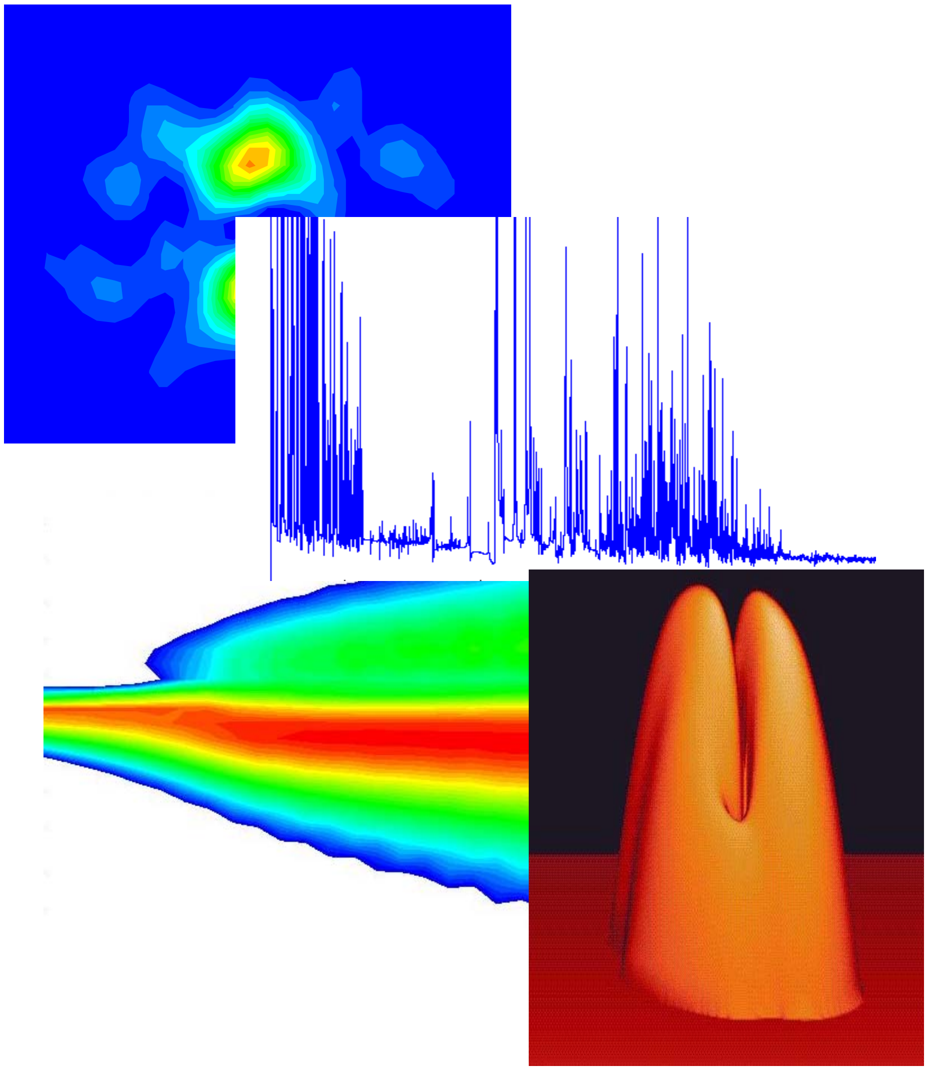
Terascale computational atomic physics for the plasma edge



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PSACI PAC

PPPL

June 5-6, 2003

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Drake University

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Nigel Badnell
Alan Whiteford
Strathclyde University
JET, UK

Phil Burke
Brendan McLaughlin
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Daresbury Laboratory

