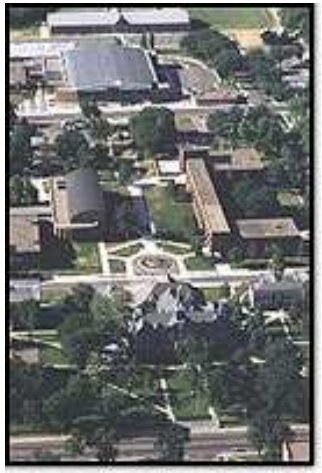
HIGH-PRECISION CROSS SECTIONS FOR LOW-ENERGY ELECTRON–ATOM COLLISIONS



Klaus Bartschat, Drake University

ICAMDATA

October 15–19, 2006

Special Thanks to:

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Alexei Grum-Grzhimailo, Don Madison, ...
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Michael Allan, Steve Buckman, Kai Franz, Hartmut Hotop, Morty Khakoo,
and all other experimentalists who are pushing us hard ...

Phil Burke, Charlotte Froese Fischer, Oleg Zatsarinny

National Science Foundation: PHY-0244470, ITR-0311161, PHY-0555226

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- Data **Wanted** vs. Data **Available**
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- **Distorted-Wave Methods**
- **The Close-Coupling Method**: Recent Developments
  - The "Convergent Close-Coupling" (**CCC**) Approach
  - The "$\mathcal{R}$-Matrix with Pseudo-States" (**RMPS**) Approach
  - The "Intermediate Energy $\mathcal{R}$-Matrix " (**IERM**) Approach
  - The "Time-Dependent Close-Coupling" (**TDCC**) Approach
  - **The "B-Spline R-Matrix" (BSR) Approach**
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III. Selected Results for Electron–Impact Excitation and Ionization

- Light Targets: **H, He**
- Quasi One-Electron Targets: **Be^+, Cs**
- Quasi Two-Electron Targets: **Zn, Hg**
- Heavy Noble-Gas Targets: **Ne, Ar, Kr, Xe**
- Complex Open-Shell Targets: **Mo, Fe^+, O**

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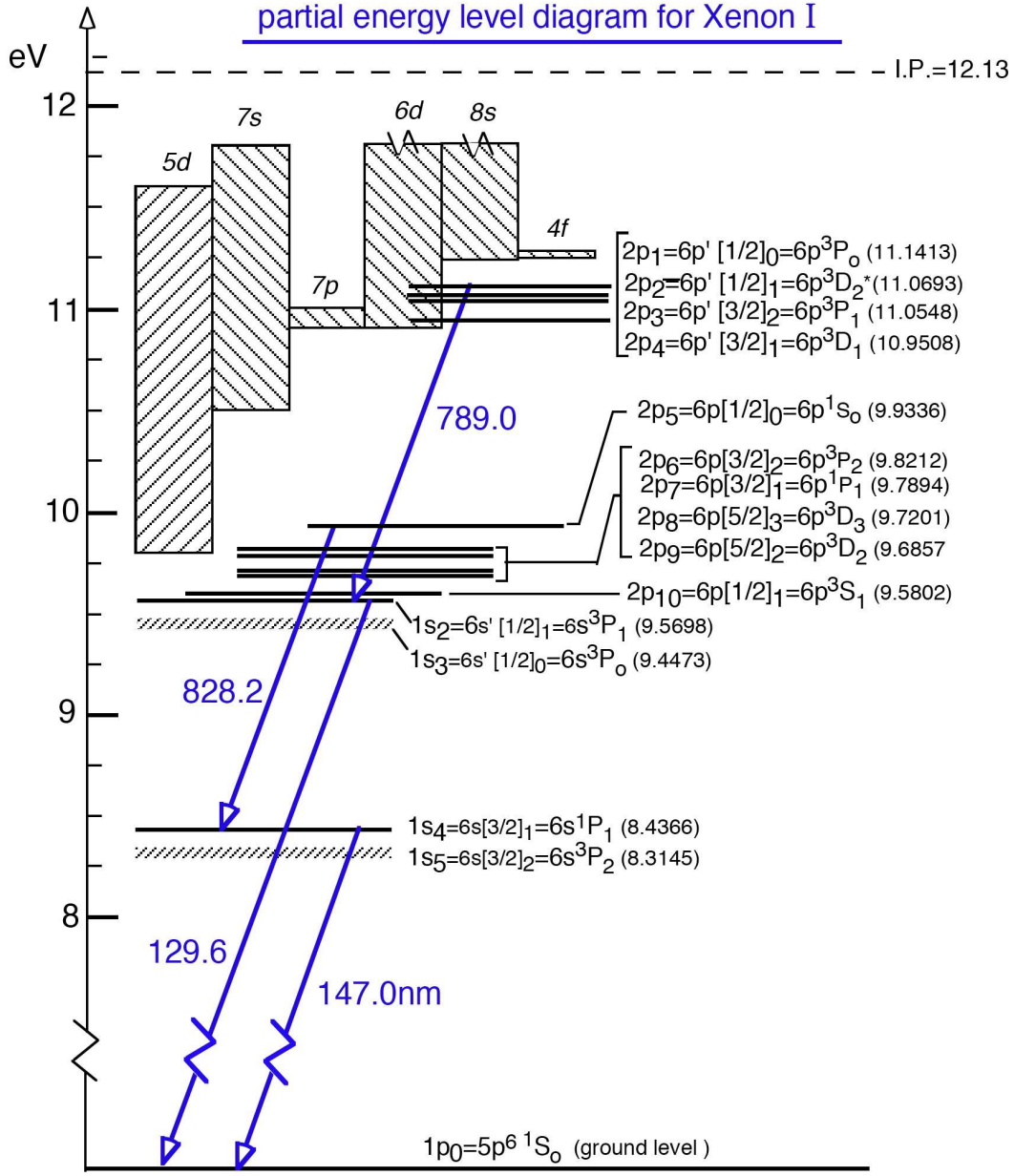
IV. Conclusions and Outlook

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

Wanted: Level-to-Level + Ionization



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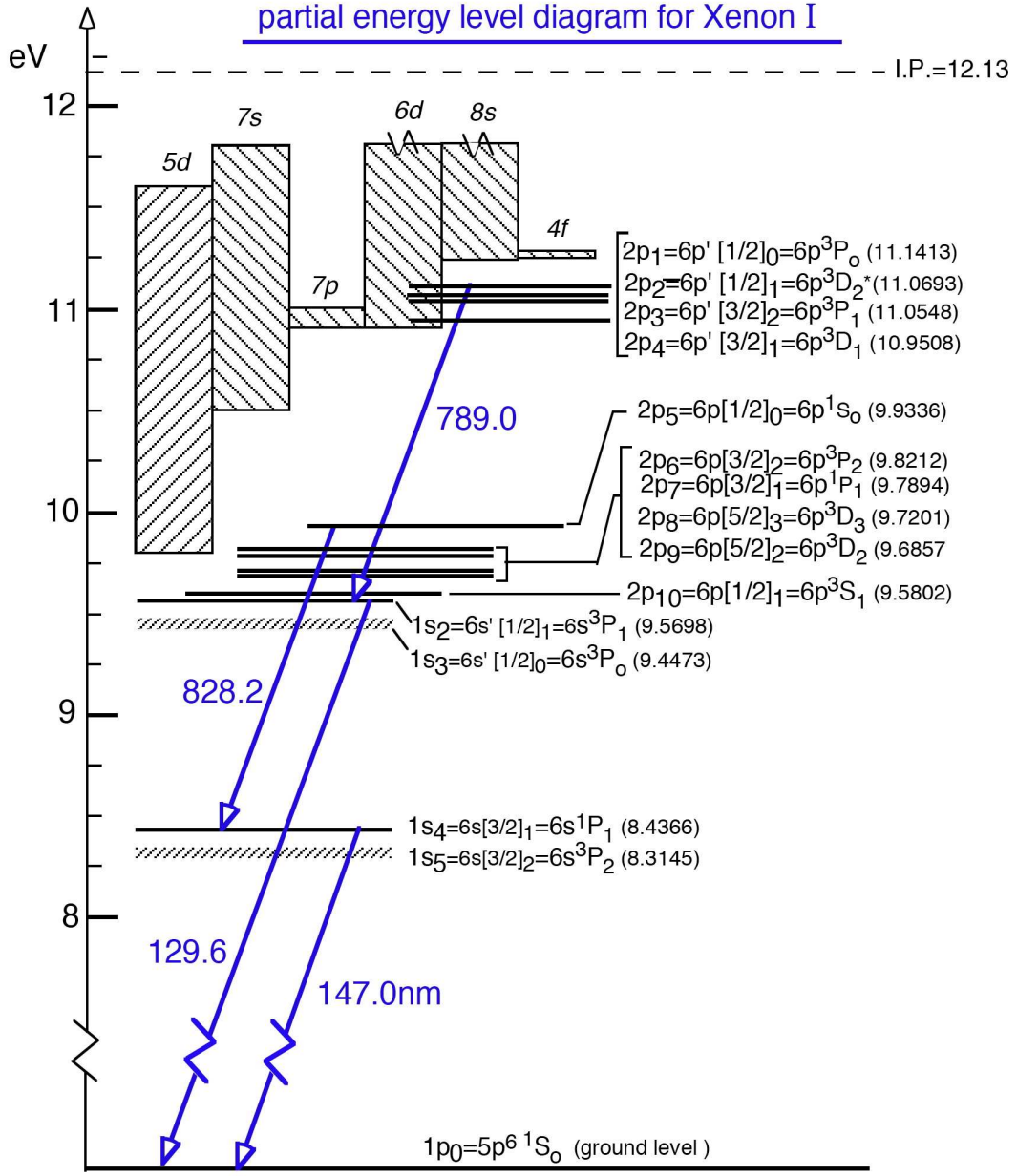
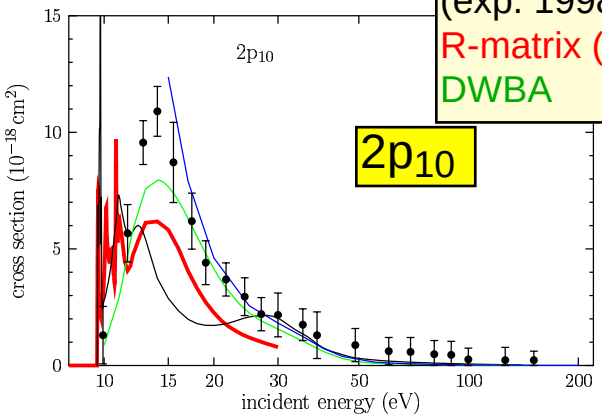
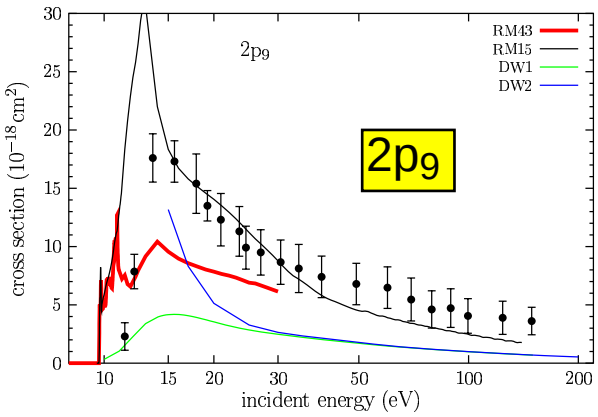
partial energy level diagram for Xenon I

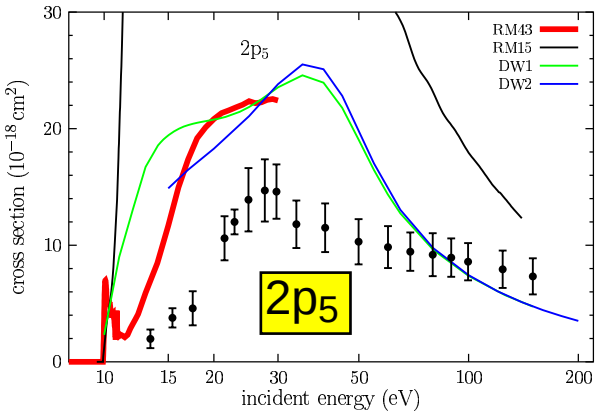


Available

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







Production and Assessment of Atomic Data

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  - **calculations** (Opacity Project, Iron Project, ...)
    - relatively cheap
    - almost any transition of interest is possible
    - often restricted to particular energy ranges:
      - high (→ Born-type methods)
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    - results could be **WRONG !**

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

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

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

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

- 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!

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Inclusion of Relativistic Effects

- **Re-coupling** of non-relativistic results (**CCC**; problematic near threshold)
- **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)

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

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[2] Department of Physics, Rollins College, Winter Park, FL 32789, USA
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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+}.

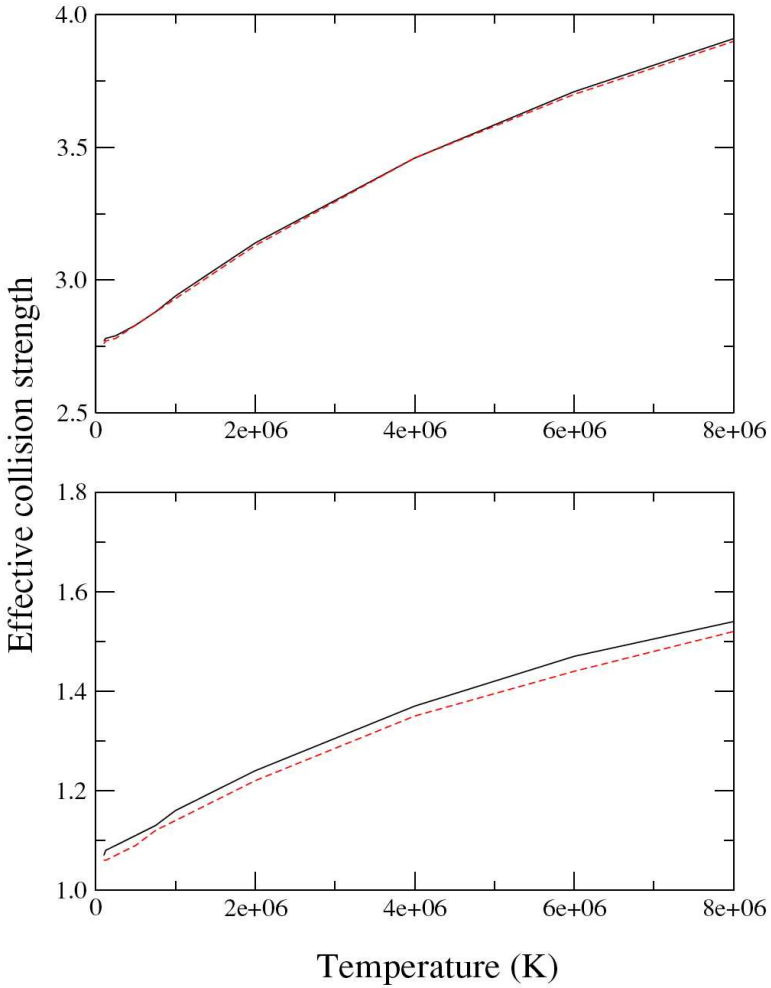

Figure 1. Effective collision strengths for two strong dipole-allowed transitions; results from the Breit–Pauli *R*-matrix calculation are represented by the solid lines and those from the Dirac *R*-matrix calculation by the dashed lines. The upper graph is for the $3s^2\ ^1S_0$–$3s3p\ ^1P_1$ transition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

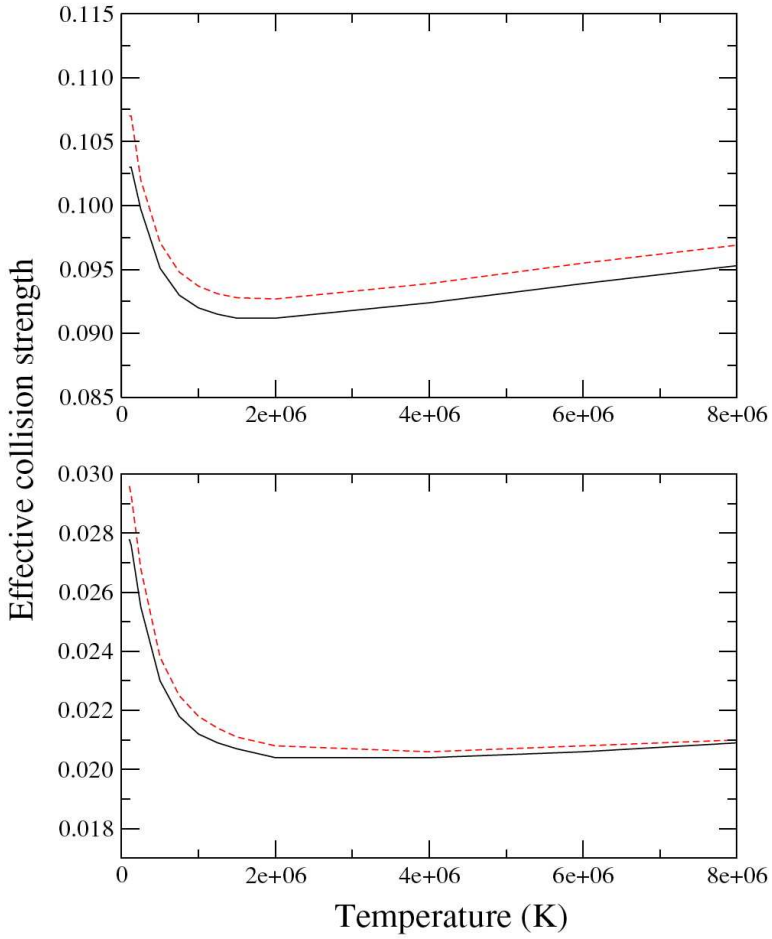

Figure 2. Effective collision strengths for two double-electron transitions; results from the Breit–Pauli *R*-matrix calculation are represented by the solid lines and those from the Dirac *R*-matrix calculation by the dashed lines. The upper graph is for the $3s^2\ ^1S_0$–$3p^2\ ^1D_2$ transition and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

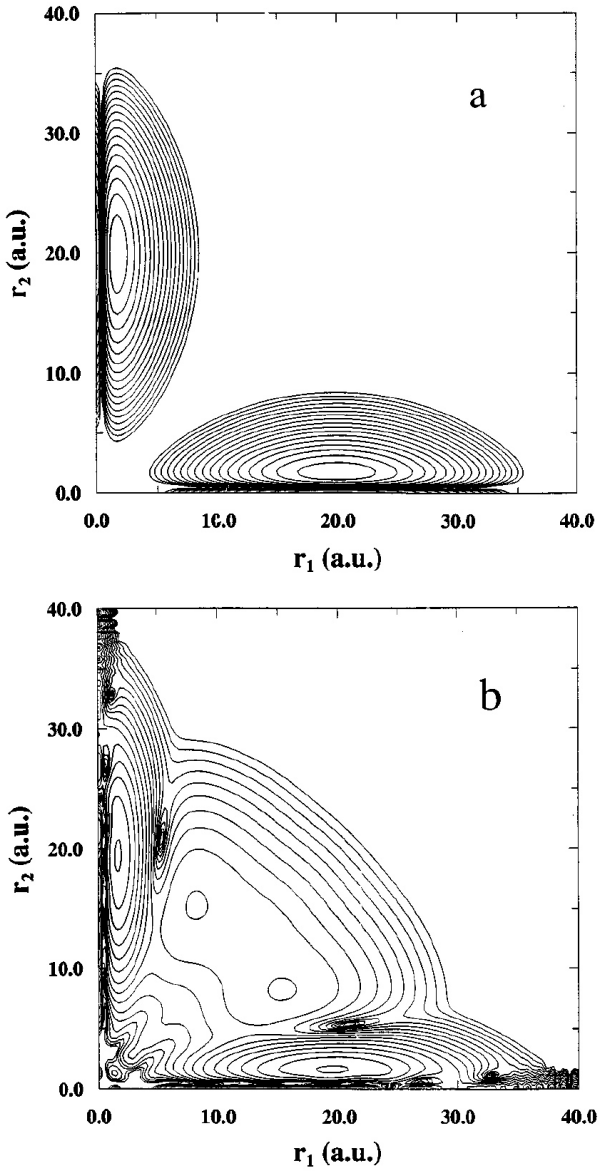
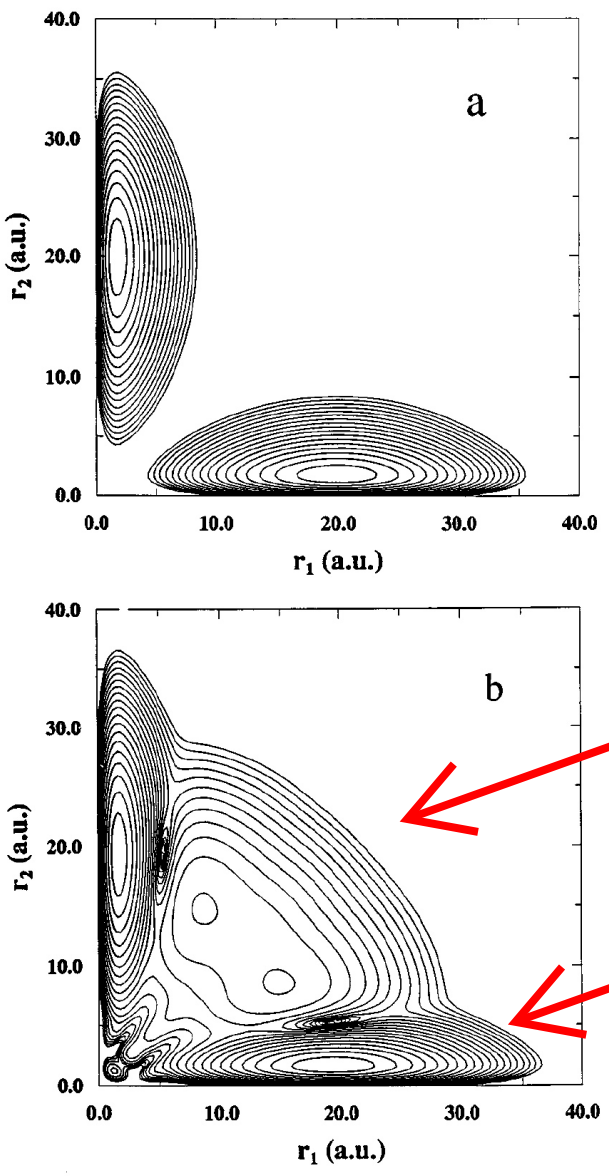


FIG. 1. ^1S partial-wave probability densities for electron-impact ionization of Be^+ at 50.0 eV using a model potential: (a) contour plot for $|P^{00}_{ss}(r_1,r_2,t=0)|^2$ and (b) contour plot for $|P^{00}_{ss}(r_1,r_2,t=20)|^2$.



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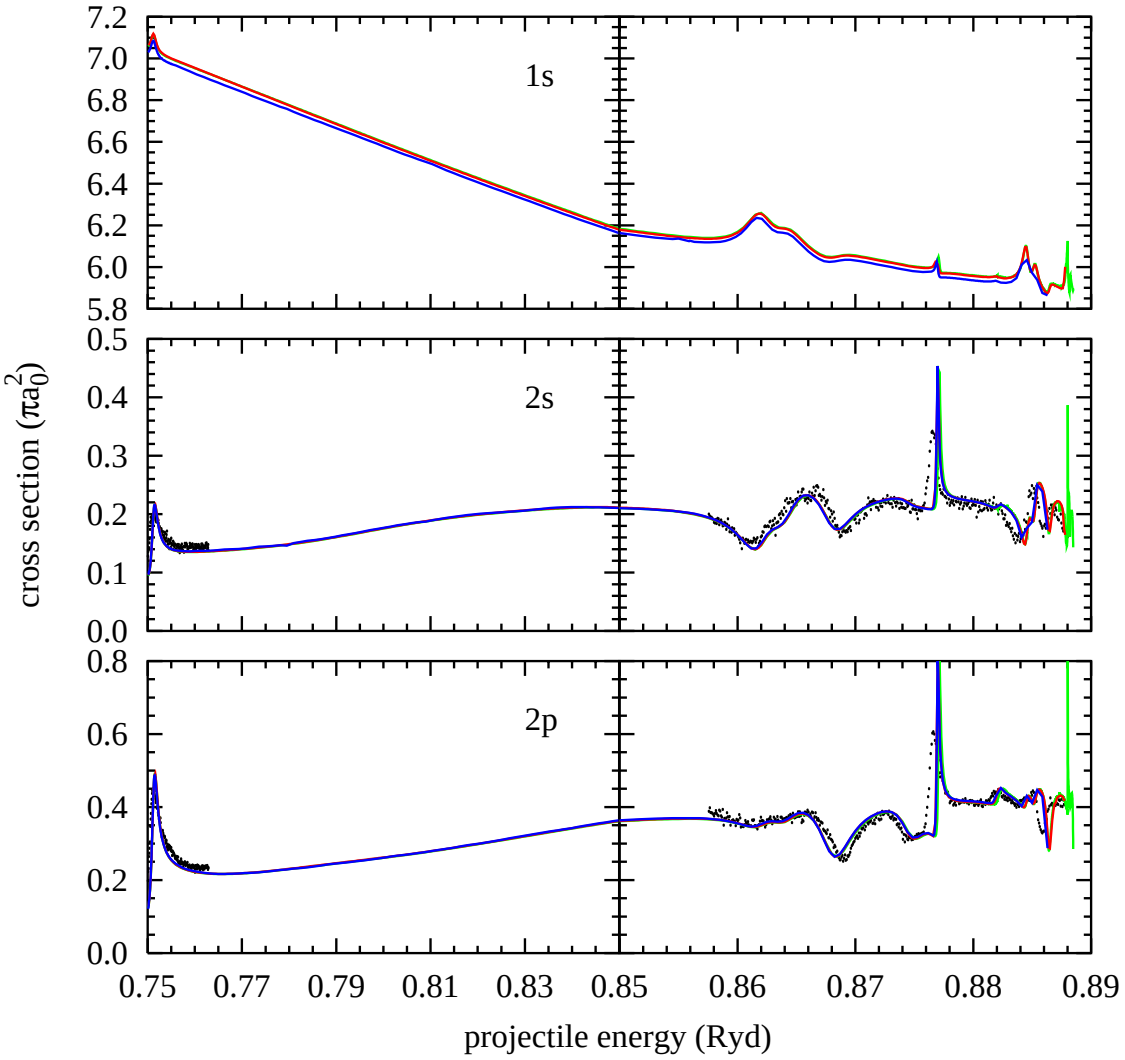
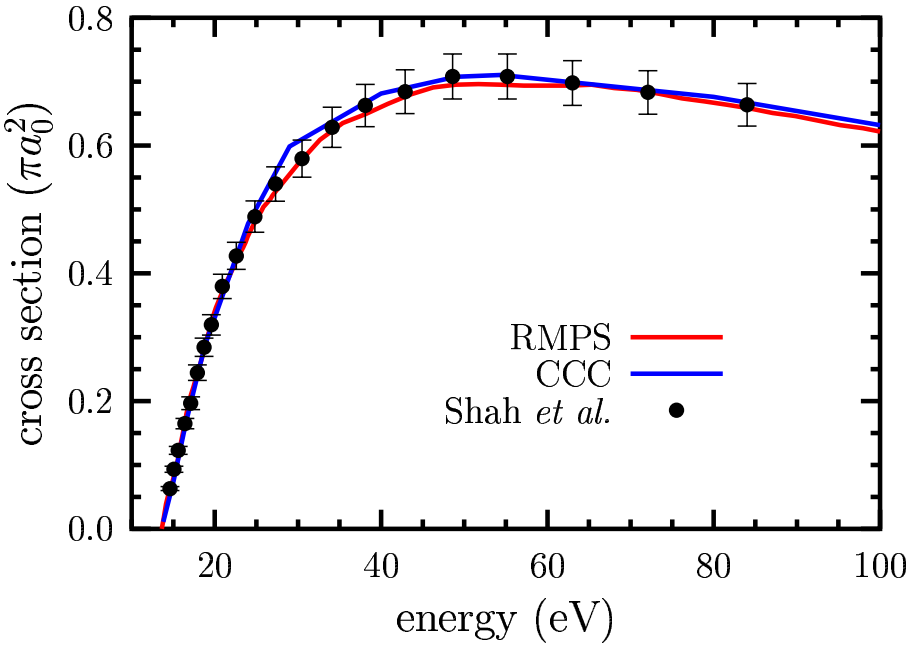
Benchmark Results for e–H Scattering

