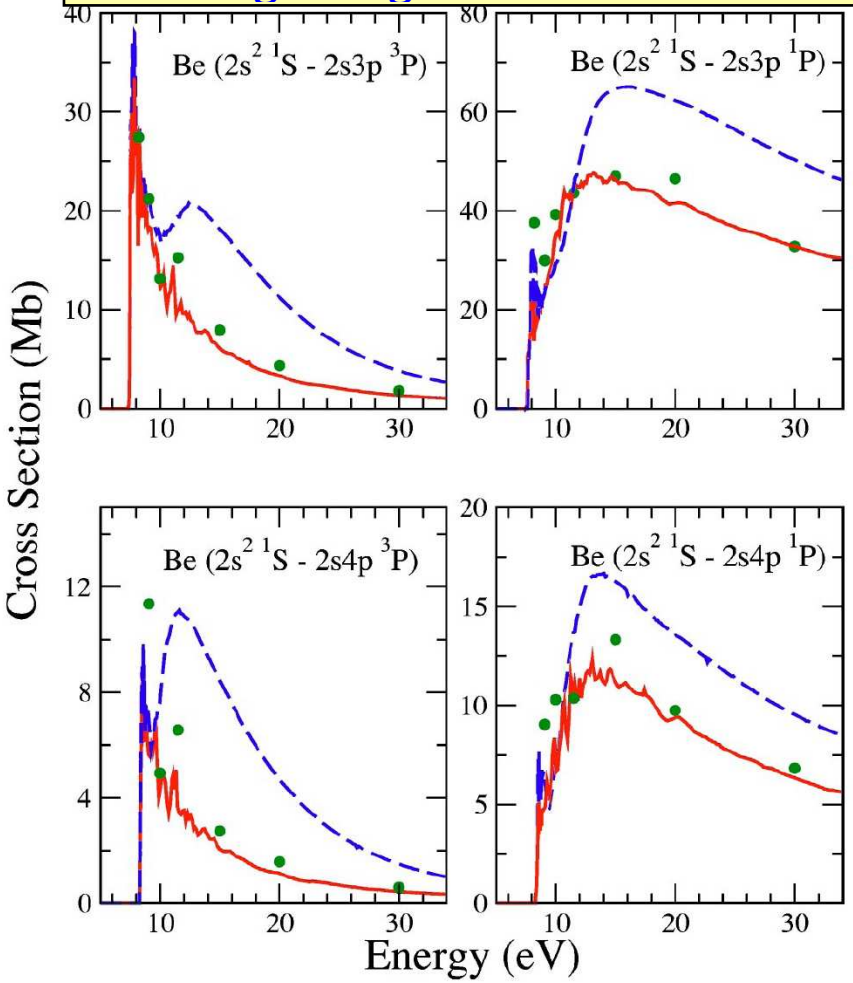


FIG. 2. Electron-impact excitation cross sections from the $2s^2\,{}^1S$ ground term of Be to the $2snp\,{}^3P$ and $2snp\,{}^1P$ excited terms for $n=3$ and 4. Dashed curves are from the present 29-term R-matrix calculation; solid curves are from the present 280-term RMPS calculation; solid circles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

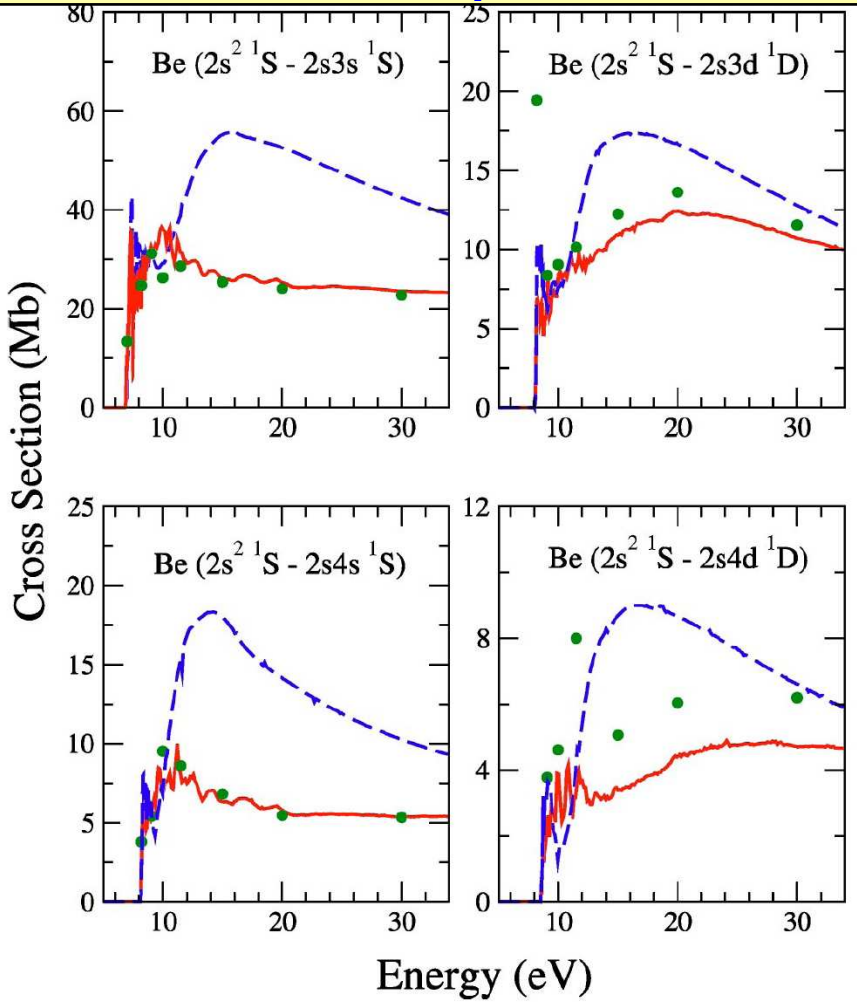
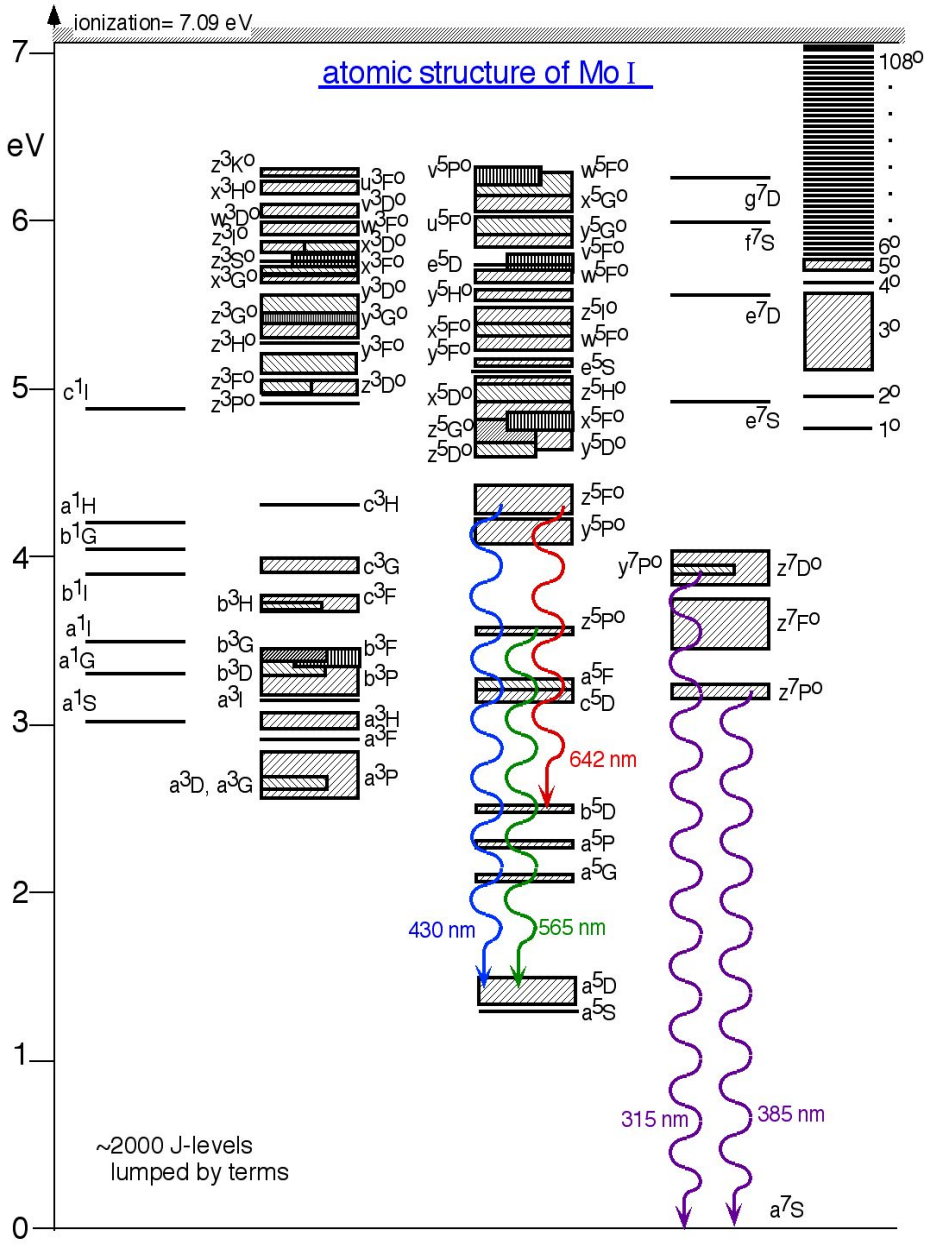


FIG. 3. Electron-impact excitation cross sections from the $2s^2\,{}^1S$ ground term of Be to the $2sns\,{}^1S$ and $2snd\,{}^1D$ excited terms. Dashed curves are from the present 29-term R-matrix calculation; solid curves are from the present 280-term RMPS calculation; solid circles are from CCC calculations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

A Grand Challenge:
Electron Collisions with Molybdenum



$Mo\text{-}O_3\text{-}Ar$ = electrodeless non-Hg discharge bulb

Experiment:

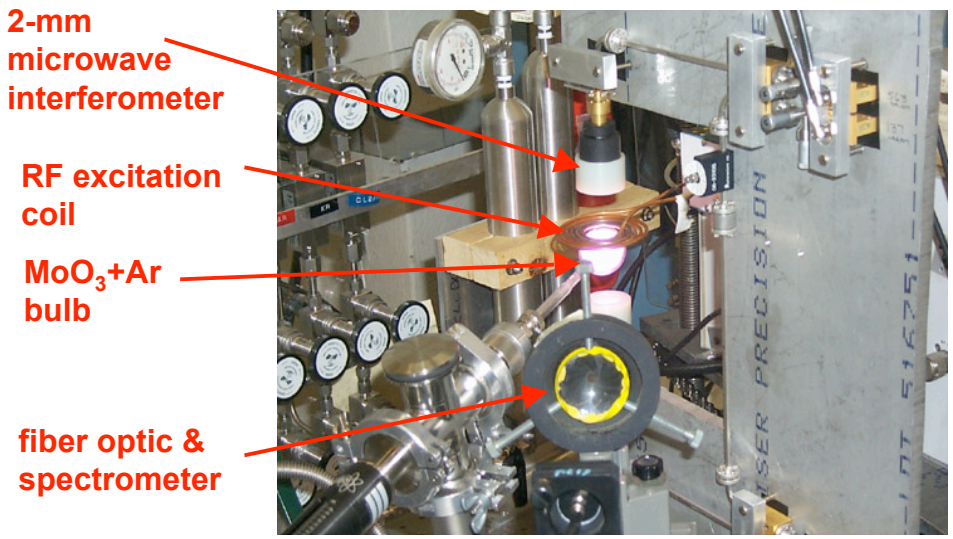
p_{Ar}= 1 Torr,
charged with MO_3 powder,
R_{bulb}=1.3 cm,
P_{RF}=200 W@ 13.6 MHz

Unique lamp properties:

Electrodeless, non-LTE,
low pressure plasma,
non-Hg, metallic emitter,
recycling chemistry,
displaying a broad spectrum
with component near optimum.

Spectrum:

Calibrated for absolute intensities.

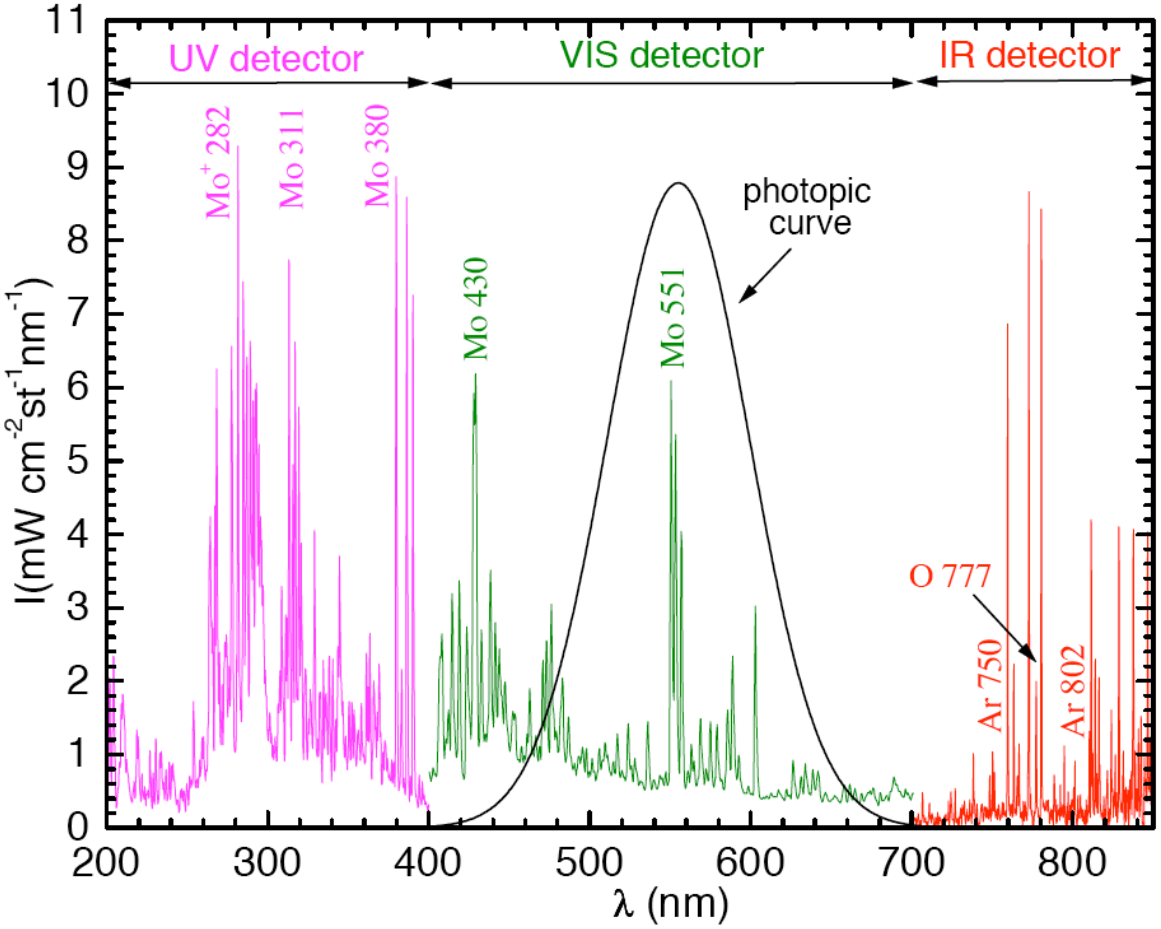


10,000 lumens, ~ 40 lpw

Giuliani, Petrov, Pechacek & Meger, Trans. Plas. Sci., **31**, 564 (2003)
Shamamian, et al., patent, 2000

Spectrum from a Moly-oxide Lamp

The Mo lamp is a low-pressure gas discharge lamp. The active element (Mo) emits direct visible light covering the UV and the whole visible domain



Reference: G M Petrov, J L Giuliani, A Dasgupta, K Bartschat and R Pechacek , *Journal of Applied Physics* **95** (2004) 5284

Excitation pathways of visible and UV emission from Mo

Motivation

Predict the most important kinetic pathways leading to emission of visible and ultraviolet radiation.

Objective

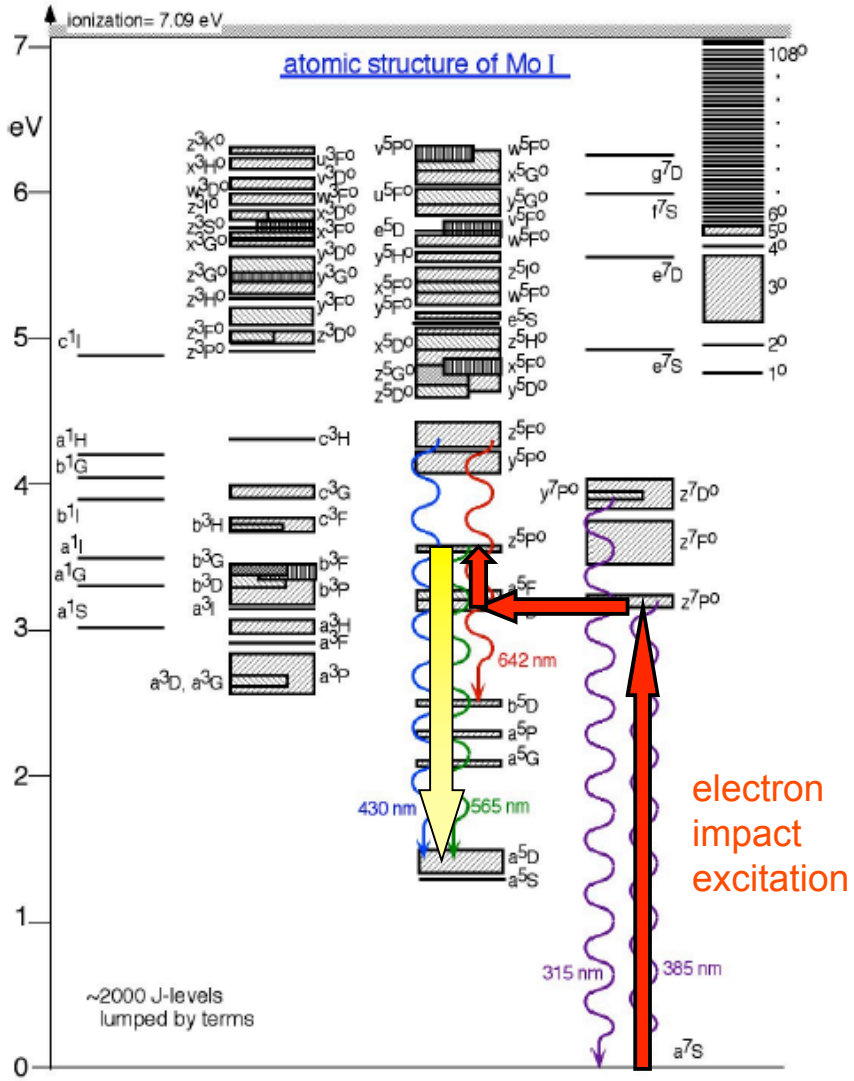
Establish the main pathways leading to emission of visible and UV radiation from Mo atoms by using a set of atomic data (excitation cross sections).

Challenge

The Mo atom has extremely complicated atomic structure. The visible radiation is a result of a sequence of transitions between the excited states of Mo with electrons.

Path #1:visible radiation with wavelengths 550–603 nm

$Mo(a^7S^e) \Rightarrow Mo(z^7P^o) \Rightarrow Mo(c^5D^e) \Rightarrow Mo(z^5P^o) \Rightarrow$ radiation.



The kinetic pathway is determined by comparing rate coefficients for electron impact out of $Mo(z^7P^o)$ to the quintet levels. The reaction with largest rate is

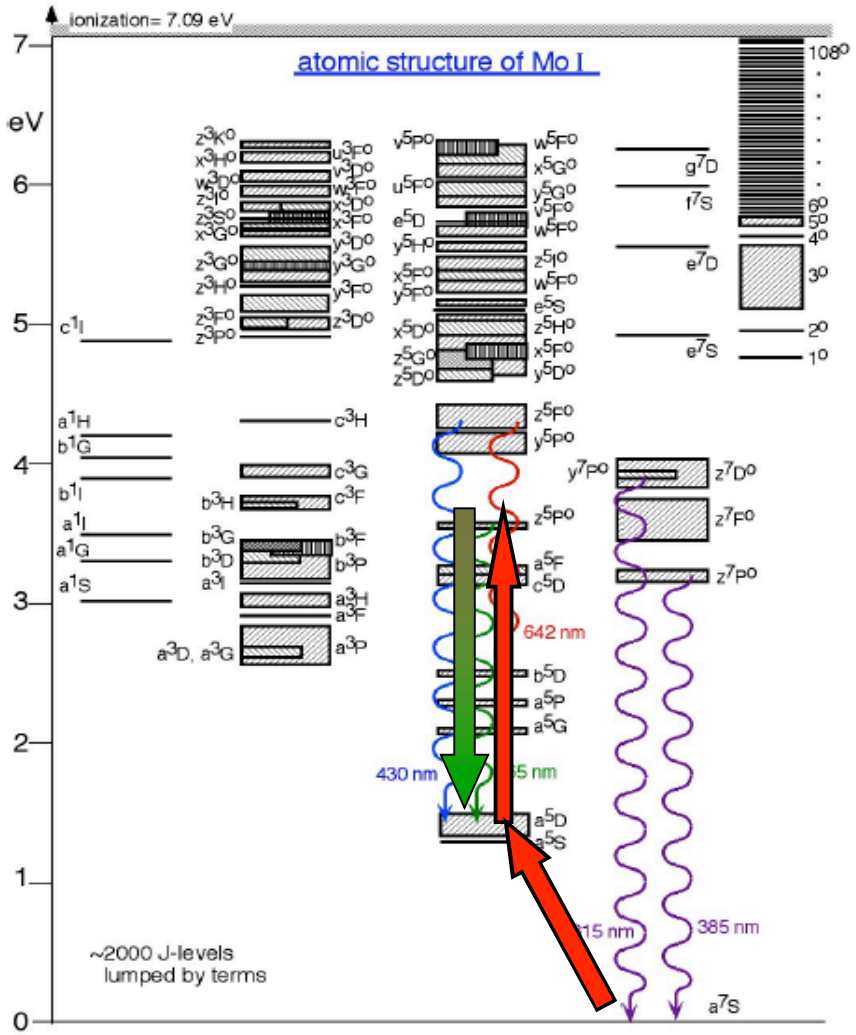
$Mo(z^7P^o) + e \rightarrow Mo(c^5D^e) + e$

Analogously, the largest rate out of $Mo(c^5D^e)$ is to $Mo(z^5P^o)$ level:

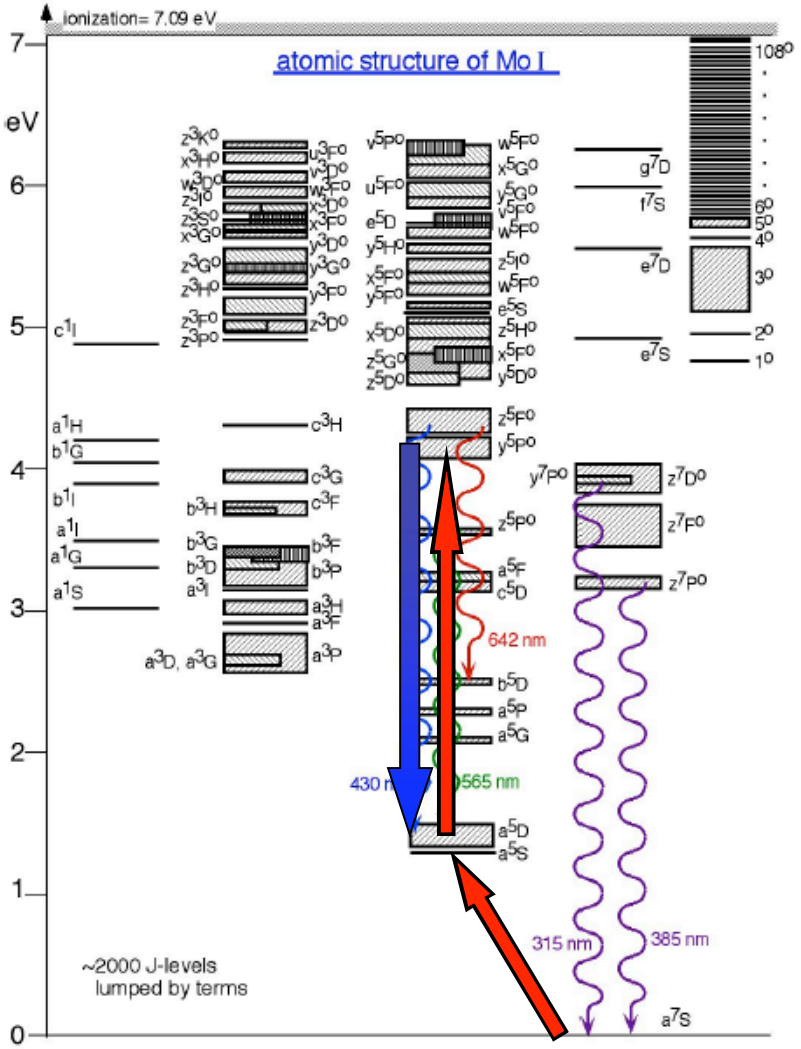
$Mo(c^5D^e) + e \rightarrow Mo(z^5P^o) + e$

Path #2-3:Visible radiation with wavelengths 550–603 and 444-446 nm

Mo(a^7S^e) ⇒ Mo(a^5S^e) ⇒ Mo(z^5P^o) ⇒radiation.



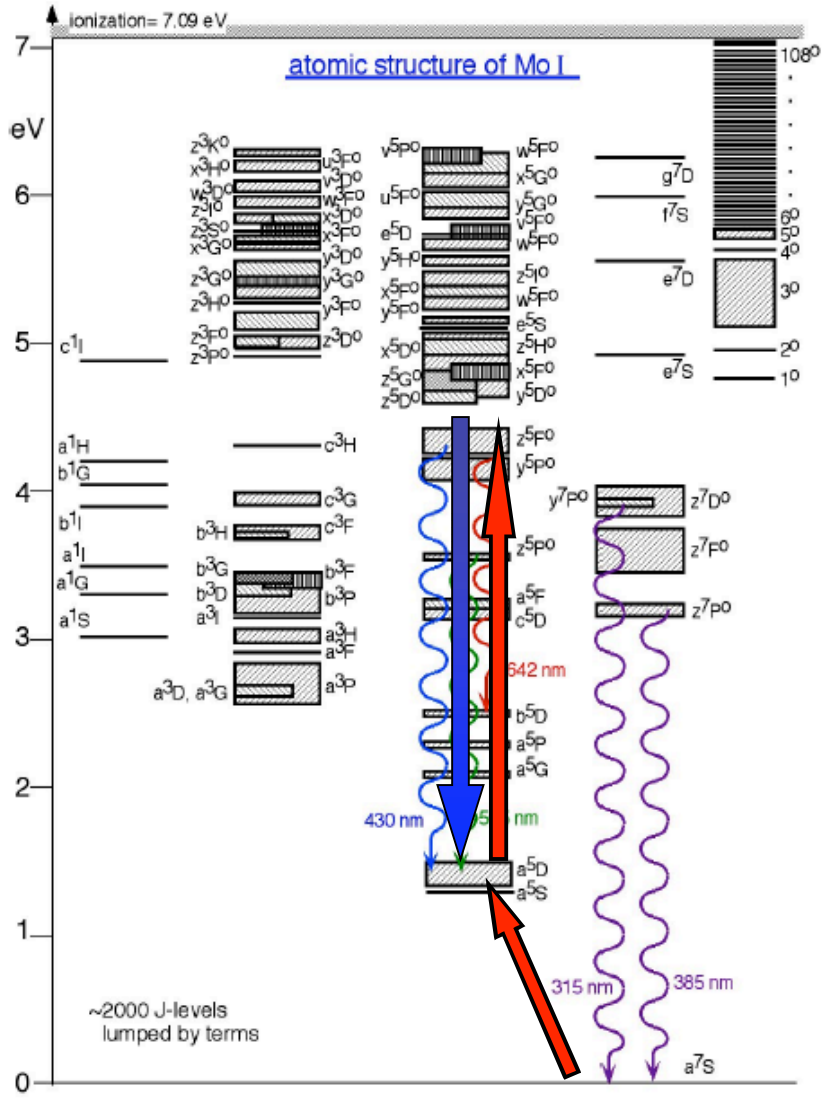
Mo(a^7S^e)⇒ Mo(a^5D^e) ⇒ Mo(y^5P^o) ⇒radiation.