Keith Berrington
Sheffield Hallam University

Direct Dissemination of Atomic Data

ATOMIC DATA FOR FUSION

Controlled Fusion Atomic Data Center, ORNL

www-cfadc.phy.ornl.gov

Atomic Data and Analysis Structure

International consortium lead by Strathclyde University and JET

adas.phys.strath.ac.uk/adas/docs/manual

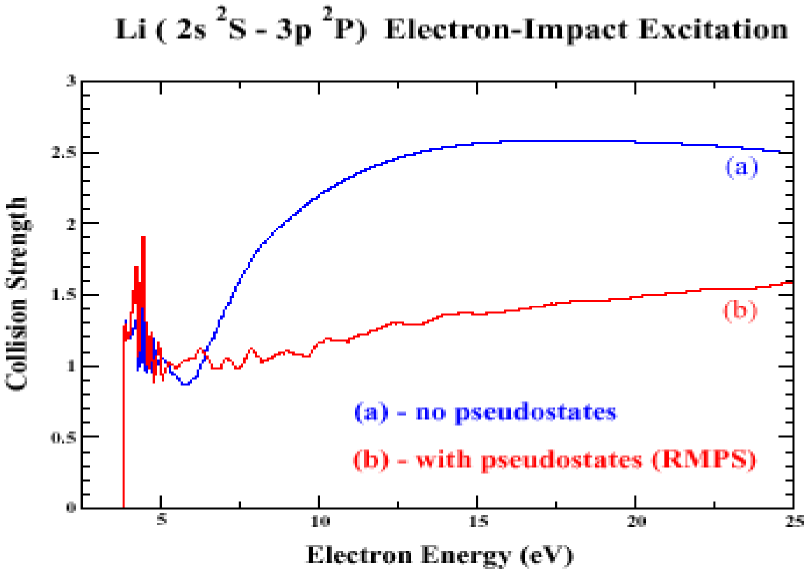
H. P. Summers, ADAS Users Manual (2nd Edition, 2003)

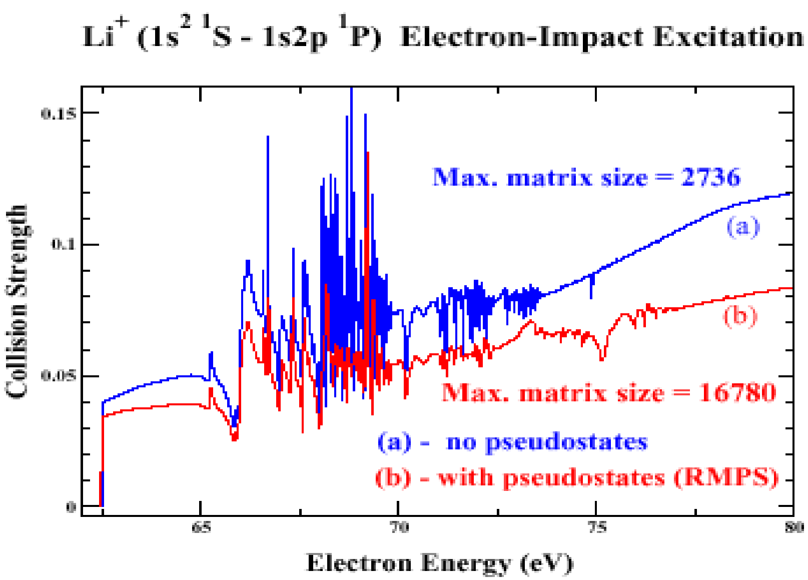
ADAS

Scientific Advances, Accomplishments

1. **Importance of continuum coupling in electron-impact excitation of light elements**
   - H (JPB 2000), He, He^+, Li (PRA 2001), …
2. **Importance of three-body dynamics in the electron-impact ionization of light elements**
   - Li, Li^* (PRL 2001), He^+ (PRA 2003), Li^{2+} (PRA 2002)
3. **Importance of correlation and coupling in the dielectronic recombination of atomic ions**
   - DR project (2003), Cl^{13+} (PRL 2003)
4. **Importance of continuum coupling in proton scattering from light elements**
   - H (PRL 1999), H (PRA 2002), Li^* (PRA 2003)
5. **Importance of three-body dynamics in the double photoionization of atoms and molecules**
   - He (JPB 2001), Be (PRA 2002), (2γ,2e) He (PRL 2002), H_2
6. **Importance of four-body dynamics in the triple photoionization of atoms**
   - Li photoionization
7. **Behavior of solitons in Bose-Einstein Condensates (JPB 2003)**
8. **Simulations of the behavior of ultracold plasmas (PRL 2002)**