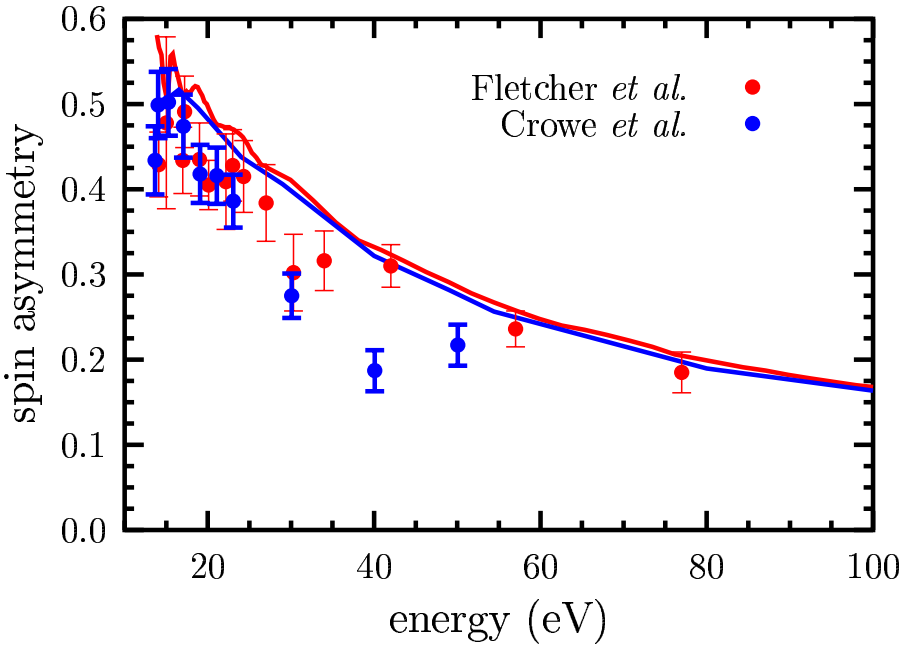
- Using a variational method, Schwartz solved the **low-energy elastic e–H scattering problem** with high accuracy in the early 1960's.
- As seen in further benchmark work in the inelastic regime, **CCC**, **RMPS**, and **IERM** predictions agree extremely well with each other, and also with the experimental 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

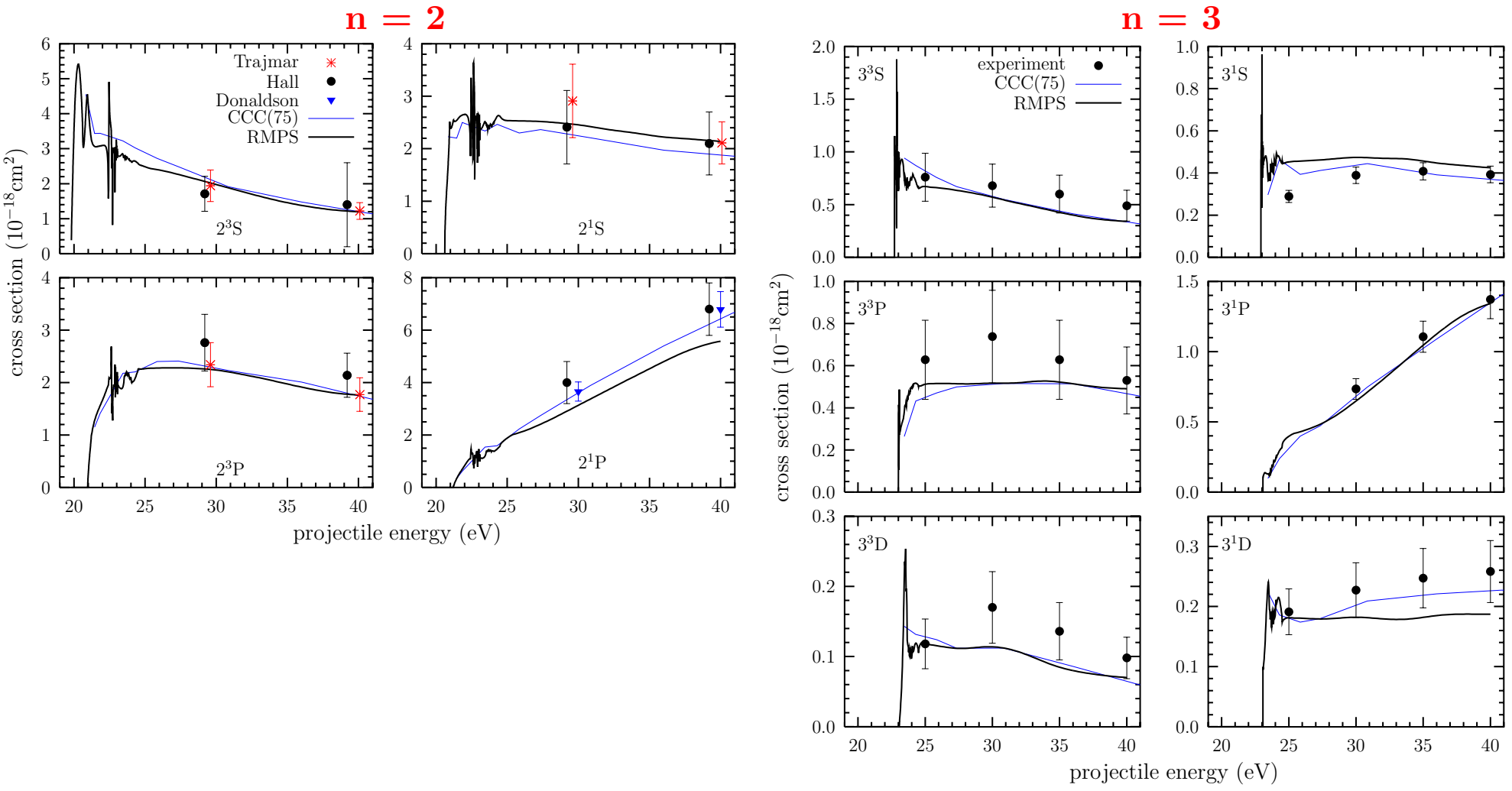
(from Bartschat and Bray 1996)





Cross Section for Electron-Impact Excitation of He($1s^2$)

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

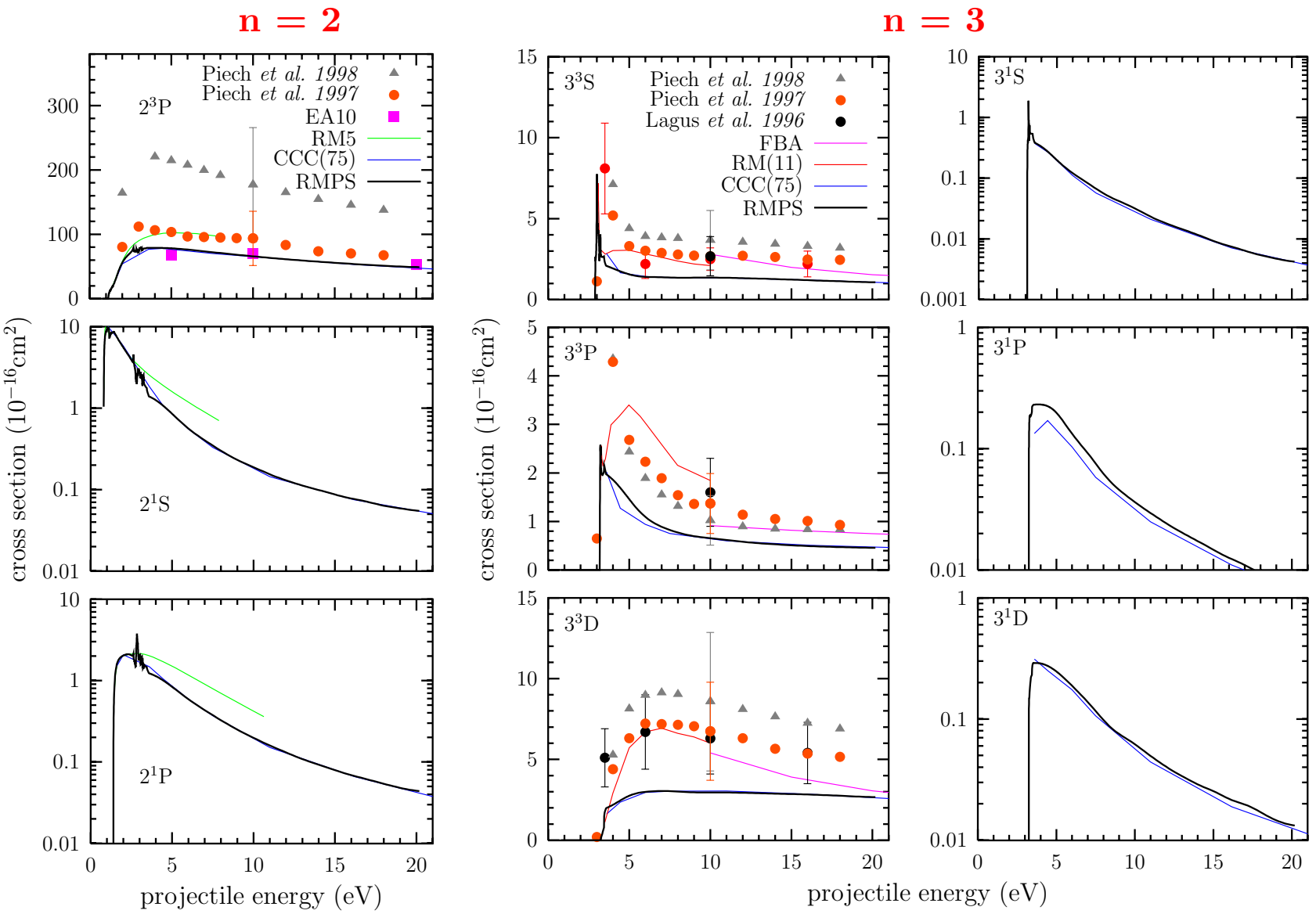


In 1998, deHeer recommends (CCC+RMPS)/2 for uncertainty of 10% or better!

(independent of experiment)

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

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



There is significant disagreement between theory and experiment !?!?!?

New Trap Measurement from Australia

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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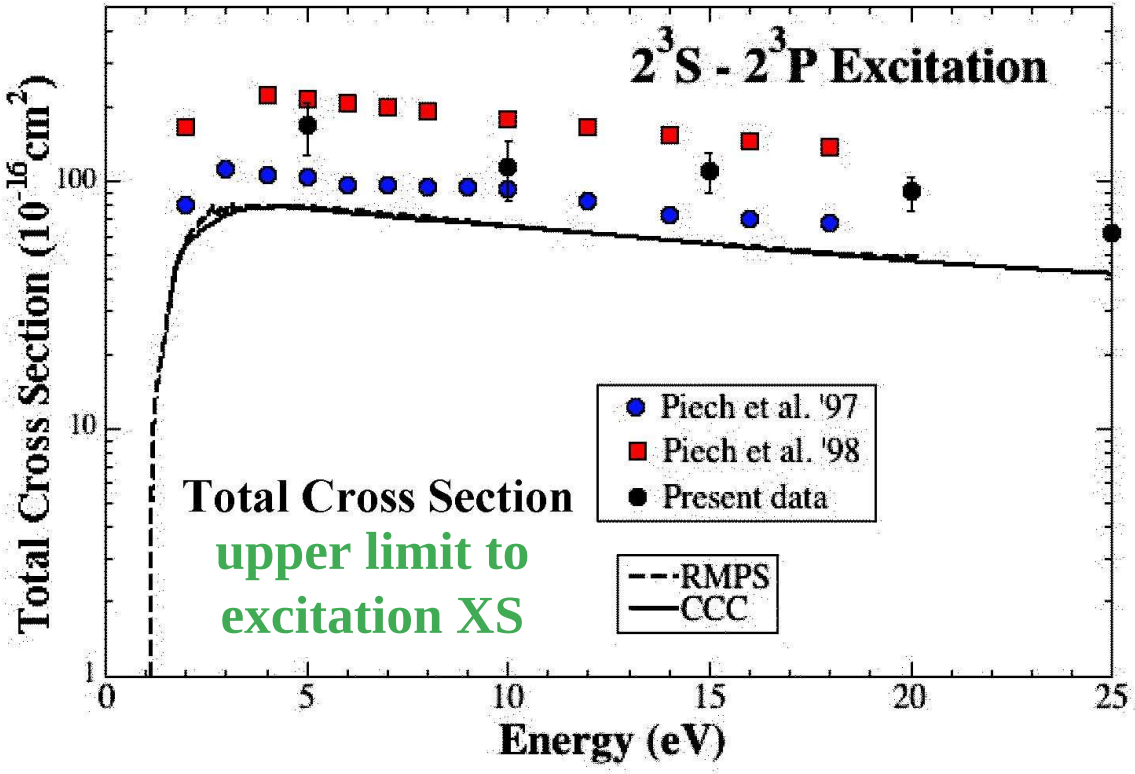

Bartschat [4] demonstrates that a total of four calculations, from an early eikonal approximation to several versions of the *R*-matrix approach, and the CCC technique all give essentially the same result, which favors the lower excitation cross section. The present total cross section result, also shown 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 !

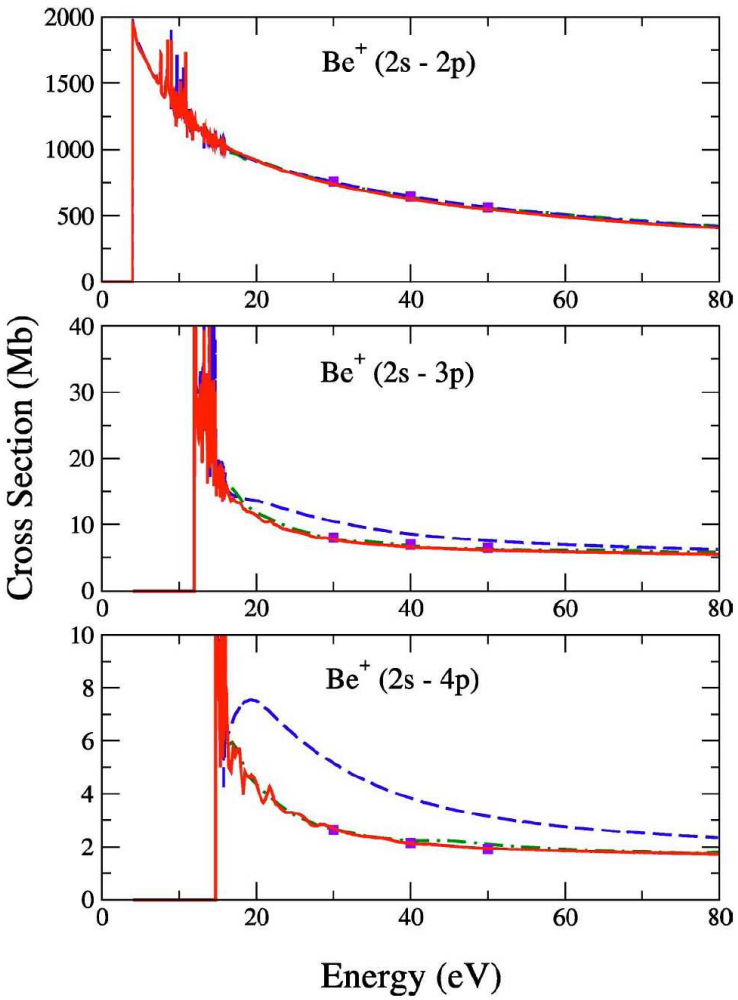

FIG. 4. Electron-impact excitation cross sections from the $2s$ ground term of Be^+ to the np excited terms. Dashed curves are from the present 14-term R-matrix calculation; solid curves are from the present 49-term RMPS calculation; solid squares are from the present TDCC calculation; dot-dashed curves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

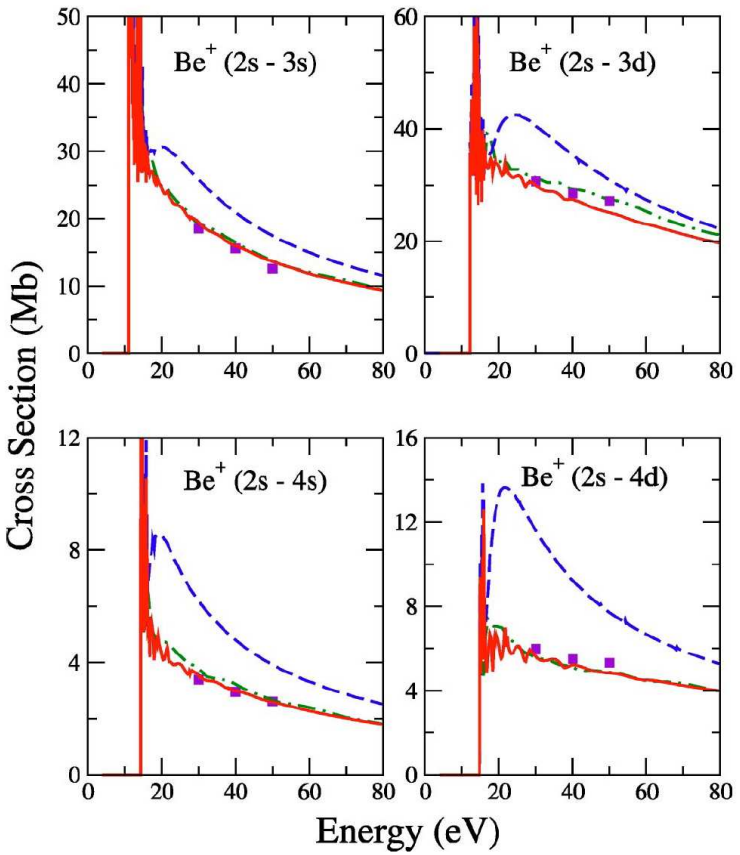

FIG. 5. Electron-impact excitation cross sections from the $2s$ ground term of Be^+ to the ns and nd excited terms. Dashed curves are from the present 14-term R-matrix calculation; solid curves are from the present 49-term RMPS calculation; solid squares are from the present TDCC calculation; dot-dashed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

e-Be: coupling to continuum most important for
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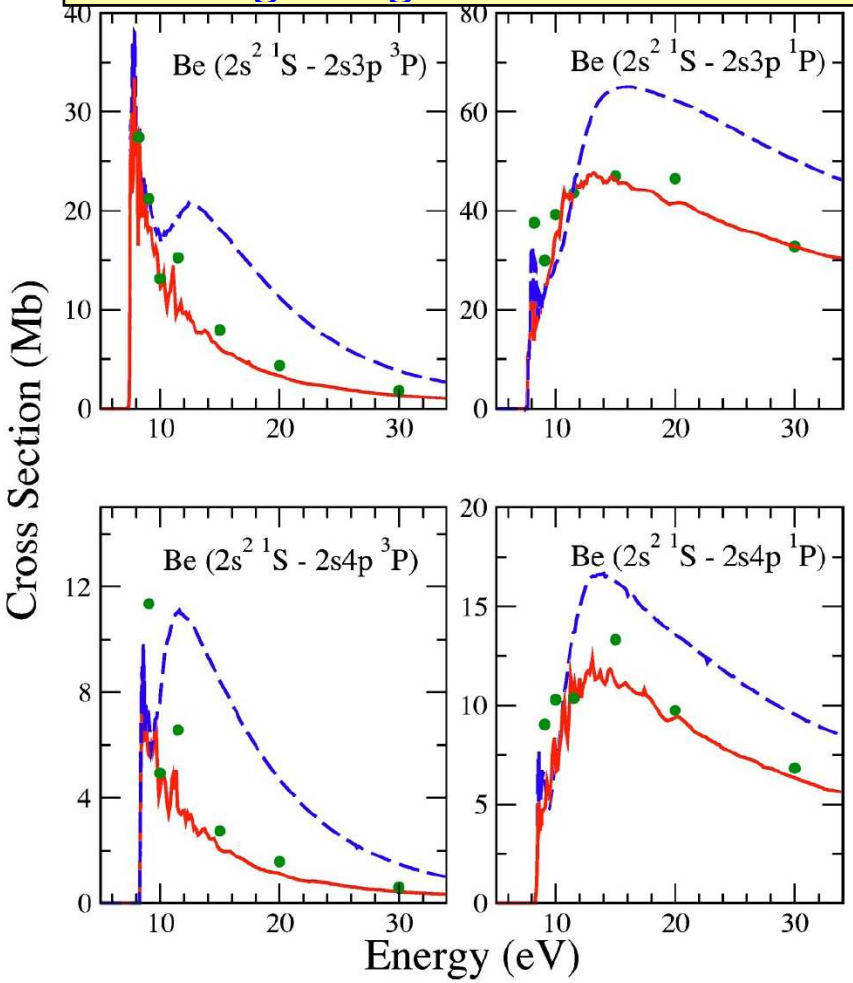


FIG. 2. Electron-impact excitation cross sections from the $2s^2\,{}^1S$ ground term of Be to the $2snp\,{}^3P$ and $2snp\,{}^1P$ excited terms for $n=3$ and 4. Dashed curves are from the present 29-term R-matrix calculation; solid curves are from the present 280-term RMPS calculation; solid circles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

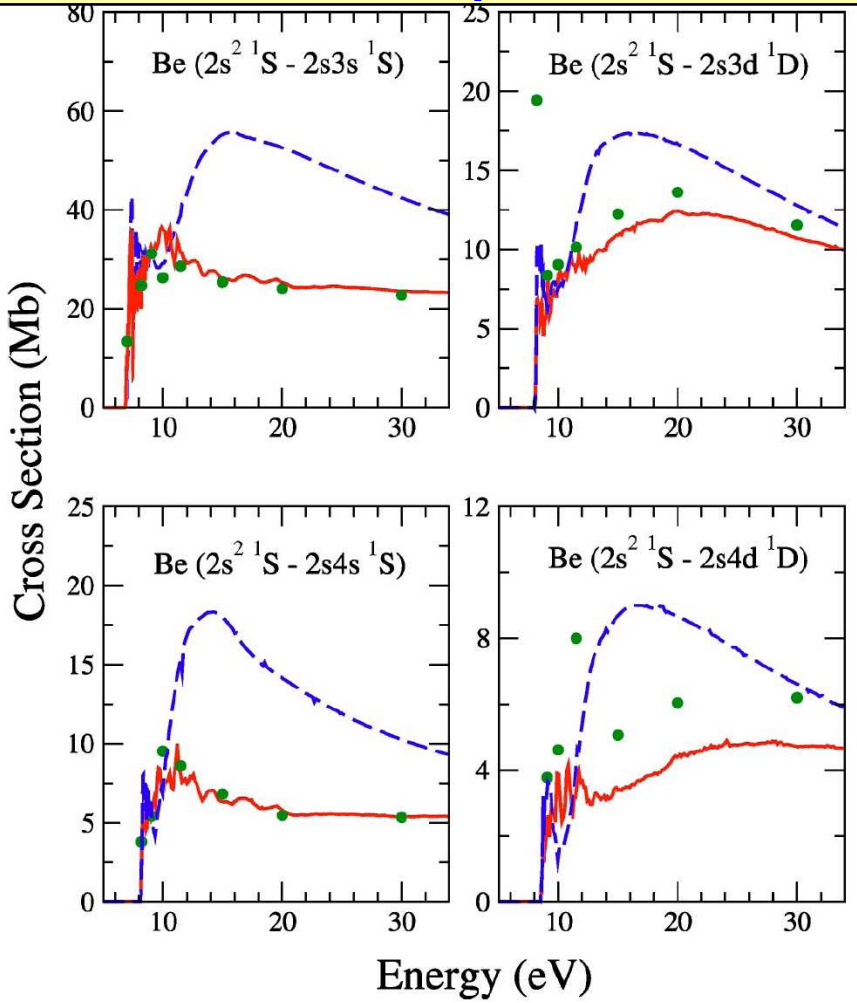
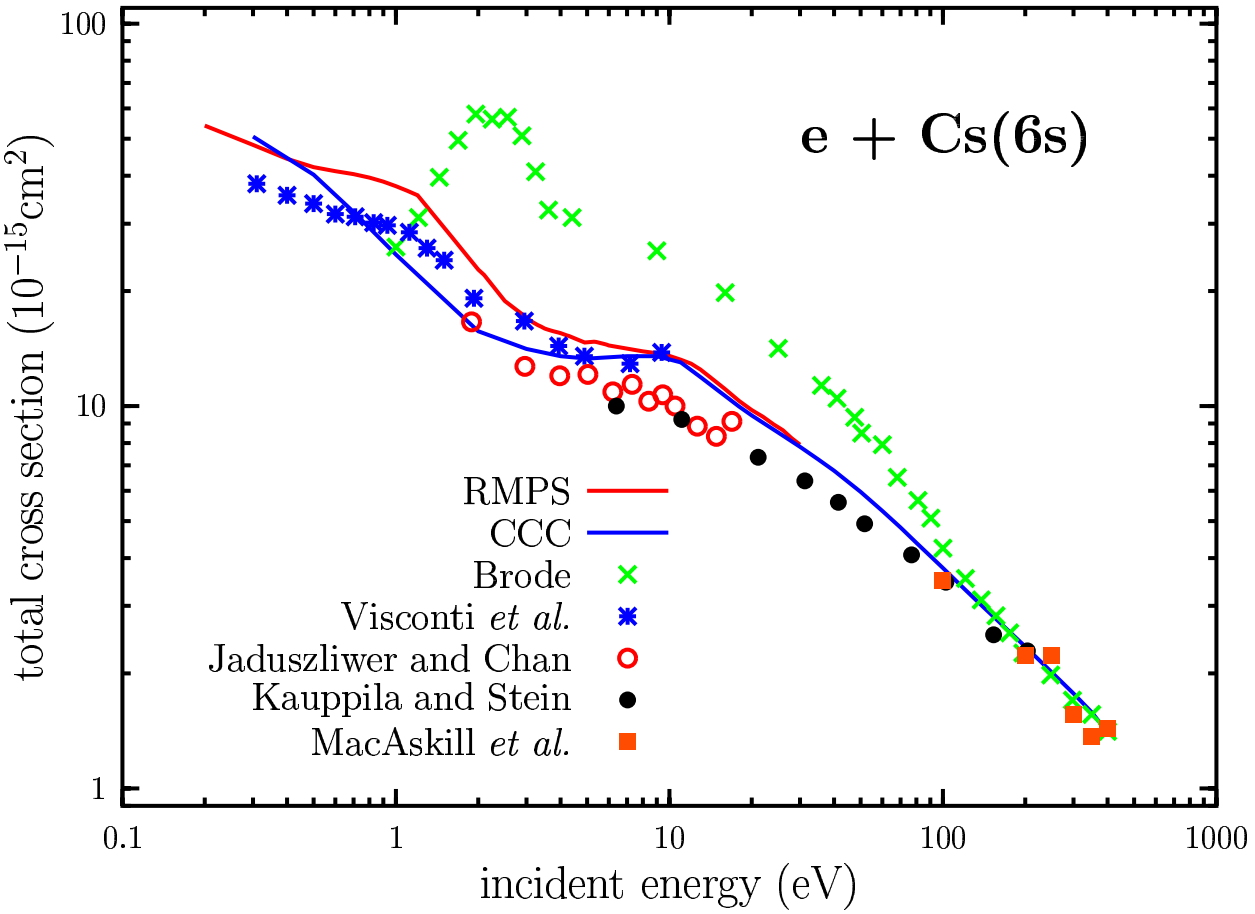