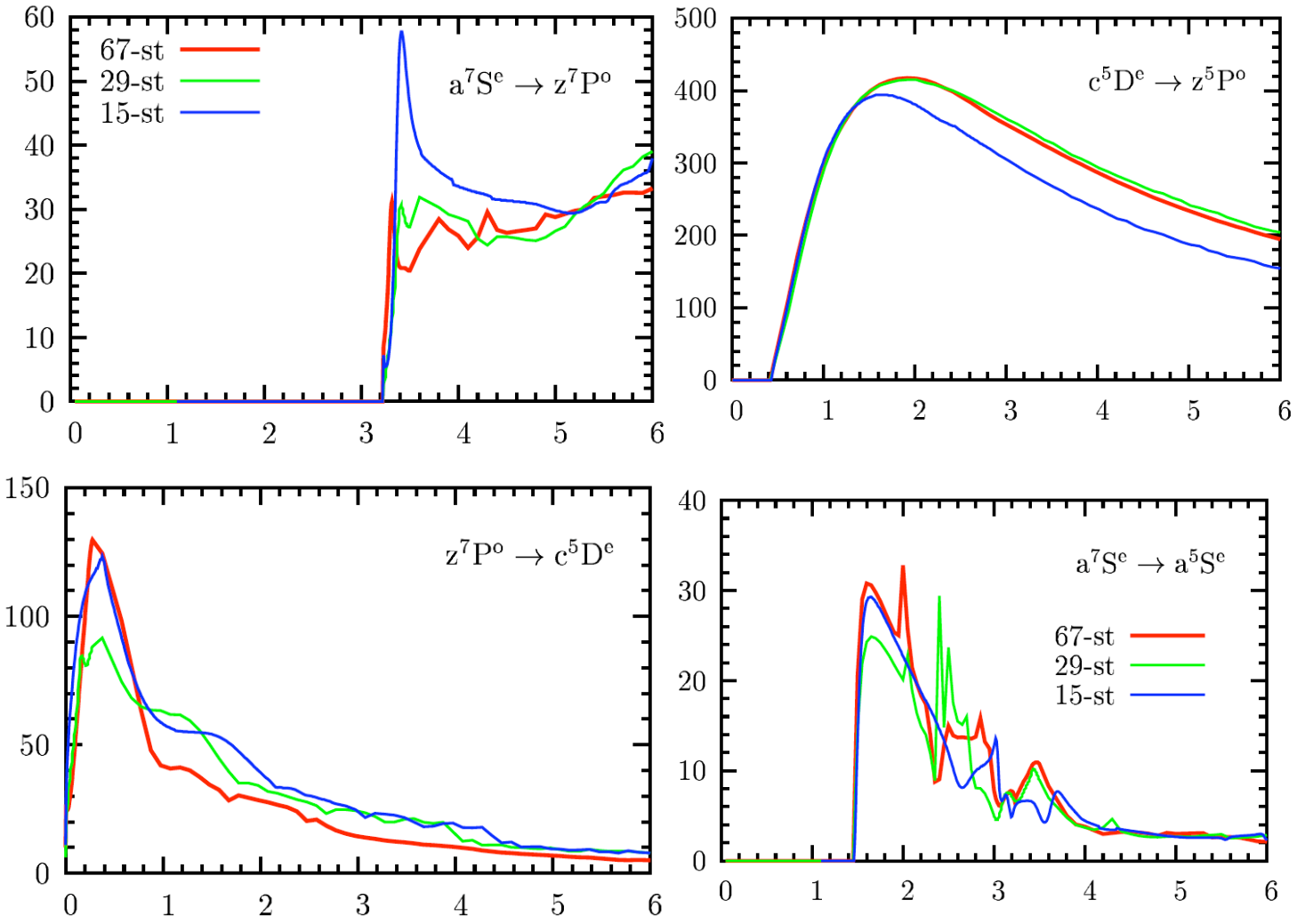
Path #4:visible radiation with wavelengths 430 nm

NRL Radiation Hydrodynamics Code 6720

$Mo(a^7S^e) \Rightarrow Mo(a^5D^e) \Rightarrow Mo(z^5F^o) \Rightarrow$ radiation.



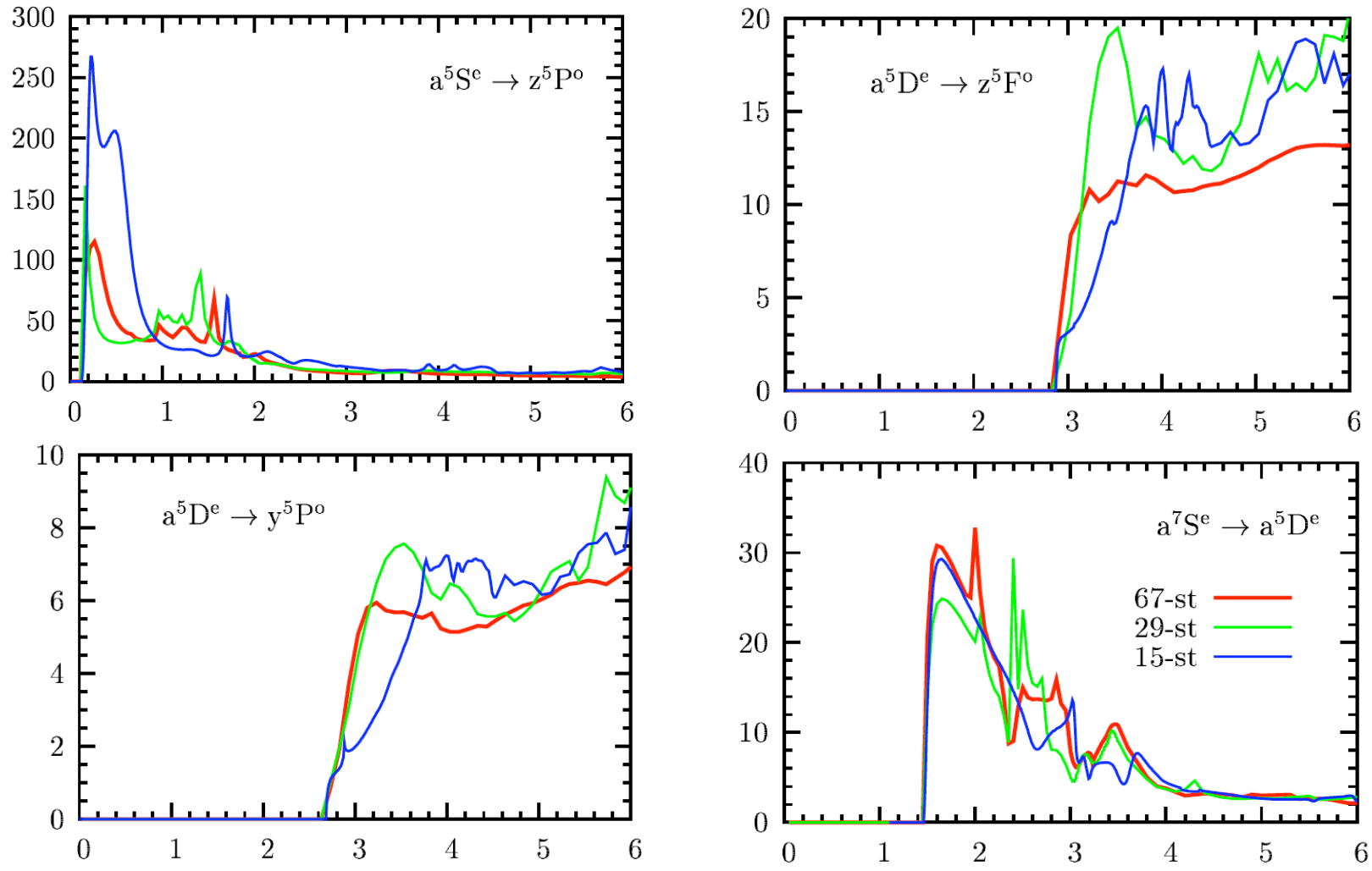
Excitation Cross sections of Mo I (R-Matrix calculations)



67-state close-coupling

Reference: K Bartschat, A Dasgupta, G M Petrov and J L Giuliani, *J. Phys. B.* **35** (2002) & *New Journal of Physics* **6** (2004) 145,

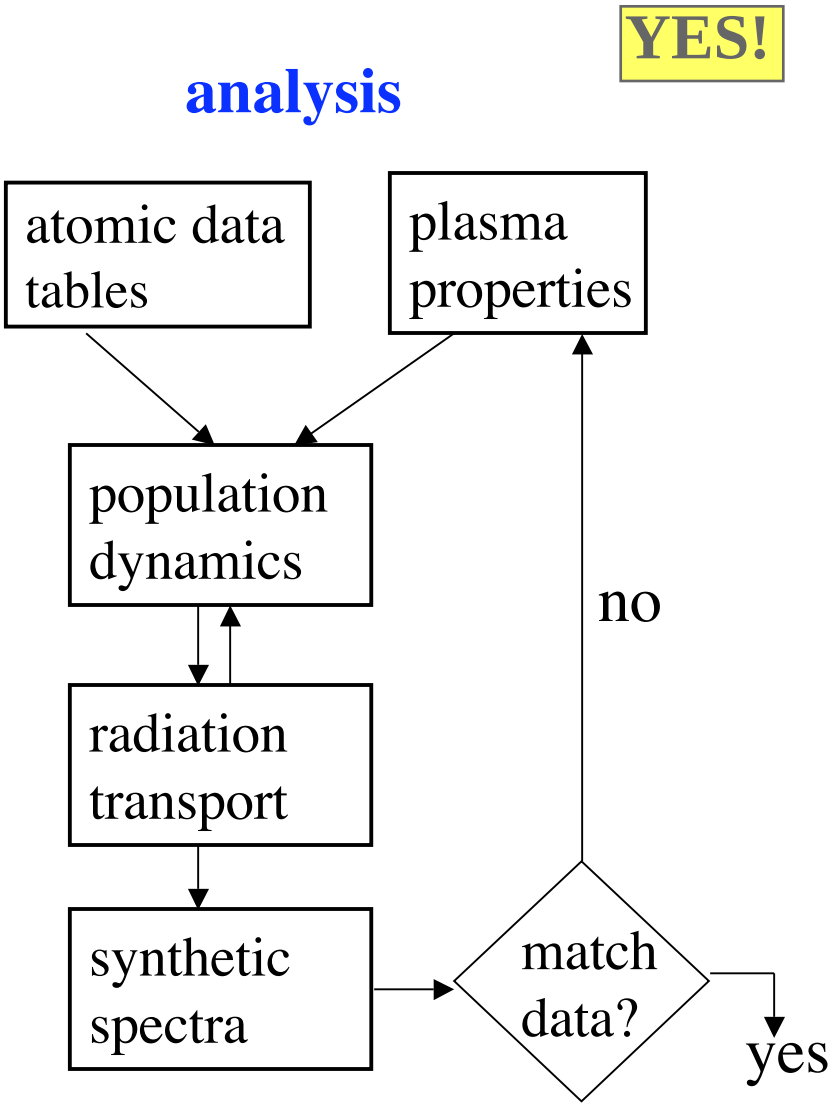
Excitation Cross sections of Mo I

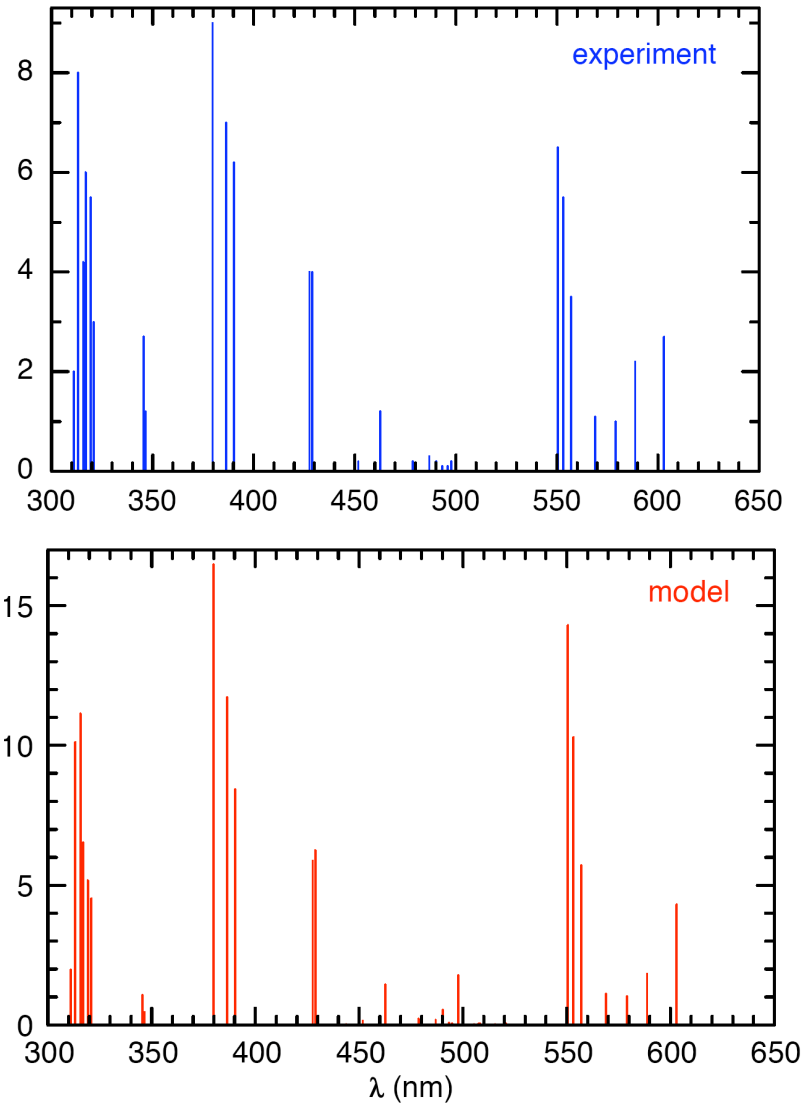


Cross sections -> Boltzmann code and chemical-diffusion model; Pathway to visible light

Does theory have any chance?

Spectra of Mo: Model vs. Experiment





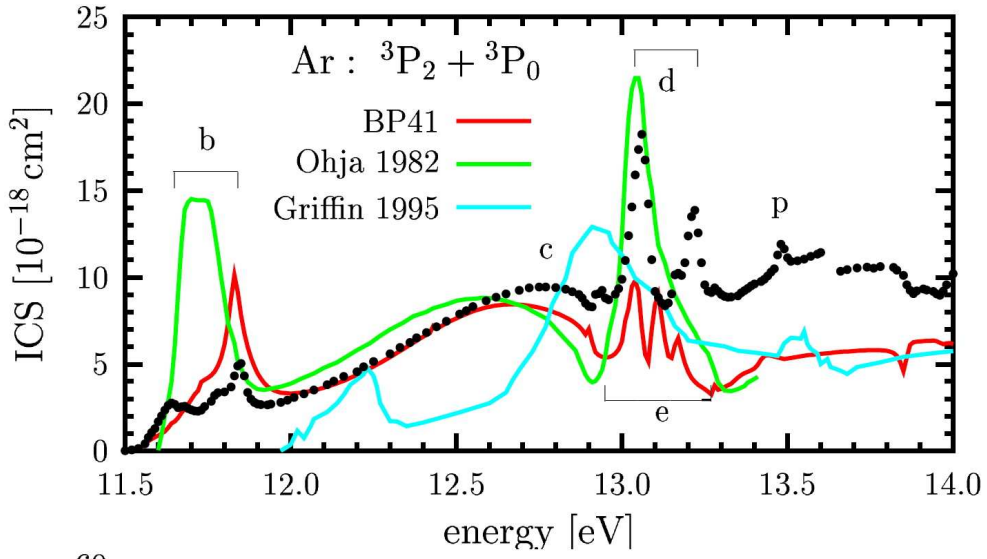
back to the noble gases ...

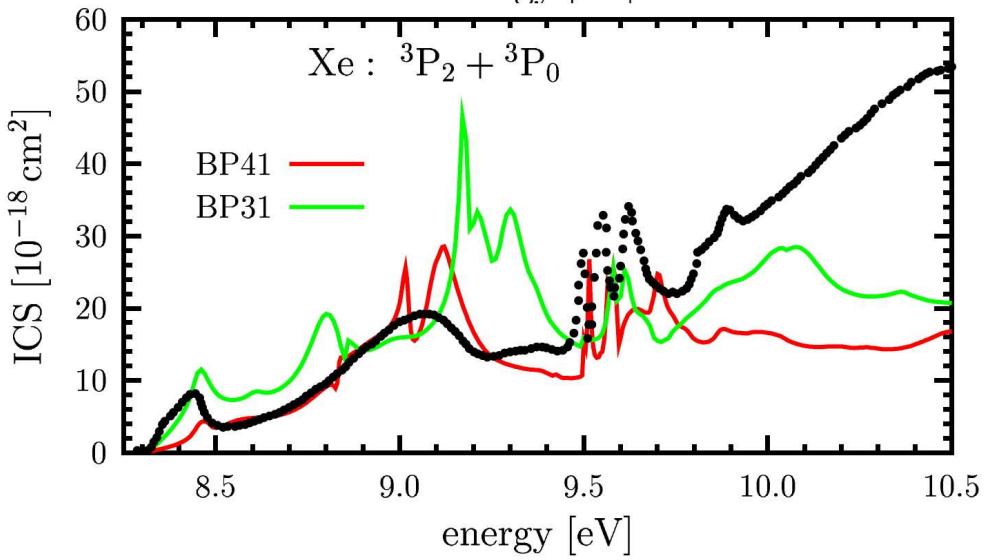
Metastable Production in Electron Collisions with Ar and Xe

theory: Breit-Pauli R-matrix
(Grum-Grzhimailo and K.B. 2001/2)
experiment: metastable count rate
(Buckman *et al.* 1983)

at best qualitative agreement between theory and experiment

significant differences in theoretical predictions



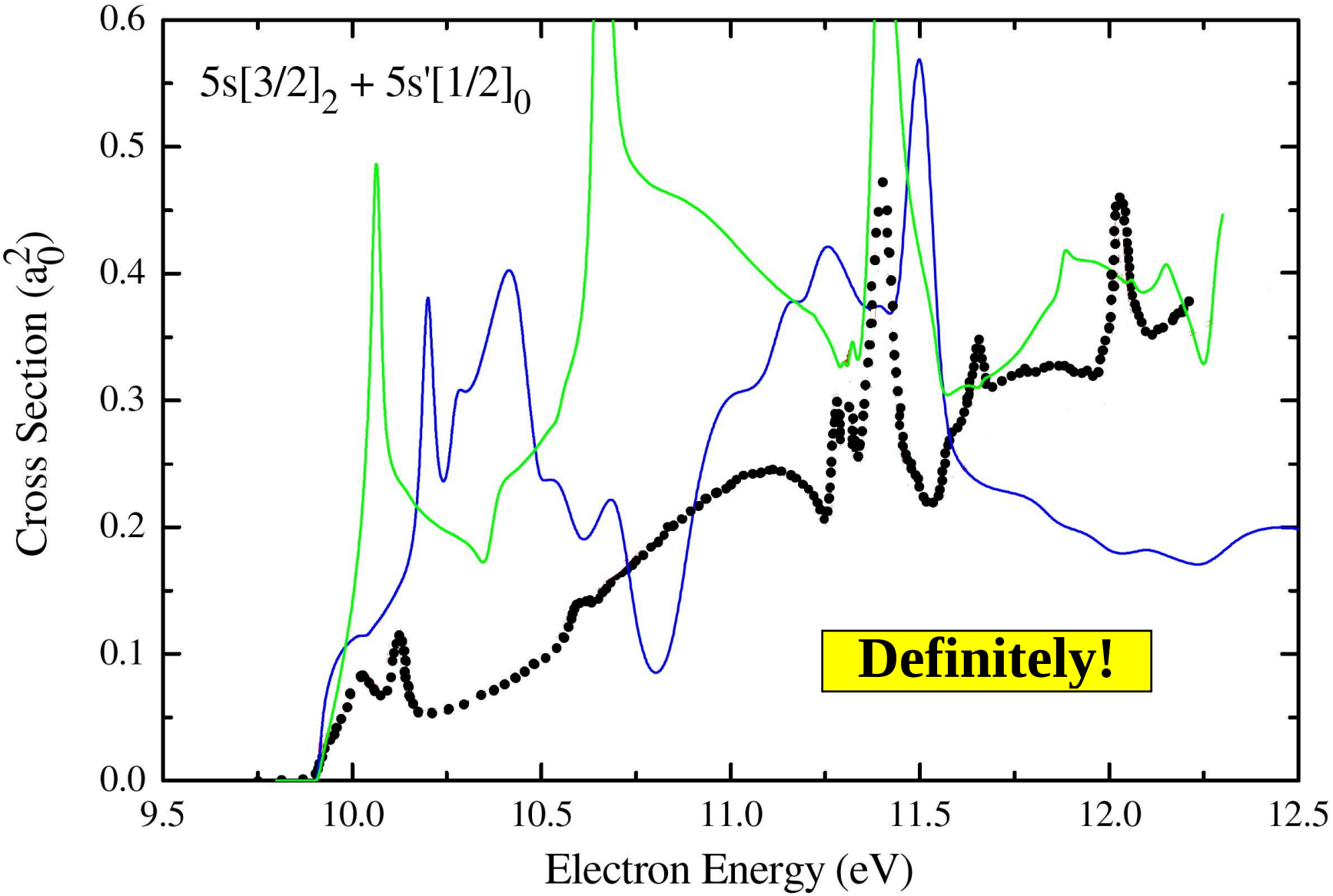


Oops — maybe we should try a bit harder?

Metastable Excitation Function in Kr

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

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



Electron-Impact Excitation of Krypton $(4p^5 5s)^3P_2$

[Phys. Rev. A 65 (2002) 042724]

Theory:

Dasgupta/Madison (DW)

Bartschat/Grum-Grzhimailo (BPRM)

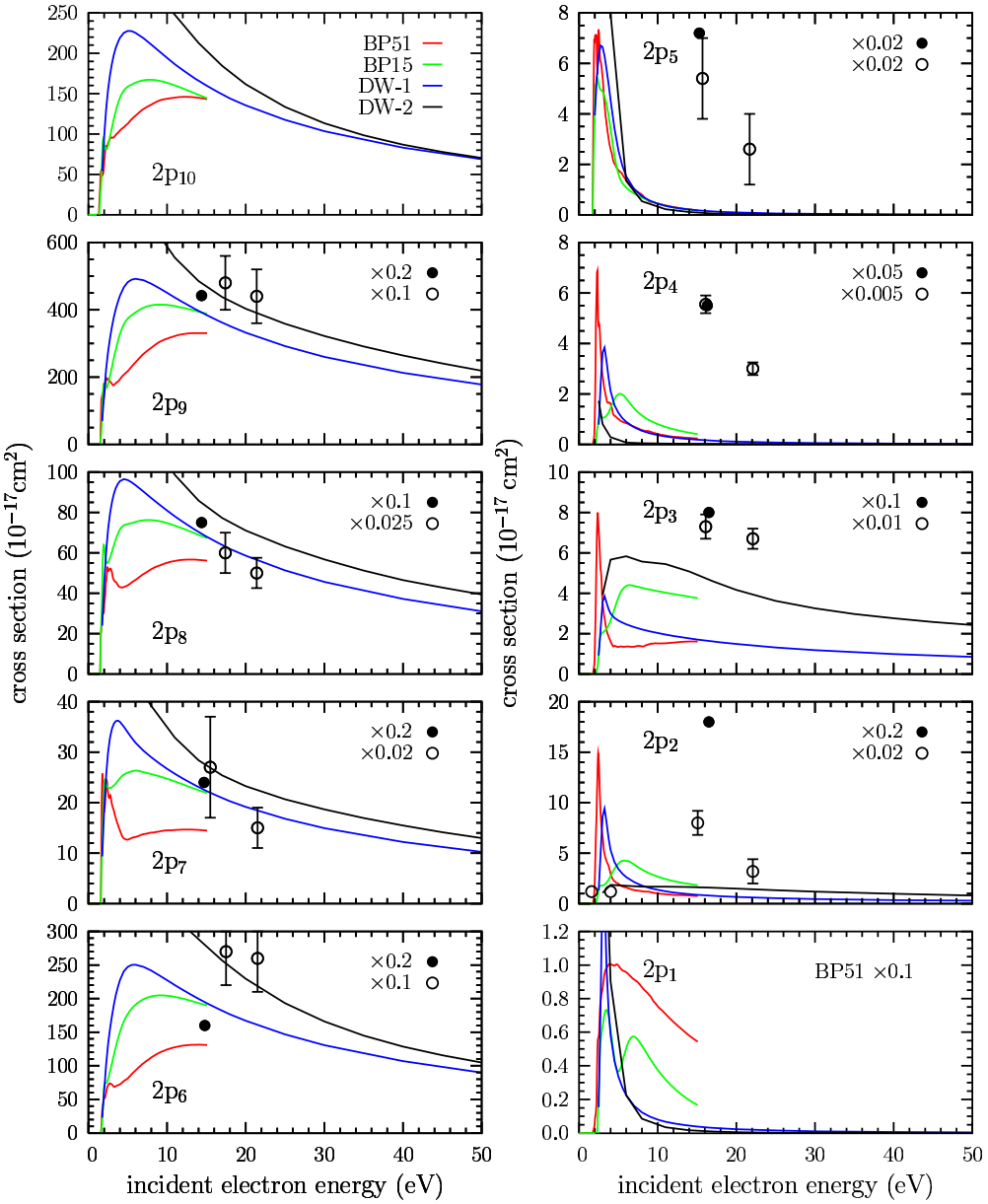
Experiment:

Kolokov and Terekhova (•)

Mityureva et al. (○)

New data from the Wisconsin group agree much better with the theoretical predictions.

The real trouble is the disagreement among the theories!