Electron-impact excitation of Li and Li^+





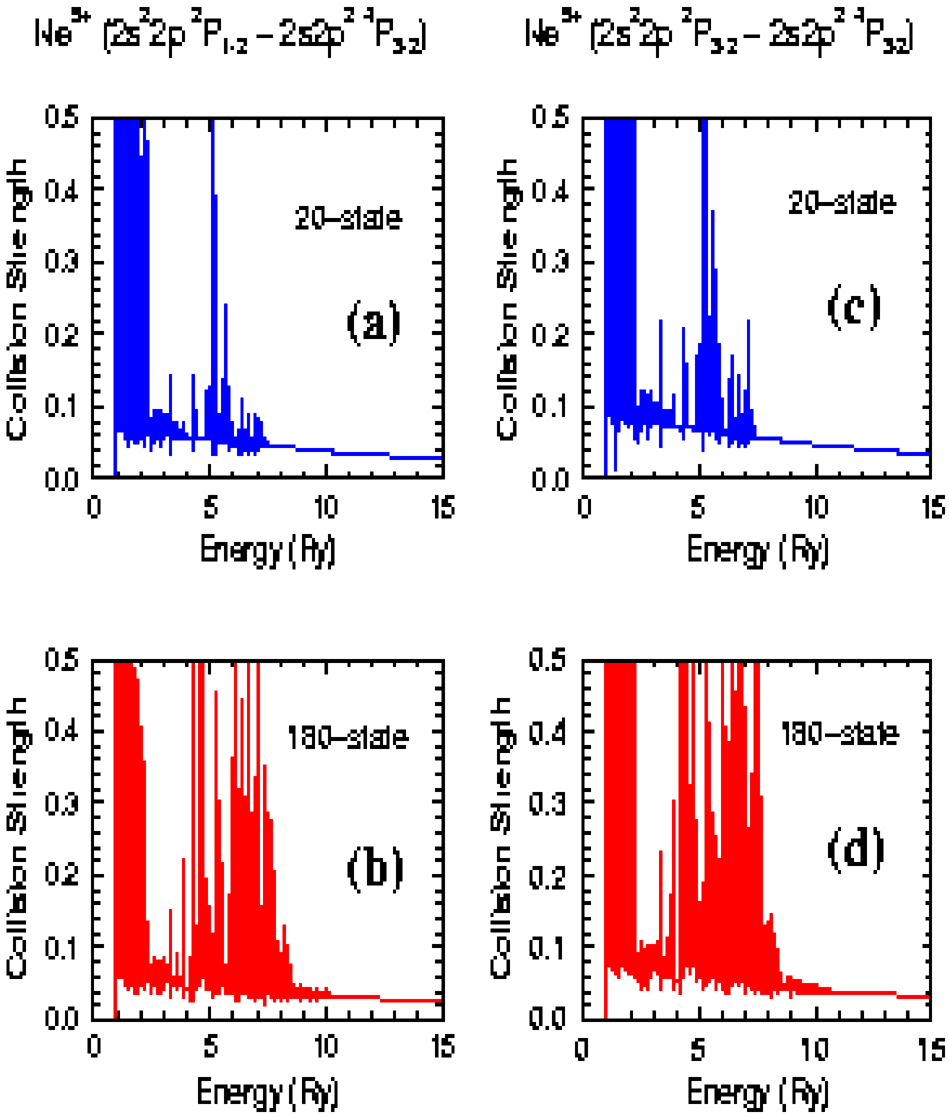
- R-matrix with Pseudo States (RMPS) method has been used for many electron-impact excitation cross section calculations

- In these calculations use of pseudo states reflected the importance of accurately representing the coupling to the continuum

- Systems of importance in fusion research, dramatic revision of accepted rate coefficients

- **Li**: Griffin et al, Phys. Rev. A (2001)
- **Li^+:** Ballance et al, J. Phys. B (2003)
- **C^{2+}:** Mitnik et al, J. Phys. B (2003)
- **C^{3+}:** Griffin et al, J. Phys. B (2000)