FIG. 3. Electron-impact excitation cross sections from the $2s^2\,{}^1S$ ground term of Be to the $2sns\,{}^1S$ and $2snd\,{}^1D$ excited terms. Dashed curves are from the present 29-term R-matrix calculation; solid curves are from the present 280-term RMPS calculation; solid circles are from CCC calculations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

Electron Collisions with Cs Atoms

Theories: semi-relativistic RMPS (Bartschat & Fang)
non-relativistic CCC (Bray)



- **While there are still some differences between the RMPS and CCC results for energies below ≈ 10 eV, the accuracy of the theoretical predictions is certainly comparable to that of experiment.**
- **The maximum in the Brode data is not confirmed by either theory nor by any of the other experimental results.**

PHYSICAL REVIEW A **74**, 032708 (2006)

Electron-impact ionization cross sections out of the ground and 6 ^2P excited states of cesium

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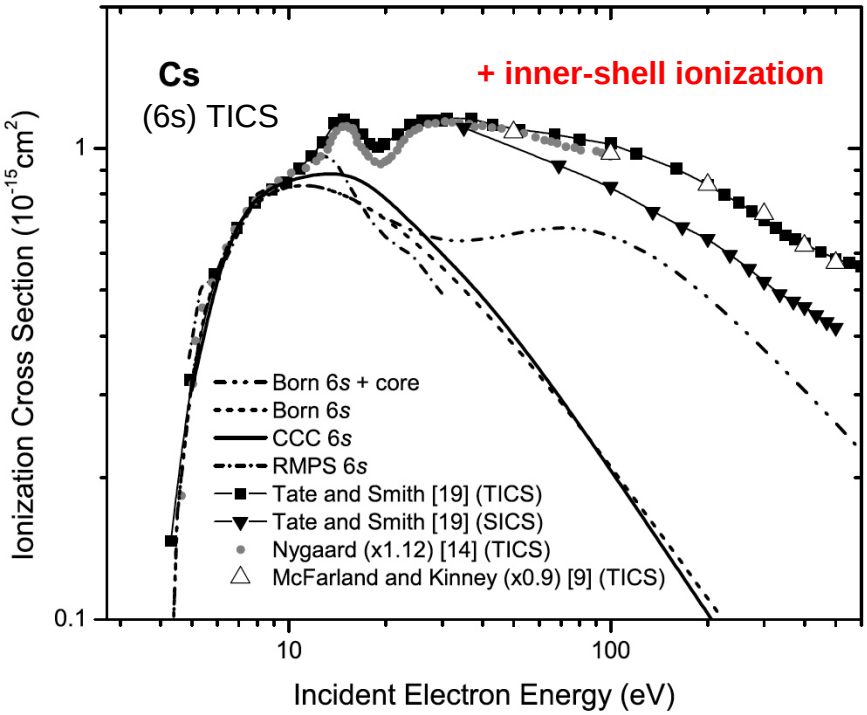


FIG. 4. Experimental TICS from the Cs ground state, rescaled to CCC and RMPS calculated SICS between 4–10 eV, as discussed in the text. The Born SICS also show the contribution from 5*p* and 5*s* core ionization, with calculated threshold energies of 22.9 and 38.0 eV, respectively. Tate and Smith's [19] rescaled SICS is also shown, indicating the contribution to the TICS from multiple ionization.

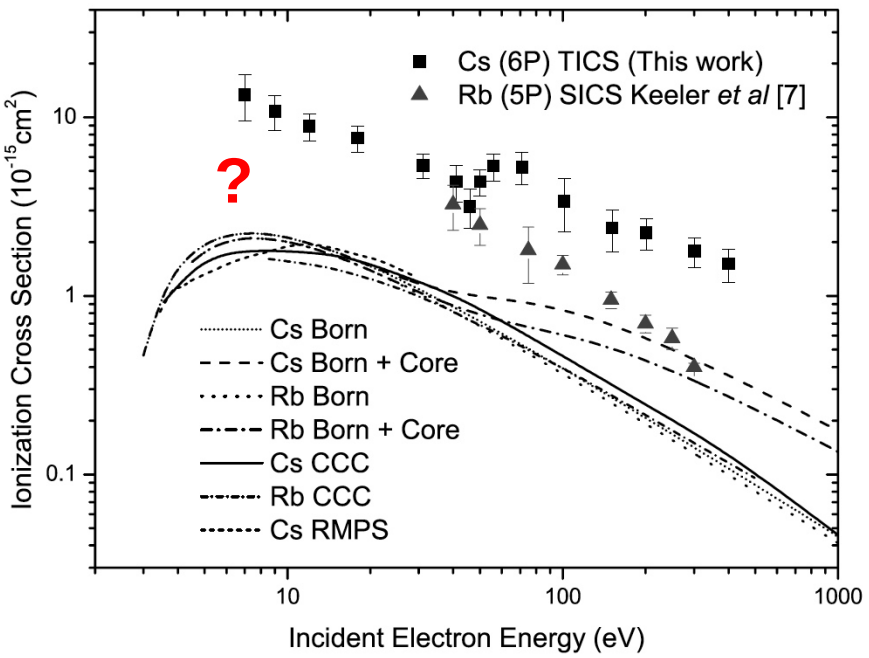
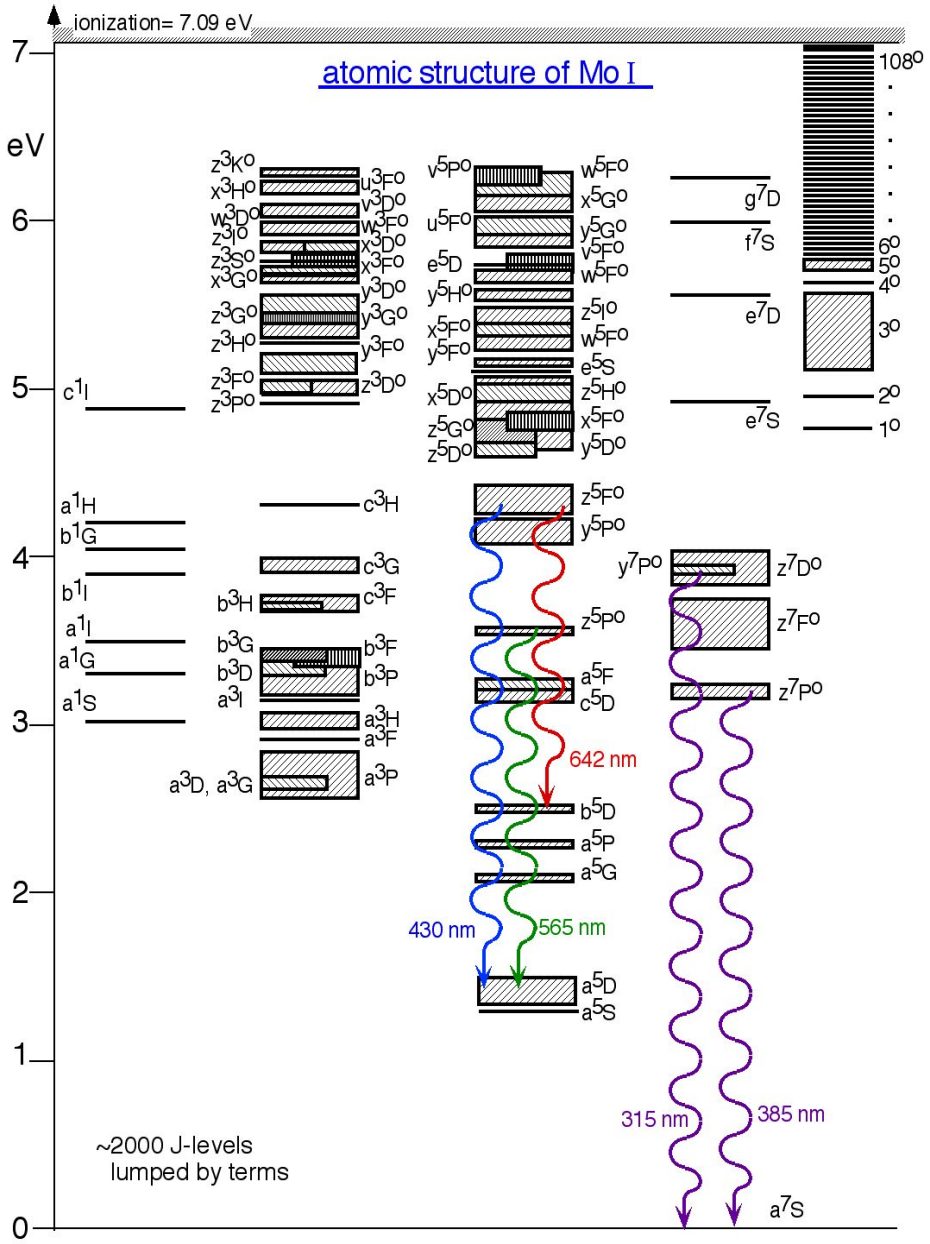


FIG. 6. The measured TICS out of the Cs 6 $^2P_{3/2}$ state compared to SICS from CCC, RMPS and Born calculations. For comparison, the results of our CCC, and Born SICS calculations for Rb 5 ^2P state are also compared to the SICS data of Keeler *et al.* [7].

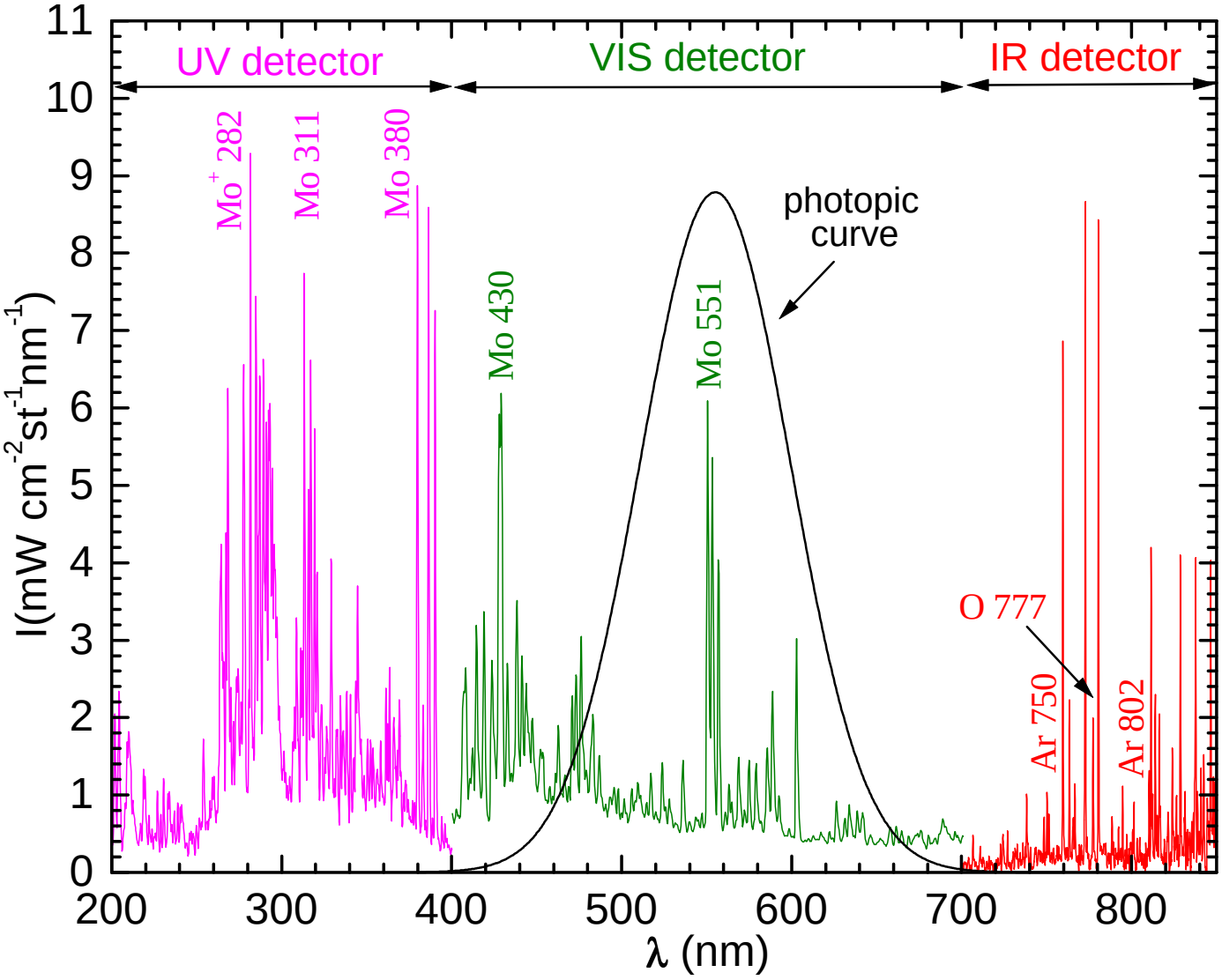
We cannot account for the large discrepancy between theory and experiment below the autoionization onset at ~11 eV; i.e., the energy region where comparison is justifiable. We are not aware of any inherent energy-dependent systematic error in the experiment.

A Grand Challenge: Electron Collisions with Molybdenum



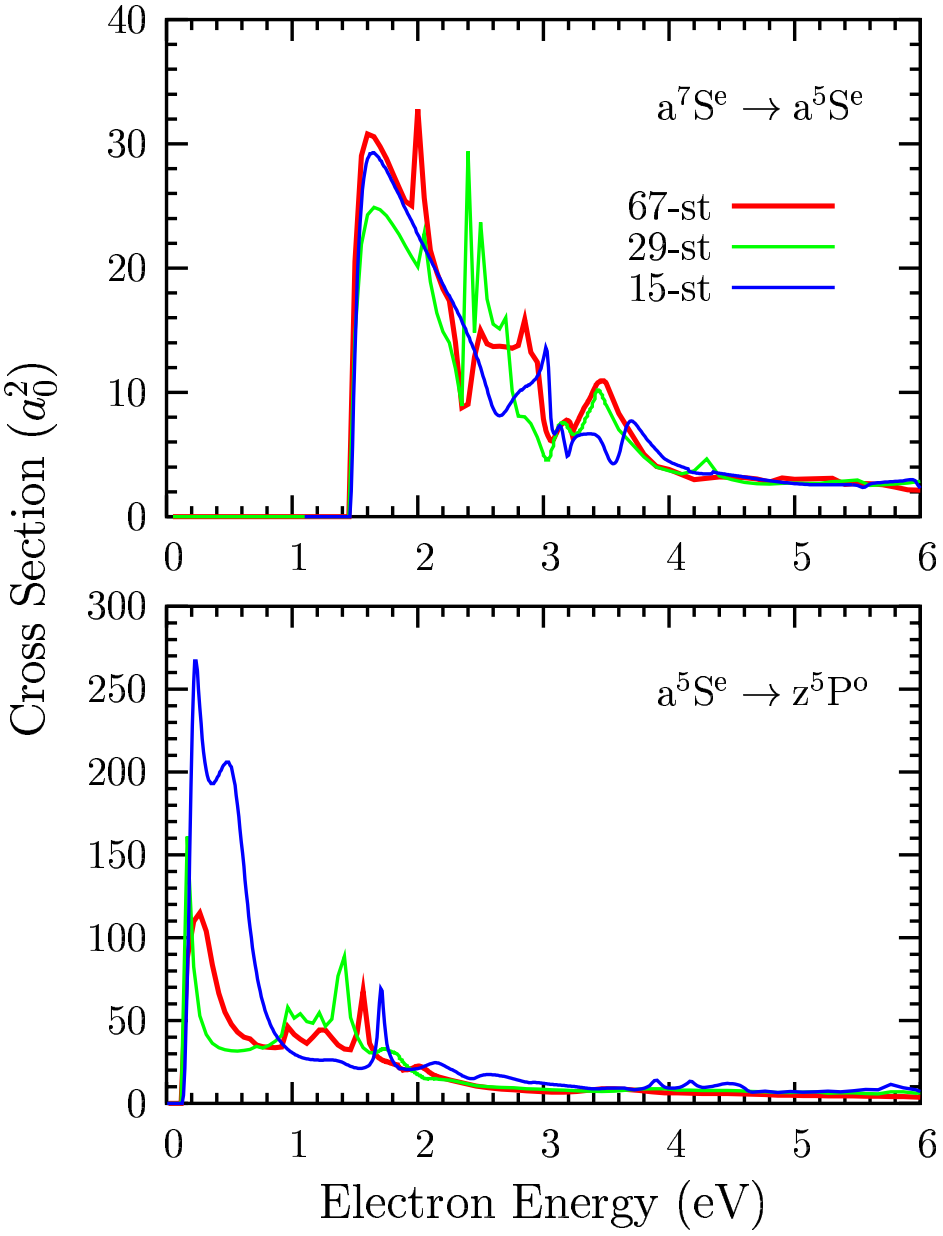
Spectrum from a Moly-Oxide Lamp

Petrov, Giuliani, Dasgupta, Bartschat and Pechacek, J. of Appl. Phys, 95 (2004) 5284



R-matrix Results for Electron Collisions with Molybdenum

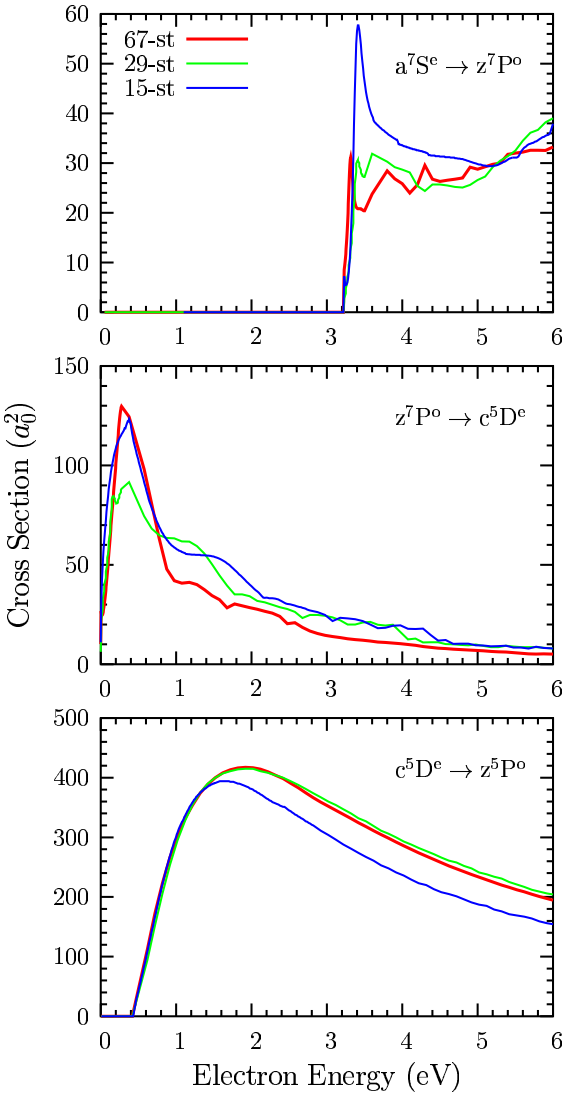
K. Bartschat, A. Dasgupta, and J.L. Giuliani, J. Phys. B 35 (2002) 2899

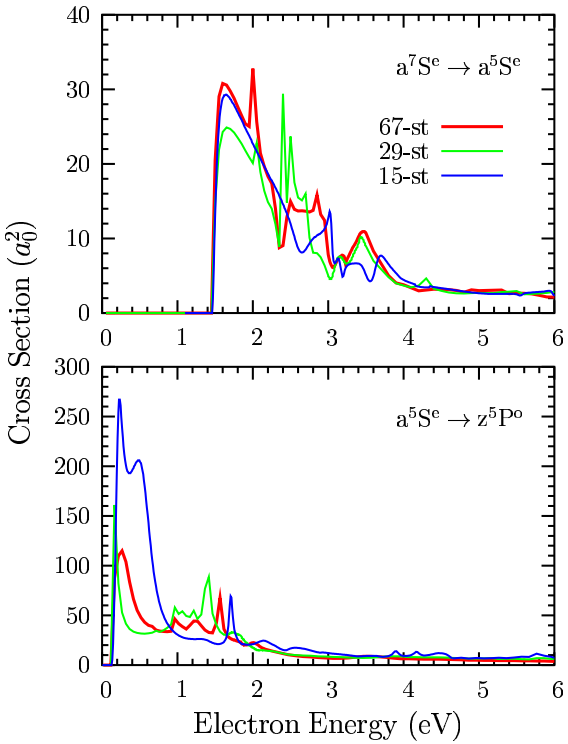


67-state R-matrix (close-coupling)

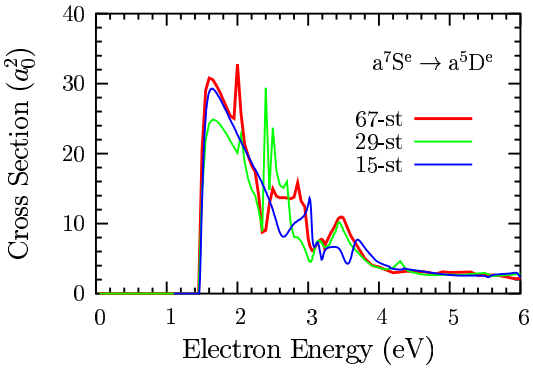
R-matrix Results for Electron Collisions with Molybdenum

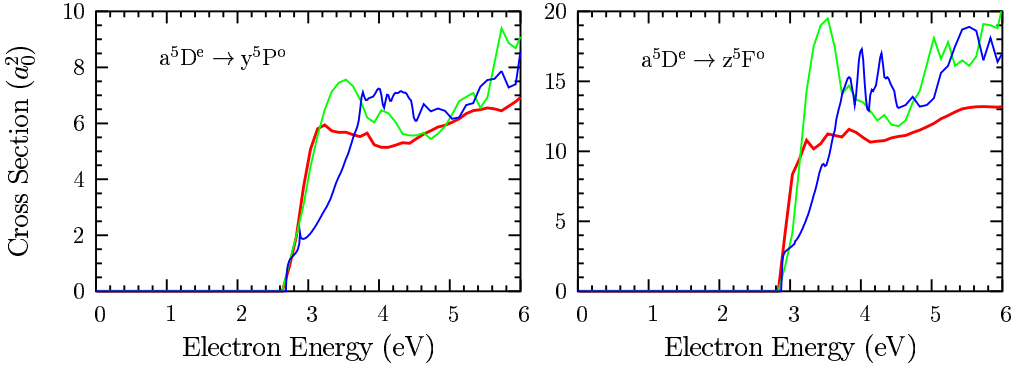
K. Bartschat, A. Dasgupta, and J.L. Giuliani, J. Phys. B 35 (2002) 2899





67-state R-matrix (close-coupling)

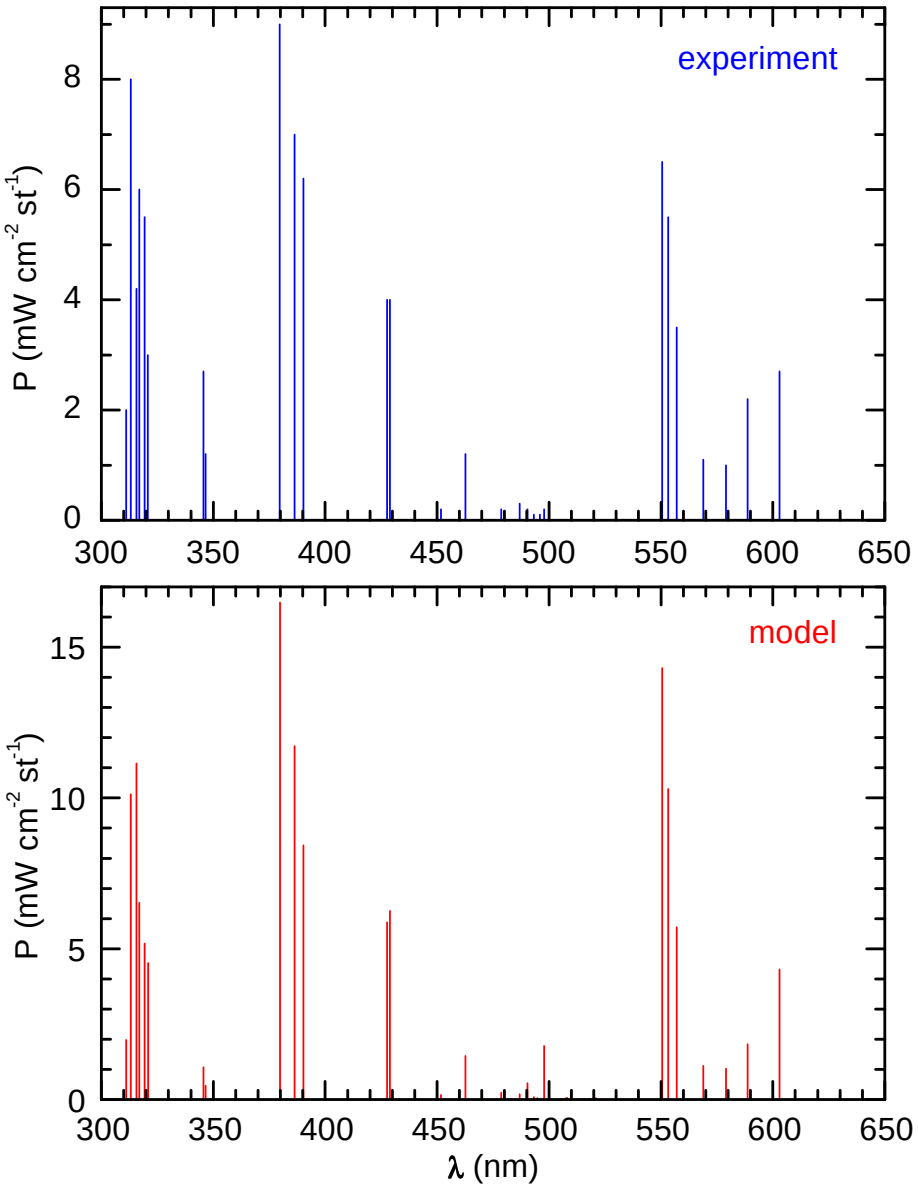




Does theory have any chance?