History of the Belfast R-Matrix Program

- **Basic Idea: Rewrite close-coupling expansion as**

$$\Psi_E(\boldsymbol{r}_1, ..., \boldsymbol{r}_{N+1}) = \sum_k A_{Ek} \Psi_k(\boldsymbol{r}_1, ..., \boldsymbol{r}_{N+1})$$

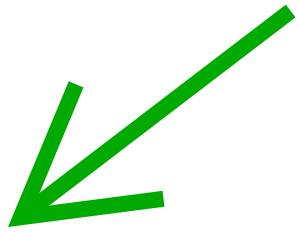
  with **energy-independent basis functions**

$$\Psi_k(\boldsymbol{r}_1, ..., \boldsymbol{r}_{N+1}) = \sum_{ij} a_{ijk} \Phi(\boldsymbol{r}_1, ..., \hat{\boldsymbol{r}}_{N+1}) u_{ij}(r)/r + \sum_j b_{jk} \chi_j(\boldsymbol{r}_1, ..., \boldsymbol{r}_{N+1})$$

- Applications to atoms:
  - Burke *et al* (1971), Burke and Robb (1975)
  - Many calculations since then; see Burke and Berrington (1993)
- **Computer Codes:**
  - **RMATRX-I:** Berrington *et al* (1995)
  - **RMATRX-II:** non-relativistic, improved angular integration (P.G. Burke, V.M. Burke)
  - **PRMAT:** parallelized version of RMATRX-II + FARM, Sunderland *et al* (2002)
  - **Badnell's RMAT:** `http://amdpp.phys.strath.ac.uk/rmatrix/`

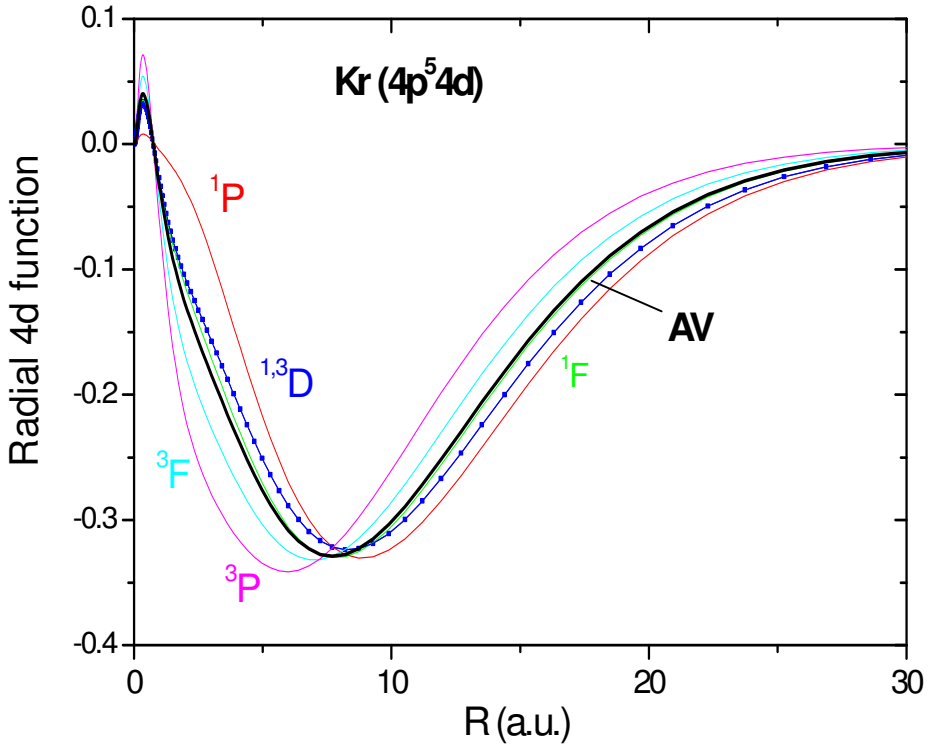
    `RMATRX-I` with possibility for radiative damping
- **Principal ingredient: a single set of orthogonal one-electron orbitals**
  - $< P_{n\ell} | u_{k\ell} >= 0 \rightarrow$ large $(N+1)$-electron expansions needed for consistency
  - $< P_{n\ell} | P_{n'\ell} >= 0 \rightarrow$ **difficulties to achieve accurate target representation**

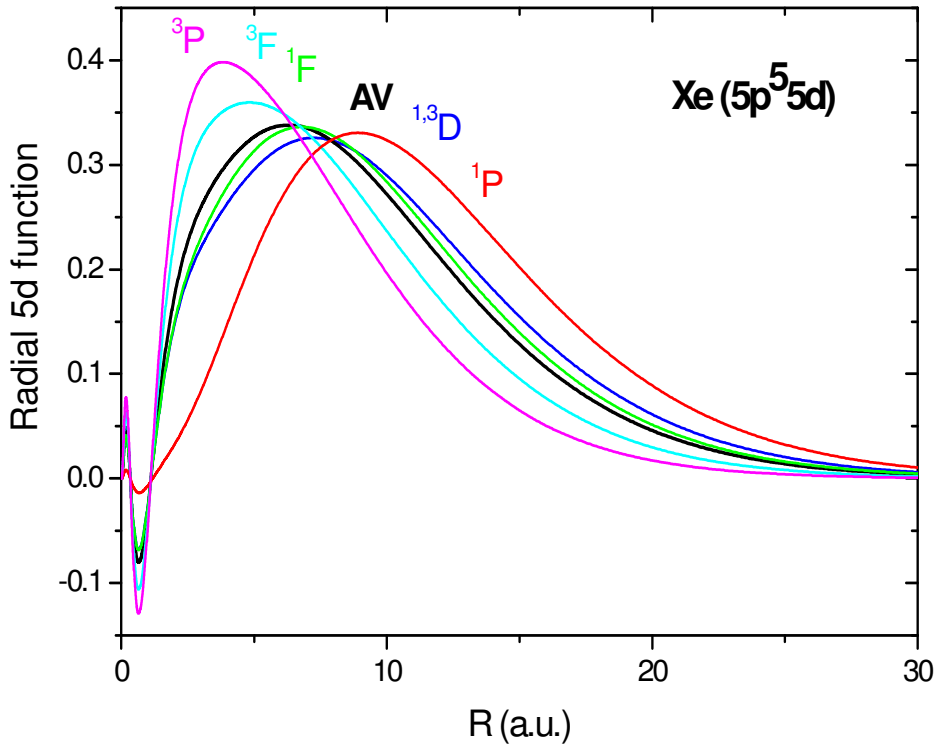
    (term-dependence, relaxation effects, correlation)
- **pseudo-orbitals can increase flexibility but also lead to pseudo-states and pseudo-resonances**



Example of Term-Dependence: 4d and 5d orbitals in Kr and Xe

- **strong term dependence** of the valence orbitals
- need to include relativistic effects due to the **fine-structure splitting** of the **np^5** core
- strong **interaction** between **$np^5(n+1)s$** and **np^5nd** levels
- **core-valence** and **inner-core** correlation





This is how BSR started at Drake

Can R-matrix (close-coupling) do better?

A general and effective program for electron collisions with atoms and ions using a B-spline approach with non-orthogonal orbitals

Oleg Zatsarinny and Klaus Bartschat

NSF Award Numbers: PHY-0311161 (ITR) and PHY-0555226

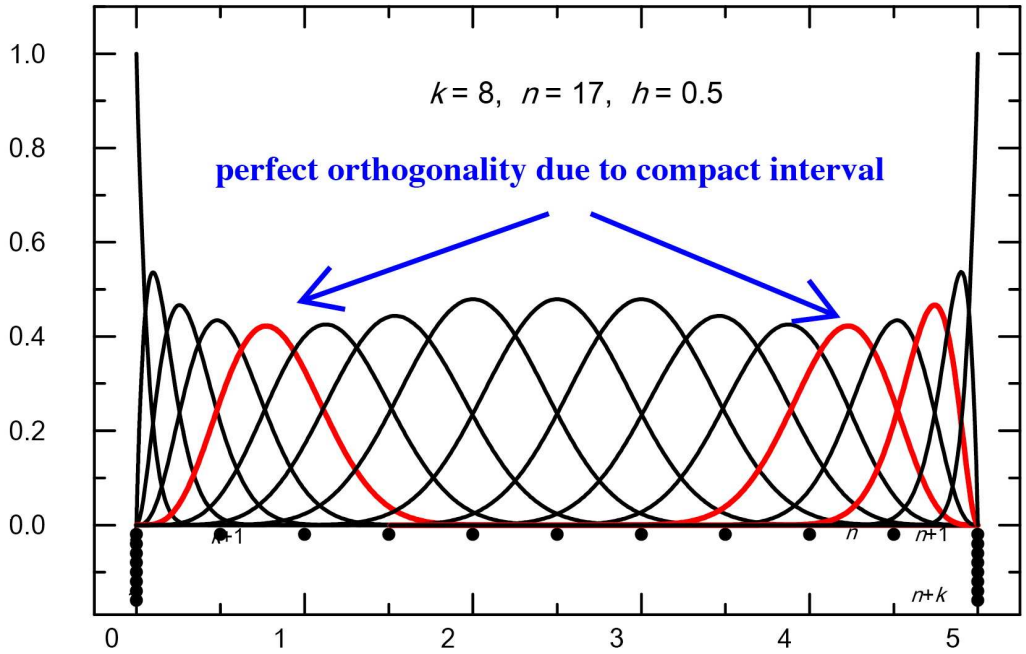
now PHY-0903818 + Teragrid

We have a great new program :):):)

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!

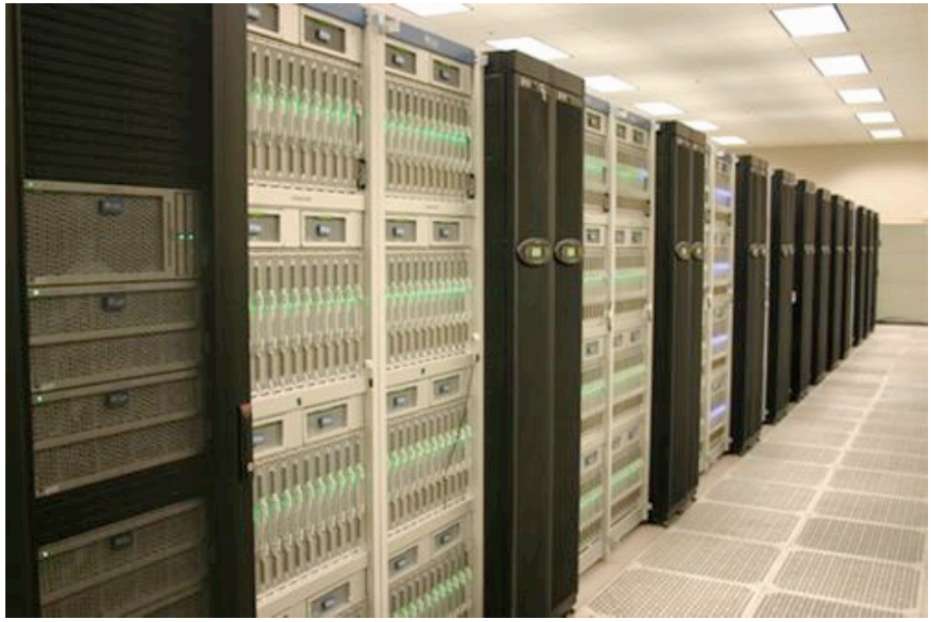


- **Consequences:**
  - **Much improved target description possible with small CI expansions**
  - **Consistent description of the *N*-electron target and (*N*+1)-electron collision problems**
  - No "Buttle correction" since *B*-spline basis is effectively complete
- **Complications:**
  - Setting up the Hamiltonian matrix can be very complicated and lengthy
  - Generalized eigenvalue problem needs to be solved
  - Matrix size typically **50,000** and higher due to size of *B*-spline basis
  - Rescue: Excellent numerical properties of *B*-splines; use of (SCA)LAPACK *et al.*

[One of] our apparatus ...

TACC TEXAS ADVANCED COMPUTING CENTER

Ranger User Guide



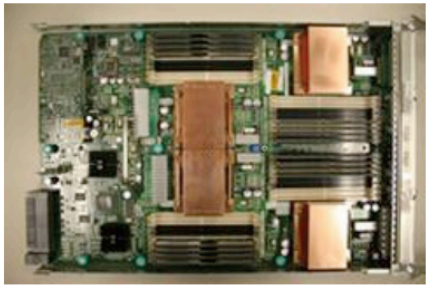


Figure 2. SunBlade x6420 motherboard (compute blade).

Operations		579 TFLOPS (Peak)
Nodes(blades)	Four Quad-Core AMD Opteron processors	3,936 Nodes / 62,976 Cores
Memory	Distributed	123 TB Aggregate
Shared Disk	Lustre, parallel File System	1.7 PB Raw

History of the B-Spline R-matrix program

- **van der Hart** (1997) shows that **the idea works very well for e−H collisions**.
- **Zatsarinny and Fischer** (1999) develop **Breit_NO**, a general program for angular integrations with non-orthogonal orbital sets.
- **Zatsarinny and Fischer** (2000) describe a **general (non-relativistic) BSR program and use it for photo-ionization of Li** .
- **Zatsarinny and Bartschat** (2004) include **relativistic effects and use it for electron-impact excitation of Ne**.
- **Zatsarinny** publishes the code in **Comp. Phys. Commun. 174 (2006) 273**.
- **Zatsarinny and Bartschat** (2008) develop a **fully relativistic version and use it for e-Cs, e-Au, e-Hg**.
- A large number (growing fast) of **calculations have now been performed for:**
  - **electron-impact excitation of complex atoms and ions**
  - **atomic structure (!)**
  - **photo-ionization and photodetachment**.

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 30 more since 2006

I will show a small selection of results ...

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

Phys. Scr. T 134 (2009) 014020

Oleg Zatsarinny and Klaus Bartschat

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

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.

Some Examples of Structure Results ...

Binding energies (NIST) and energy differences (computed – observed) in eV for low-lying levels in Ne, Ar, Kr and Xe .

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
3s'[1/2]0	4.849	0.014	4s'[1/2]0	4.036	0.099	5s'[1/2]0	3.437	0.136	6s'[1/2]0	3.118	0.061
3s'[1/2]1	4.716	0.014	4s'[1/2]1	3.932	0.095	5s'[1/2]1	3.356	0.127	6s'[1/2]1	2.996	0.071
		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**
3p'[3/2]1	2.871	-0.012	4p'[3/2]1	2.477	0.020	5p'[3/2]1	1.899	0.042	6p'[3/2]1	1.608	0.040
3p'[3/2]2	2.860	-0.010	4p'[3/2]2	2.457	0.025	5p'[1/2]1	1.859	0.034	6p'[3/2]2	1.511	0.057
3p'[1/2]1	2.838	-0.012	4p'[1/2]1	2.432	0.023	5p'[3/2]2	1.856	0.039	6p'[1/2]1	1.496	0.053
3p'[1/2]0	2.599	-0.009	4p'[1/2]0	2.280	0.018	5p'[1/2]0	1.743	0.048	6p'[1/2]0	1.424	0.065
		0.075			**0.120**			**0.130**			**0.120**

Binding energies (NIST) and energy differences (computed – observed) in eV for low-lying levels in Ne, Ar , Kr and Xe .

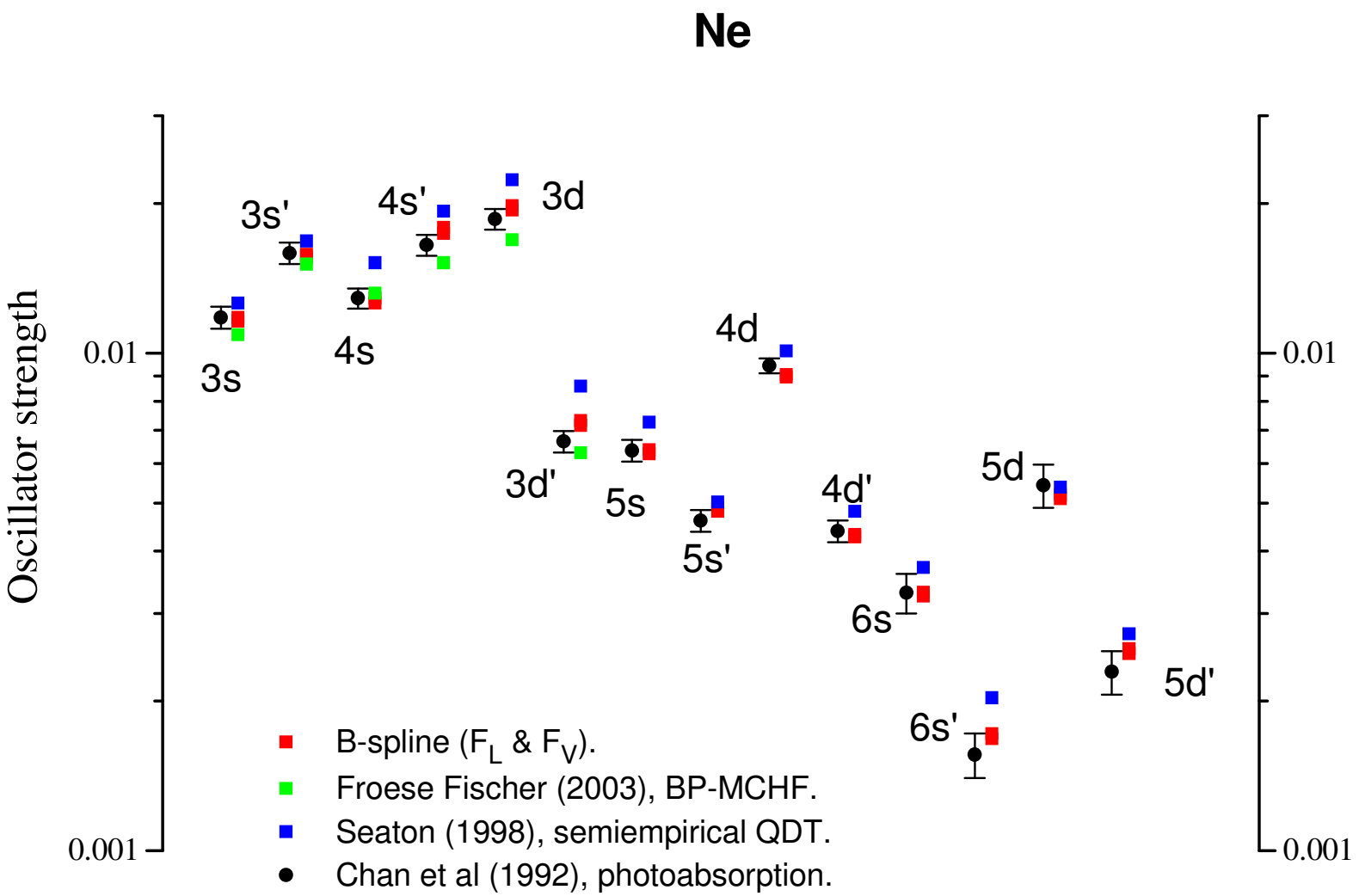
Ne	NIST	Diff.	Ar	NIST	Diff.	Kr	NIST	Diff.	Xe	NIST	Diff.
3d [1/2]0	1.540	-0.004	$3d[1/2]_0$	1.915	0.116	4d [1/2]0	2.001	0.116	5d[1/2]0	2.675	0.014
3d [1/2]1	1.538	-0.004	$3d[1/2]_1$	1.896	0.113	4d [1/2]1	1.963	0.112	5d[1/2]1	2.648	0.066
3d [7/2]4	1.530	-0.001	$3d[3/2]_2$	1.856	0.105	4d [3/2]2	1.888	0.101	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]2	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**
3d'[5/2]2	1.428	-0.009	$3d'[5/2]_2$	1.546	0.054	4d'[3/2]2	1.196	0.041	5d'[5/2]2	1.264	0.034
3d'[5/2]3	1.428	-0.008	$3d'[3/2]_2$	1.526	0.045	4d'[5/2]2	1.174	0.042	5d'[3/2]2	1.227	0.020
3d'[3/2]2	1.427	-0.008	$3d'[5/2]_3$	1.524	0.048	4d'[5/2]3	1.142	0.038	5d'[5/2]3	1.190	0.035
3d'[3/2]1	1.425	-0.007	$3d'[3/2]_1$	1.456	0.025	4d'[3/2]1	0.995	0.019	5d'[3/2]1	0.958	0.016
		0.010			**0.150**			**0.160**			**0.225**
4s [3/2]2	1.901	0.007	$5s[3/2]_2$	1.691	0.028	6s [3/2]2	1.647	0.020	7s[3/2]2	2.003	0.034
4s [3/2]1	1.876	0.006	$5s[3/2]_1$	1.670	0.026	6s [3/2]1	1.614	0.023	7s[3/2]1	1.972	0.034
4s'[1/2]0	1.804	0.005	$5s'[1/2]_0$	1.519	0.018	6s'[1/2]0	0.970	0.026	7s'[1/2]0	0.697	0.039
4s'[1/2]1	1.785	0.006	$5s'[1/2]_1$	1.505	0.019	6s'[1/2]1	0.963	0.023	7s'[1/2]1	0.688	0.039
		0.040			**0.070**			**0.080**			**0.075**

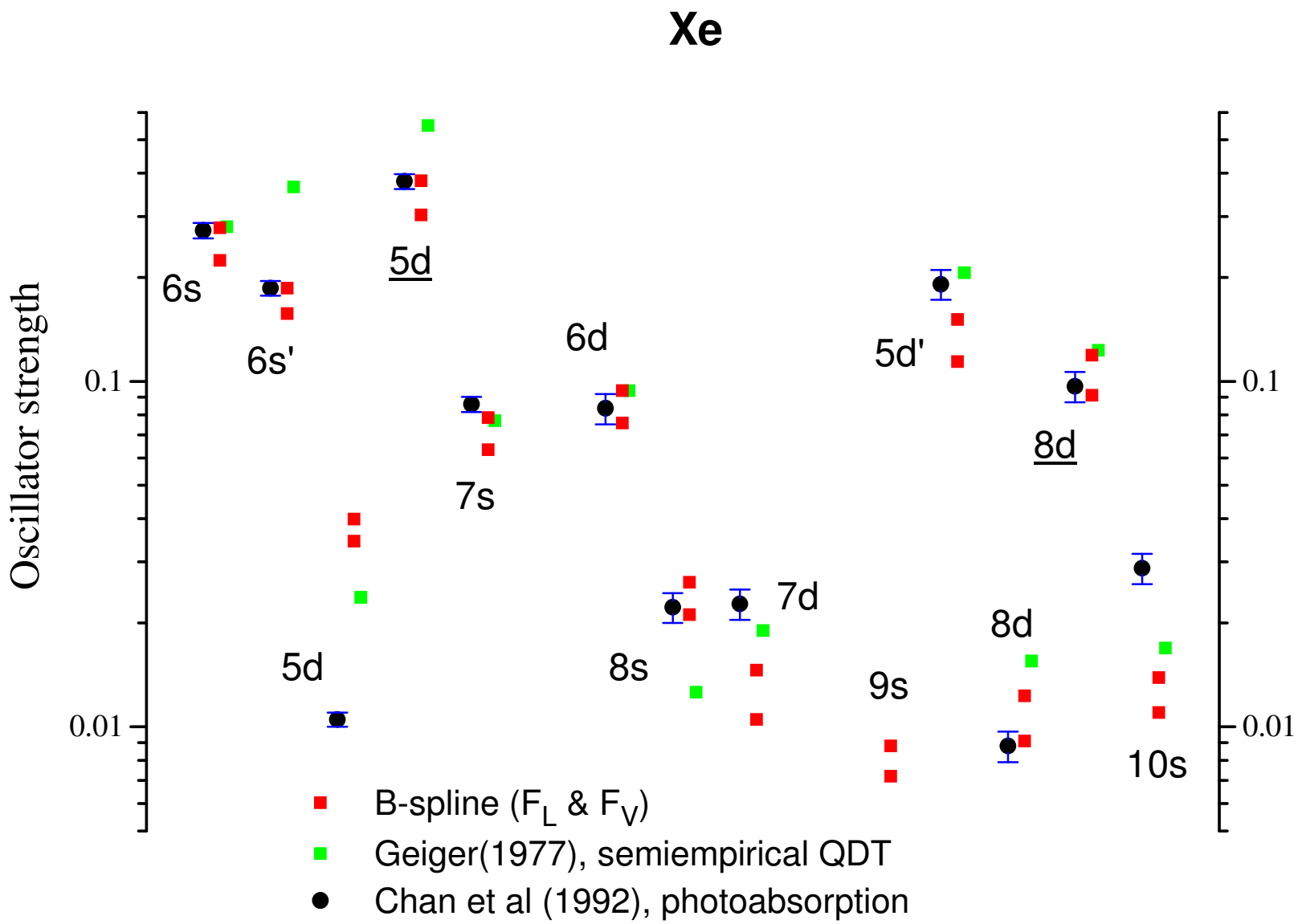
Ne

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, respectively.

Upper level	F_L	Fv	Froese Fischer (2003)	Seaton (1998)	NIST	Chan *et al* (1992)	Zhong *et al* (1997)
$3s[3/2]_1$	0.0118	0.0116	0.0109	0.0126	0.0118	0.0118(6)	0.0124(38)
$3s'[1/2]_1$	0.0158	0.0156	0.0151	0.0168	0.0149	0.0159(8)	0.0156(9)
$4s[3/2]_1$	0.0126	0.0129	0.0132	0.0152	0.0086	0.0129(6)	0.0126(6)
$4s'[1/2]_1$	0.0174	0.0179	0.0152	0.0193	0.013	0.0165(8)	0.0167(7)
$3d[1/2]_1+3d[3/2]_1$	0.0194	0.0198	0.0169	0.0223		0.0186(9)	0.0183(8)
$3d'[3/2]_1$	0.00716	0.00732	0.00631	0.00859	0.0065	0.00665(33)	0.00687(32)
$5s[3/2]_1$	0.00628	0.00640		0.00727		0.00637(32)	0.00645(18)
$5s'[1/2]_1$	0.00481	0.00490		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)	

Seaton (1998) – semiempirical QDT;
Froese Fischer (2003) – Breit-Pauli MCHF;
Chan *et al* (1992) – photoabsorption
Zhong *et al* (1997) – electron-impact study.


Ne
Oscillator strength
0.01
0.001
3s
3s'
4s
4s'
3d
3d'
5s
5s'
4d
4d'
6s
6s'
5d
5d'
B-spline (F_L & F_V).
Froese Fischer (2003), BP-MCHF.
Seaton (1998), semiempirical QDT.
Chan et al (1992), photoabsorption.


Xe
Oscillator strength
0.1
0.01
6s
6s'
5d
5d
7s
6d
8s
7d
5d'
9s
8d
8d
10s
B-spline (F_L & F_V)
Geiger(1977), semiempirical QDT
Chan et al (1992), photoabsorption

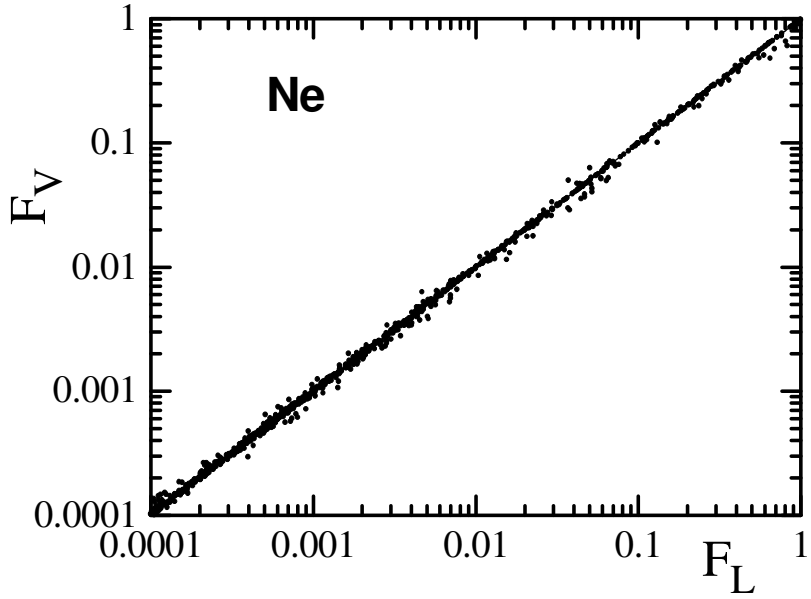
Xe

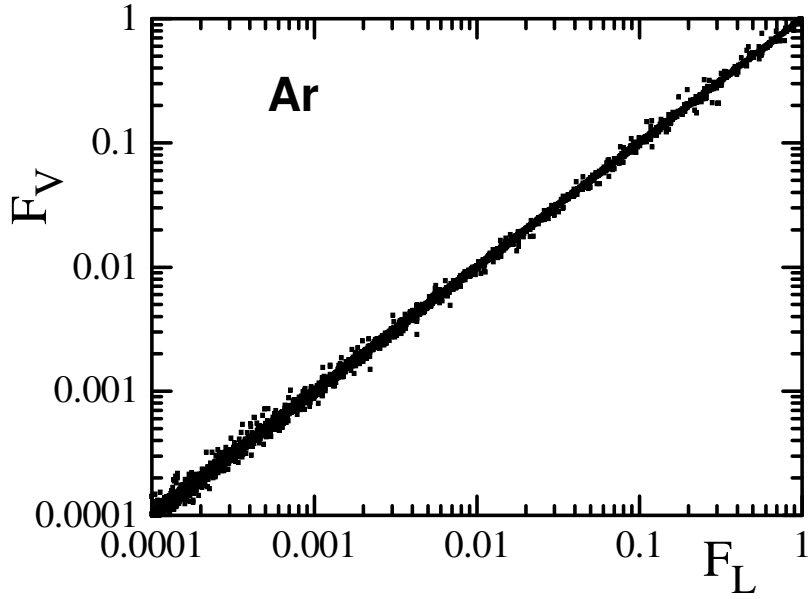
Oscillator strengths for excitation from the ground state in **Xe**.

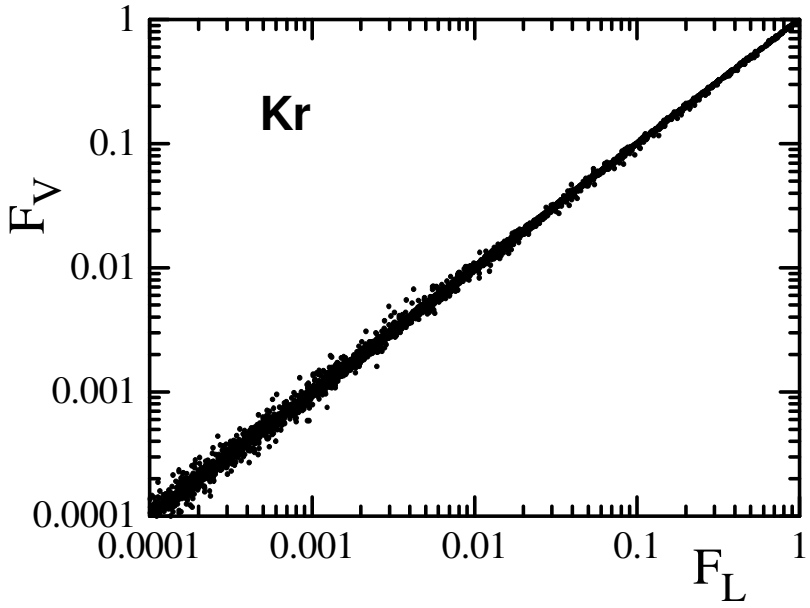
Upper level	Breit-Pauli		Dirac		Chan *et al* (1992)	Suzuki *et al* (1996)
	F_L	F_V	F_L	F_V		
$6s[3/2]_1$	0.278	0.224	0.260	0.258	0.273	0.0222
$6s'[1/2]_1$	0.186	0.157	0.188	0.189	0.186	0.158
$5d[1/2]_1$	0.0399	0.0345	0.0083*	0.0071	0.0105	
$5d[3/2]_1$	0.380	0.303	0.303	0.327	0.379	0.298
$7s[3/2]_1$	0.0785	0.0633	0.0791	0.0783	0.0859	0.0738
$6d[1/2]_1$	0.0001	0.0002	0.0003	0.0005	< 0.001	
$6d[3/2]_1$	0.0939	0.0758	0.0987	0.0873	0.0835	
$8s[3/2]_1$	0.0262	0.0211	0.0201	0.0192	0.0222	
$7d[1/2]_1$	0.0146	0.0105	0.0395	0.0441	0.0227	
$7d[3/2]_1$	0.0088	0.0072	0.0064	0.0081	< 0.001	
$9s[3/2]_1$	0.0001	0.0002	0.0002	0.0003	< 0.001	
$5d'[3/2]_1$	0.151	0.114	0.167	0.170	0.191	
$8d[1/2]_1$	0.0123	0.0091	0.0068	0.0071	0.0088	
$8d[3/2]_1$	0.119	0.091	0.0846	0.0835	0.0967	
$10s[3/2]_1$	0.0139	0.0110	0.0139	0.0134	0.0288	

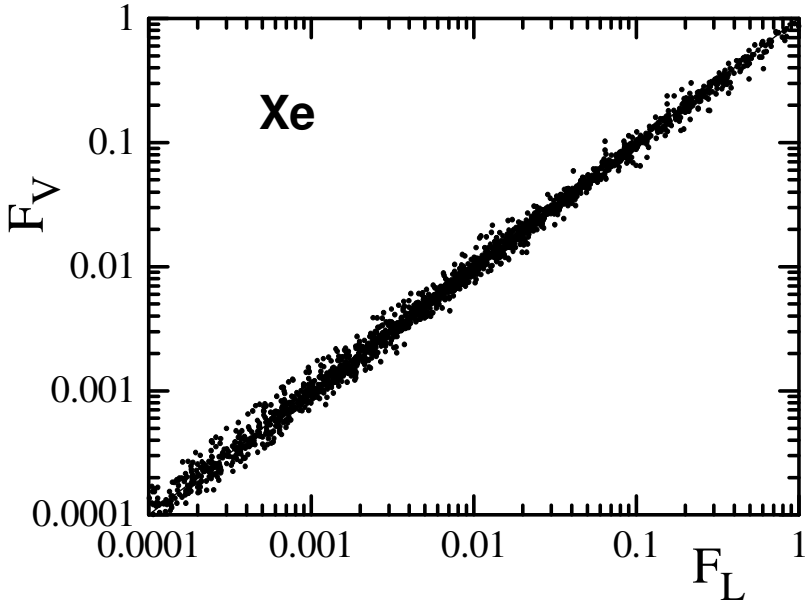
Chan *et al*, Phys.Rev. A **46**, 149 (1992) - Photoabsorption
Suzuki *et al*, Phys.Rev. **53**, 4138 (1996) - Electron-impact study