Moly-Lines from a Moly-Oxide Lamp

Petrov, Giuliani, Dasgupta, Bartschat and Pechacek, J. of Appl. Phys, 95 (2004) 5284
Bartschat, Dasgupta, Petrov and Giuliani, New Journal of Physics 6 (2004) 145



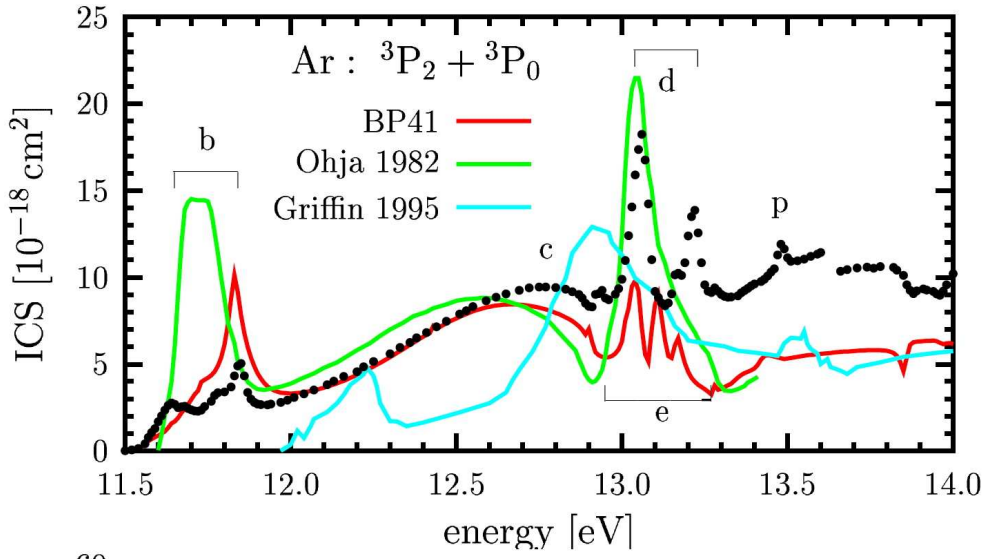
YES!

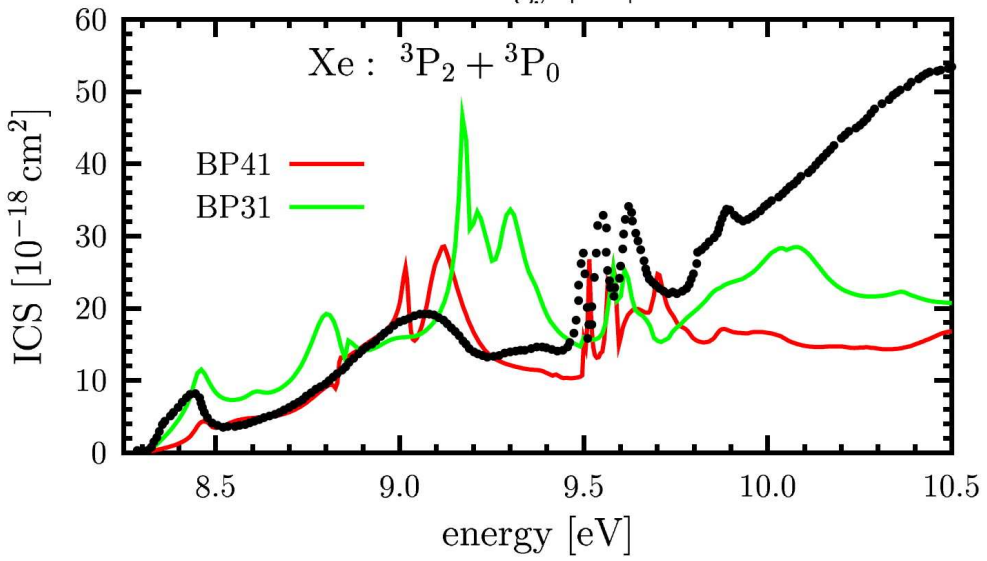
Metastable Production in Electron Collisions with Ar and Xe

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





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

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

Theory:

Dasgupta/Madison (DW)

Bartschat/Grum-Grzhimailo (BPRM)

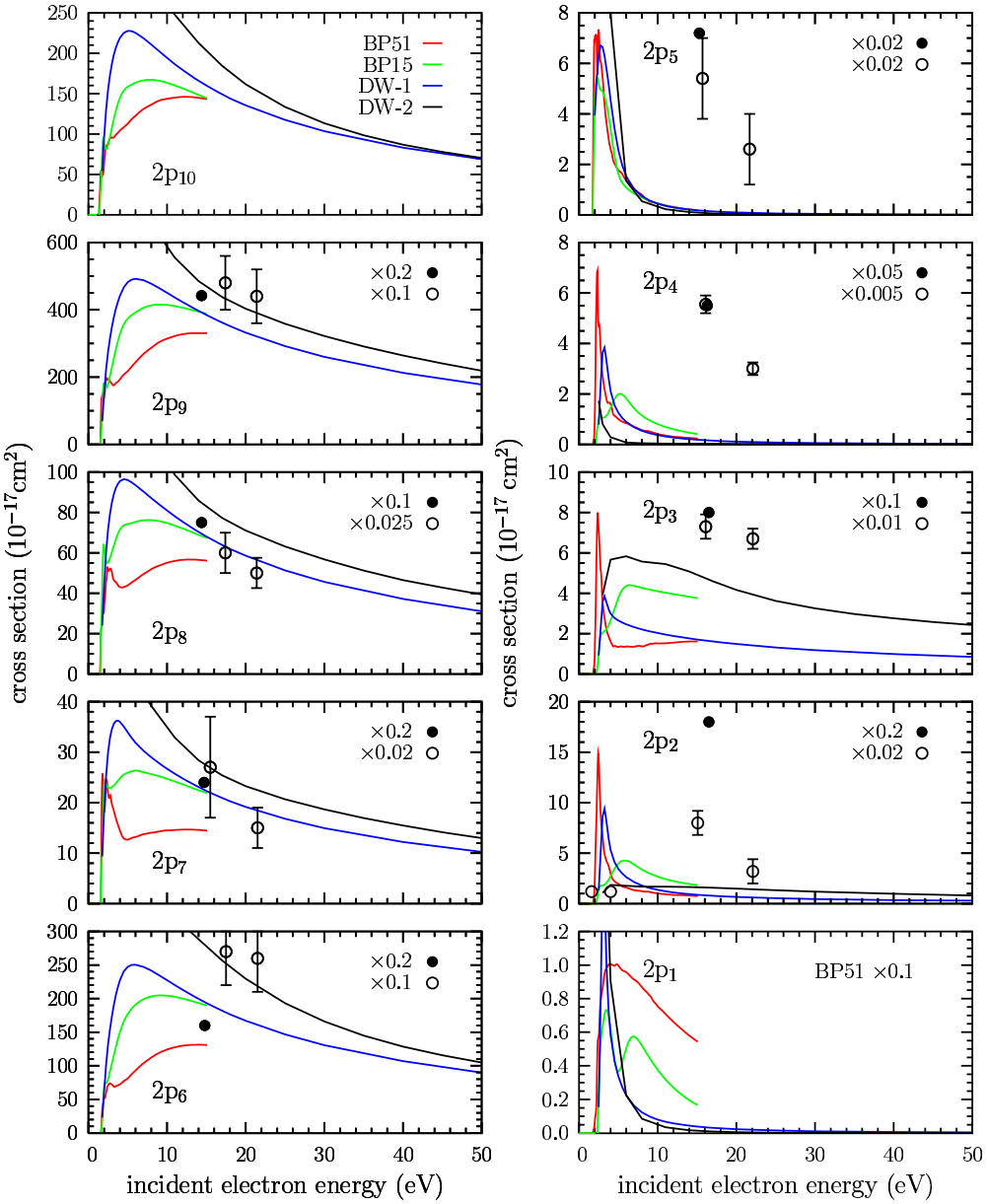
Experiment:

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!



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

History of the Belfast R-matrix program

R-matrix technique

First implementation to atoms - Burke *et al.* (1971), Burke and Robb (1975)

Enormous amount of calculations - Burke and Berrington (1993)

Set of programs:

RMATRX–I: Berrington *et al.* (1995)

RMATRX–II: non-relativistic, with 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

One of the principal ingredients of the above-mentioned programs is the usage of a single set of orthogonal one-electron orbitals.

Major problems

i) the difficulties in describing all target states of interest for a given calculation to sufficient accuracy

ii) the likely occurrence of unphysical structures, so-called "pseudo-resonances", when an attempt is made to address the former problem

iii) numerical difficulties due to an ill-conditioned orthogonalization procedure and the need to modify the so-called "Buttle correction".

New general R-matrix program BSR

Key Ideas

close-coupling expansion

- use **B-spline** functions as universal basis set to represent the continuum orbitals
- allow for **non-orthogonal orbitals** to represent both bound and continuum radial functions

R-matrix basis functions ($\Gamma \equiv \alpha LSM_L M_S \pi$) :

$$\Psi_k^\Gamma(x_1,\ldots,x_{N+1}) = \mathrm{A}\sum_{ij}\overline{\Phi}_i^\Gamma(x_1,\ldots,x_N;\boldsymbol{r}_{N+1}\sigma_{N+1})r_{N+1}^{-1}u_j(r_{N+1})a_{ijk}^\Gamma + \sum_i \chi_i^\Gamma(x_1,\ldots,x_{N+1})b_{ik}^\Gamma$$

$$u_j(r) = \sum_m c_{im}B_m(r), \qquad 0 < r < a$$

Orthogonality conditions on the one-electron radial functions

Target states: $\Phi_i = \sum_{j=1}^{m} c_{ij}\phi_j, \qquad \phi_j \rightarrow \{P_{nl}\}$

P_{nl} – physical (spectroscopic) orbitals;

$\underline{P}_{nl}$ – correlated or pseudo-orbitals (to improve the target eigenstates; to represent the pseudo-states)

$\langle P_{nl}|P_{n'l}\rangle = 0$

$\langle P_{nl}|u_{kl}\rangle = 0$

difficult to achieve accurate target representation (term-dependence, relaxation effects, correlation)

large (N+1)-electron expansions; pseudo-resonances;

$$\chi_i^\Gamma(x_1,\ldots,x_{N+1}) = A\{\phi_i(x_1,\ldots,x_N)\times P_{nl}(r_{N+1})\}$$

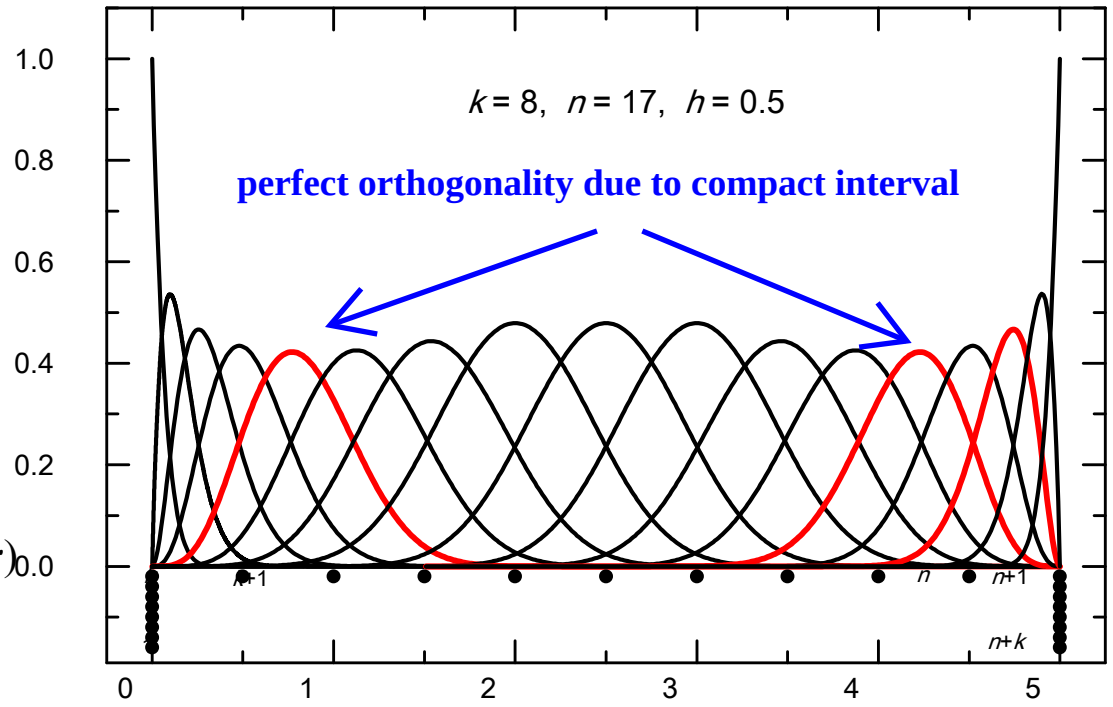
B-splines

$[0,R] \rightarrow [t_i], \quad i = 1,2,\ldots,n+k,$

$t_1=t_2=\ldots=t_k, \quad t_{n+1}=t_{n+2}=\ldots=t_{n+k}$

$$B_{i,1} = \begin{cases} 1, & t_i \le r \le t_{i+1} \\ 0, & \text{otherwise} \end{cases}$$

$$B_{i,k}(r) = \frac{r-t_i}{t_{i+k-1}-t_i} B_{i,k-1}(r) + \frac{t_{i+k}-r}{t_{i+k}-t_{i+1}} B_{i+1,k-1}(r)$$



Advantages of B-splines

- **Excellent numerical properties**; machine accuracy with Gaussian quadratures; flexibility in the choice of radial grid; avoid finite-difference algorithms; banded structure; established **Linear Algebra packages** available

- Effective **completeness** of B-spline basis – no Buttle correction required.

— First B-spline R-matrix calculation: e–H (van der Hart, 1997)

— Recent exponential growth of B-spline applications; see Bachau *et al.*, Rep. Prog. Phys. **64** (2001) 1815

The BSR program

Present implementation

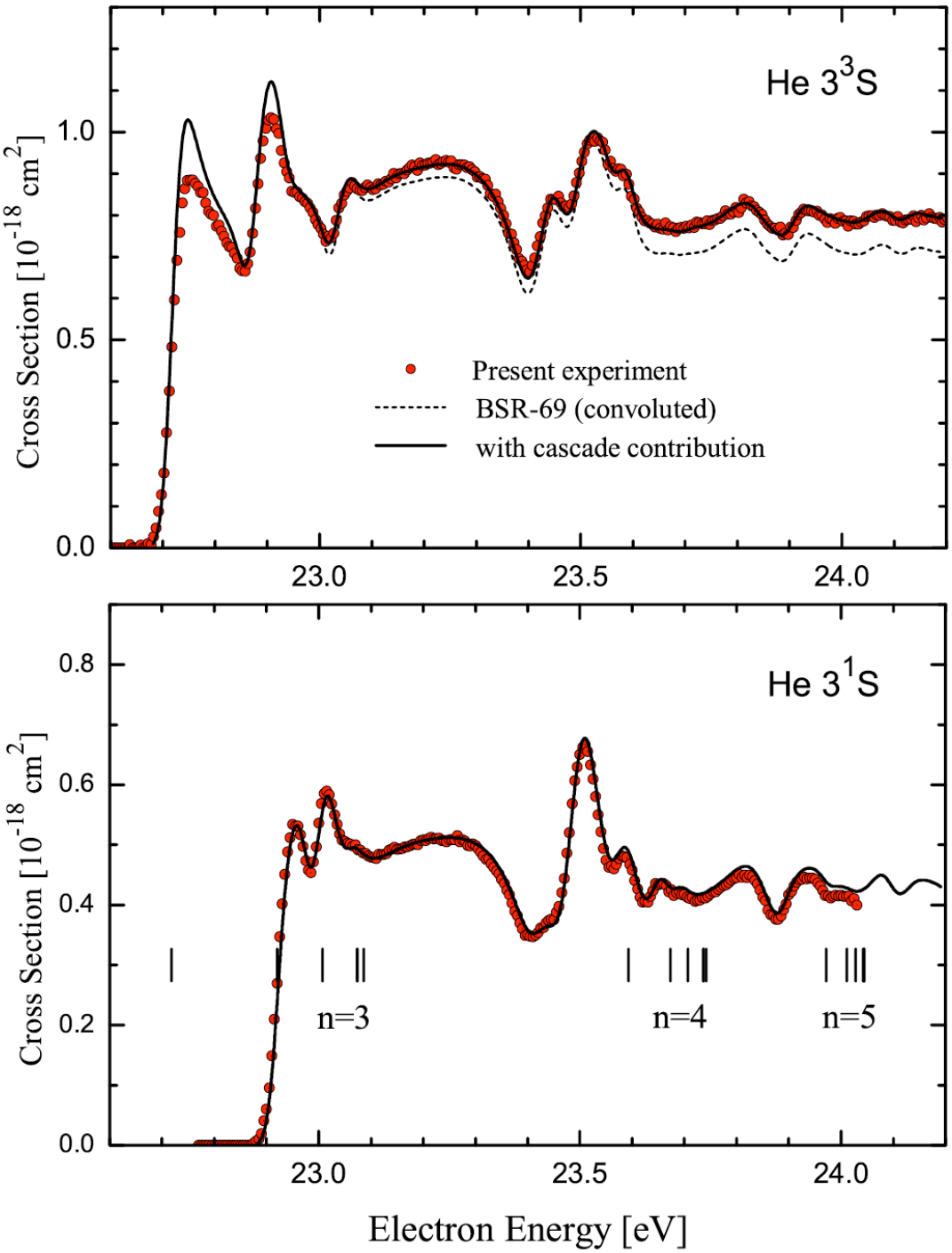
- based on general programs for angular integration with non-orthogonal orbitals (BREIT_NO, Zatsarinny and Froese Fischer 1999)
- abandon orthogonality constraints; **restricted orthogonality** of $u_{kl}(r)$ to closed-shell core orbitals
- independent generation of different target states allows for an **accurate target description** through direct account for **term dependence in one-electron orbitals**
- no (N+1)-electron terms in the close-coupling expansion yields consistent treatment of N-electron target and (N+1)-electron collision problems; **pseudo-resonance structure is greatly reduced**
- Outer region: FARM (Burke & Noble 1995), STGF (Seaton 1985, Badnell 1999)

Difficulties

- Setting up the Hamiltonian matrix can be very complicated and lengthy.
- Generalized eigenvalue problem needs to be solved ($H\Psi = E\ S\ \Psi$).
- Matrix size is typically big (~10,000) due to large size of B-spline basis (50-100).

Resonances in e–He collisions (excitation of $3^{3,1}S$)

(from Stepanovic *et al.*, J. Phys. B 39 (2006) 1547)



Computational model for e-Ne collisions

[Zatsarinny and Bartschat, *J. Phys. B* **37** 2173 (2004)]

Problems:

- strong term dependence of the valence orbitals
- we need to include relativistic effects due to fine-structure splitting of the Ne^+ core
- simultaneous importance of channel-coupling effects

Target states $2p^6$, $2p^5nl$ were generated as various sets of non-orthogonal state-dependent valence ***nl*** orbitals using a B-spline box-based close-coupling method, with expansion:

$$\Phi(2s^2 2p^5 nl, J) = A\sum_{i,LS}\{\phi(2s^2 2p^5)P(n_i l_i)\}^{LSJ} + A\sum_{j,LS}\{\phi(2s2p^6)P(n_j l_j)\}^{LSJ}$$
$$+ \sum_{i,j,LS}\chi(2s^2 2p^4 \bar{n}_i l_i \bar{n}_j l_i, LSJ) + \sum_{i,j,LS}\chi(2s2p^5 \bar{n}_i l_i \bar{n}_j l_i, LSJ)$$

- The Hamiltonian to be diagonalized was chosen as $\boldsymbol{H_{BP} = H_{NR} + H_{mass} + H_{D1} + H_{SO} + H_{SOO}}$
- Theoretical binding energies differed from experiment by no more than 30 meV

Scattering model:

- Close-coupling expansion included 31 states in the *jK* coupling scheme, with configurations $2p^6$, $2p^5 3s$, $2p^5 3p$, $2p^5 3d$, and $2p^5 4s$.
- + $2p^5\underline{4d}$ and $2p^5\underline{5s}$ ^1P pseudostates reproduced polarizability of the ground state.
- (N+1)-electron terms in the R-matrix expansion were avoided completely.
- The largest number of coupled channels was 126, resulting (with $N_s = 96$) in matrix dimension of nearly 10,000 in the generalized eigenvalue problem. Such calculations can still be performed on a fast desktop PC with 2 Gb of RAM.

Energy Levels in Ne

Table 1. Calculated and observed energy levels for the lowest 31 states of neon.

State	Theory [a.u.]	Experiment [eV]	Difference [eV]
$(2p^6)^1S_0$	−128.7454364	0	−0.091
$3s[3/2]_2$	−128.1309482	16.619	0.011
$3s[3/2]_1$	−128.1289358	16.671	0.014
$3s'[1/2]_0$	−128.1272471	16.715	0.016
$3s'[1/2]_1$	−128.1217922	16.848	0.031
$3p[1/2]_1$	−128.0654904	18.382	0.030
$3p[5/2]_3$	−128.0596727	18.555	0.015
$3p[5/2]_2$	−128.0589268	18.576	0.014
$3p[3/2]_1$	−128.0574642	18.613	0.017
$3p[3/2]_2$	−128.0566791	18.637	0.014
$3p'[3/2]_1$	−128.0543692	18.693	0.021
$3p'[3/2]_2$	−128.0540267	18.704	0.019
$3p[3/2]_0$	−128.0536576	18.711	0.022
$3p'[1/2]_1$	−128.0530935	18.726	0.022
$3p'[1/2]_0$	−128.0437159	18.966	0.038
$4s[3/2]_2$	−128.0196244	19.664	−0.004
$4s[3/2]_1$	−128.0187096	19.688	−0.004
$4s'[1/2]_0$	−128.0159254	19.761	0
$4s'[1/2]_1$	−128.0152029	19.780	0
$3d[1/2]_0$	−128.0063773	20.025	−0.005
$3d[1/2]_1$	−128.0063083	20.026	−0.005
$3d[7/2]_4$	−128.0060234	20.035	−0.005
$3d[7/2]_3$	−128.0060055	20.035	−0.005
$3d[3/2]_2$	−128.0059251	20.037	−0.004
$3d[3/2]_1$	−128.0057907	20.040	−0.004
$3d[5/2]_2$	−128.0055058	20.048	−0.004
$3d[5/2]_3$	−128.0055022	20.048	−0.005
$3d'[5/2]_1$	−128.0021312	20.136	−0.001
$3d'[5/2]_3$	−128.0021214	20.136	0
$3d'[3/2]_2$	−128.0020691	20.138	0
$3d'[3/2]_1$	−128.0019986	20.139	0

Oscillator Strengths in Ne

Table 2. Calculated and observed oscillator strengths for selected transitions in neon. The subscripts L and V denote the length and velocity forms, respectively.

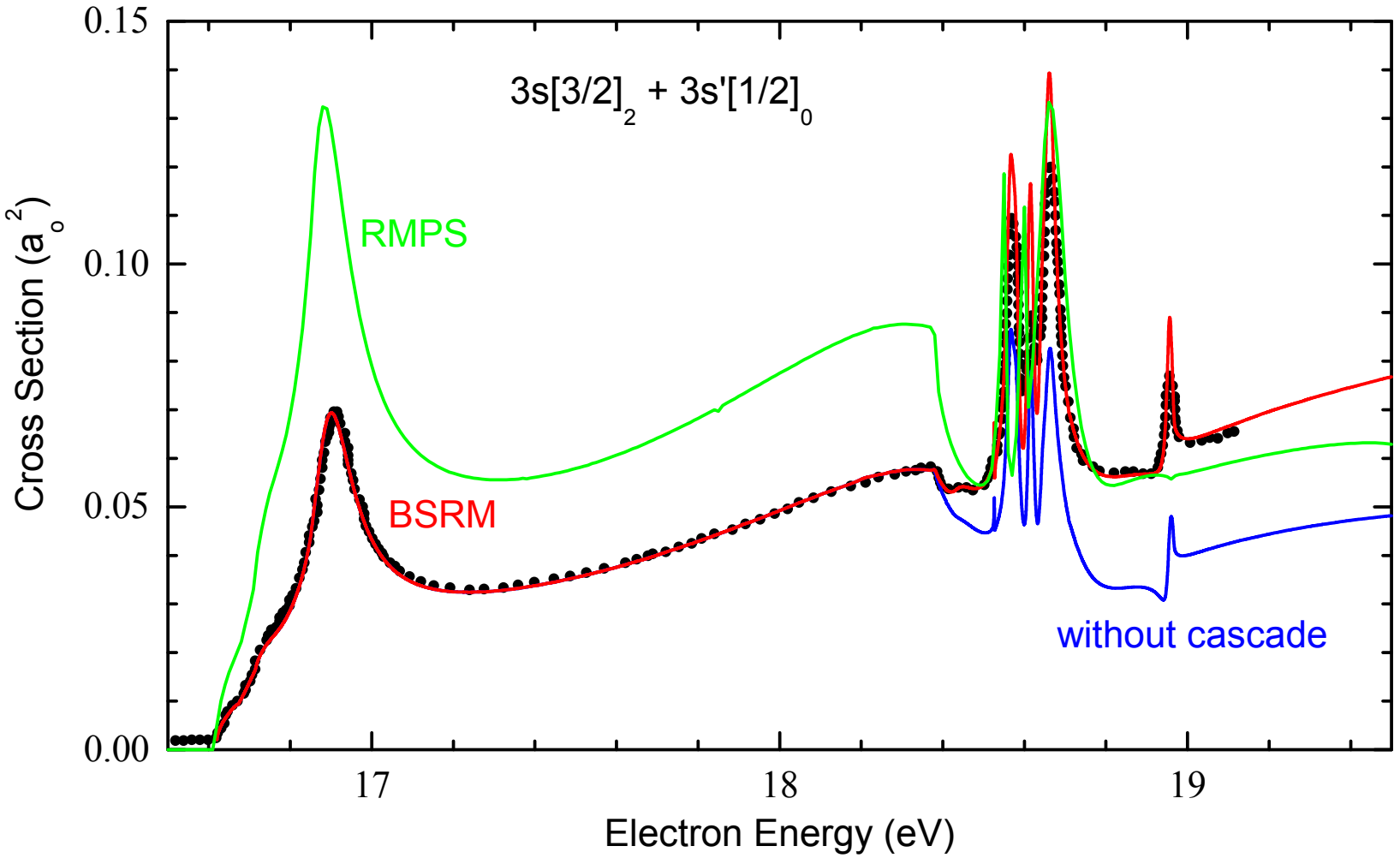
Initial	Final	f_L	f_V	NIST	del Val *et al* (2000)	Seaton (1998)
$(2p6)^1S_0$	$3s[3/2]_1$	1.14E-2	1.02E-2	1.18E-2		1.26E-2
$(2p6)^1S_0$	$3s'[1/2]_1$	1.65E-1	1.48E-1	1.49E-1		1.68E-1
$(2p6)^1S_0$	$4s[3/2]_1$	1.42E-2	1.29E-2	8.6E-3		
$(2p6)^1S_0$	$4s'[1/2]_1$	1.78E-2	1.62E-2	1.3E-2		
$(2p6)^1S_0$	$3d[1/2]_1$	4.01E-3	5.16E-3	5.7E-3		5.58E-3
$(2p6)^1S_0$	$3d[3/2]_1$	1.22E-2	1.56E-2	1.6E-2		1.67E-2
$(2p6)^1S_0$	$3d'[3/2]_1$	5.96E-3	7.64E-3	6.5E-3		8.59E-3
$3s[3/2]_2$	$3p[1/2]_1$	1.24E-1	1.37E-1	1.13E-1	1.13E-1	1.10E-1
$3s[3/2]_2$	$3p[3/2]_1$	2.21E-2	2.21E-2	2.22E-2	2.33E-2	2.12E-2
$3s[3/2]_2$	$3p'[3/2]_1$	1.05E-2	1.12E-2			1.06E-2
$3s[3/2]_2$	$3p'[1/2]_1$	3.40E-2	3.44E-2			3.42E-2
$3s[3/2]_2$	$3p[5/2]_2$	9.38E-2	9.05E-2	9.69E-2	9.62E-2	9.68E-2
$3s[3/2]_2$	$3p[3/2]_2$	1.67E-1	1.70E-1	1.6E-1	1.64E-1	1.58E-1
$3s[3/2]_2$	$3p'[3/2]_2$	6.50E-2	6.98E-2	5.99E-2	5.40E-2	5.80E-2
$3s[3/2]_2$	$3p[5/2]_3$	4.54E-1	4.29E-1			4.28E-1
$3s[3/2]_1$	$3p[3/2]_0$	1.09E-1	1.12E-1	1.11E-1	1.06E-1	1.05E-1
$3s[3/2]_1$	$3p'[1/2]_0$	1.05E-3	9.52E-4			9.70E-4
$3s[3/2]_1$	$3p[1/2]_1$	8.18E-2	9.20E-2	7.36E-2	7.40E-2	7.37E-2
$3s[3/2]_1$	$3p[3/2]_1$	2.02E-1	1.96E-1	1.96E-1	2.24E-1	1.94E-2
$3s[3/2]_1$	$3p'[3/2]_1$	2.78E-3	3.56E-3			3.73E-3
$3s[3/2]_1$	$3p'[1/2]_1$	3.35E-2	3.59E-2	3.06E-2	2.94E-2	2.86E-2
$3s[3/2]_1$	$3p[5/2]_2$	3.27E-1	3.08E-1	3.18E-1	3.17E-1	3.09E-1
$3s[3/2]_1$	$3p[3/2]_2$	2.64E-2	2.86E-2	4.37E-2	4.57E-2	4.2E-2
$3s[3/2]_1$	$3p'[3/2]_2$	1.87E-1	1.87E-1	1.68E-1	1.63E-1	1.63E-1
$3s'[1/2]_0$	$3p[1/2]_1$	6.29E-2	7.19E-2	5.75E-2	6.70E-2	5.75E-2
$3s'[1/2]_0$	$3p[3/2]_1$	2.05E-1	1.87E-1	2.07E-1	2.13E-1	1.91E-1
$3s'[1/2]_0$	$3p'[3/2]_1$	4.44E-1	4.37E-1	4.4E-1	4.63E-1	4.27E-1
$3s'[1/2]_0$	$3p'[1/2]_1$	2.58E-1	2.69E-1	2.5E-1	2.55E-1	2.42E-1
$3s'[1/2]_1$	$3p[3/2]_0$	5.69E-4	6.6E-4			8.07E-4
$3s'[1/2]_1$	$3p'[1/2]_0$	1.21E-1	1.19E-1			1.08E-1
$3s'[1/2]_1$	$3p[1/2]_1$	7.53E-4	1.05E-3			1.01E-3
$3s'[1/2]_1$	$3p[3/2]_1$	1.73E-2	1.76E-2	1.4E-2	1.60E-2	1.48E-2
$3s'[1/2]_1$	$3p'[1/2]_1$	1.49E-1	1.50E-1	1.52E-1	1.56E-1	1.47E-1
$3s'[1/2]_1$	$3p'[3/2]_1$	1.57E-1	1.54E-1	1.47E-1	1.57E-1	1.47E-1
$3s'[1/2]_1$	$3p[3/2]_2$	2.36E-1	2.24E-1	2.09E-1	2.22E-1	2.11E-1
$3s'[1/2]_1$	$3p[5/2]_2$	5.61E-2	5.44E-2	3.69E-2	4.24E-2	3.93E-2
$3s'[1/2]_1$	$3p'[3/2]_2$	2.47E-1	2.39E-1			2.59E-1

Metastable yield in e-Ne collisions

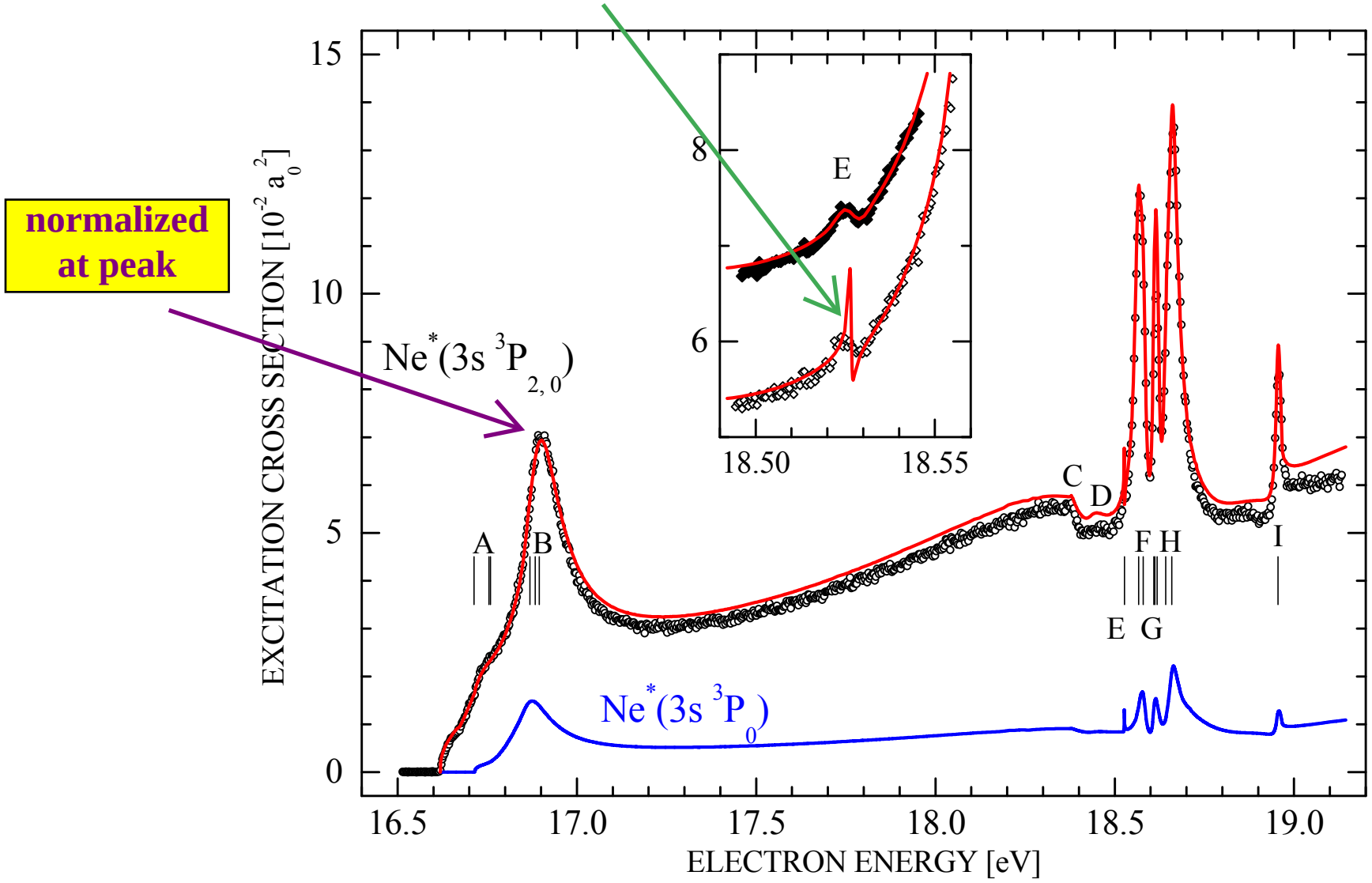
Experiment: Buckman *et al.* (1983) [x 0.78]

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

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

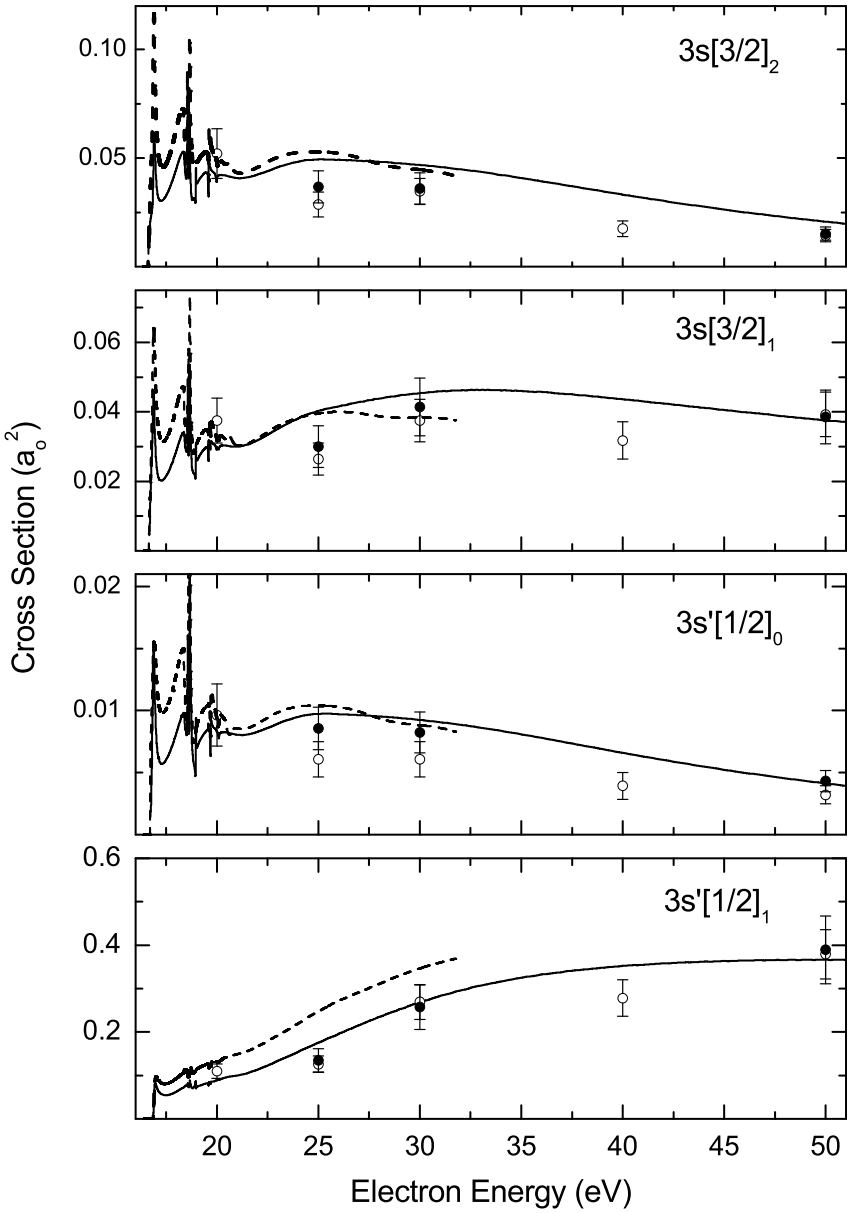


position of resonance predicted to 1 meV accuracy !!!



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)

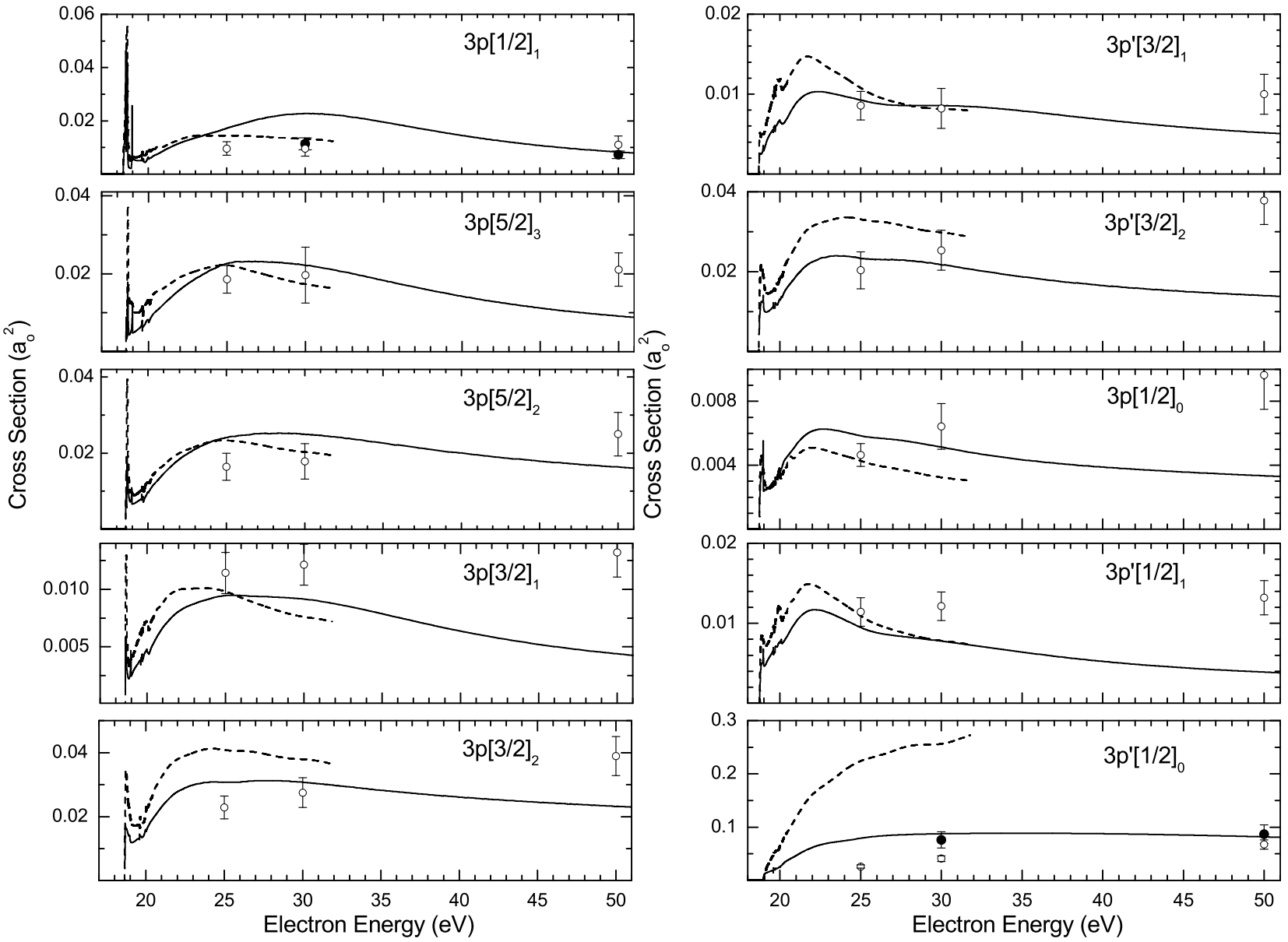
Electron-Impact Excitation of Ne ($2p^5 3s$)



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?

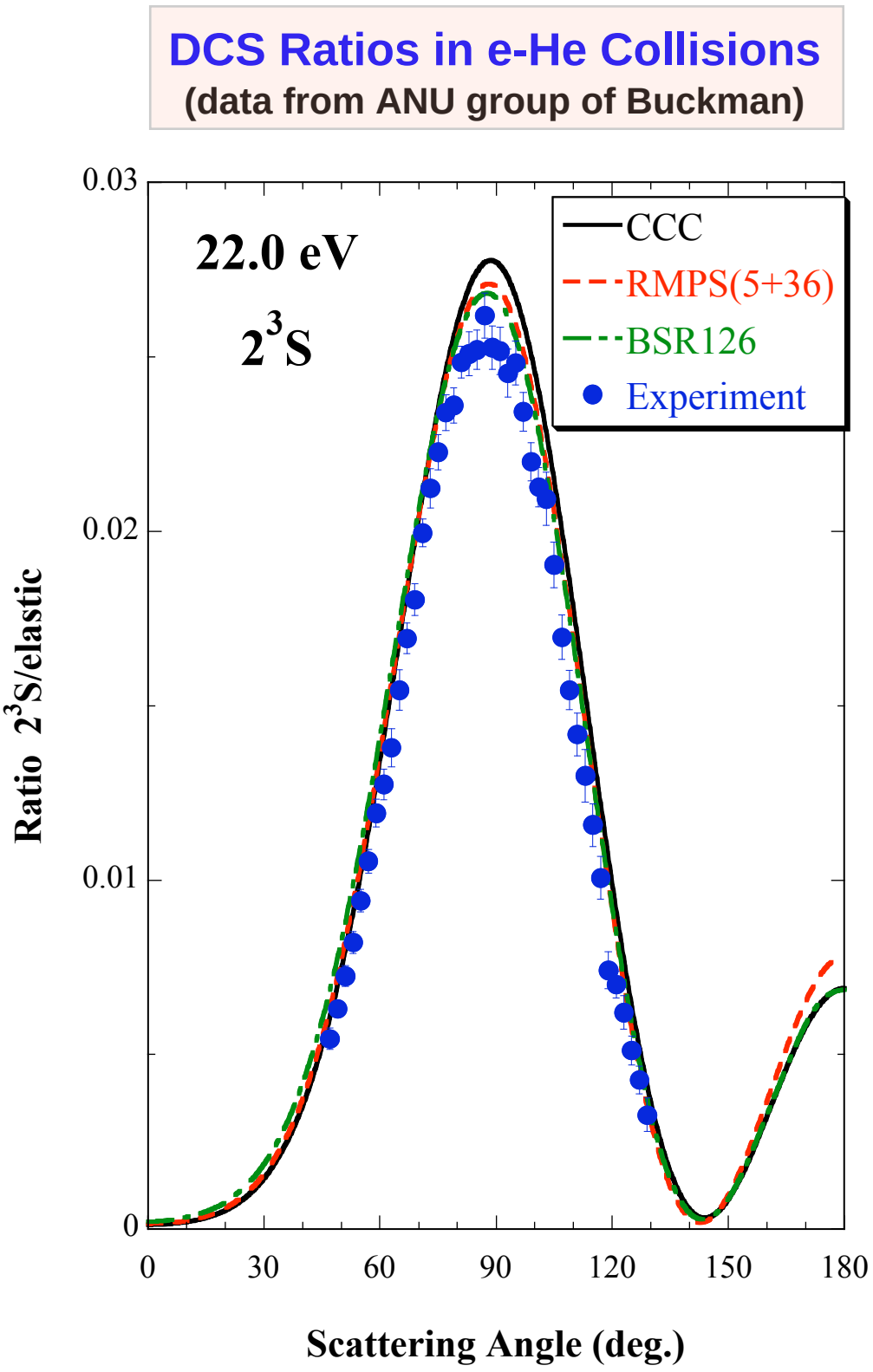
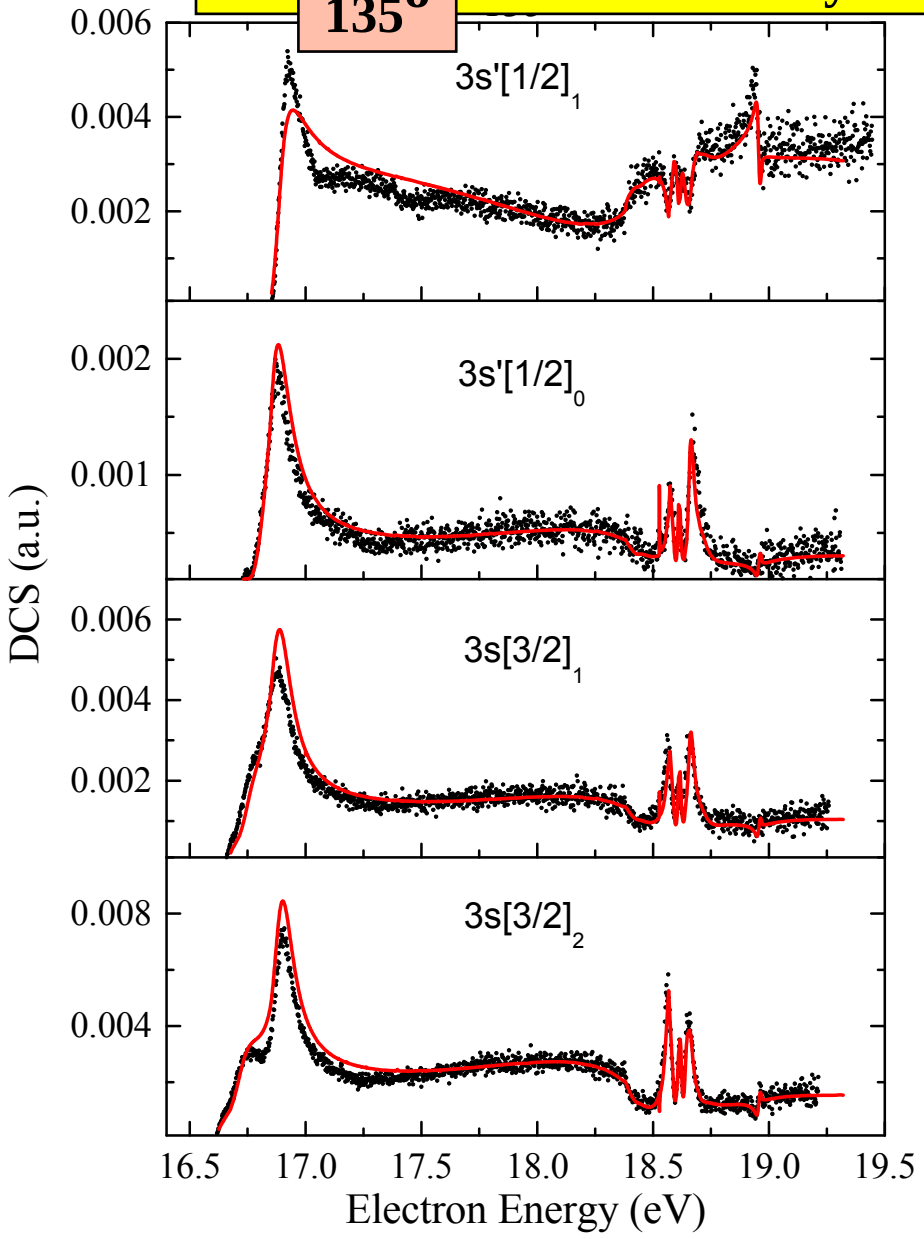
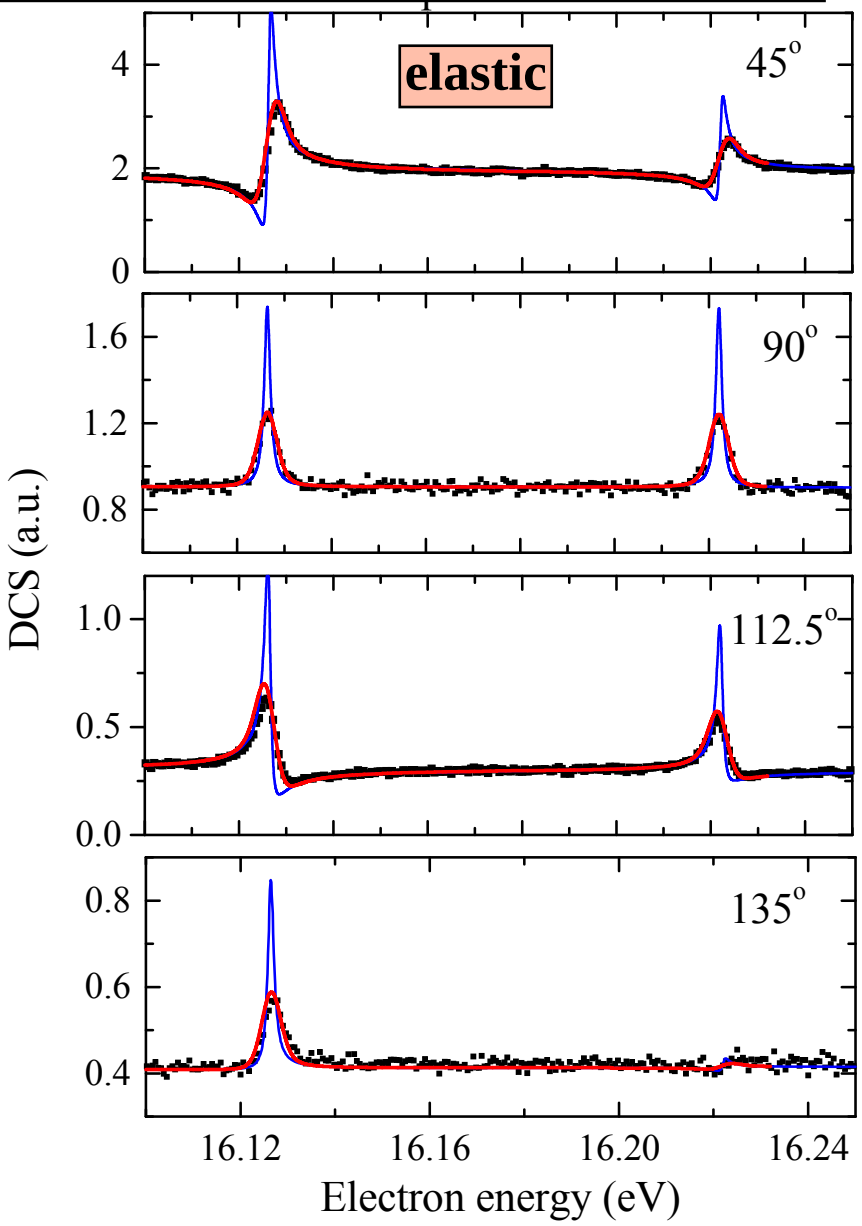

DCS Ratios in e-He Collisions
(data from ANU group of Buckman)
22.0 eV
2^3S
CCC
RMPS(5+36)
BSR126
Experiment
Ratio 2^3S/elastic
0.03
0.02
0.01
0
0
30
60
90
120
150
180
Scattering Angle (deg.)