Length vs. Velocity Results
An Estimate for the Accuracy









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
```

That's a lot of numbers!

- **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

Phys. Scr. T 134 (2009) 014020

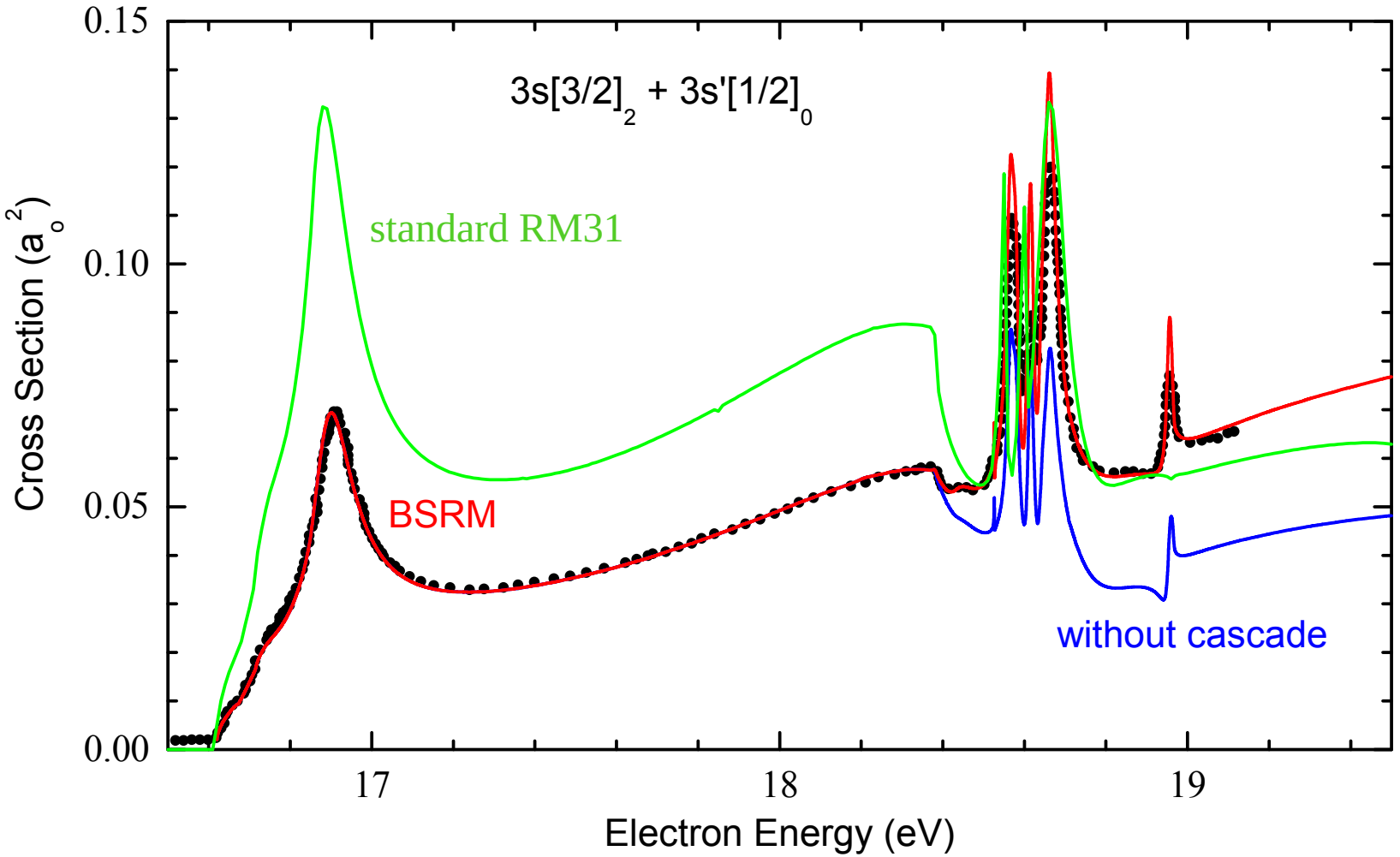
Let's move on to Collisions ...

Metastable yield in e-Ne collisions

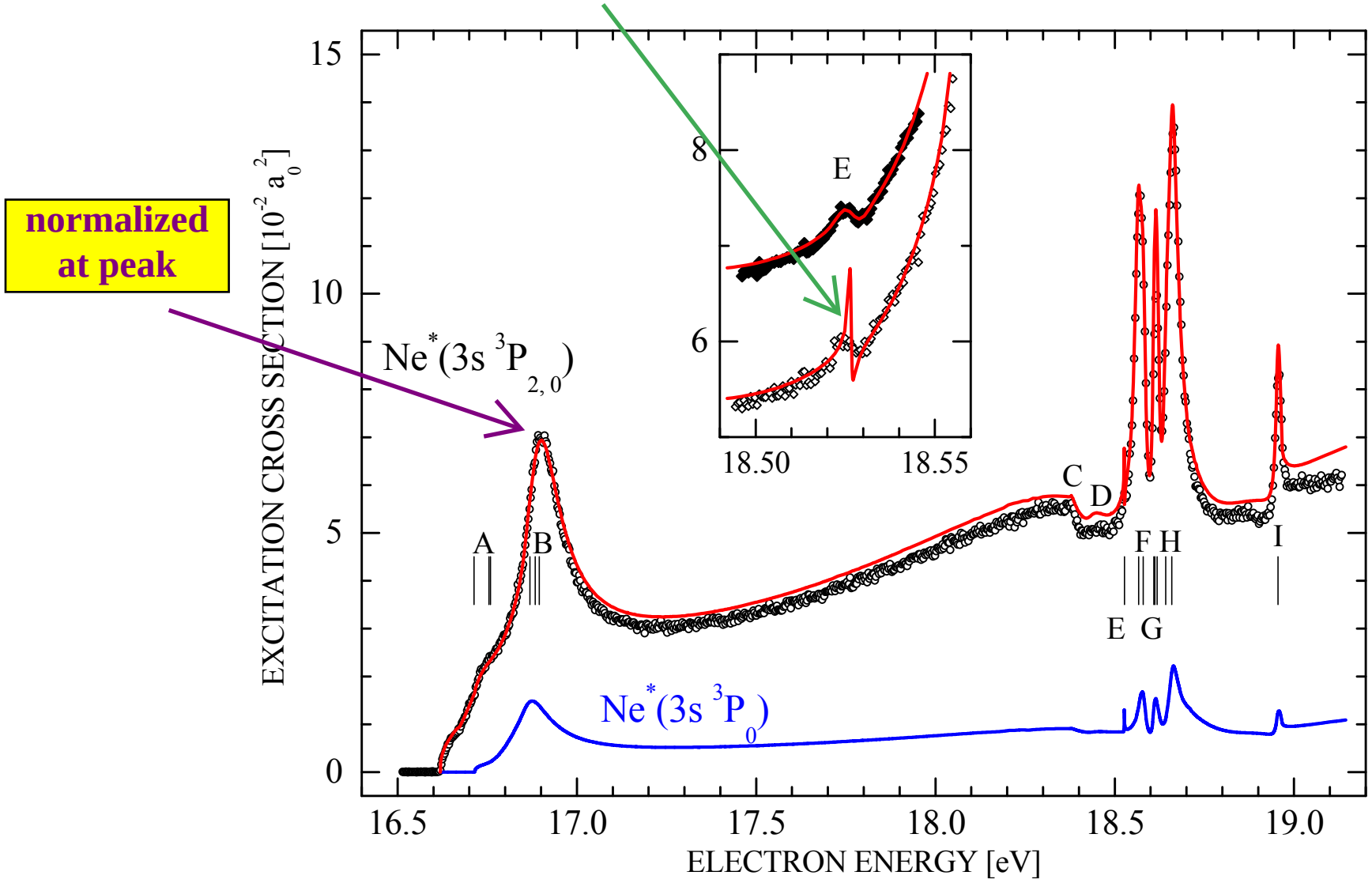
Experiment: Buckman *et al.* (1983) [x 0.78]

Theories: 31-state Breit-Pauli R-matrix (Zeman & Bartschat 1997)

31-state B-spline R-matrix (Zatsarinny & Bartschat 2004)

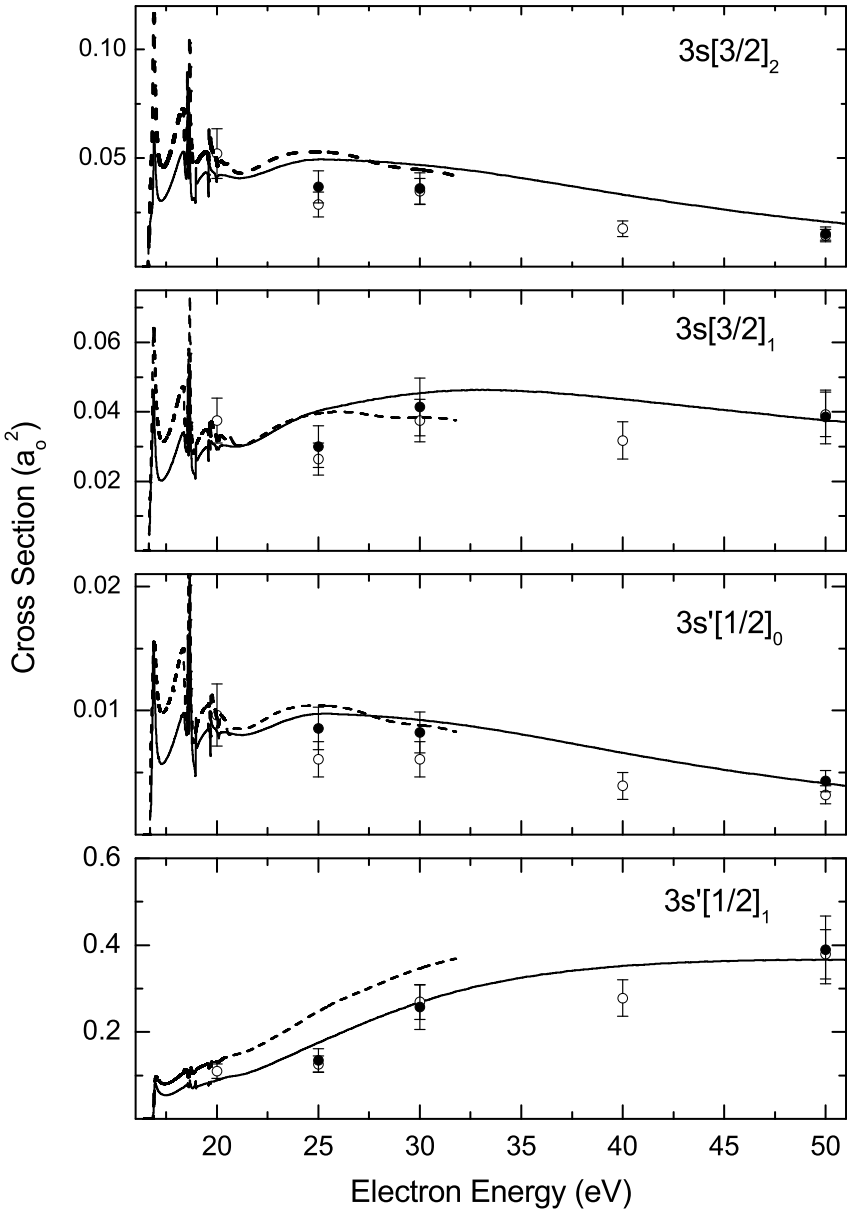


position of resonance predicted to 1 meV accuracy !!!



Bömmels J, Franz K, Hoffman T H, Gopalan A, Zatsarinny O, Bartschat K, Ruf M.-W., and Hotop H
Low-lying resonances in electron-neon scattering: measurements at 4 meV resolution and comparison with theory
Phys. Rev. A **71**, 012704 (2005)

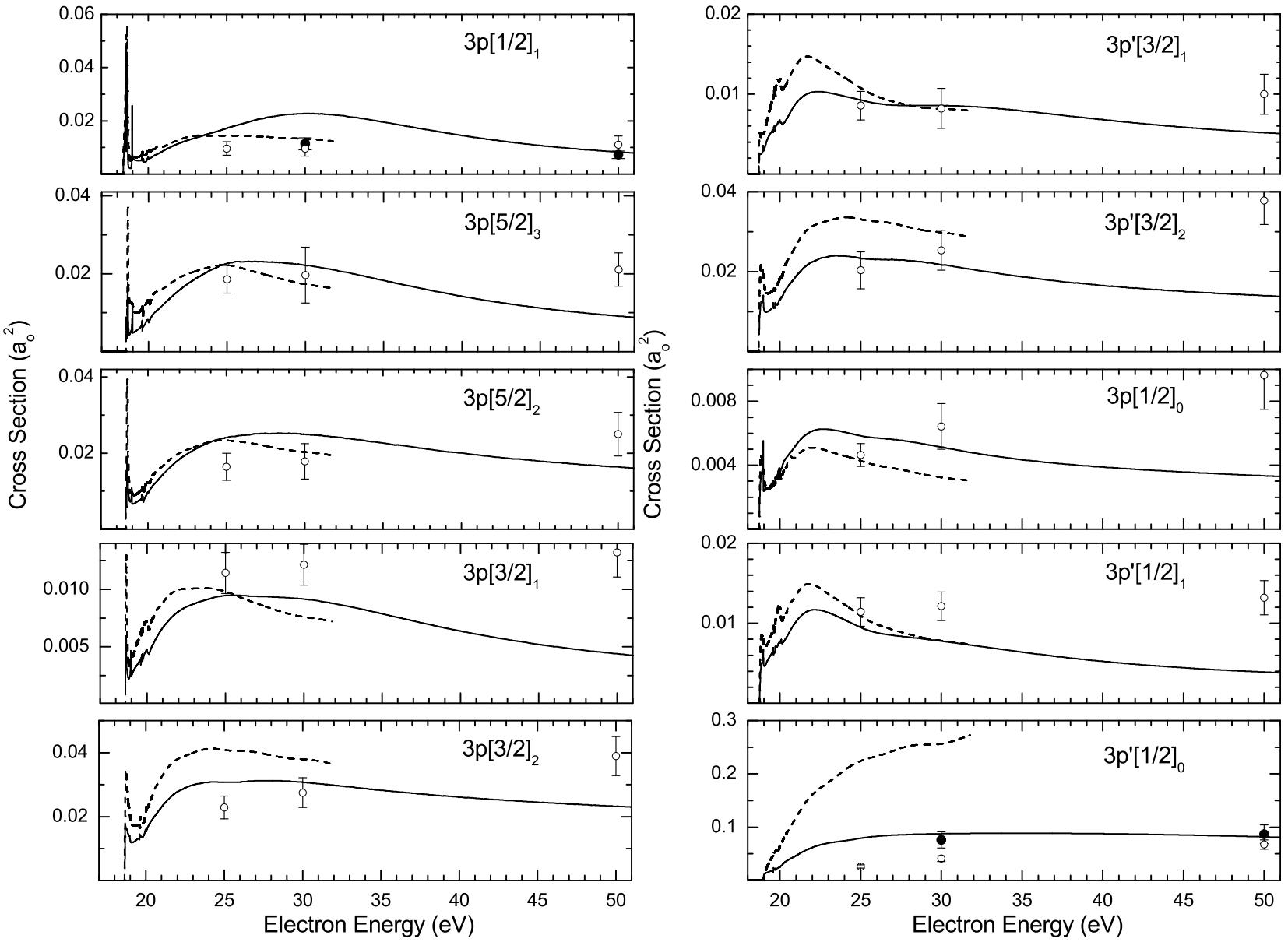
Electron-Impact Excitation of Ne ($2p^5 3s$)



solid line: BSRM
dashed line: RM31

experiments:
Register *et al.*, Khakoo *et al.*

Electron-Impact Excitation of Ne ($2p^5 3p$)



experiments: Khakoo *et al.*, Chilton *et al.*

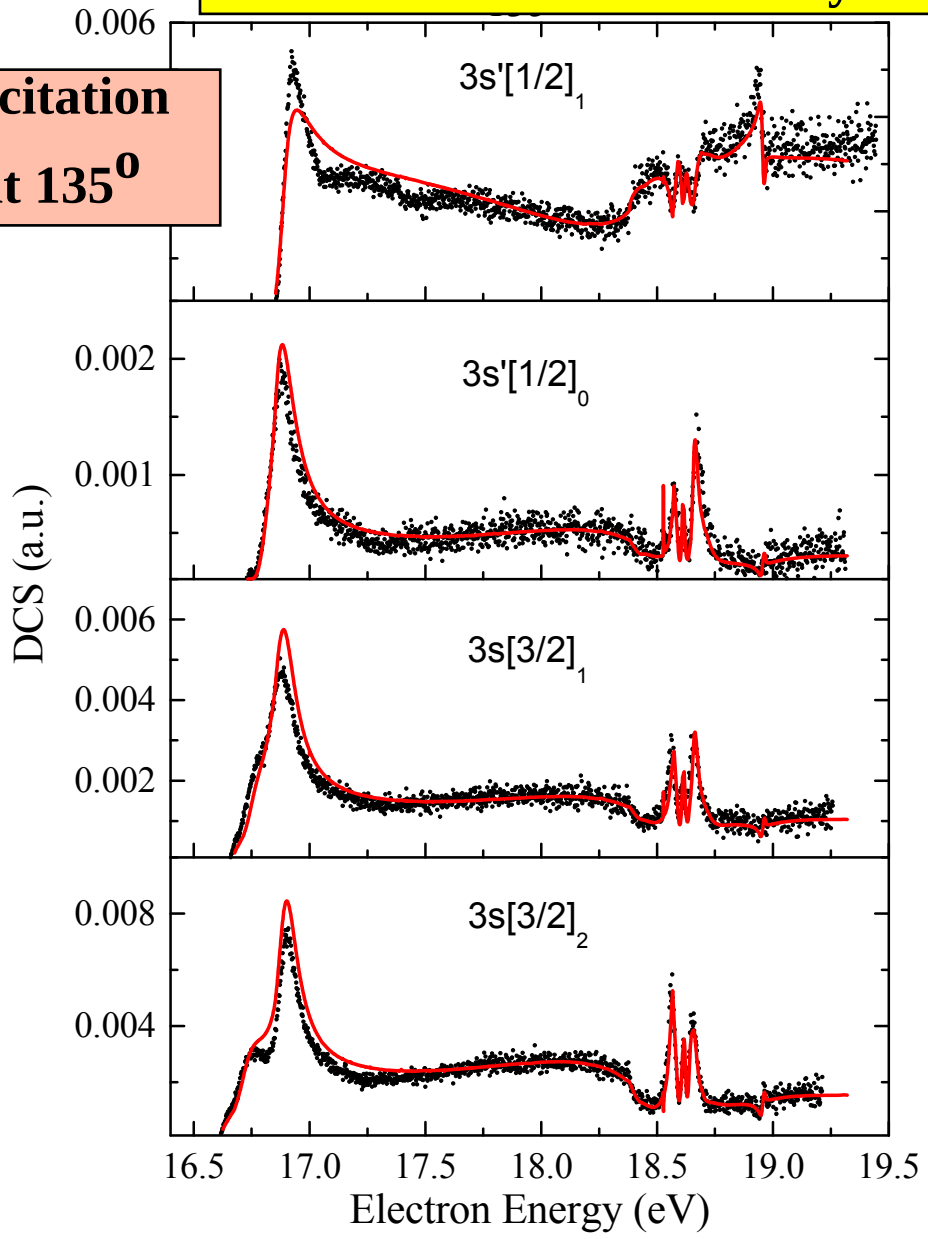
solid line: BSRM
dashed line: RM31

How about angle-differential measurements?

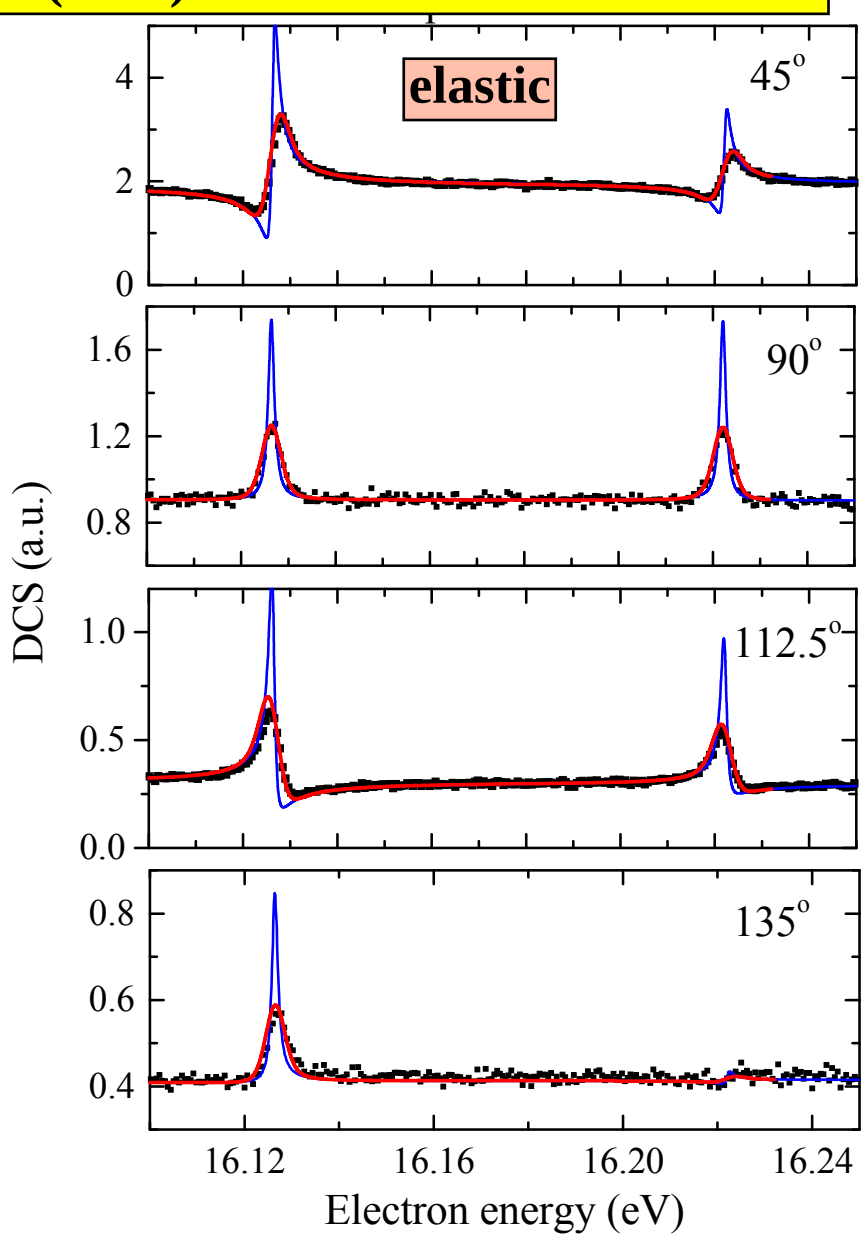
How about higher energies?

Angle-differential measurements: Allan, Franz, Hotop, OZ & KB
J. Phys. B 39 (2006) L139

excitation at 135^o



Experiment - K. Franz *et al.* (next talk)

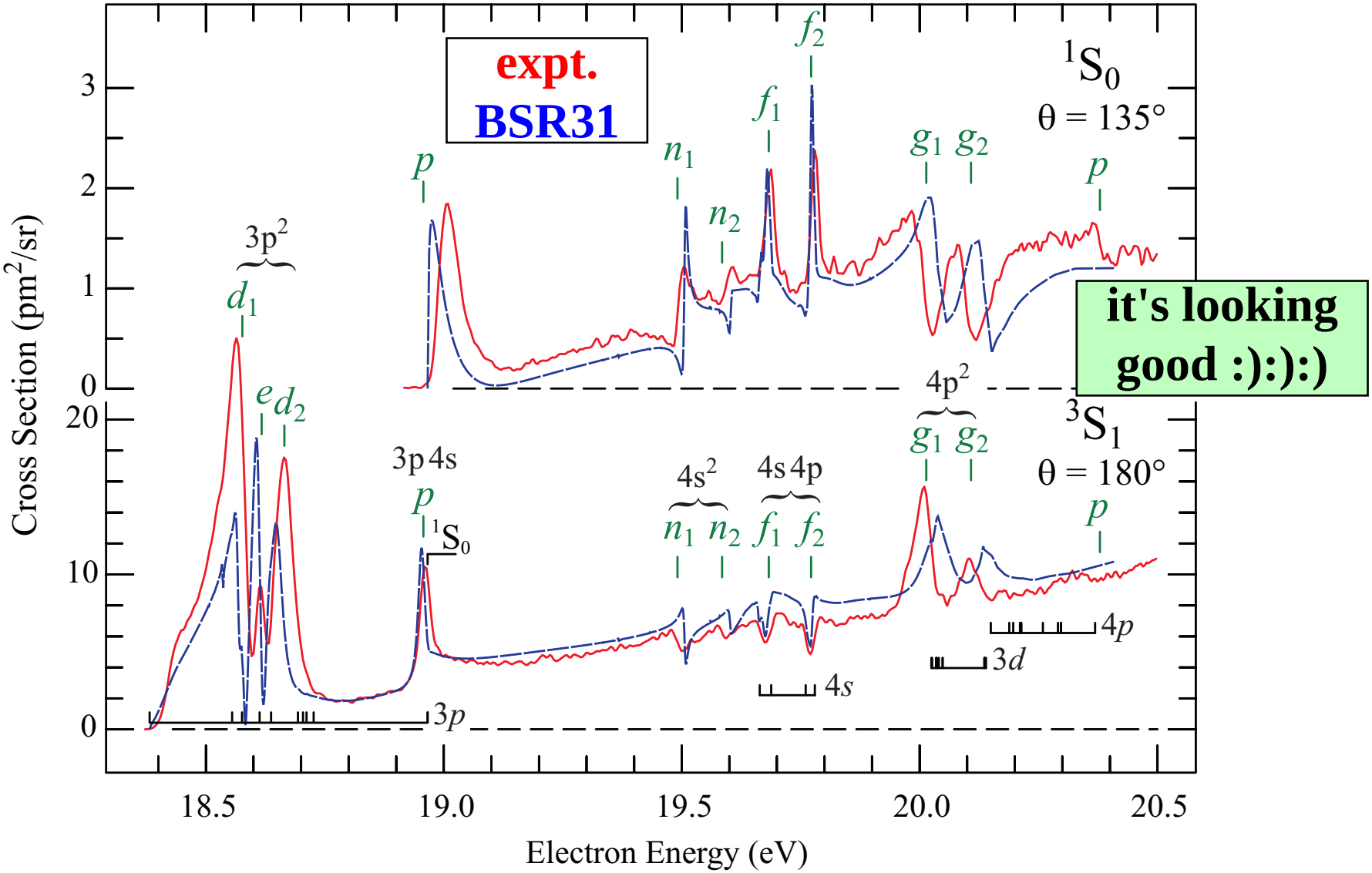


Experiment - Bömmels *et al.* (2005)

Compared to BSRM and BSRM-convoluted

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

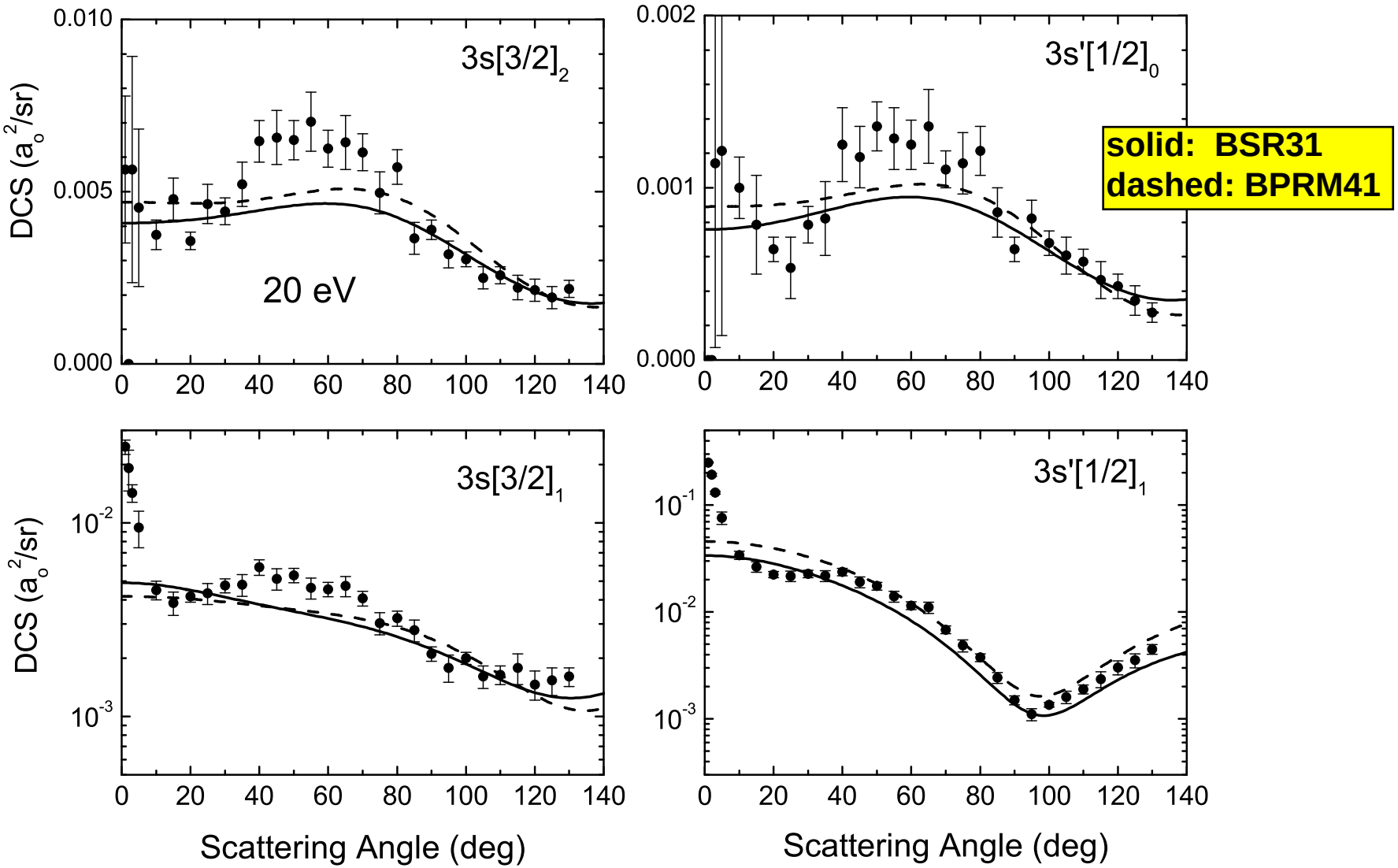
Allan, Franz, Hotop, Zatsarinny, Bartschat (2009), J. Phys. B 42, 044009



it's looking good :):):)

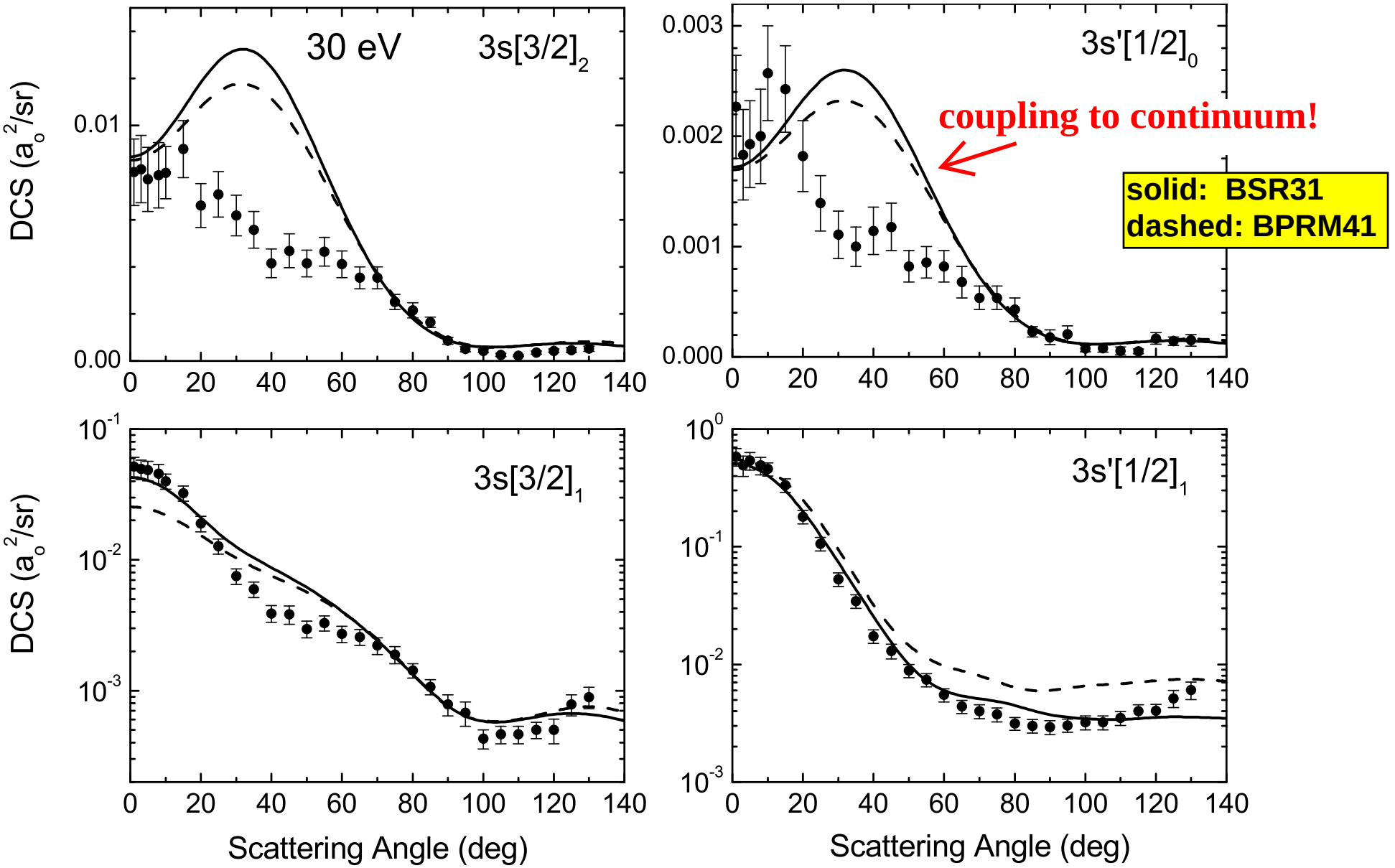
Expanded view of the resonant features in selected cross sections for the excitation of the 3p states. Experiment is shown by the more ragged red line, theory by the smooth blue line. The present experimental energies, labels (using the notation of Buckman *et al*. (1983), and configurations of the resonances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

Electron-Impact Excitation of Ne ($2p^5 3s$): Differential Cross Sections at 20 eV



Experiment: Khakoo *et al.*

Electron-Impact Excitation of Ne ($2p^5 3s$): Differential Cross Sections at 30 eV



Experiment: Khakoo *et al.*

J. Phys. B: At. Mol. Opt. Phys. **37** (2004) 2943–2957 PII: S0953-4075(04)80339-0

Electron-impact excitation of neon: a pseudo-state convergence study

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doi:10.1088/0953-4075/37/14/008

Abstract

A number of convergent close-coupling and R-matrix with pseudo-state (RMPS) calculations for H-like, He-like, Li-like and Be-like ions have demonstrated that coupling to the target continuum can have large effects on the electron-impact excitation cross sections of neutral and low-charge species. However, no one has yet attempted such advanced calculations on a system as complex as neutral neon. We report on a series of RMPS calculations of electron-impact excitation of Ne using recently developed parallel Breit–Pauli R-matrix programs. Our largest calculation included 235 spectroscopic and pseudo-state levels in the close-coupling expansion of the target. Although the results clearly reveal the importance of coupling to the target continuum in this atom, the pseudo-state expansion is not yet sufficiently complete to provide reliable cross sections for energies above the ionization limit. However, this is the largest intermediate-coupling calculation that can be performed with present computer resources. Thus, we have also carried out a series of RMPS calculations in LS coupling with different pseudo-state expansions. Comparisons of these results have allowed us to determine the approximate size of the pseudo-state expansion required to achieve convergence in future intermediate-coupling calculations for neon.

pseudo-thresholds

coupling to continuum!

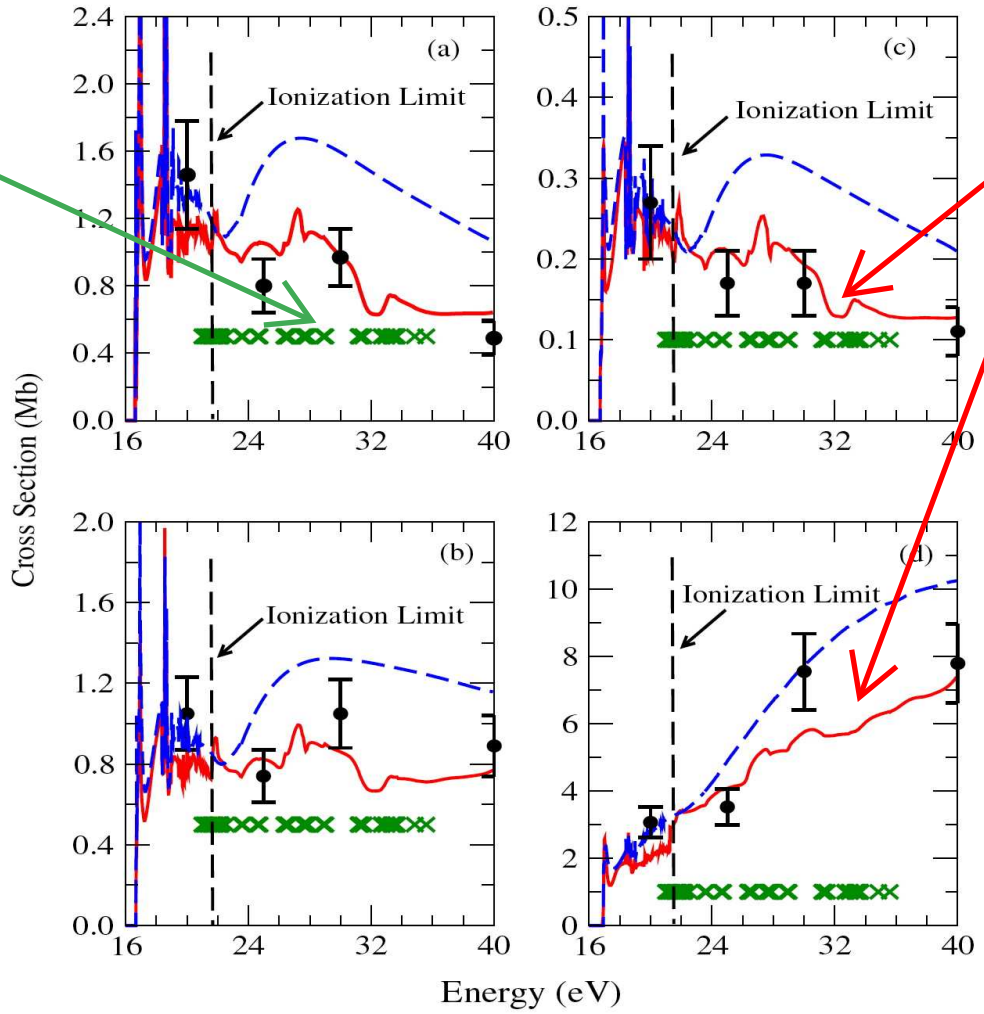

Figure 1. Breit–Pauli calculations of cross sections for excitation from the $2p^6\ ^1S_0$ ground level of neon to the $2p^5 3s\ 3/2[3/2]_2$ level in (a); to the $2p^5 3s\ 3/2[3/2]_1$ level in (b); to the $2p^5 3s\ 1/2[1/2]_0$ level in (c); and to the $2p^5 3s\ 1/2[1/2]_1$ level in (d). The dashed curves are from the present 115-level *R*-matrix calculation; the solid curves are from the present 235-level RMPS calculation; the solid circles are from the experimental results of Khakoo *et al* [4]; and the X show the energy distribution of the pseudo states in the RMPS calculation.

Application !!!

Reconstruction of Electron Energy Distribution Functions from Optical Emission Spectroscopy

Dirk Dodt[1], Andreas Dinklage[1], Rainer Fischer[1], Klaus Bartschat[2],Oleg Zatsarinny[2]

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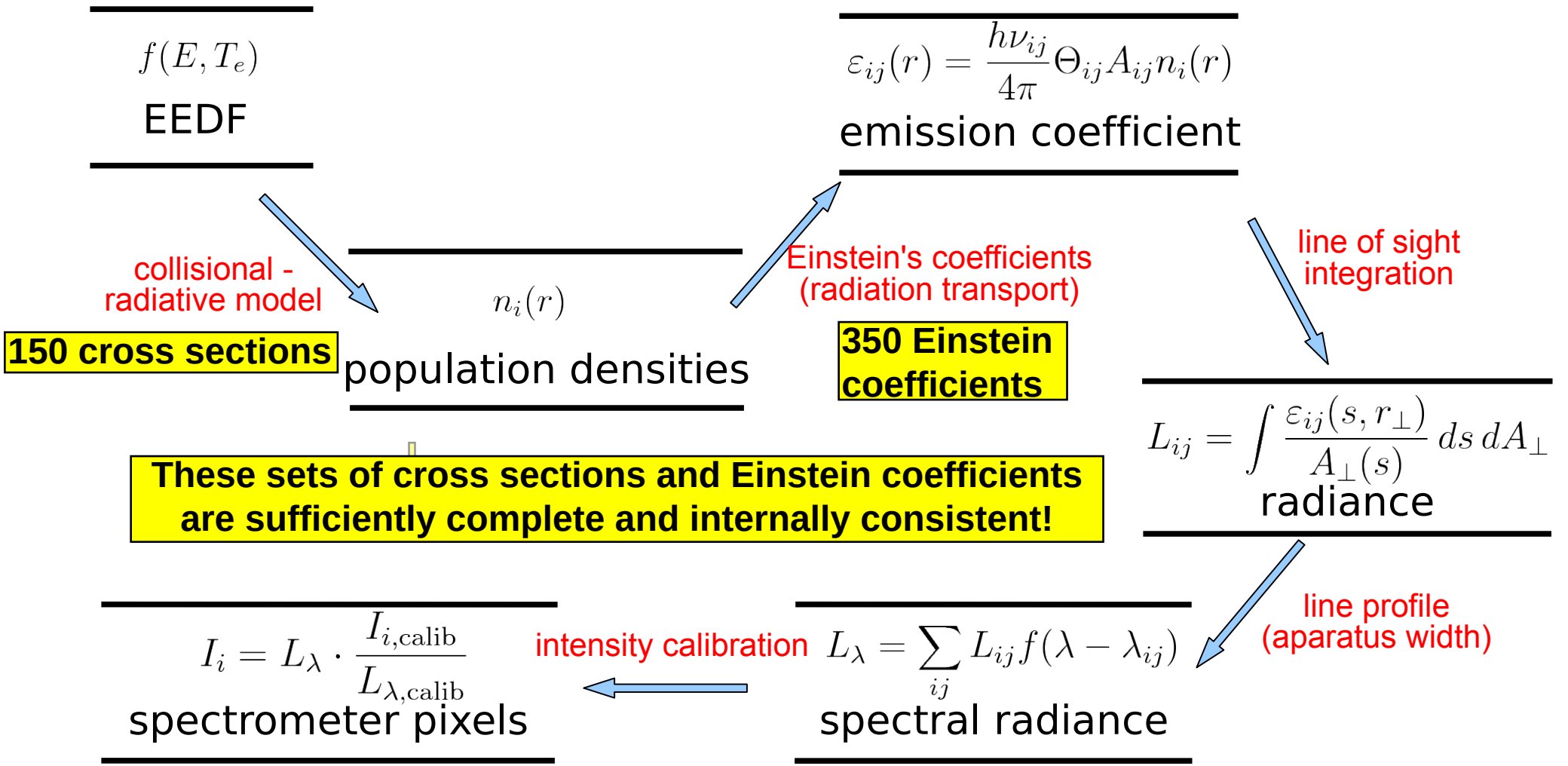
[1]Max-Planck-Institut für Plasmaphysik (IPP)

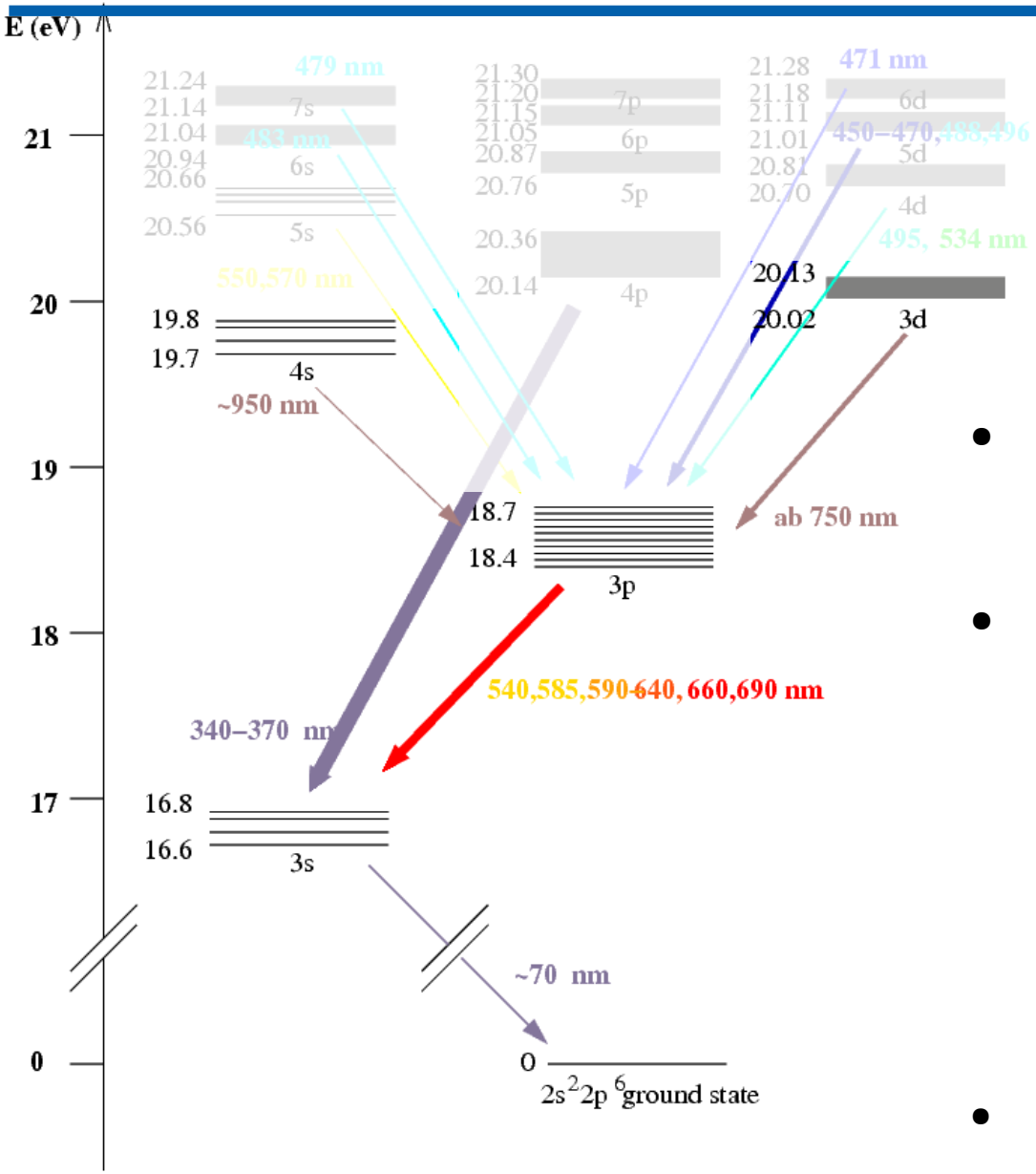
[2]Drake University, Des Moines

Forward Model

Let's use these data in a real plasma model! (Dirk Dodt's PhD Thesis)



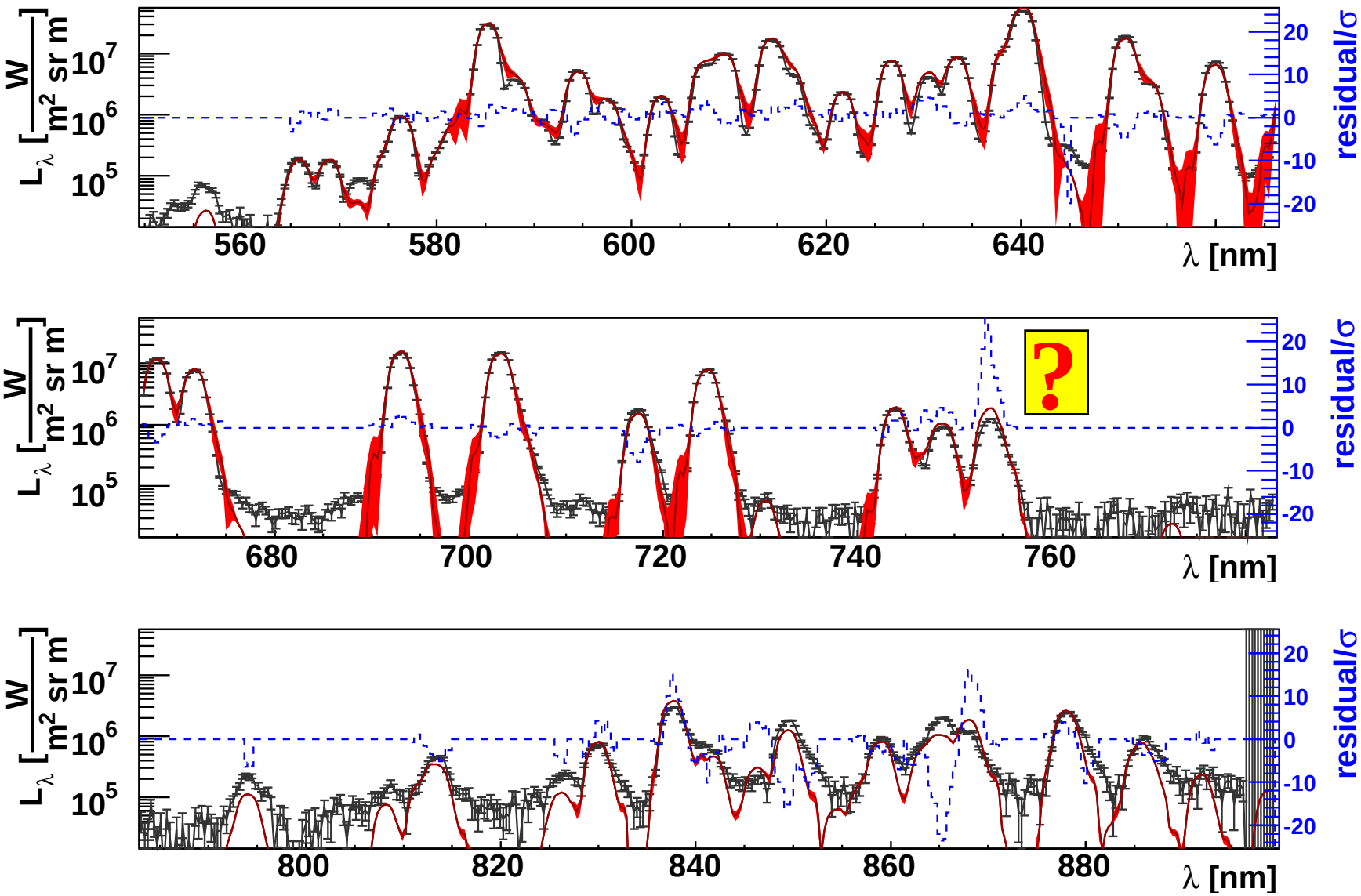
Collisional Radiative Model



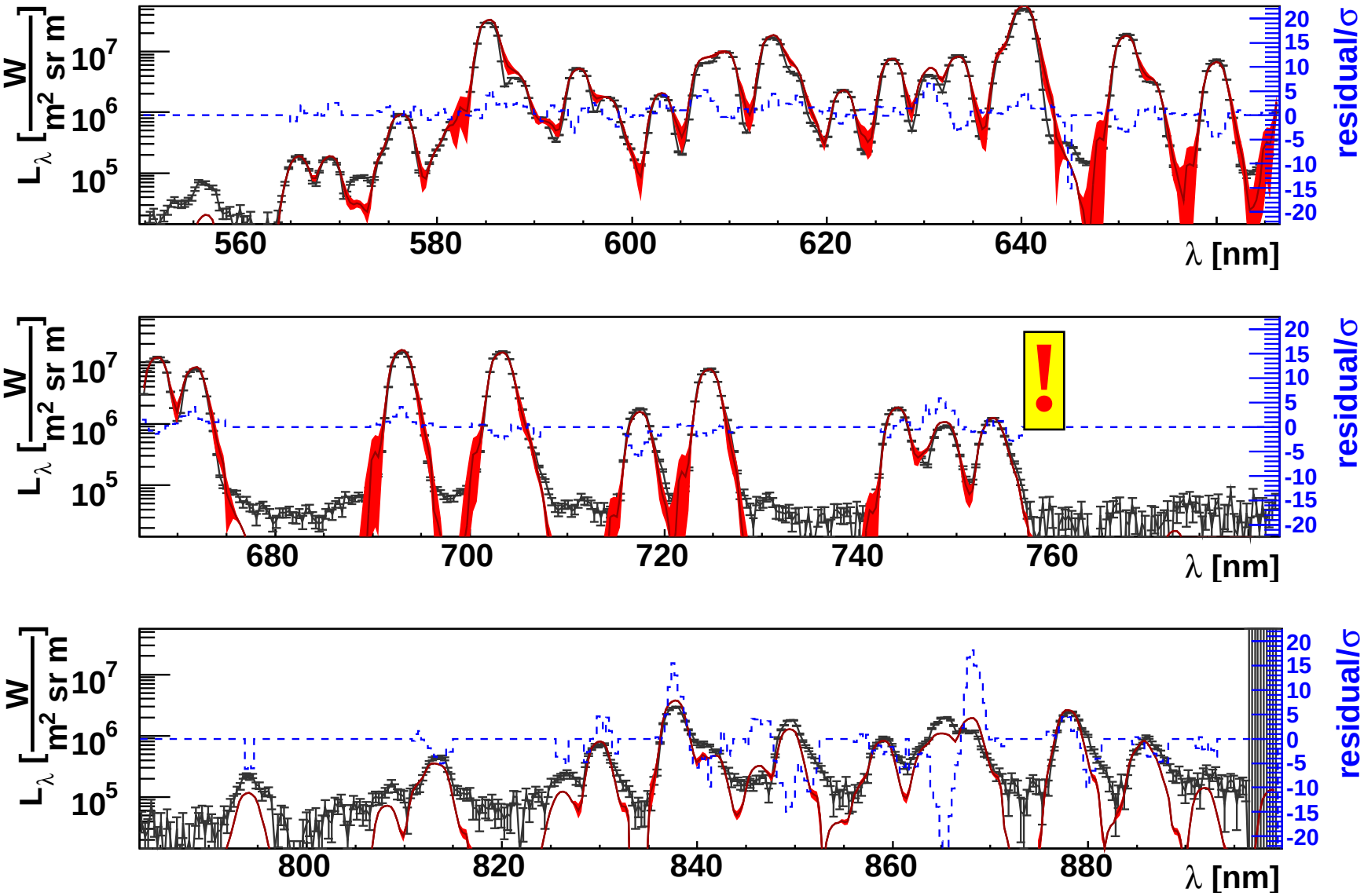
$$\dot{n}_i = P_i + L_i$$

- Balance equation for each excited state density
- Elementary processes:
  - Electron impact (de)excitation
  - Radiative transitions
  - Atom collisions
  - Wall losses
- Linear equation for n_i

Modeled Spectrum Without Uncertainty in Atomic Data

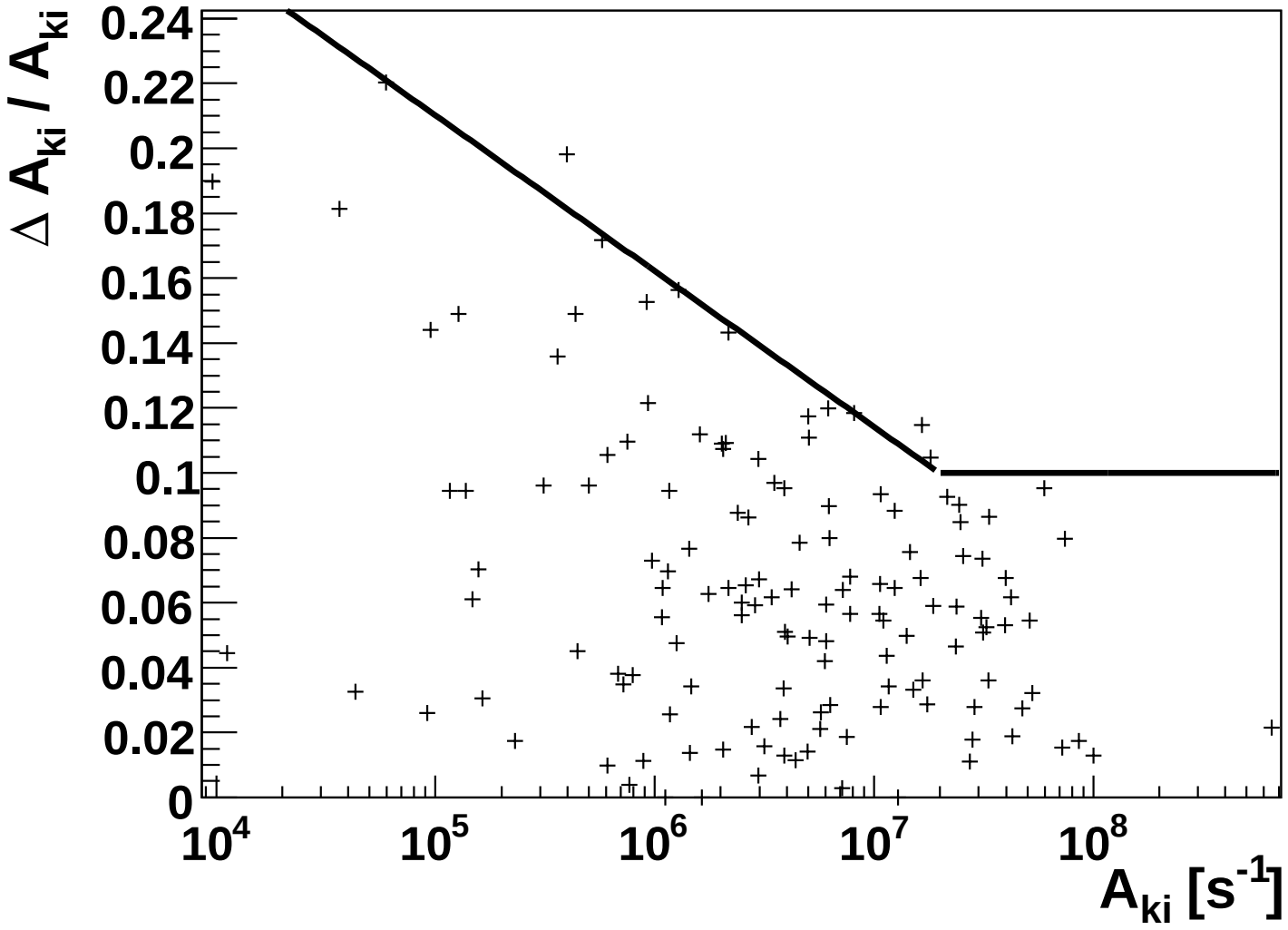


Modeled Spectrum — One Cross Section x 0.4



Although we are are [almost] perfect, let's allow for some uncertainty ...

Uncertainty Estimate of Oscillator Strengths



Uncertainty Estimate of Cross Sections

Estimated uncertainties of the excitation cross sections.

final state	width of prior distribution (relative error)
$2p^5 3s,\ J = 1$	10%
$2p^5 3s,\ J = 2$	20%
$2p^5 3p$	40%
$2p^5 4s$	60%
$2p^5 3d$	60%

These corrections are implemented by allowing for an energy-independent correction factor.

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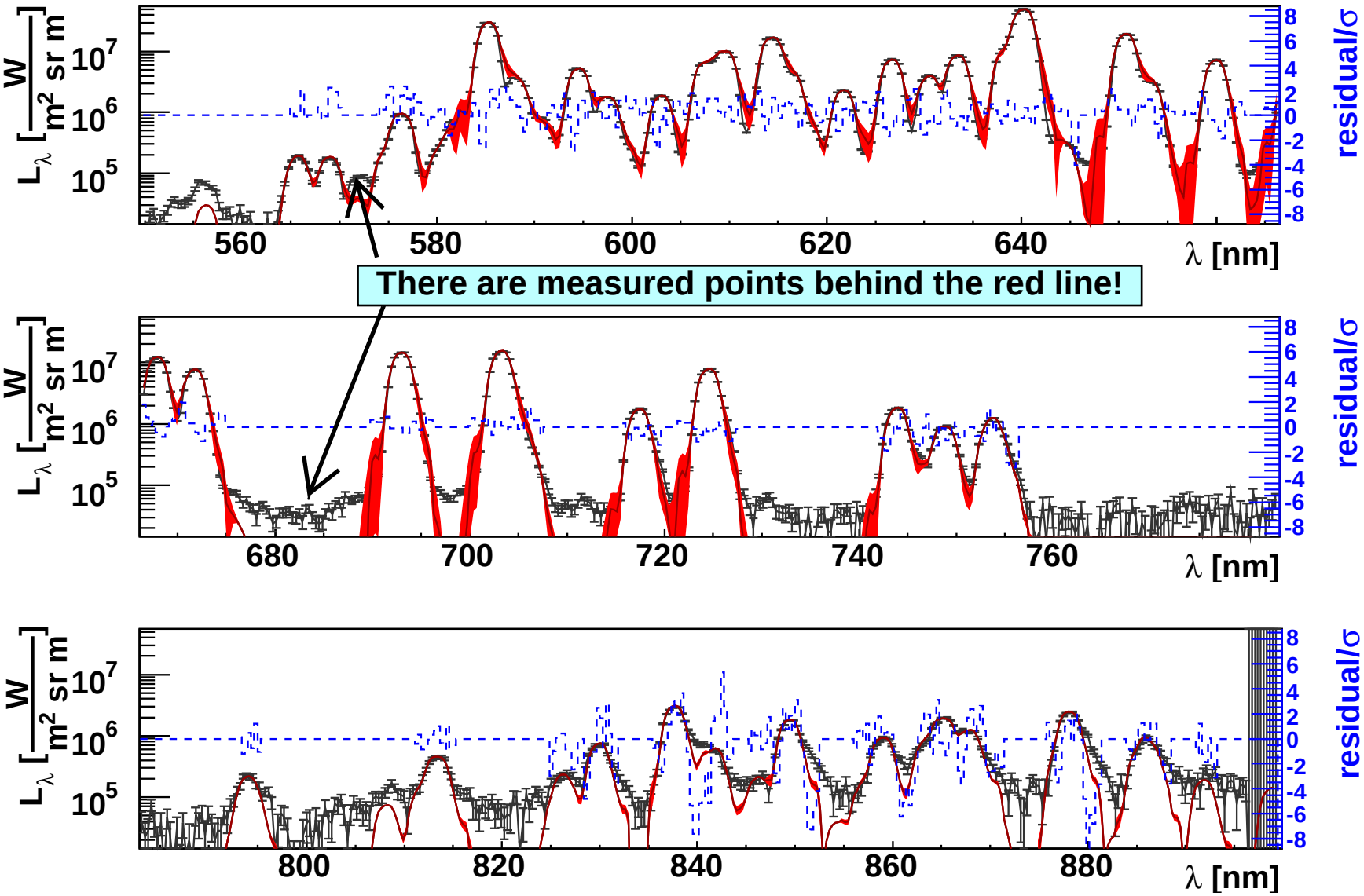
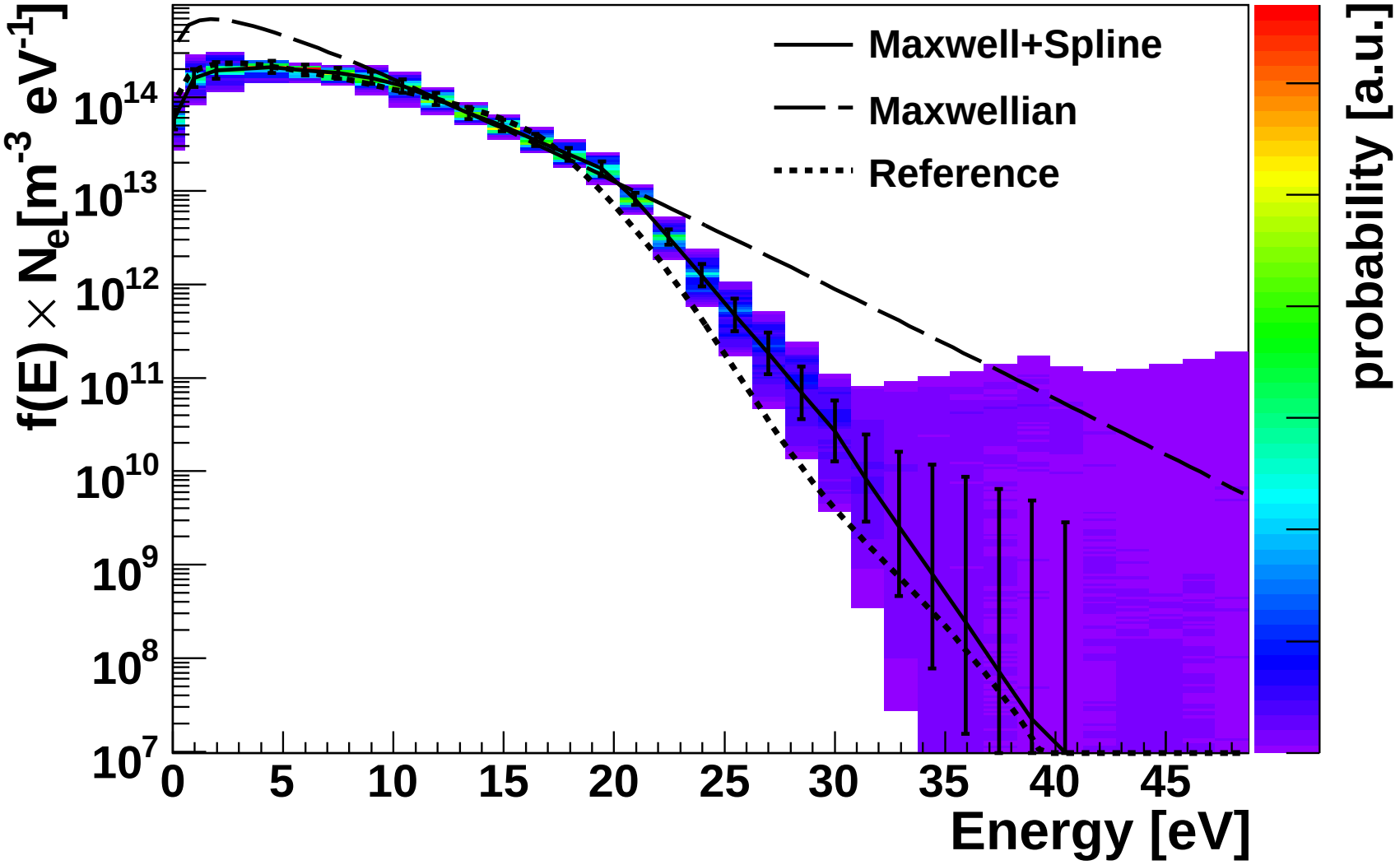
Modeled Spectrum With "Reasonable Uncertainty in Atomic Data"



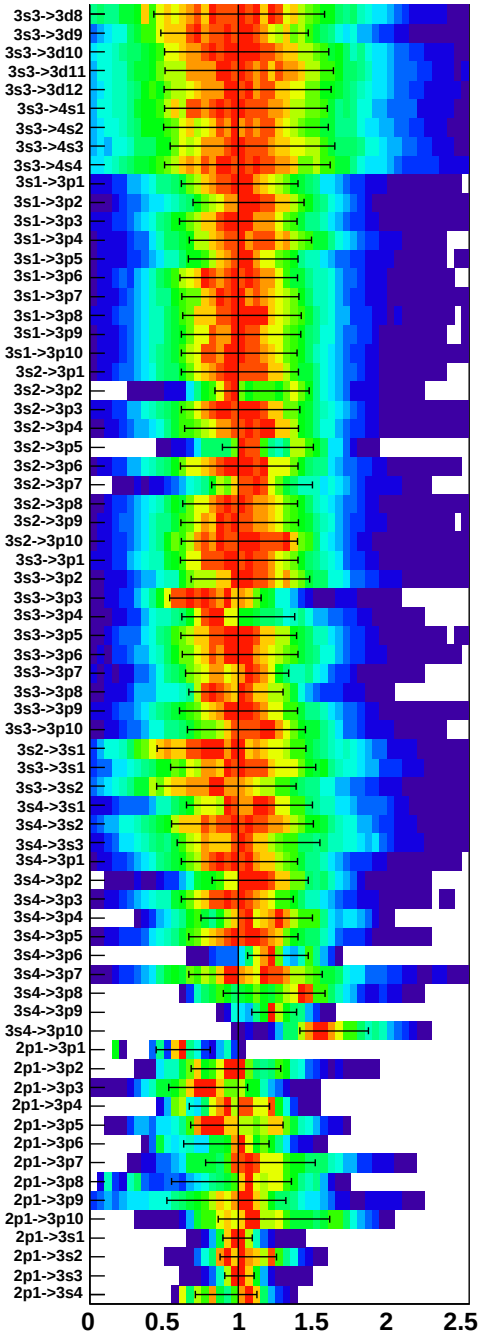
Reconstructed EEDF With Uncertainty in Atomic Data

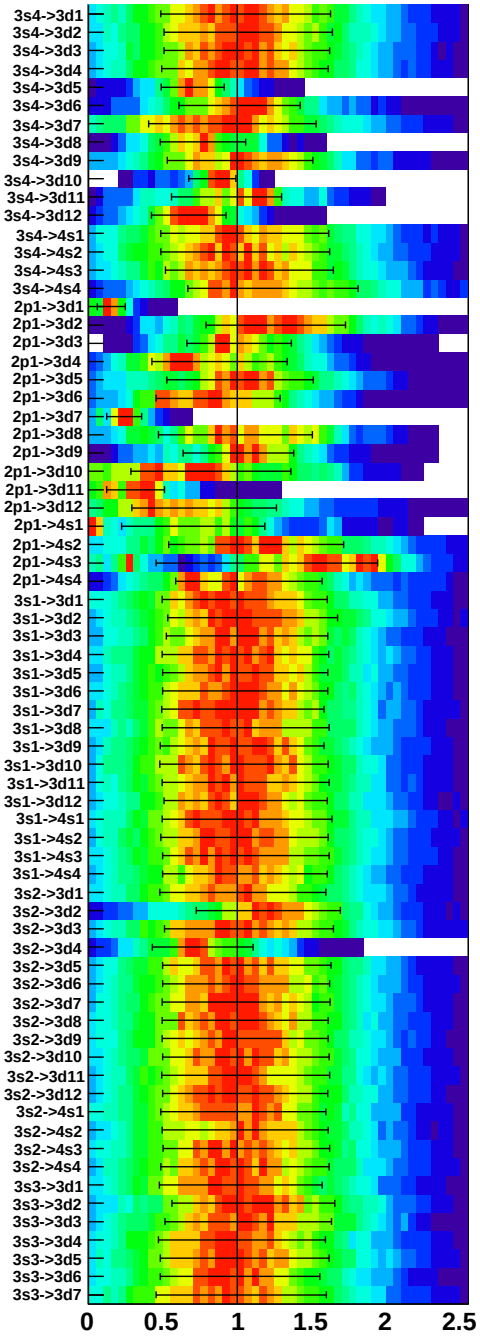
Reference: Uhrlandt and Franke, J. Phys. D 35 (2002), 680



This is the real check!

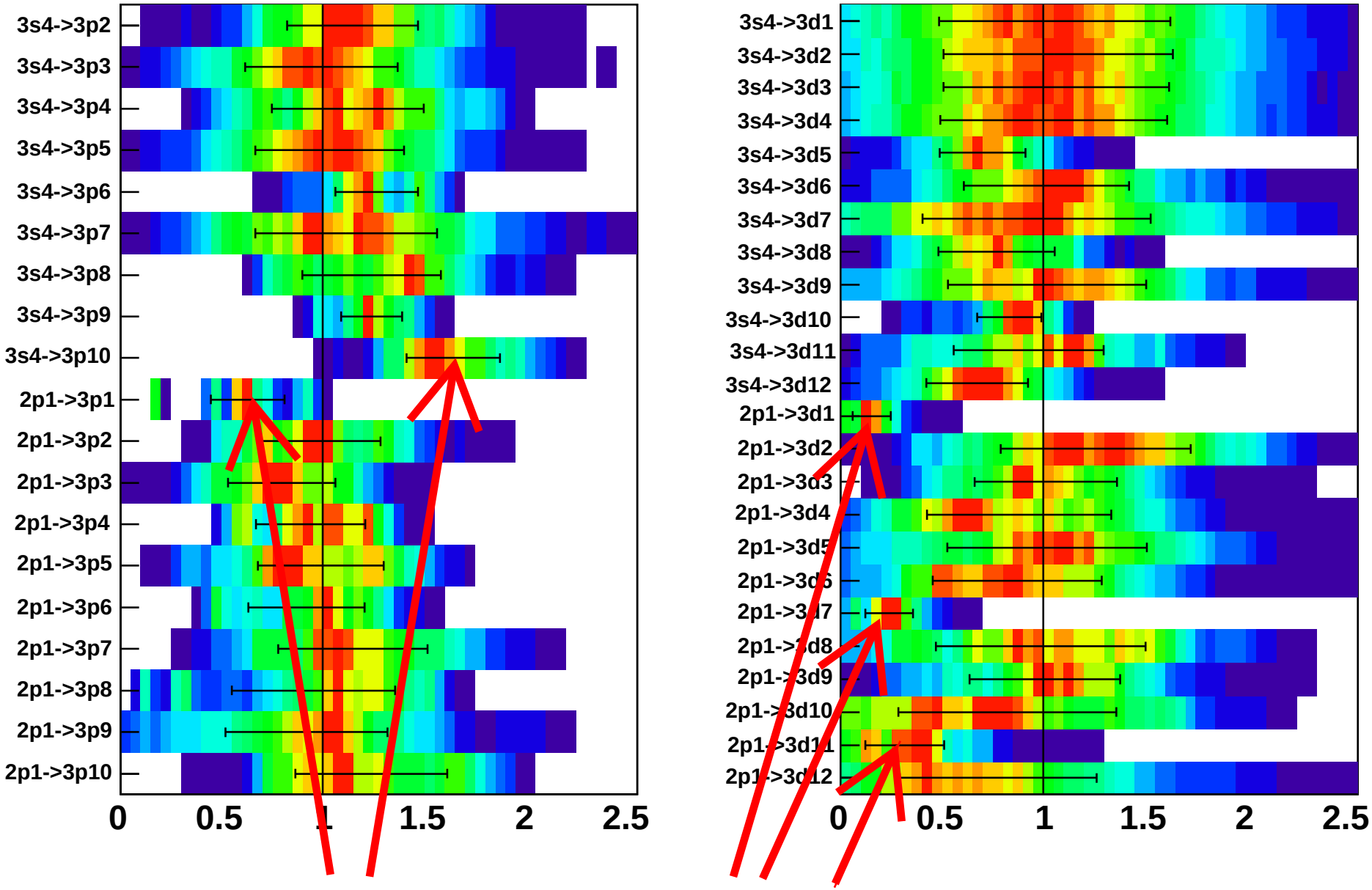
Results: Are the Atomic Data Consistent?





looks pretty good; correction factors mostly consistent with 1.0

Let's Zoom In ...



OOPS ?!?!?!

Results: Significant Correction Factors for a Few Transitions

Most significant corrections obtained from the measured spectral data. The corrections are given for cross sections of excitation from the *ground* state and the *lowest 3s* state.

final state:	*initial state:* ground	$2p^5(^2P^\circ_{3/2})\,3s\,^2[\frac{3}{2}]^\circ,\ J=2$
$2p^5(^2P^\circ_{3/2})\,3d\,^2[\frac{1}{2}]^\circ,\ J=1$	$0.43^{+0.3}_{-0.27}$	
$2p^5(^2P^\circ_{3/2})\,3d\,^2[\frac{3}{2}]^\circ,\ J=1$	$0.27^{+0.17}_{-0.14}$	
$2p^5(^2P^\circ_{1/2})\,3d\,^2[\frac{3}{2}]^\circ,\ J=1$	$0.17^{+0.15}_{-0.11}$	
$2p^5(^2P^\circ_{3/2})\,3p\,^2[\frac{1}{2}],\ J=1$		$1.3^{+0.2}_{-0.16}$
$2p^5(^2P^\circ_{1/2})\,3p\,^2[\frac{1}{2}],\ J=0$	$0.66^{+0.28}_{-0.21}$	

Explanation: The results for these transitions are very sensitive to the inclusion of continuum coupling! (already suggested in 2004 by Ballance and Griffin)