Figure 2(a)

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



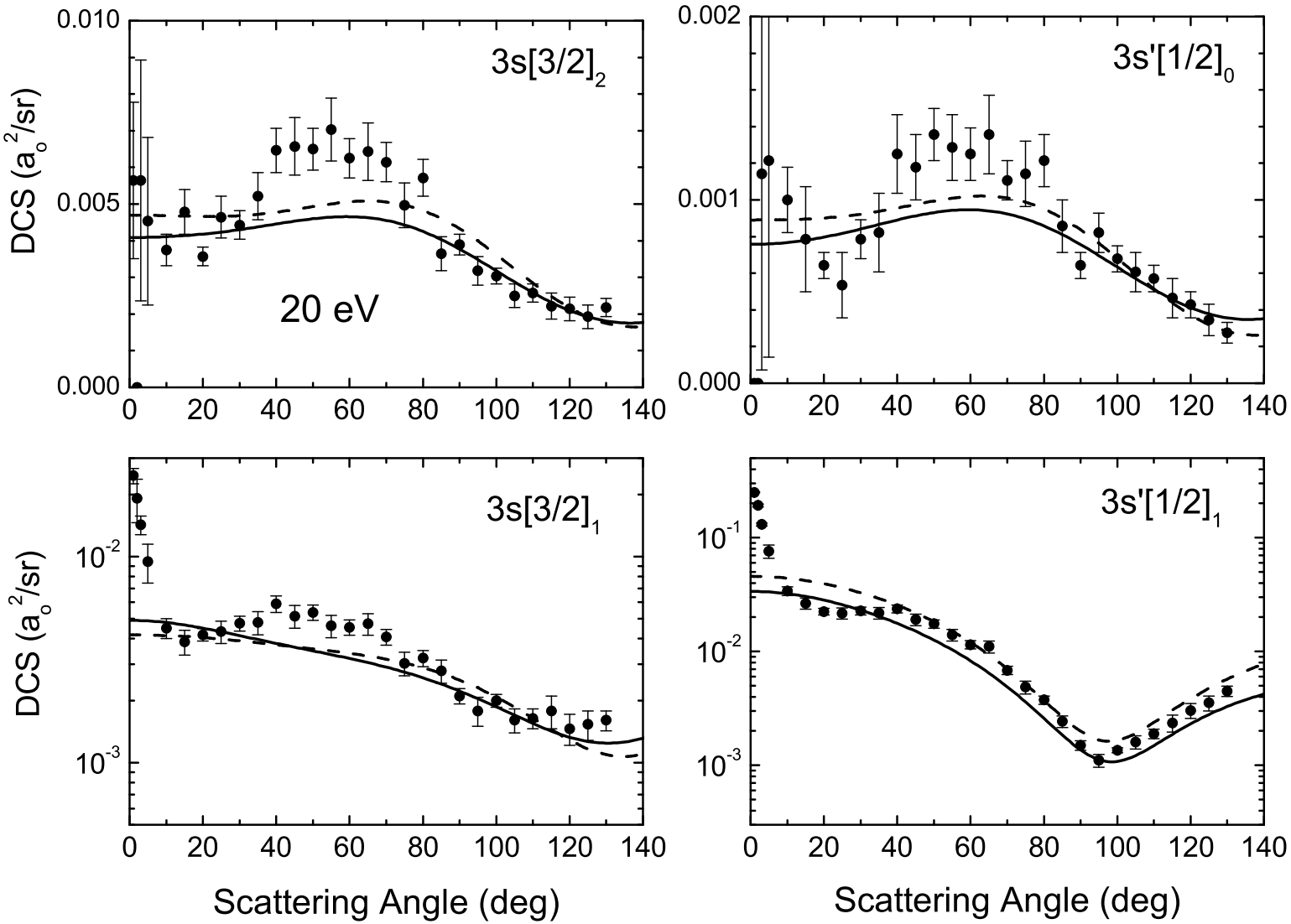
Experiment - K. Franz *et al.* (next talk)



Experiment - Bömmels *et al.* (2005)

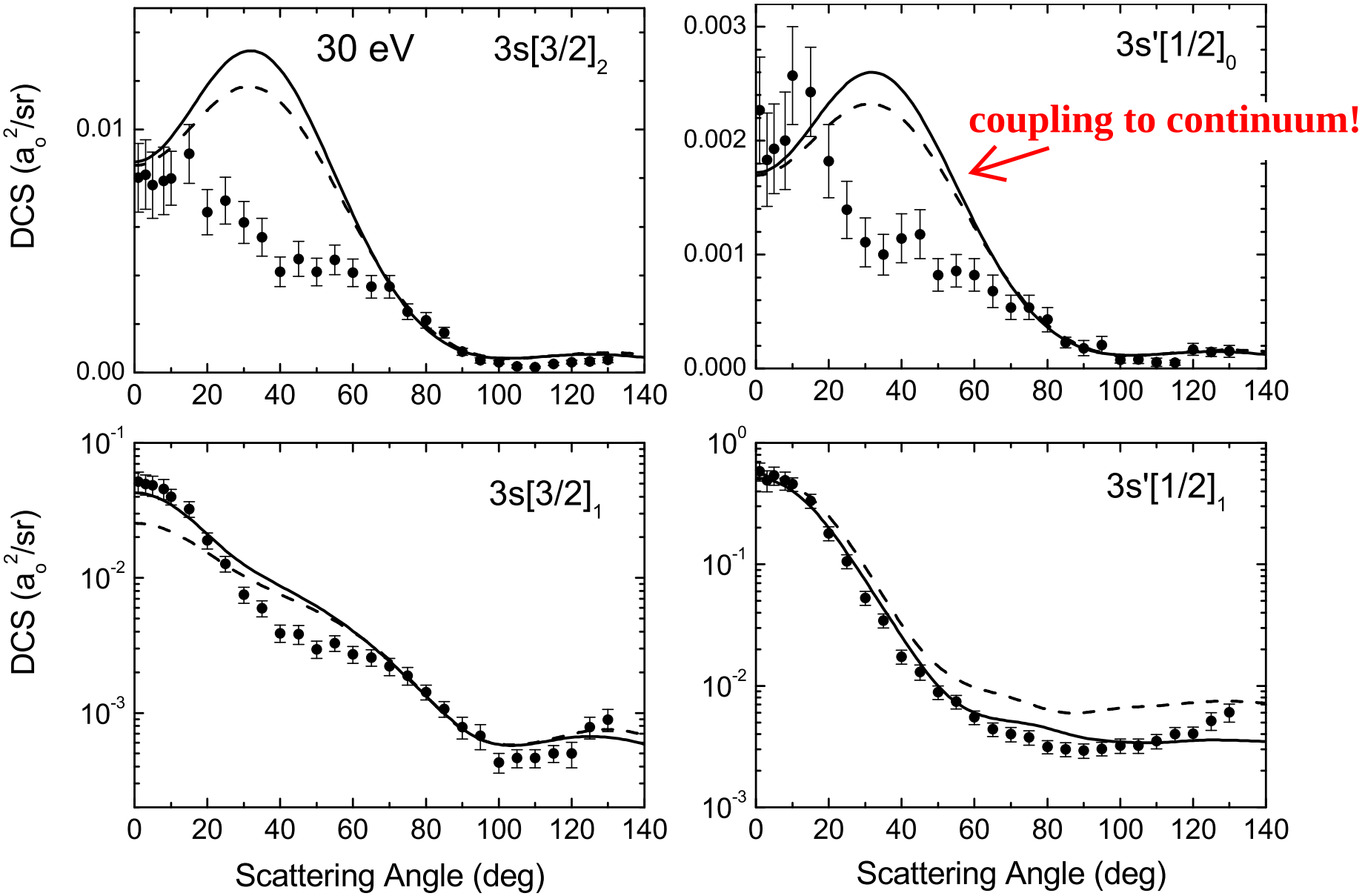
Compared to BSRM and BSRM-convoluted

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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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!

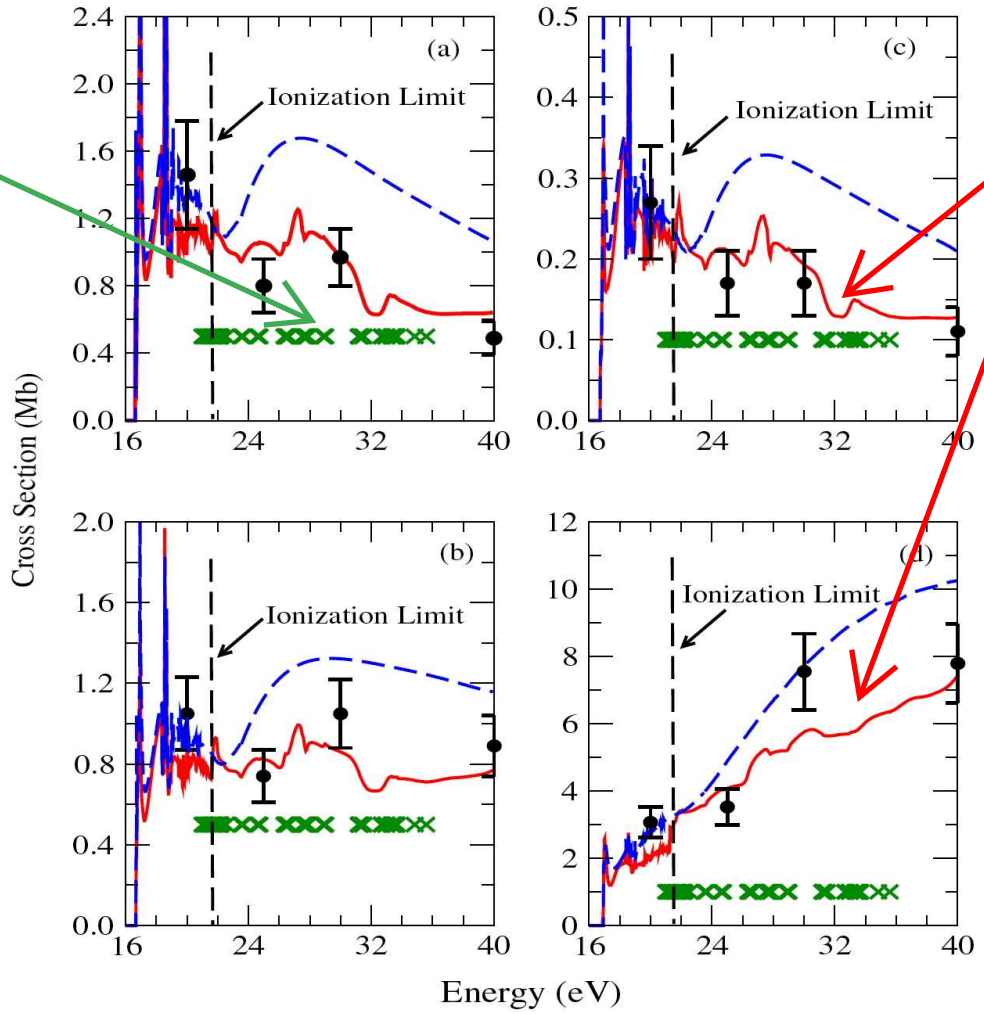
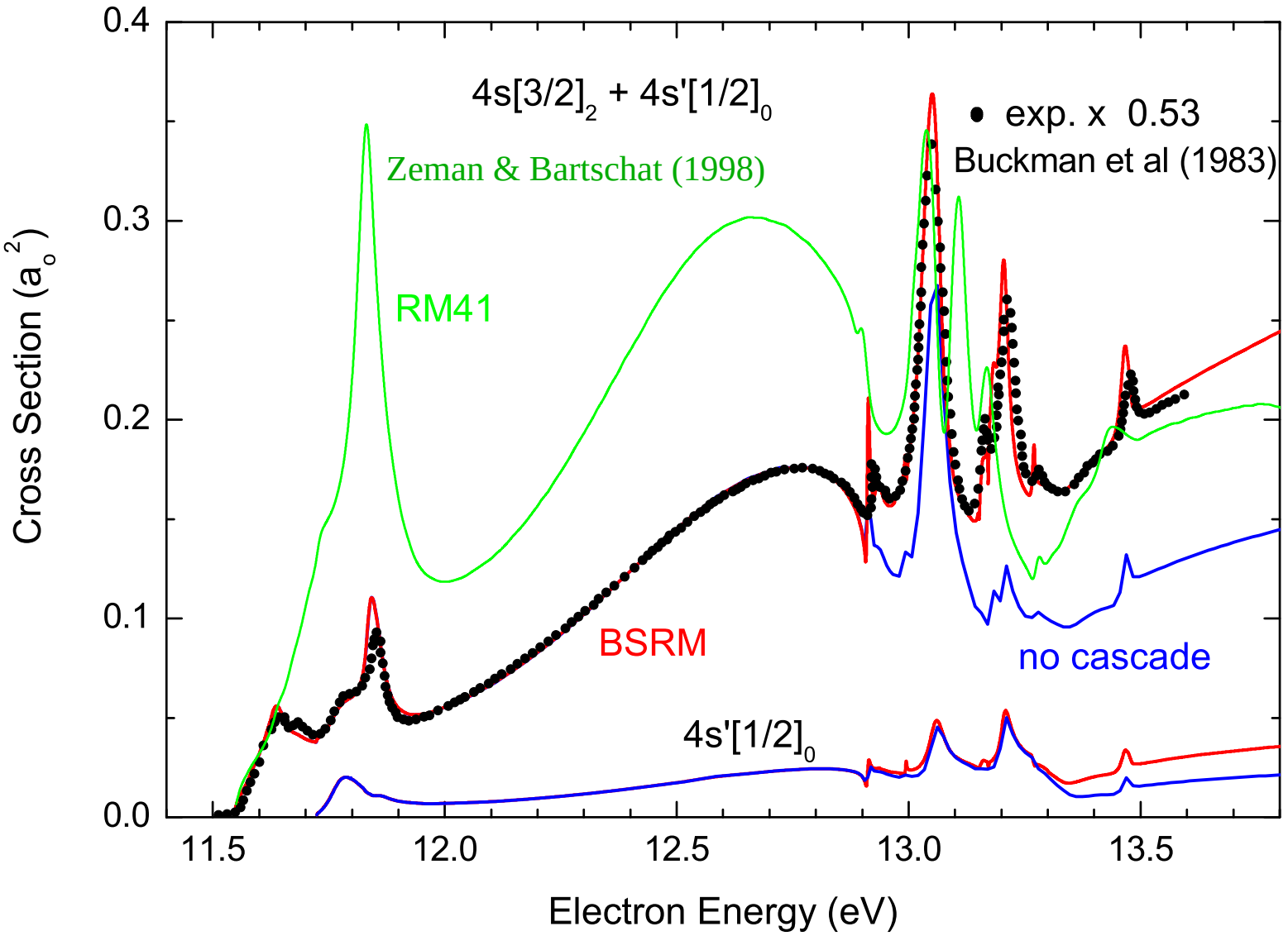
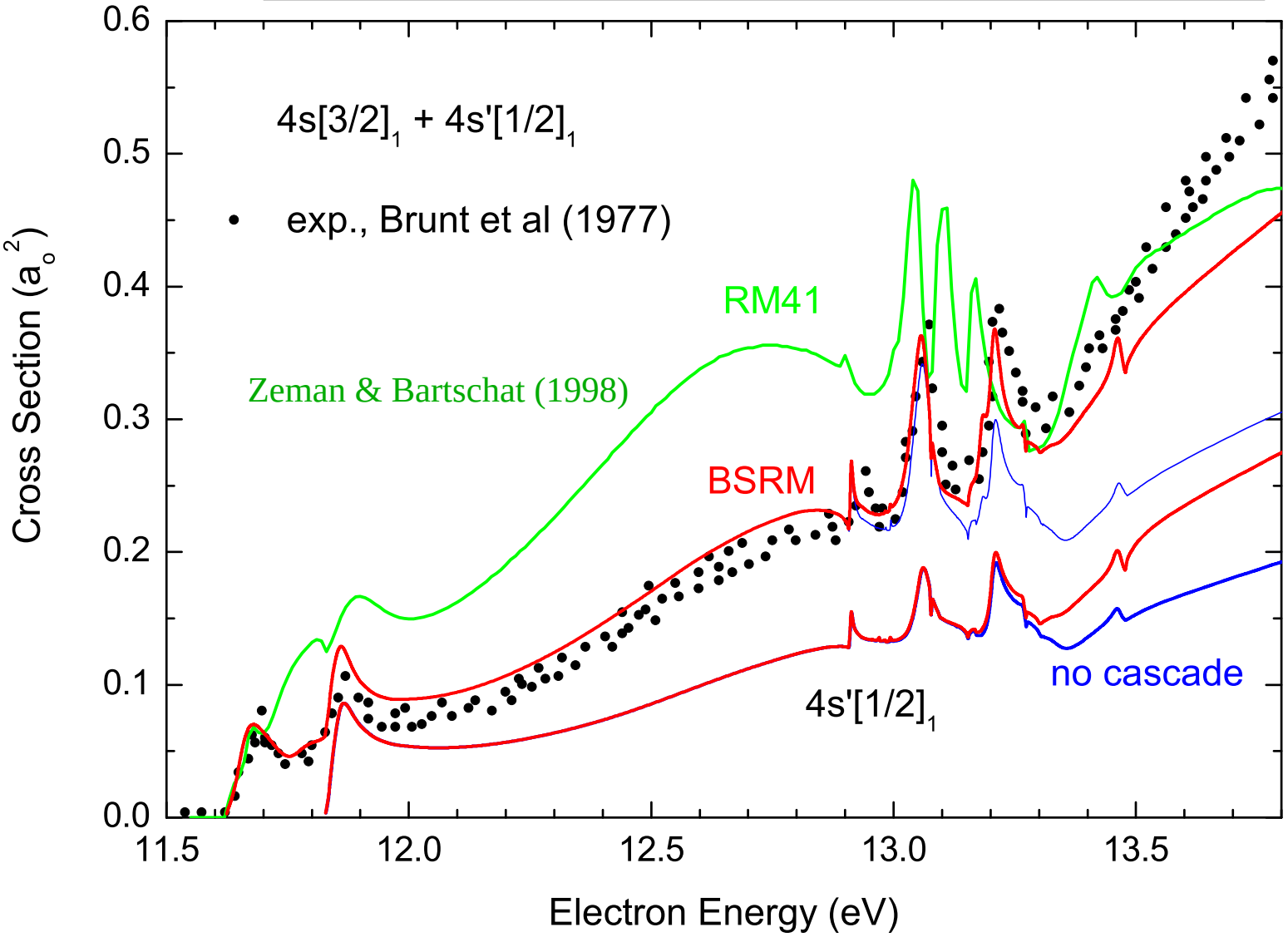


Figure 1. Breit–Pauli calculations of cross sections for excitation from the $2p^6\ ^1S_0$ ground level of neon to the $2p^5 3s\ 3/2[3/2]_2$ level in (a); to the $2p^5 3s\ 3/2[3/2]_1$ level in (b); to the $2p^5 3s\ 1/2[1/2]_0$ level in (c); and to the $2p^5 3s\ 1/2[1/2]_1$ level in (d). The dashed curves 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.

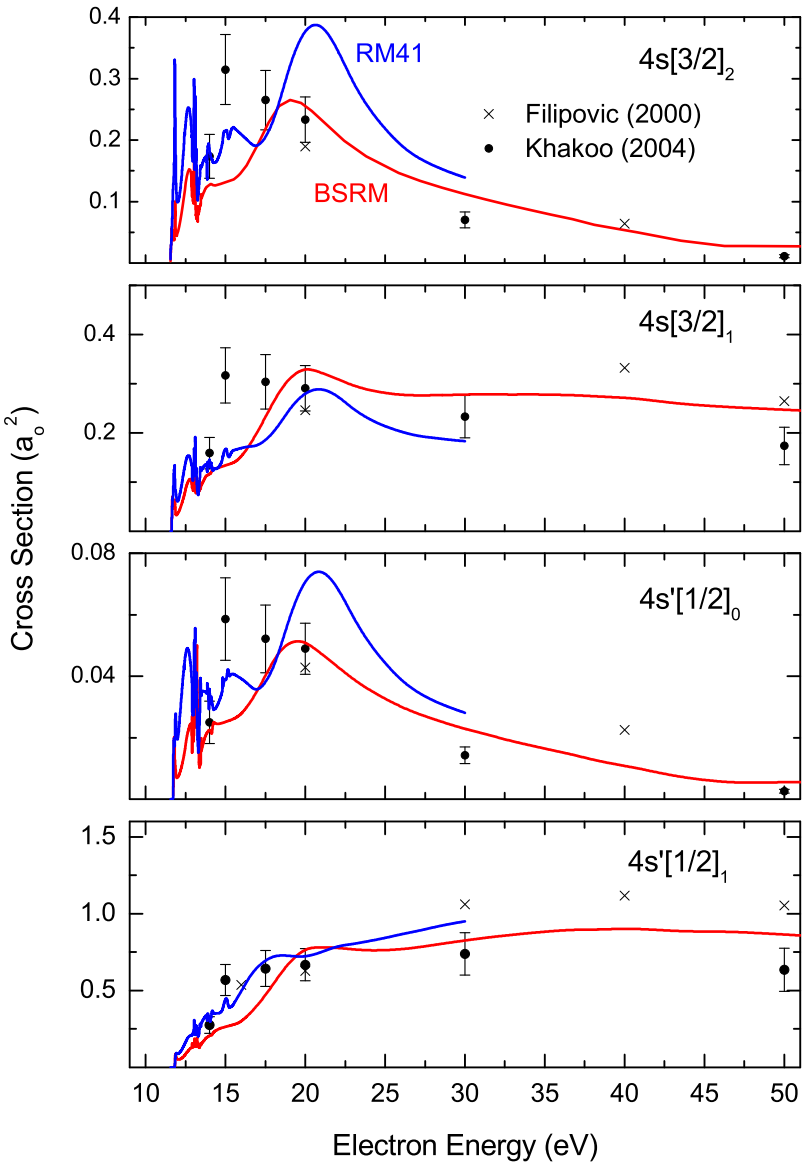
Metastable yield in e-Ar collisions



UV excitation function for e-Ar



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

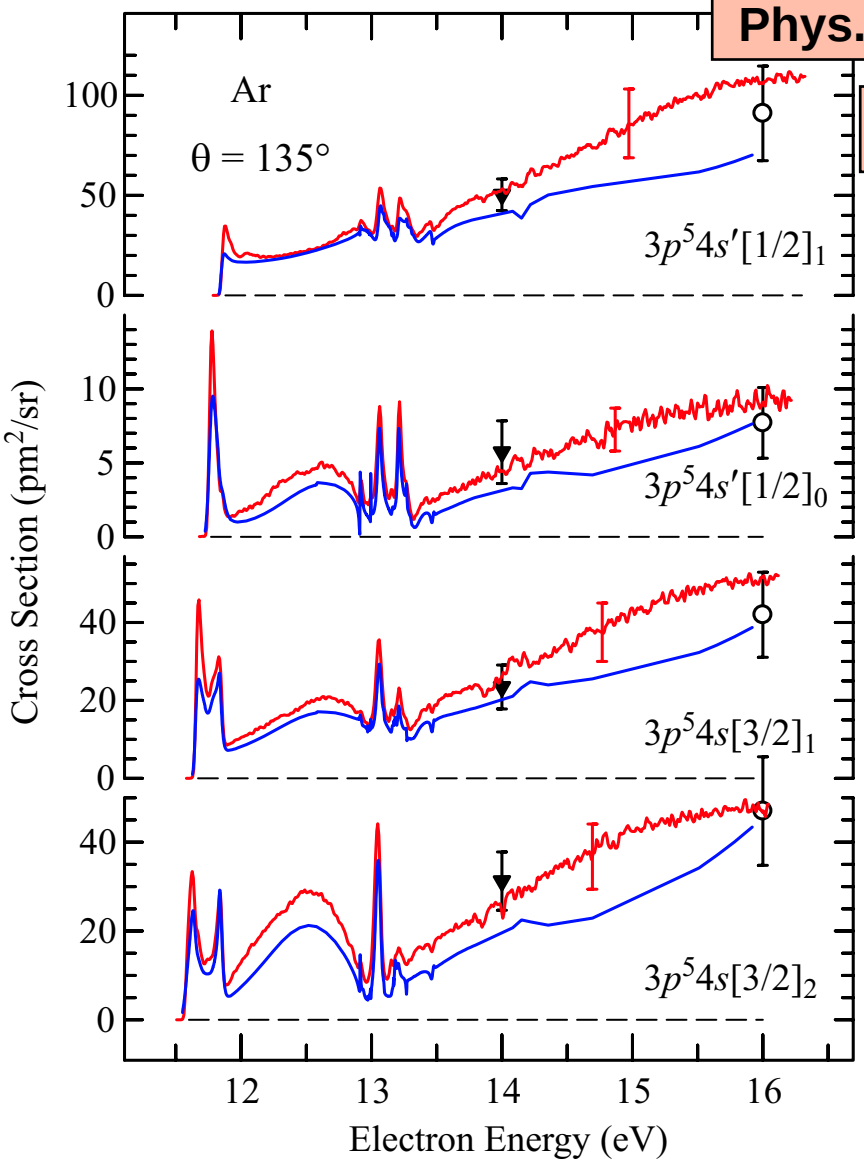


experiments: Filipovic *et al.*, Khakoo *et al.*,

e-Ar: energy scan at 135^o

Phys. Rev. A 74 (2006) 030701(R)

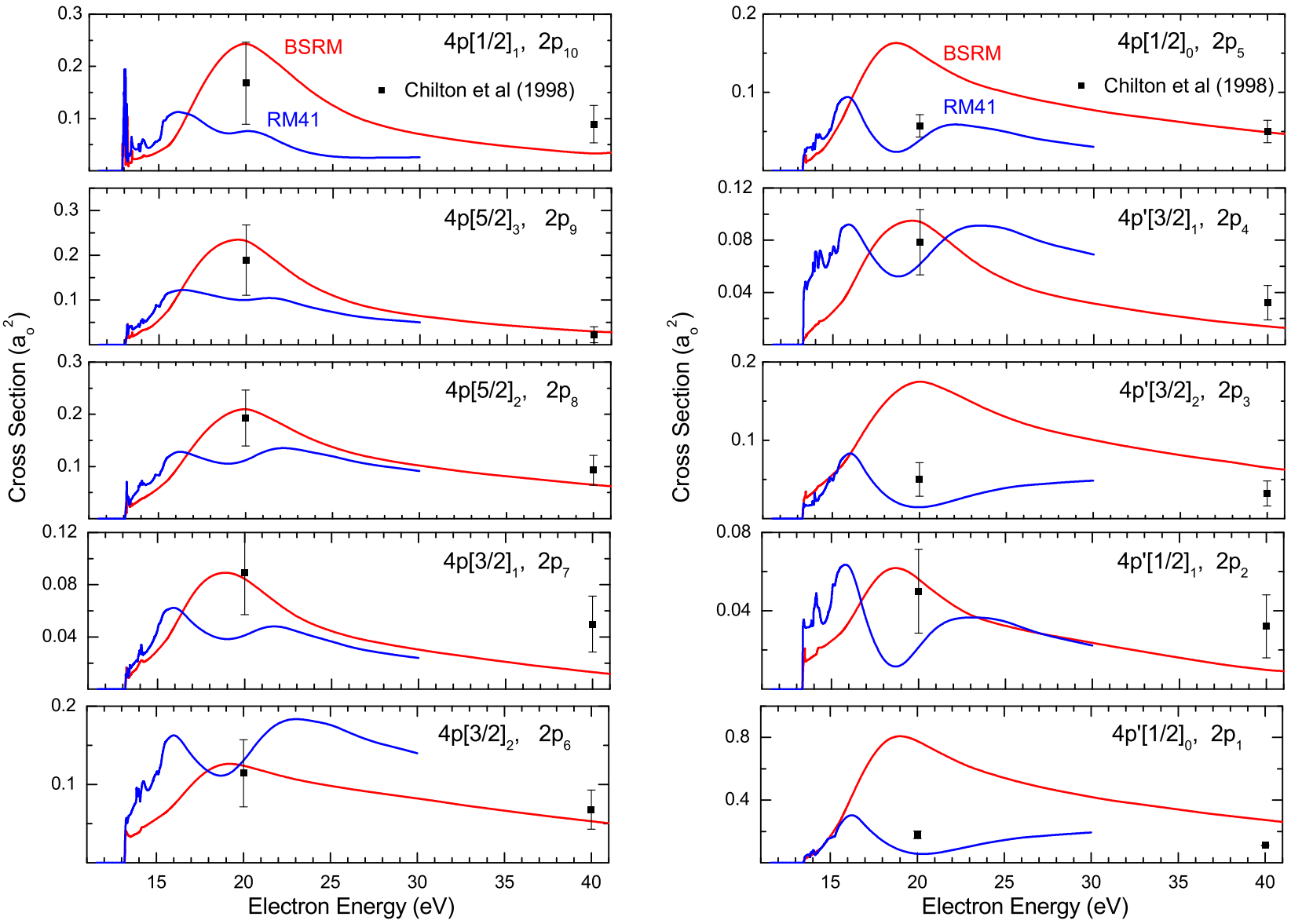
Michael Allan's experiment



Angle-differential cross sections for electron-impact excitation of the lowest four states of argon as a function of impact energy at a fixed scattering angle of 135°.

present experiment; BSR theory. Circles: Chutjian and Cartwright (1981); triangles: Khakoo *et al.* (2004), reduced by 1.45 due to different elastic DCS.

Electron-Impact Excitation of Ar ($3p^5 4p$)



experiment: Chilton *et al.*

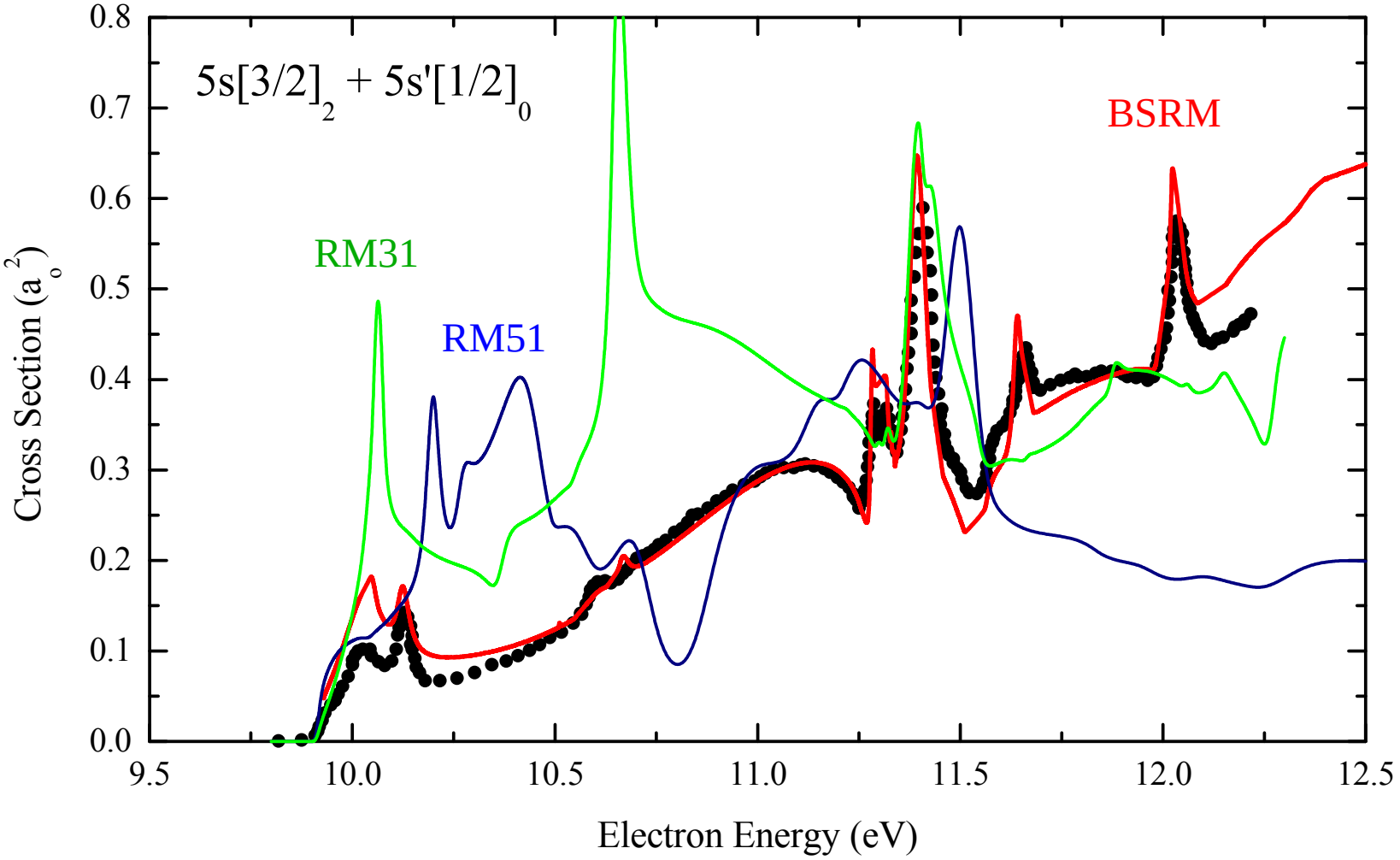
Metastable yield in e-Kr collisions

Experiment: Buckman *et al.* (1983) [x 0.84]

Theories: 31-state Breit-Pauli R-matrix (Zeman & Bartschat 1998)

51-state Breit-Pauli R-matrix (Bartschat & Grum-Grzhimailo 2000)

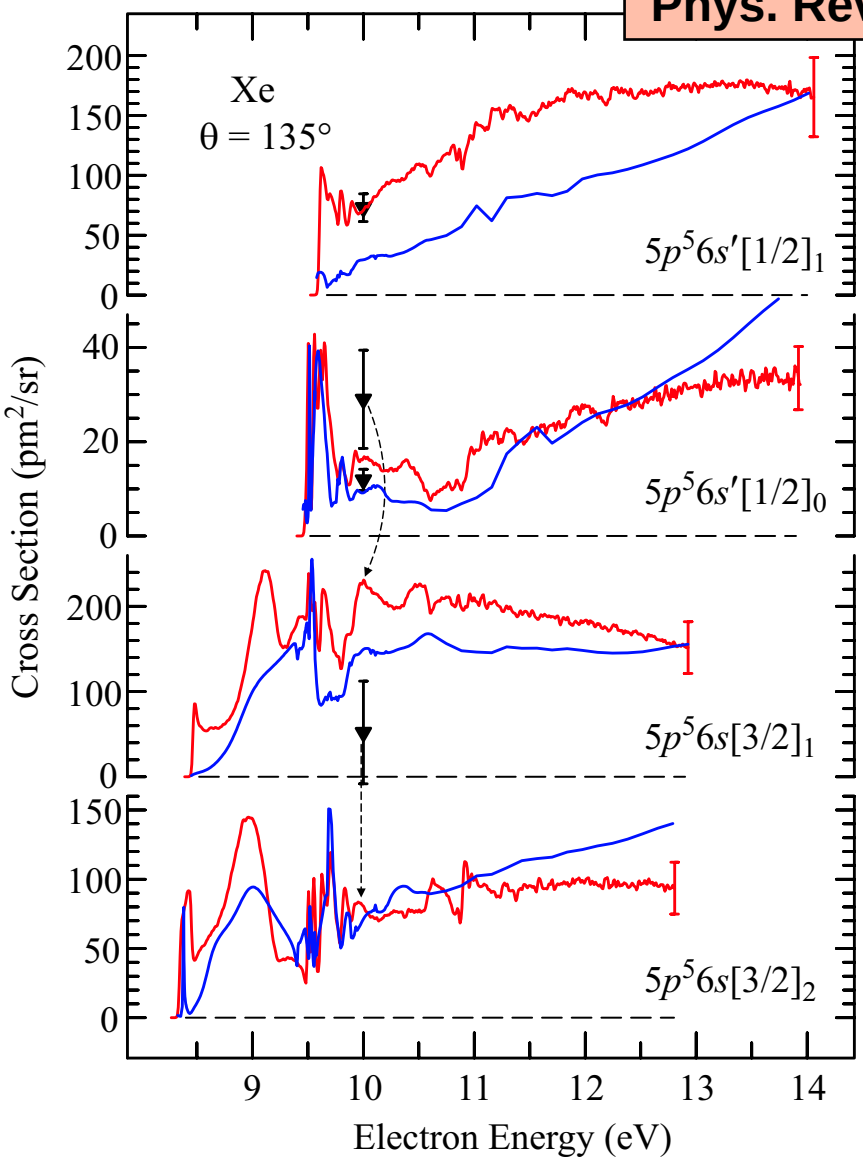
31-state B-spline R-matrix



e-Xe: energy scan at 135^o

Phys. Rev. A 74 (2006) 030701(R)

Michael Allan's experiment



Angle-differential cross sections for electron-impact excitation of the lowest four states of xenon as a function of impact energy at a fixed scattering angle of 135°.

present experiment; BSR theory. Triangles: Khakoo *et al.* (1996).

Resonances in e-Zn collisions

O. Zatsarinny and K. Bartschat (Phys. Rev. A **71**, 022716, 2005)

Experiment:

Sullivan J P, Burrow P D, Newman D S, Bartschat K, Panajotovic R, Moghbelalhossein M, McEachran R P and Buckman S J
New Journal of Physics **5** (2003) 159.1
"An experimental and theoretical study of transient negative ions in Mg, Zn, Cd and Hg"

Calculations:

1. RMPS, 25 target states, 11 spectroscopic (semi-empirical core-potential approach)
2. BSRM, 49 target states, 11 spectroscopic (*ab initio*)

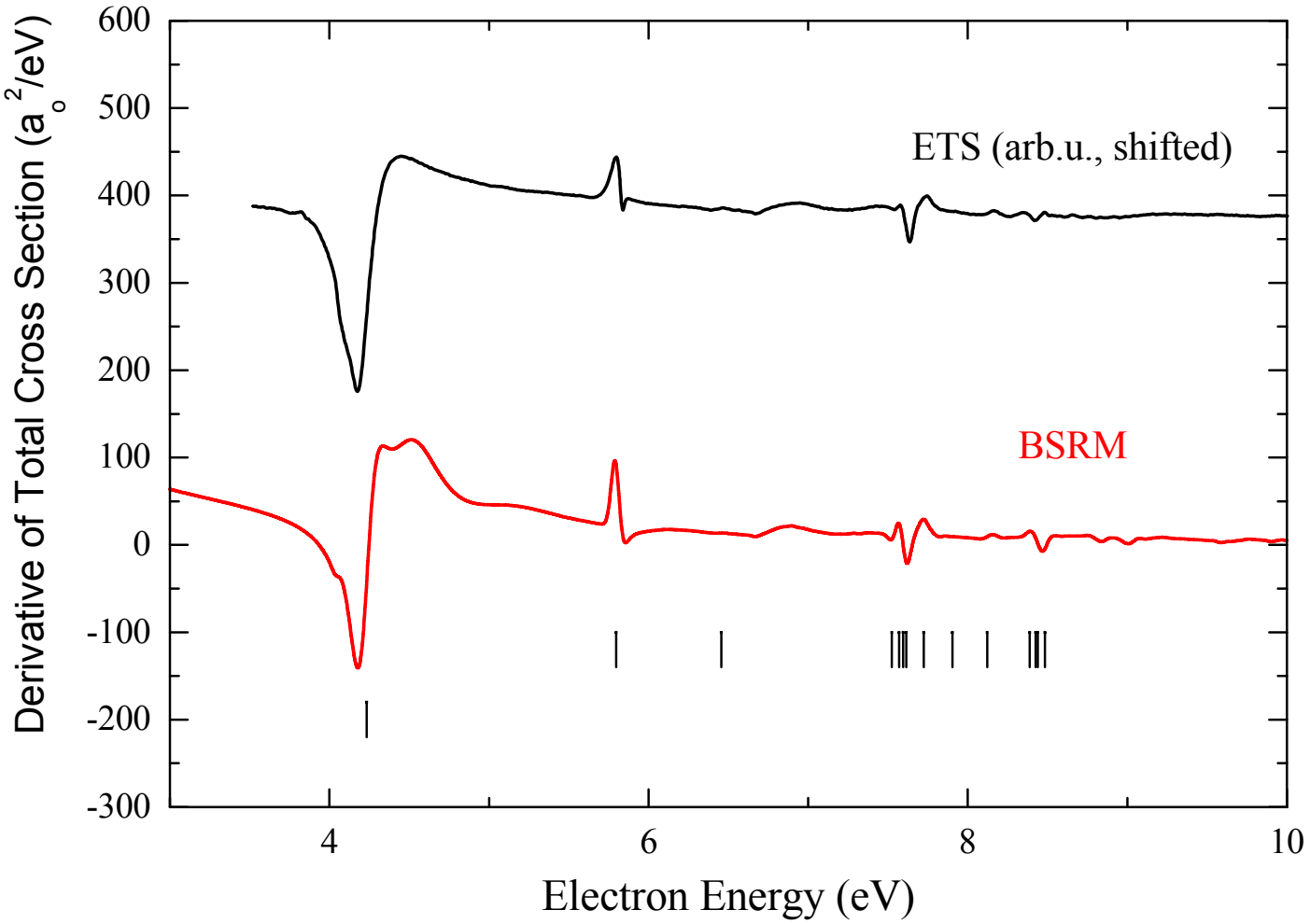
Target states were obtained in the B-spline bound state calculations

$$\Phi(3d^{10}4snl, LS) = A\sum_i \{\phi(3d^{10}4s)P(n_i l_i)\}^{LS} + A\sum_i \{\phi(3d^{10}4p)P(n_i l_i)\}^{LS}$$
$$+ A\sum_i \{\phi(3d^{10}5s)P(n_i l_i)\}^{LS} + A\sum_i \{\phi(3d^{10}4d)P(n_i l_i)\}^{LS}$$
$$+ A\sum_i \{\phi(3d^{9}4s^{2})P(n_i l_i)\}^{LS} + \sum_{i,6l} \chi(3d^{9}n_i l_i 6l'6l'', LS)$$

Theoretical excitation energies differed from experiment by no more than 80 meV.
Polarizability of ground state: 36.8 a_o^3; exp.: 38.8 (0.8) a_o^3.

Electron transmission spectroscopy in e-Zn collisions

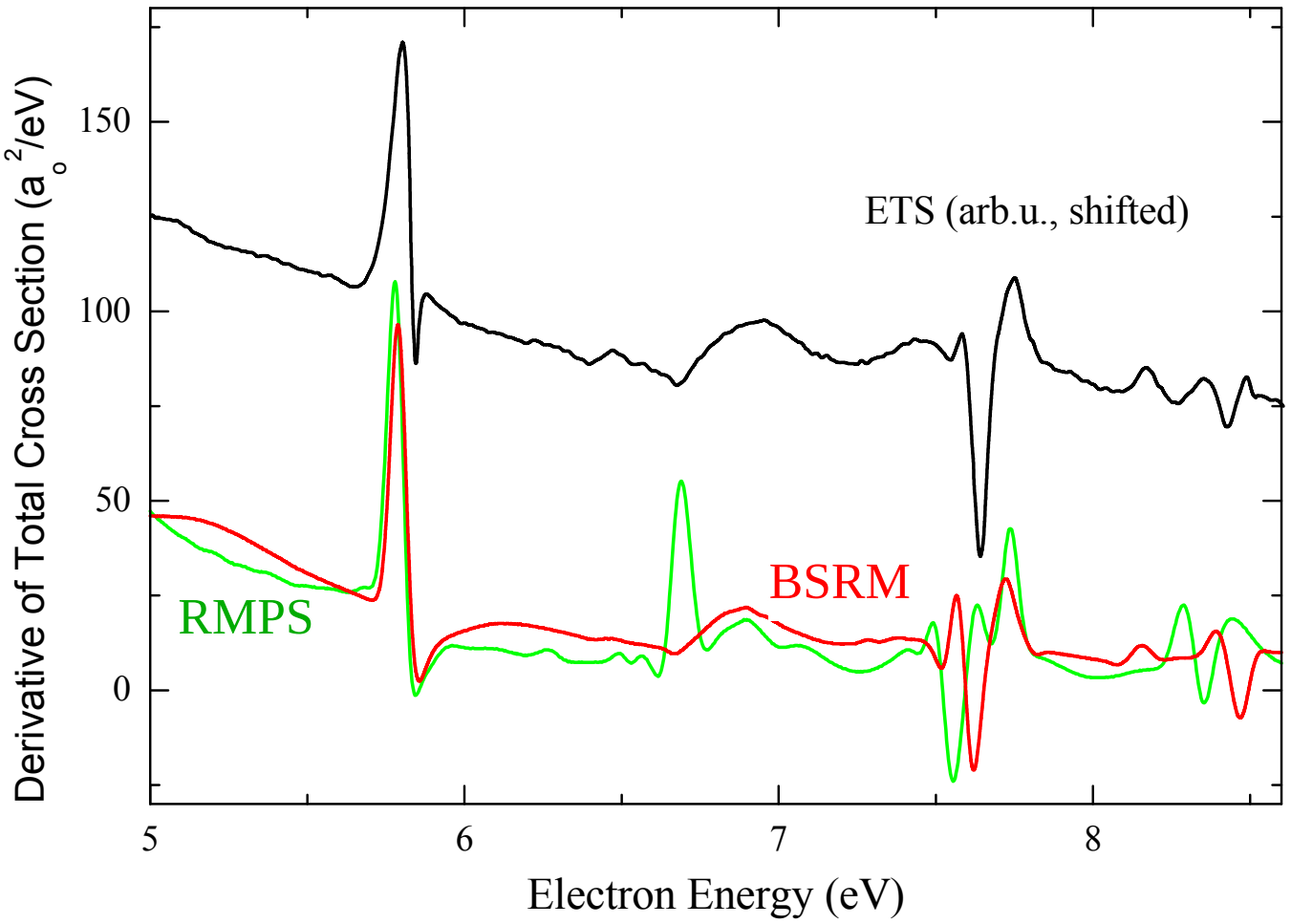
Experiment: Sullivan, Burrow *et al.*, New Journal of Physics (2003)
Theory: 49 states B-spline R-matrix (Zatsarinny & Bartschat 2005)



We predicted and identified 15 resonances!

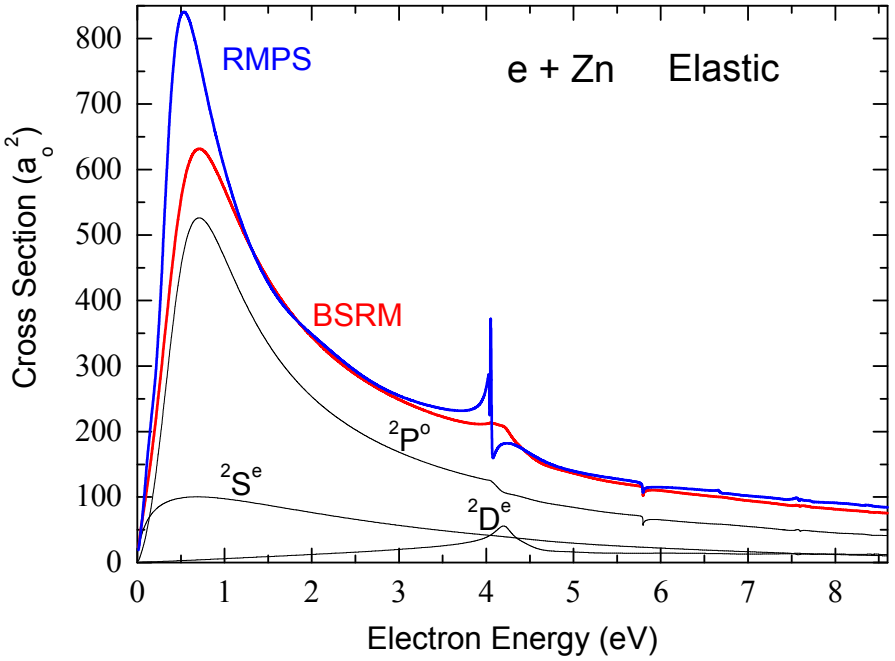
Electron transmission spectroscopy in e-Zn collisions

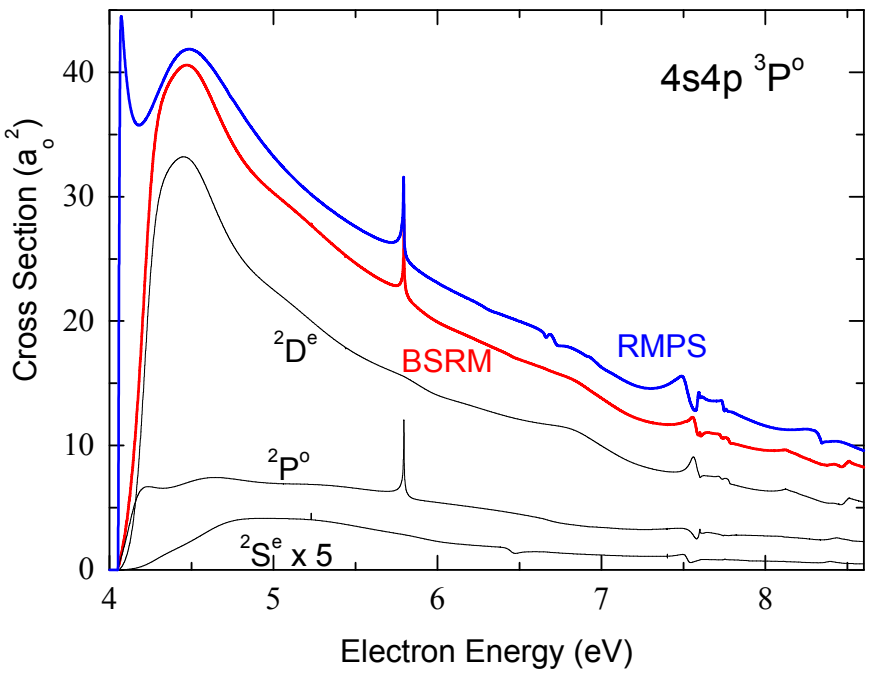
Experiment: Sullivan, Burrow *et al.*, New Journal of Physics (2003)
Theory: **49-state B-spline R-matrix**
25-state R-matrix with pseudo-states

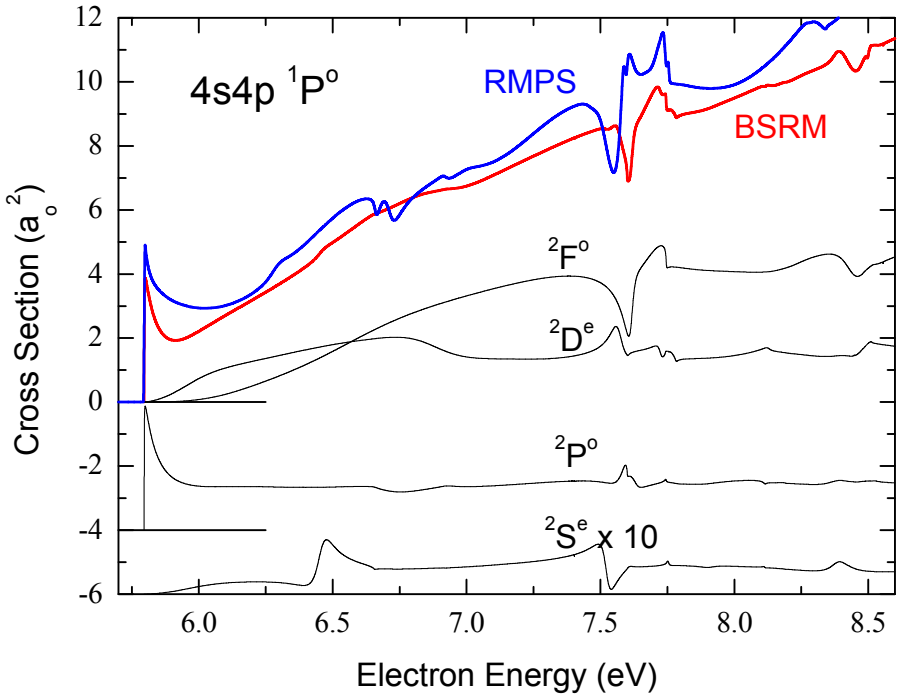


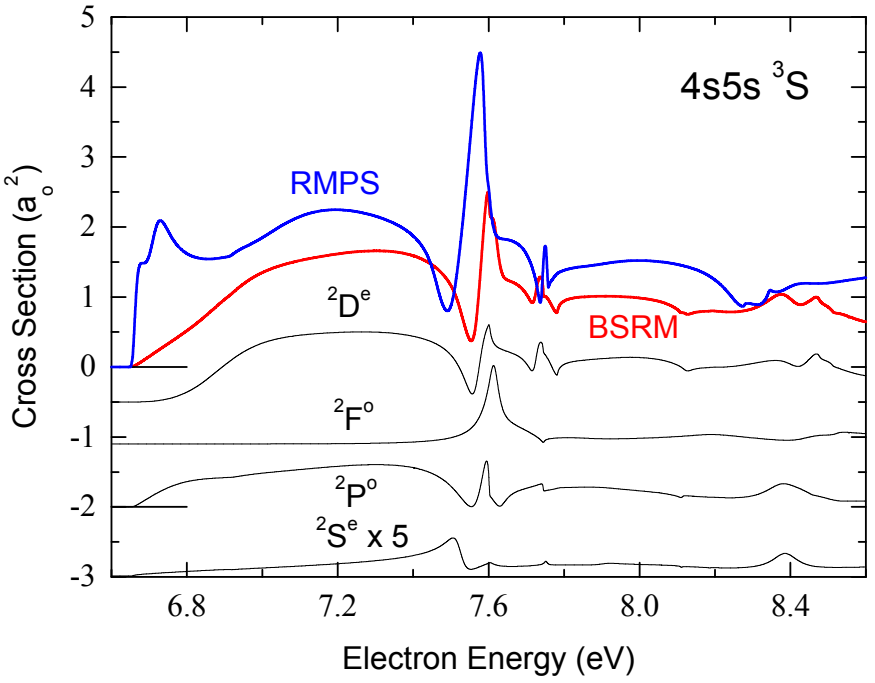
We predicted and identified 15 resonances!