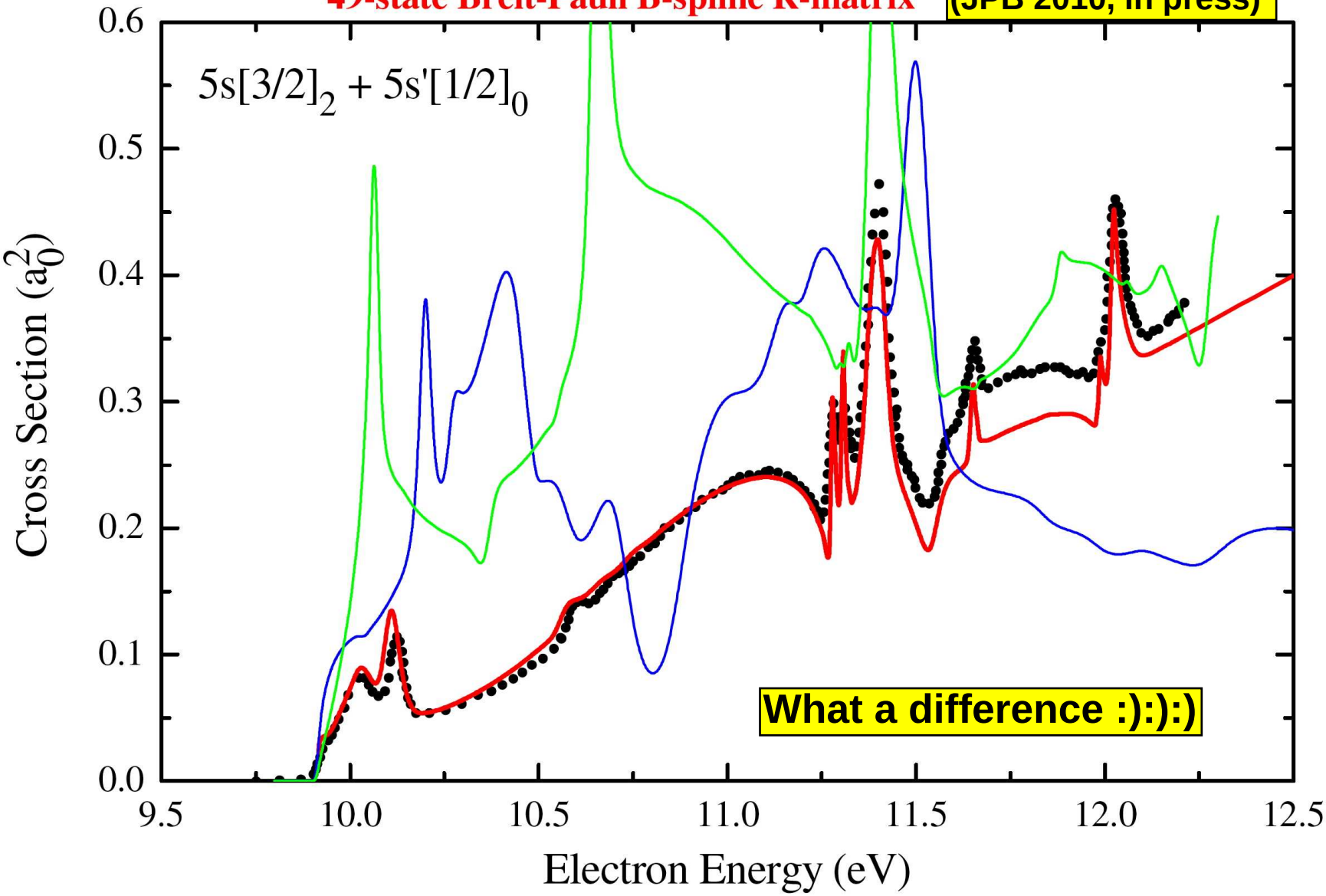
Collaboration between Data Producers and Data Users is Beneficial for Both!

One of Many Remaining Problems: Heavy Targets

Metastable Excitation Function in Kr

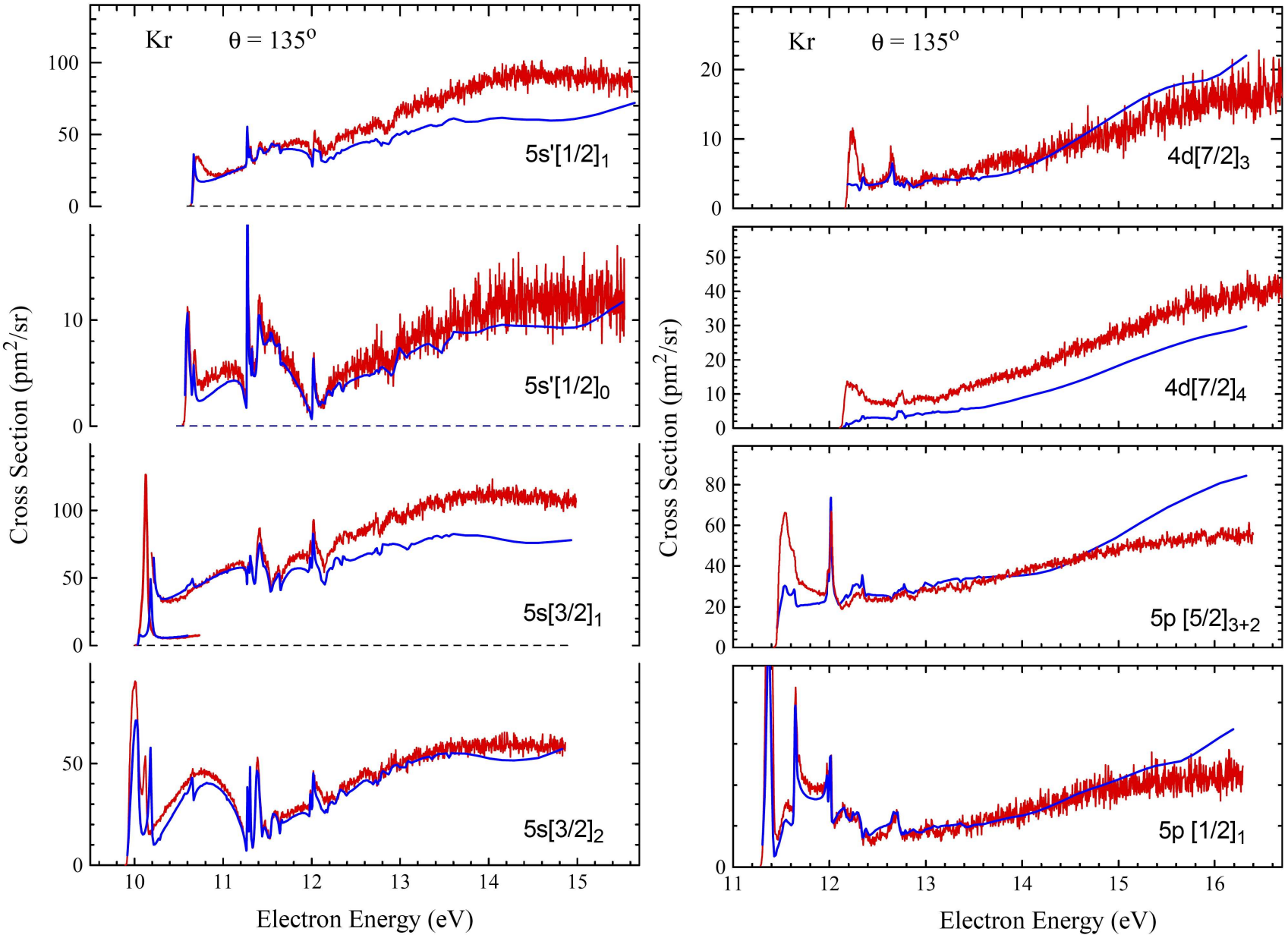
Experiment: Buckman *et al* (1983), multiplied by 0.67

Theories: 31-state Breit-Pauli R-matrix (Zeman & Bartschat 1998)
51-state Breit-Pauli R-matrix (Bartschat & Grum-Grzhimailo 2000)
49-state Breit-Pauli B-spline R-matrix (JPB 2010, in press)



Angle-Differential Cross Sections for e-Kr Excitation

Experiment: M. Allan (2010)



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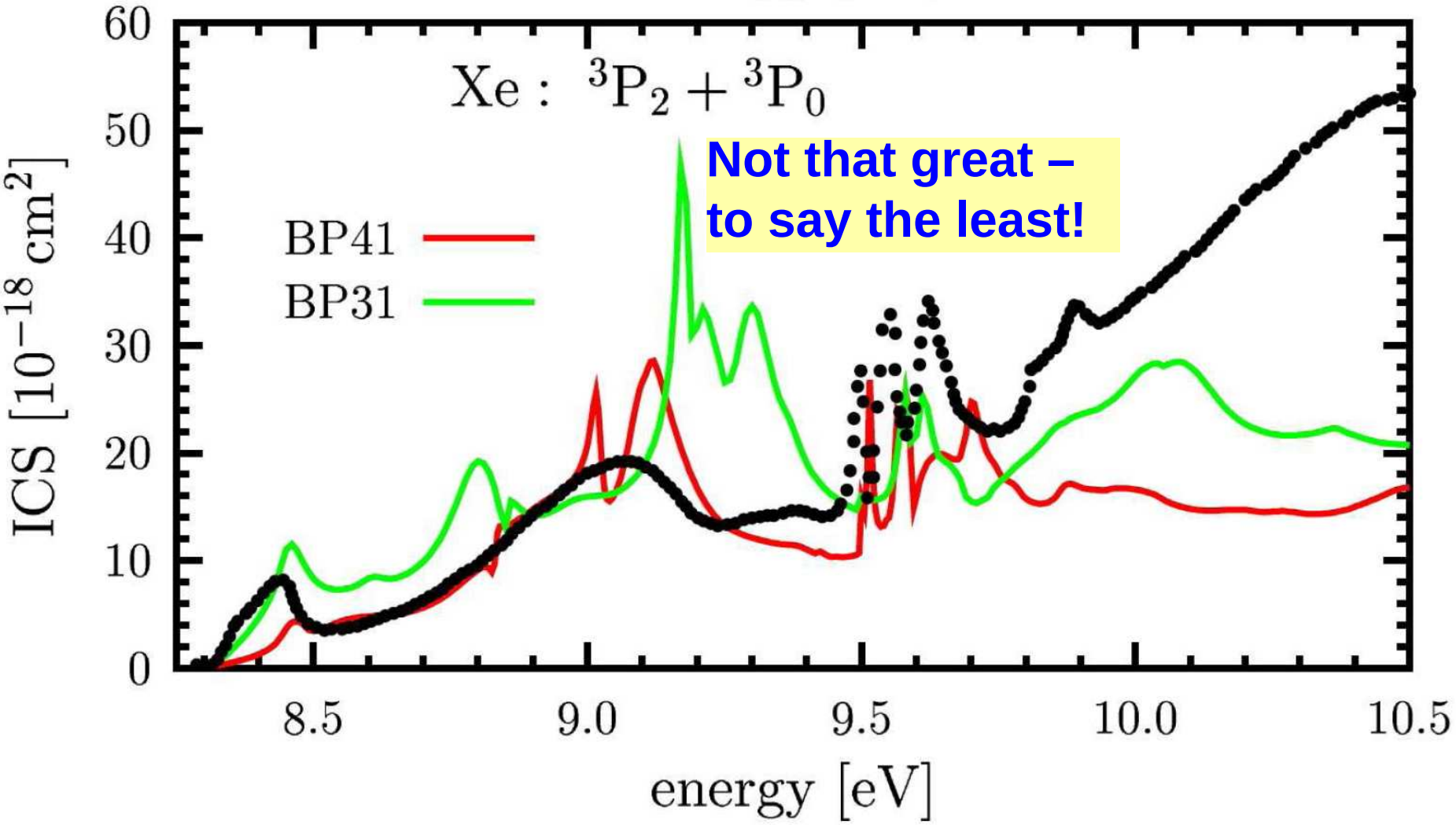
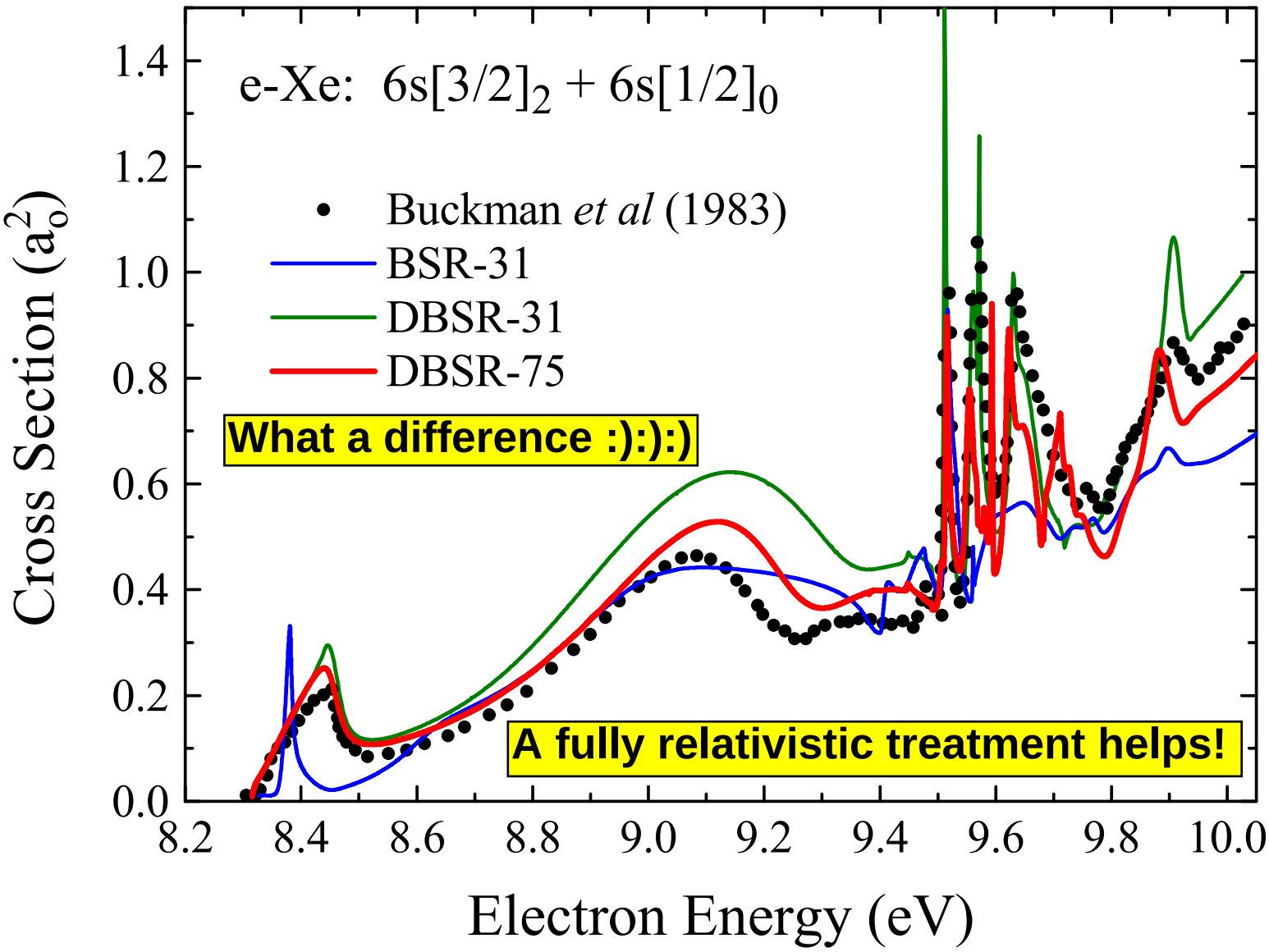
Reminder: e-Xe is difficult!

Calculations are extremely difficult!

- **Experiment: Buckman *et al.* (1983) – not absolute**
- **Theory: Semi-relativistic Breit-Pauli *R*-matrix (close-coupling) models**



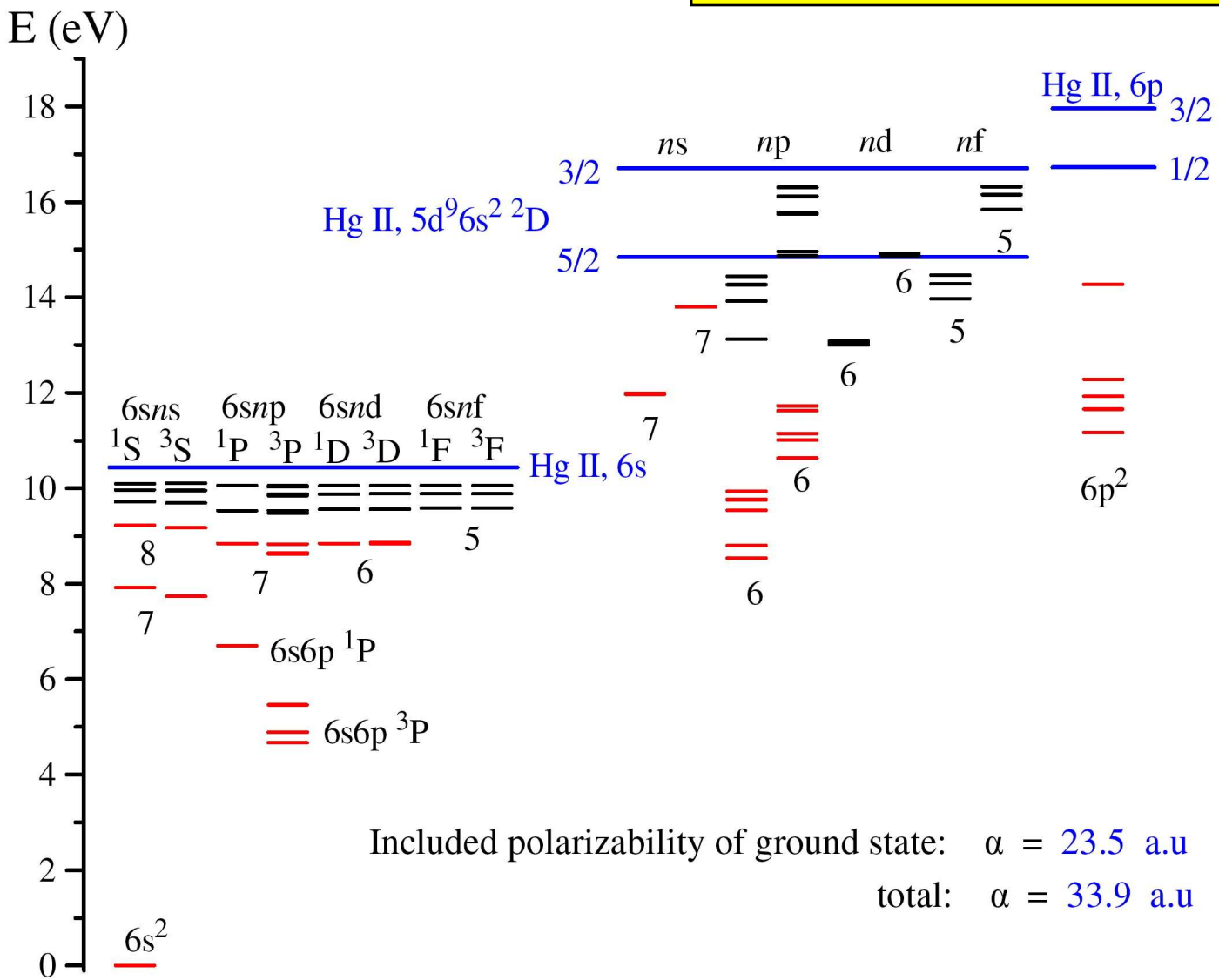
Metastable Excitation Function in Xe



Energy spectrum of Hg

Scattering models - 36CC and 90CC

A Really Heavy Target

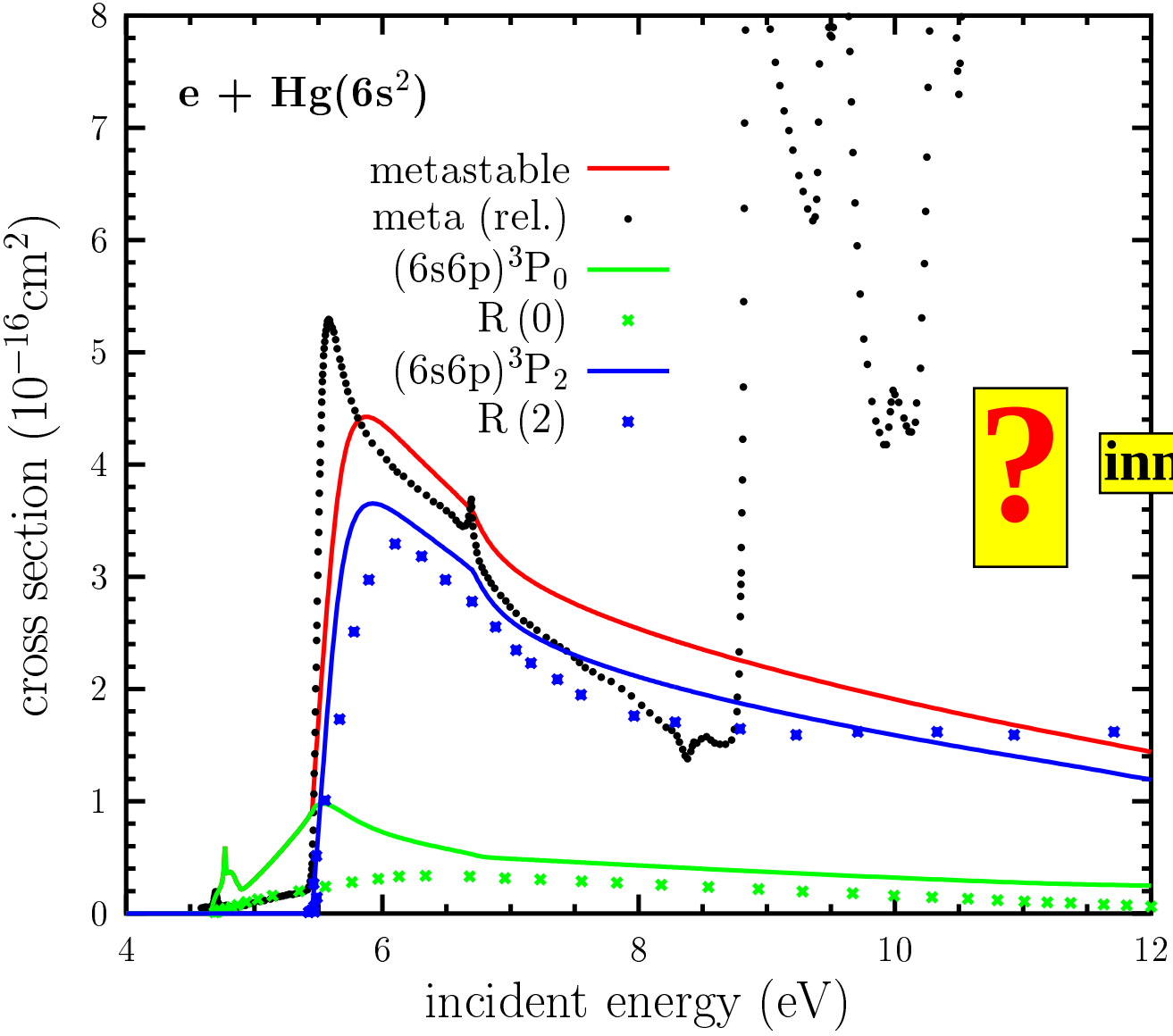


Included polarizability of ground state: α = 23.5 a.u

total: α = 33.9 a.u

Popular Datasets for e-Hg Collisions in 2002
Metastable Excitation Function

- experiment: Newman *et al.*
- semi-empirical Rockwood "R"

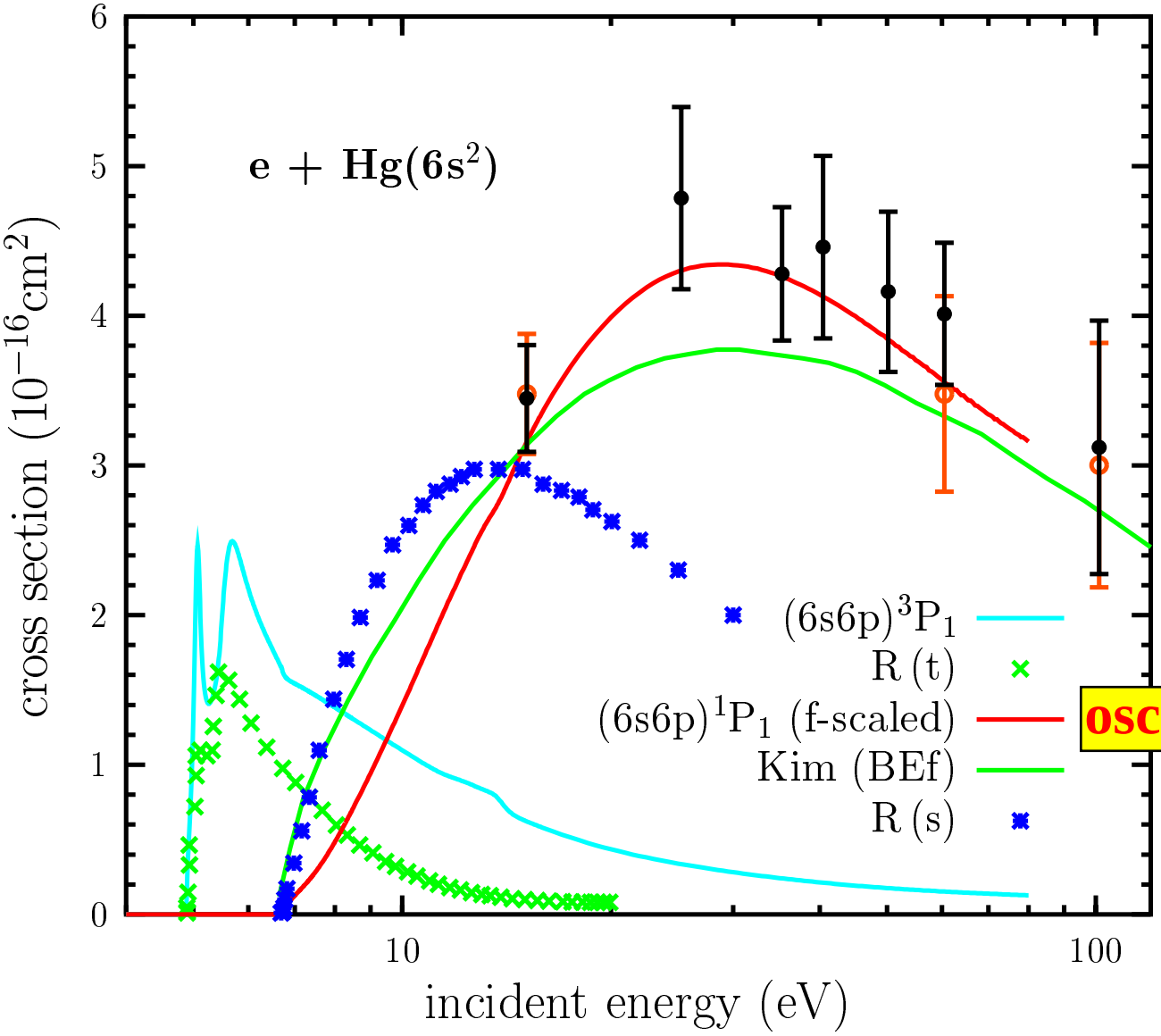


?

inner-shell excitation

Popular Datasets for e-Hg Collisions in 2002
VUV Excitation Function

- experiment: Peitzmann and Kessler
- semi-empirical Rockwood "R"



oscillator strength ?!?!

There seems to be room for improvement in the dataset.

Tables

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TABLE I: Target states of Hg used in the DBSR model. Most of the experimental energies are taken from the NIST database [C. E. Moore, *Atomic Energy Levels* Vol. 3, NSRDS-NBS 35, 1971] with an asterisk. The latter were [illegible] Phys. B **4**, 1236 (1971)].

energy levels

Configuration	Term	Expt. (eV)	Theory (eV)	Diff. (eV)
$6s^2$	$^1S_0$	0.000	0.000	0.000
$6s6p$	$^3P^o_0$	4.667	4.590	-0.078
$6s6p$	$^3P^o_1$	4.887	4.821	-0.065
$6s6p$	$^3P^o_2$	5.461	5.401	-0.060
$6s6p$	$^1P^o_1$	6.704	6.848	0.144
$6s7s$	$^3S_1$	7.730	7.794	0.064
$6s7s$	$^1S_0$	7.926	7.953	0.027
$5d^96s^26p$	$^3P^o_2$	8.541	8.533	-0.007
$6s7p$	$^3P^o_0$	8.619	8.613	-0.006
$6s7p$	$^3P^o_1$	8.637	8.630	-0.007
$5d^96s^26p$	$^3D^o_3$	8.794*	8.816	0.021
$6s7p$	$^3P^o_2$	8.829	8.842	0.014
$6s7p$	$^1P^o_1$	8.839	8.845	0.006
$6s6d$	$^3D_1$	8.845	8.847	0.002
$6s6d$	$^1D_2$	8.844	8.850	0.006
$6s6d$	$^3D_2$	8.852	8.866	0.014
$6s6d$	$^3D_3$	8.856	8.868	0.011
$6s8s$	$^3S_1$	9.170	9.169	-0.001
$6s8s$	$^1S_0$	9.225	9.215	-0.010
$5d^96s^26p$	$^3F^o_4$	9.540	9.513	-0.027
$5d^96s^26p$	$^1D^o_2$	9.755	9.730	-0.025
$5d^96s^26p$	$^1P^o_1$	9.772	9.745	-0.027
$5d^96s^26p$	$^1F^o_3$	9.934*	9.877	-0.057
$5d^96s^26p$	$^3F^o_3$		9.908	
ionization limit		10.438		
$5d^96s^26p$	$^3F^o_2$		10.602	
$5d^96s^26p$	$^3P^o_1$	11.005	11.104	0.099
$5d^96s^26p$	$^3P^o_0$		11.111	
$6p^2$	$^3P_0$	11.170	11.224	0.054
$5d^96s^26p$	$^3D^o_1$	11.622	11.583	-0.039
$5d^96s^26p$	$^3D^o_2$		11.703	
$6p^2$	$^3P_1$	11.652	11.787	0.135
$6p^2$	$^3P_2$	11.926*	11.897	-0.029
$5d^96s^27s$	$^3D^o_3$	12.039*	11.939	-0.100
$5d^96s^27s$	$^3D^o_2$	12.065*	11.963	-0.102
$6p^2$	$^1D_2$		12.253	
$6p^2$	$^1S_0$		14.248	

TABLE II: Contributions to the static dipole polarizability of the Hg ground state in the DBSR model. Here kp, kf and np, nf stand for contributions from the ionization continuum and the remain[illegible] or strengths are g[illegible] of experimental values. See Migdalek [Physica Scripta **T100**, 47 (2002)] for references and more details.

oscillator strengths

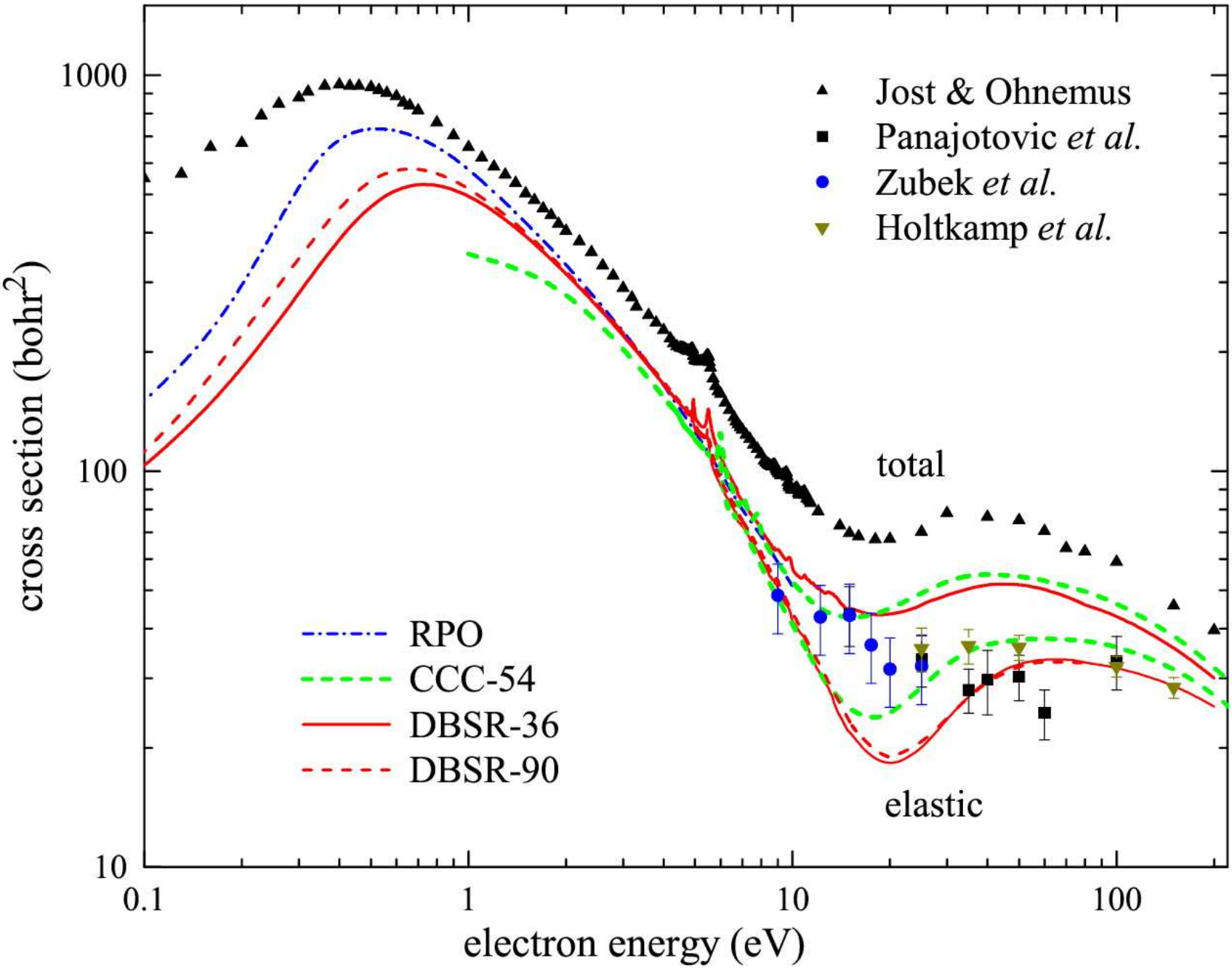