Low-energy elastic and excitation cross sections for e-Zn

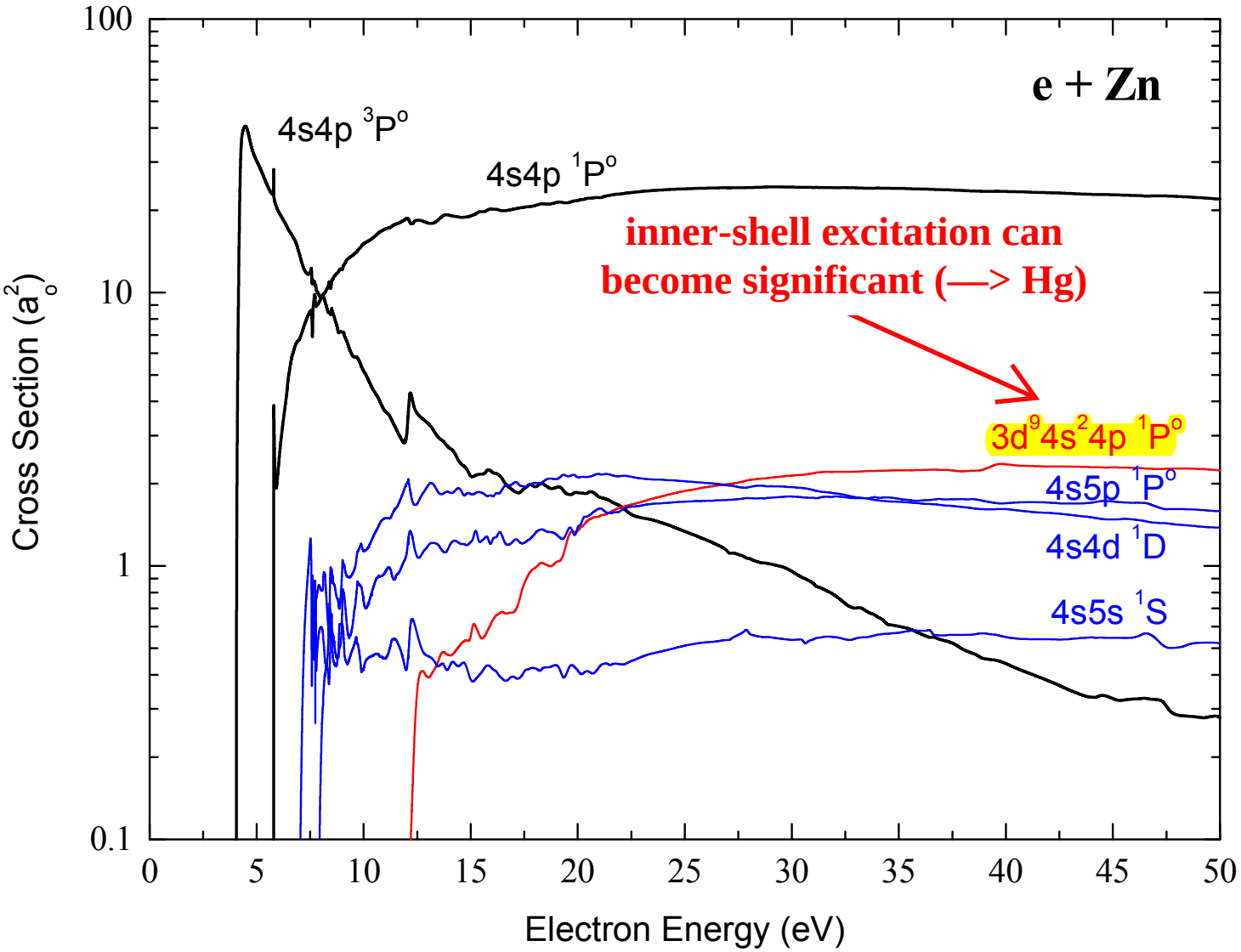








Intermediate-energy excitation cross sections for e-Zn



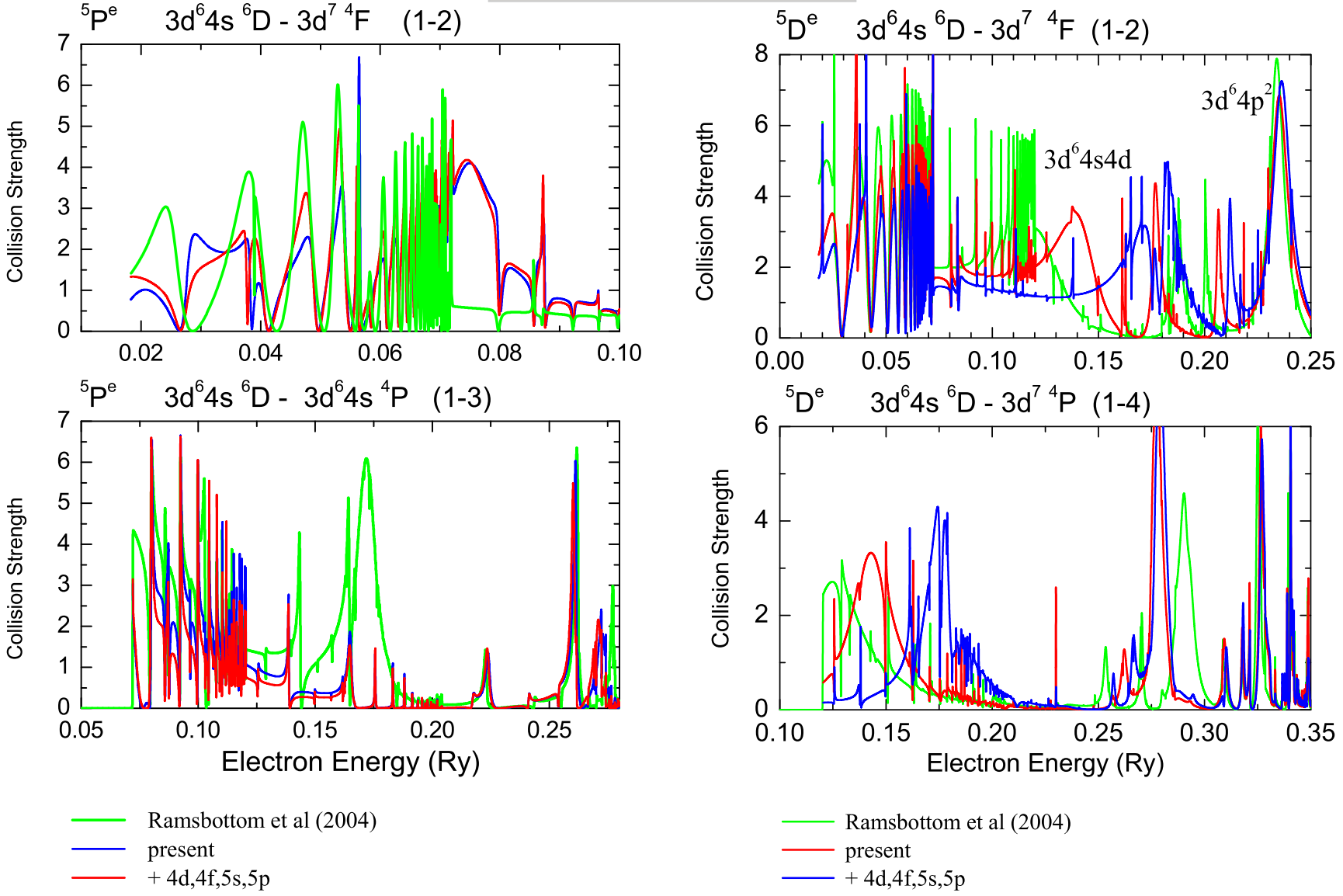
Good agreement with recent experiment and CCC calculations of Fursa and Bray (2005) for excitation of the 4s4p ^1P and 4s5p ^1P levels.

A Problem from Astrophysics: e–FeII

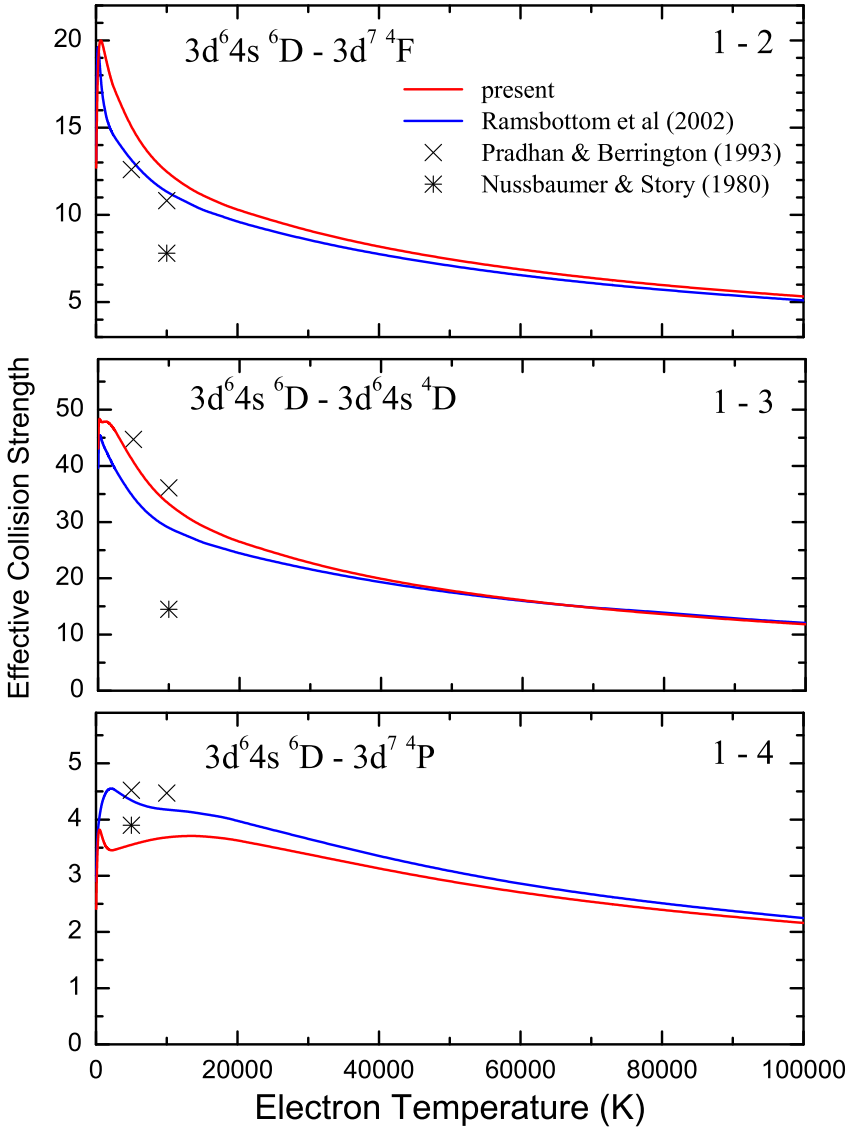
Observed and calculated term energies of Fe II (in Ry × 10^{-4}) relative to the ground state.

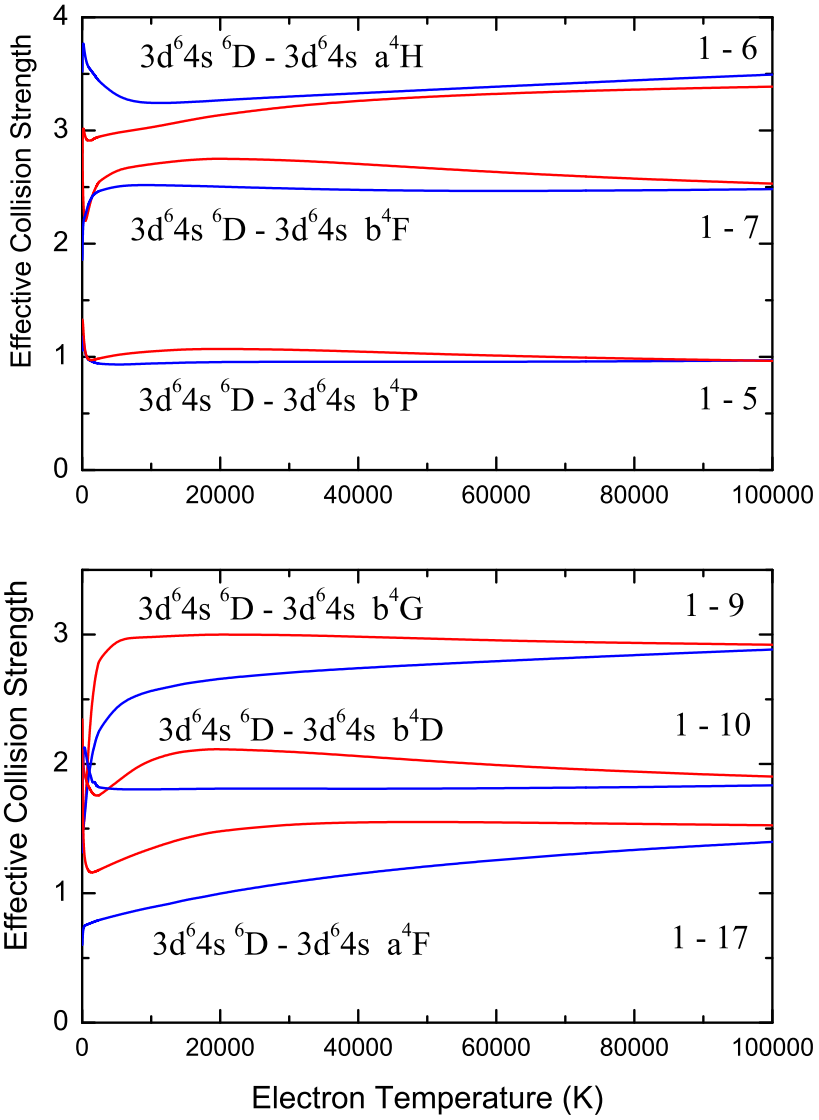
	State	Term	Observed term energy	Present data difference	Ramsbottom et al (2004) difference	Ramsbottom et al (2002) difference
1	$3d^6(^5D)4s$	a ^6D	0	0	0	0
2	$3d^7$	a ^4F	182	16	-33	-14
3	$3d^6(^5D)4s$	a ^4D	720	-19	5	-1
4	$3d^7$	a ^4P	1203	49	17	143
5	$3d^6(^3P_2)4s$	b ^4P	1914	-46	250	547
6	$3d^6(^3H)4s$	a ^4H	1918	8	423	282
7	$3d^6(^3F^2)4s$	b ^4F	2040	-2	317	467
8	$3d^54s^2$	a ^6S	2087	1	394	
9	$3d^6(^3G)4s$	a ^4G	2310	1	414	429
10	$3d^6(^3D)4s$	b ^4D	2825	-24	400	658
11	$3d^6(^5D)4p$	z ^6Do	3490	-82	-229	-371
12	$3d^6(^5D)4p$	z ^6Fo	3805	-82	-187	-327
13	$3d^6(^5D)4p$	z ^6Po	3886	-2	-162	-208
14	$3d^6(^5D)4p$	z ^4Fo	4037	46	-144	-172
15	$3d^6(^5D)4p$	z $^4D^o$	4039	-75	-116	-205
16	$3d^6(^5D)4p$	z $^4P^o$	4265	63	-64	-127
17	$3d^6(^3P_1)4s$	c ^4P	4499	60	592	1247
18	$3d^6(^3F_1)4s$	c ^4F	4532	-5	594	1148
19	$3d^54s^2$	b ^4G	4907	21	737	
20	$3d^54s^2$	d ^4P	5199	22	611	
21	$3d^6(^3P_2)4p$	z $^4S^o$	5399	-58	104	291
22	$3d^54s^2$	c ^4D	5463	43	767	
23	$3d^6(^3P_2)4p$	y $^4P^o$	5504	-3	27	247
24	$3d^6(^3H)4p$	z $^4G^o$	5504	-1	163	-1
25	$3d^6(^3H)4p$	z $^4H^o$	5516	-51	249	12
26	$3d^6(^3H)4p$	z $^4I^o$	5565	1	210	-70

Collision Strengths



Effective Collision Strengths



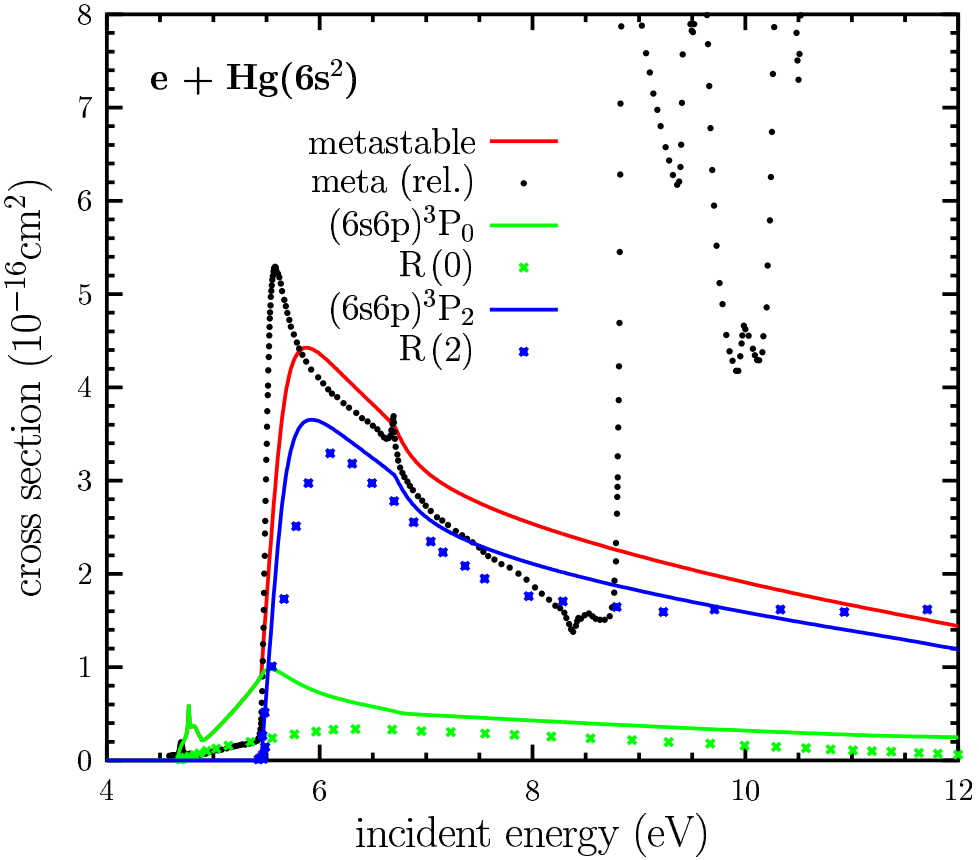


List of calculations with the BSR code (rapidly growing)

***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)
e + He	Stepanovic *et al. J. Phys. B* **39** 1547 (2006)
	Lange M *et al. J. Phys. B* **39** in preparation (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: At. Mol. Opt. Phys.* **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 *Phys. Rev. A* in preparation (2006)
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)

Electron Collisions with Hg Atoms: Metastable Production

data sources: **5-state semi-relativistic RMPS**
indirect from transport data (Rockwood 1973)
metastable count rate (Newman *et al.* 1985)

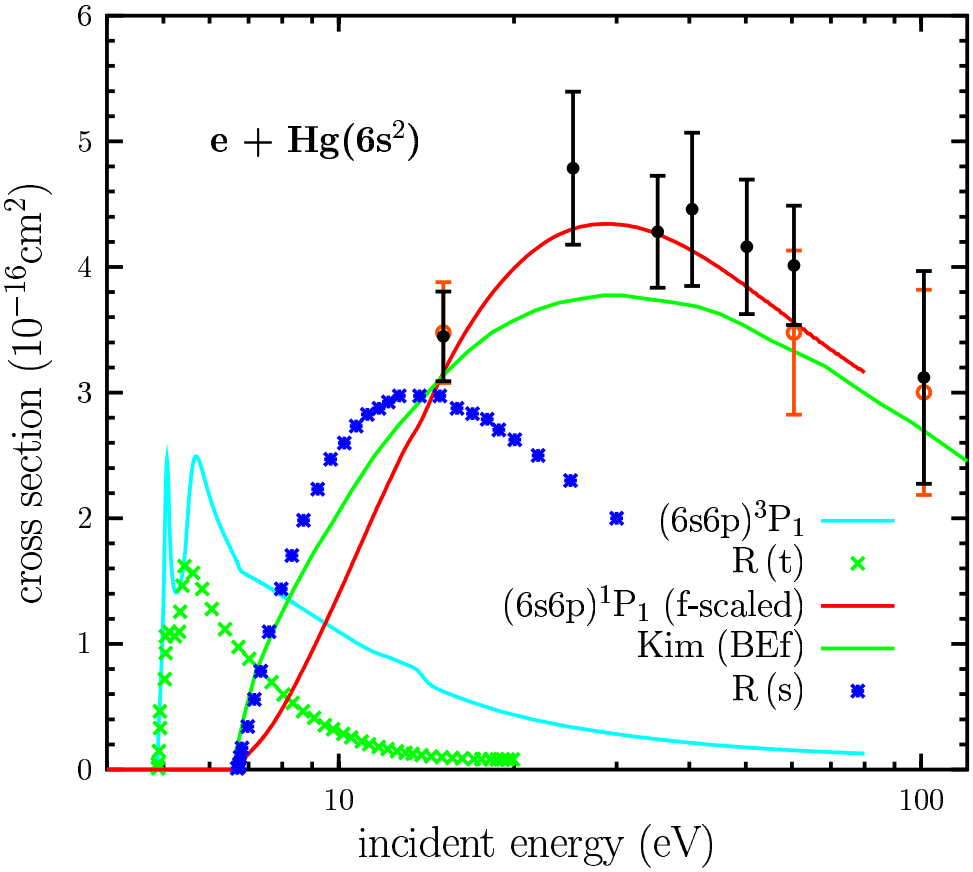


- **At higher energies, the data set suggested by Rockwood violates the well-known energy dependence of cross sections for forbidden transitions.**
- **Since the wavefunctions for the triplet states are expected to be good, we can normalize the Newman *et al.* data.**
- **Above ≈ 8 eV, the metastable yield is affected by inner-shell excitation and cascading (not yet included).**

Electron Collisions with Hg Atoms: (V)UV Production

data sources: 5-state semi-relativistic R-Matrix
indirect from transport data (Rockwood 1973)

Experiments: Peitzmann & Kessler (1990)
Panajatovic *et al.* (1993)



- The data set suggested by Rockwood does not seem reliable.
- The f-scaling (→ Kim) works well and is needed for $^1P_1$.
- There is more evidence (→ Franck-Hertz) of a very strong $(6s6p^2)^4P_{5/2}$ resonance at $(6s6p)^3P_1$ threshold.

Cross sections for electron scattering from the ground state of mercury

J. Phys. B: At. Mol. Opt. Phys. **36** (2003) 4255–4271

Dmitry V Fursa[1], Igor Bray[2] and Graeme Lister[3]

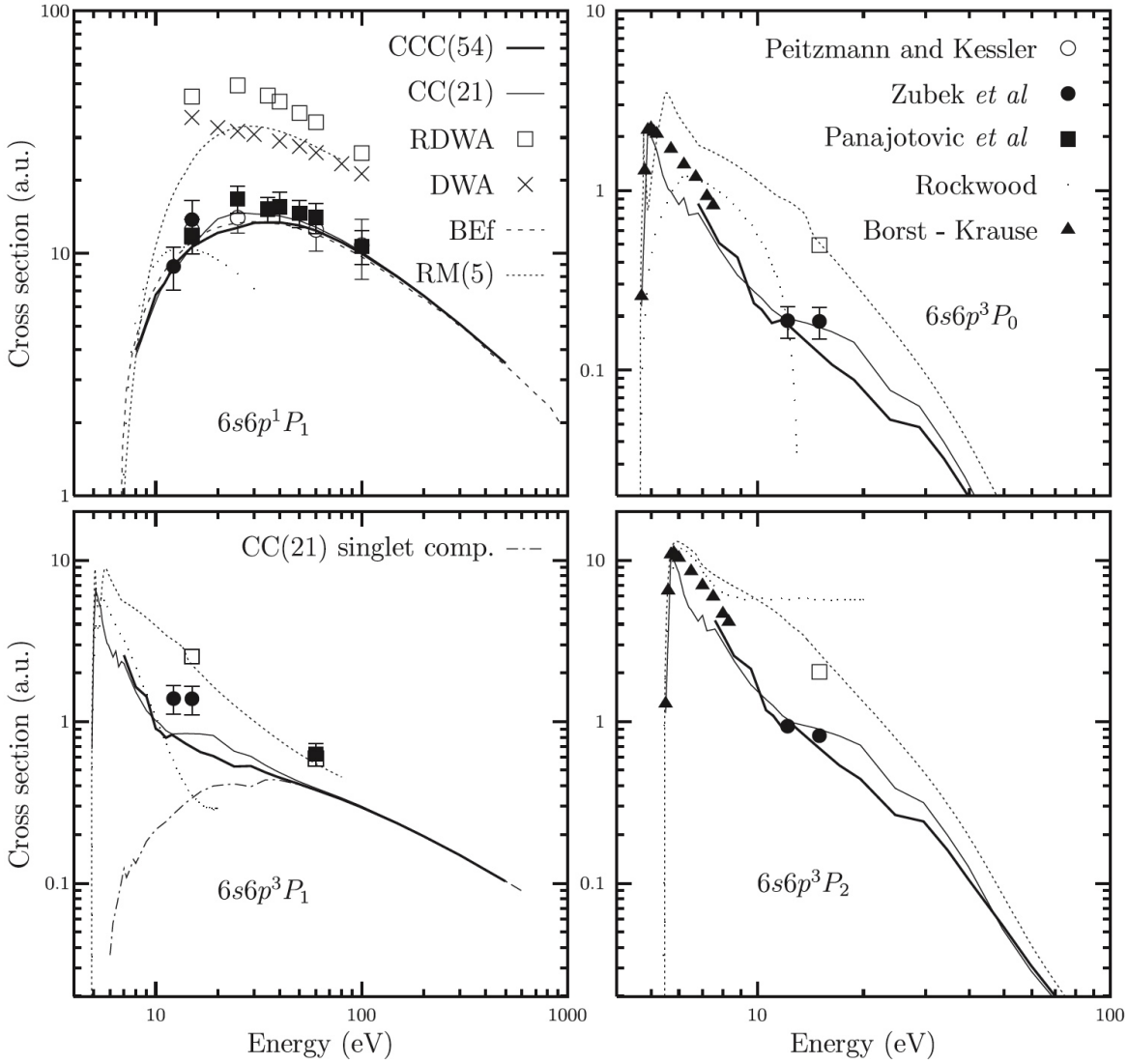


Figure 9. Electron-impact ICSs for the 6s6p $^1P_1$ and 6s6p $^3P_{0,1,2}$ states of mercury from the ground state. Theory and experiment are as in figure 3. In addition, RM(5) calculations are due to Bartschat (2002), BEf results are due to Kim (2001) and the experimental data for the 6s6p $^3P_{0,2}$ states are due to Borst (1969) and Krause *et al* (1977).

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THANK YOU — and LET'S TALK!