Upper level	oscillator strength	polarizability (a_0^3)	experiment
$(5d^{10}6s6p)^1P^o_1$	1.147	18.474	1.16
$(5d^{10}6s6p)^3P^o_1$	0.018	0.435	0.024
$(5d^{10}6s7p)^1P^o_1$	0.022	0.208	
$(5d^{10}6s8p)^1P^o_1$	0.019	0.154	
$(5d^96s^26p)^1P^o_1$	0.203	1.583	
$(5d^96s^26p)^3P^o_1$	0.495	2.976	
$(5d^96s^26p)^3D^o_1$	0.182	0.994	
$(5d^96s^27p)^1P^o_1$	0.086	0.386	
$(5d^96s^28p)^1P^o_1$	0.027	0.110	
$(5d^96s^27p)^3P^o_1$	0.044	0.154	
$6skp$		3.426	
$5d^96s^2(np+kp)$		2.143	
$5d^96s^2(nf+kf)$		2.993	
Total		34.036	33.9

TABLE III: Positions and widths of the $6s6p^2$ negative-ion resonances. The experimental data are taken from Sullivan *et al.*. [New Journal of Physics **5**, 1 (2003)]

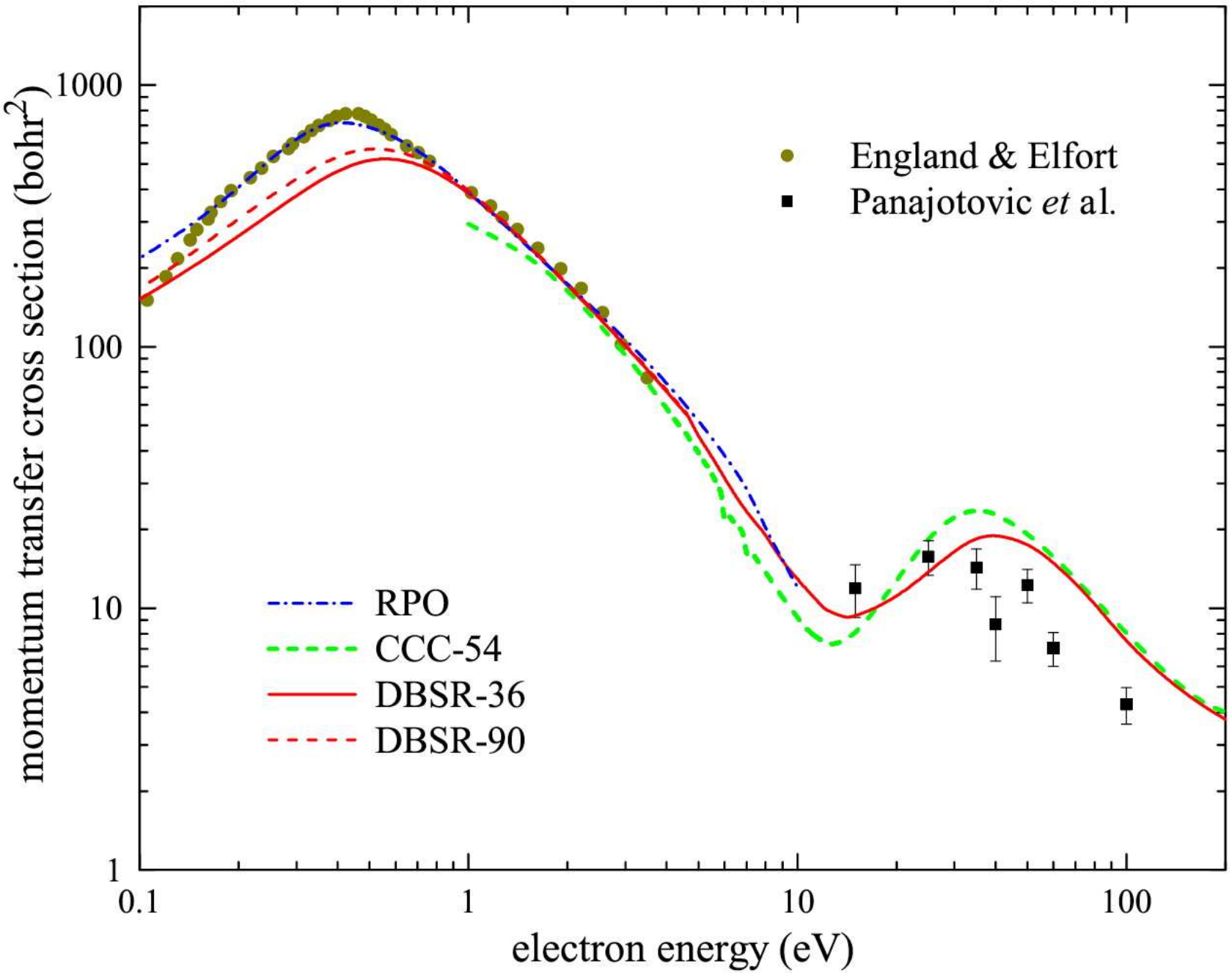
resonances

Resonance	Energy (eV)	Width (meV)	Expt.	
$(6s6p^2)^4P_{1/2}$	4.614	0.04	4.550	0.46
$(6s6p^2)^4P_{3/2}$	4.712	36	4.670	14.7
$(6s6p^2)^4P_{5/2}$	4.938	65	4.915	60
$(6s6p^2)^2D_{3/2}$	4.904	300	5.12	290
$(6s6p^2)^2D_{5/2}$	5.483	148	5.53	280

Elastic and Total Cross Section



Momentum-Transfer Cross Section



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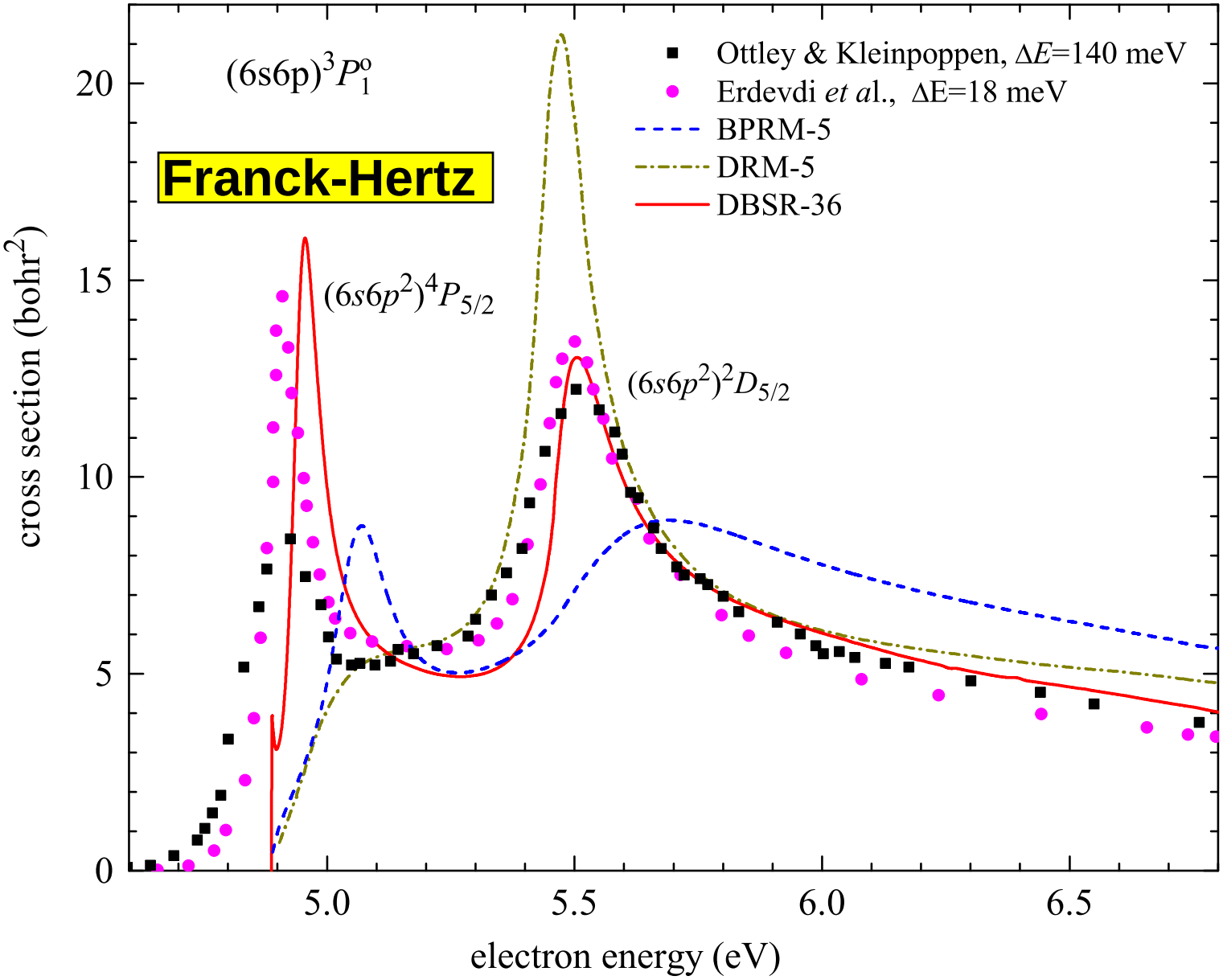
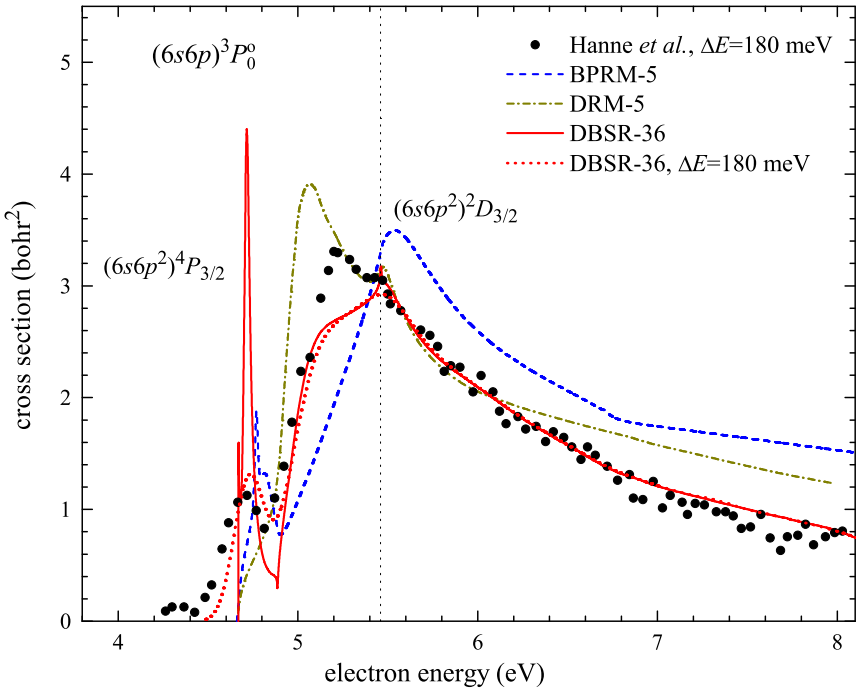
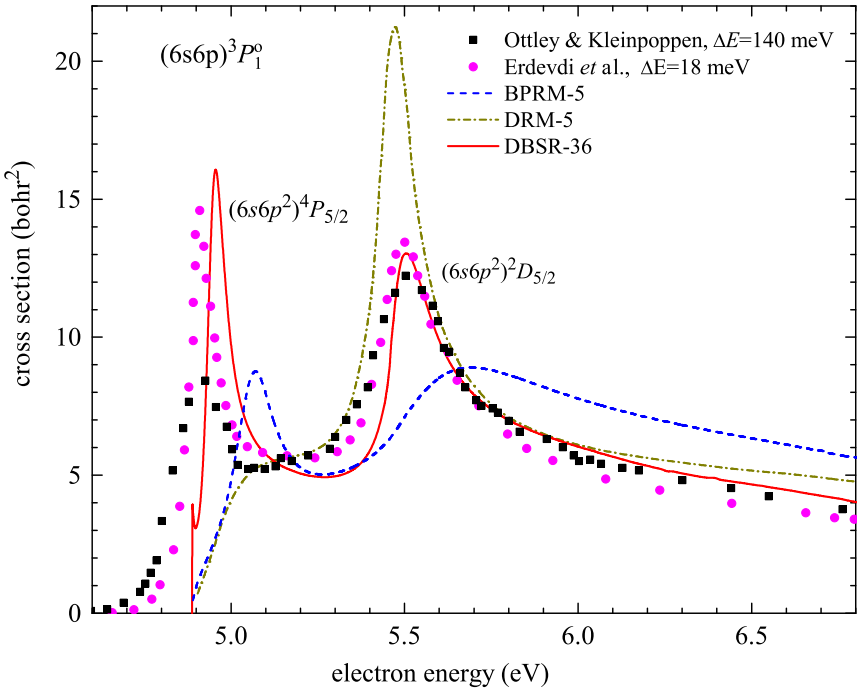
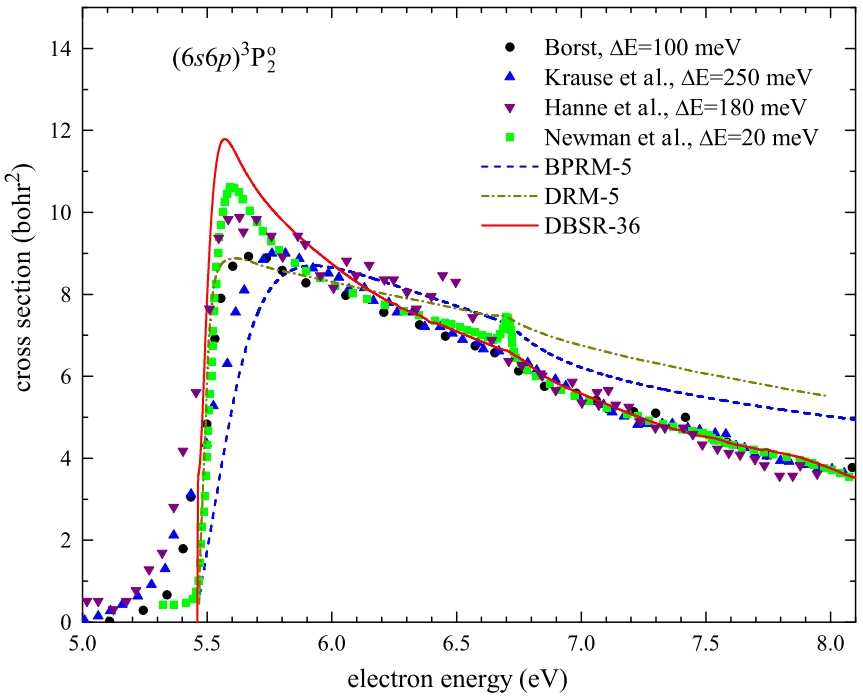
Angle-Integrated Cross Sections for the $(6s6p)^3P_1$ State

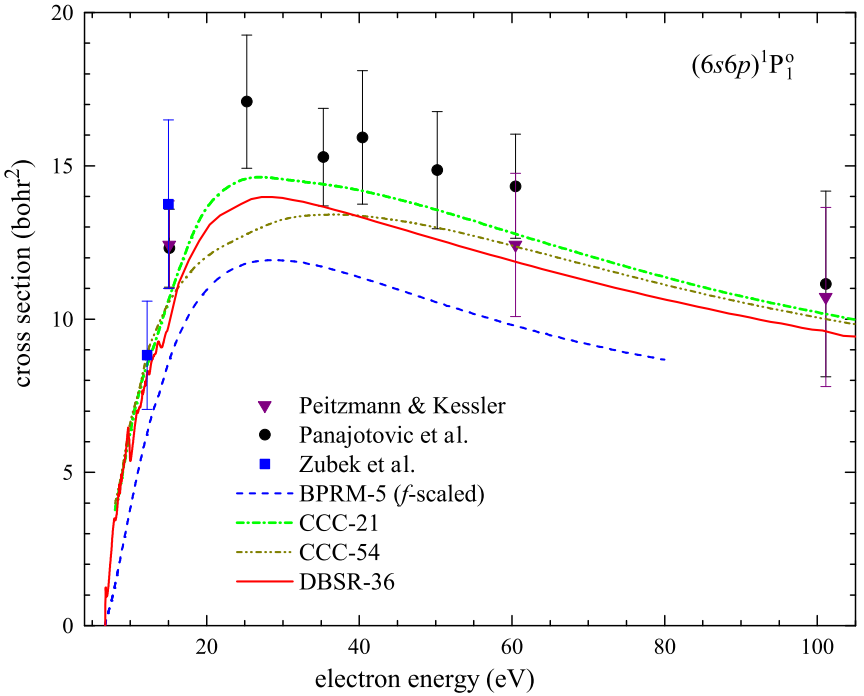


Angle-Integrated Cross Sections for the (6s6p) States









Conclusions and Outlook

- Much progress has been made in **calculating the structure of and electron-induced collision processes in noble gases — and other complex targets (C, O, F, ..., Cu, Zn, Cs, Au, Hg, Pb).**
- **Time-independent close-coupling (*R*-matrix)** seems to be the way to go.
- **Other sophisticated methods (CCC, TDCC, ECS, ...) are still restricted to simple targets**. These methods are have **essentially solved the (quasi-)one- and (quasi-)two-electron problems** for excitation and ionization.
- **Perturbative** (Born) methods are still being used, but **be careful about the accuracy!**
- For calculations on noble gases other than helium, the **target structure problem** should not be ignored!
- For such complex targets, the **BSR method with non-orthonal orbitals has achieved a breakthrough in the description of near-threshold phenomena.** The major advantages are:
  - **highly accurate target description**
  - **consistent description** of the N-electron target and (N+1)-electron collision problems
  - ability to give **"complete" datasets** for atomic structure and electron collisions

Conclusions and Outlook (continued)

- After setting up a **detailed model of a Ne discharge with a large number of observed lines, we validated most atomic BSR input data** (oscillator strengths and collision cross sections).
- The validation method provides a valuable **alternative for data assessment and detailed plasma diagnostics** — especially when no absolute cross sections from beam experiments are available.
- This is a nice example of a very fruitful and **mutually beneficial collaboration between data producers and data users**.

- **We can provide atomic data for (almost) any system**. **Practical limitations** are:
  - expertise of the operator/developer — **Oleg, please stop smoking!**
  - further **necessary code development** (pseudo-states, better parallelization)
  - computational resources (**Many Thanks to Teragrid!**)
- We are currently preparing **fully relativistic *R*-matrix with pseudo-states calculations on massively parallel platforms**.
- We don't have a company (yet). If you really want/need specific data, you can
  - **ask us really nicely and hope for the best** (preferred by most colleagues)
  - **give us $$$ and increase your priority on the list** (preferred by us)

THANK YOU!