Electron-impact excitation of heavier ions



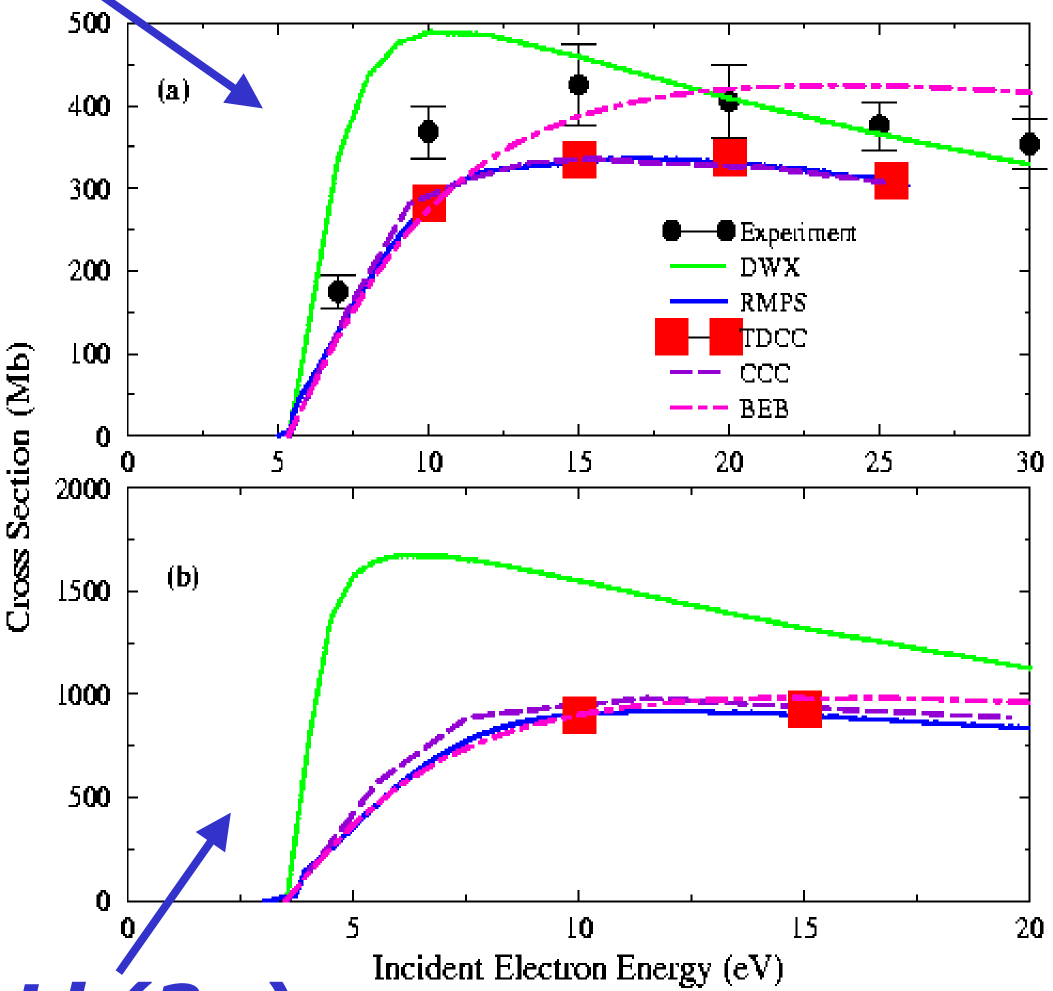
- Large R-matrix calculations (with no pseudo states) contain many levels to represent the low-lying bound states accurately

- Ne^{+}: Griffin et al, J. Phys. B (2001)
- Ne^{4+}: Griffin et al, J. Phys. B (2000)
- Ne^{5+}: Mitnik et al, J. Phys. B (2001)

- Fe^{20+}: Badnell & Griffin, J. Phys. B (2001)
- Fe^{21+}: Badnell et al, J. Phys. B (2001)
- Fe^{23+}: Whiteford et al, J. Phys. B (2002)
- Fe^{24+}: Whiteford et al, J. Phys. B (2002)
- Fe^{25+}: Ballance et al, J. Phys. B (2002)

Electron-impact ionization of lithium

Li (2s)



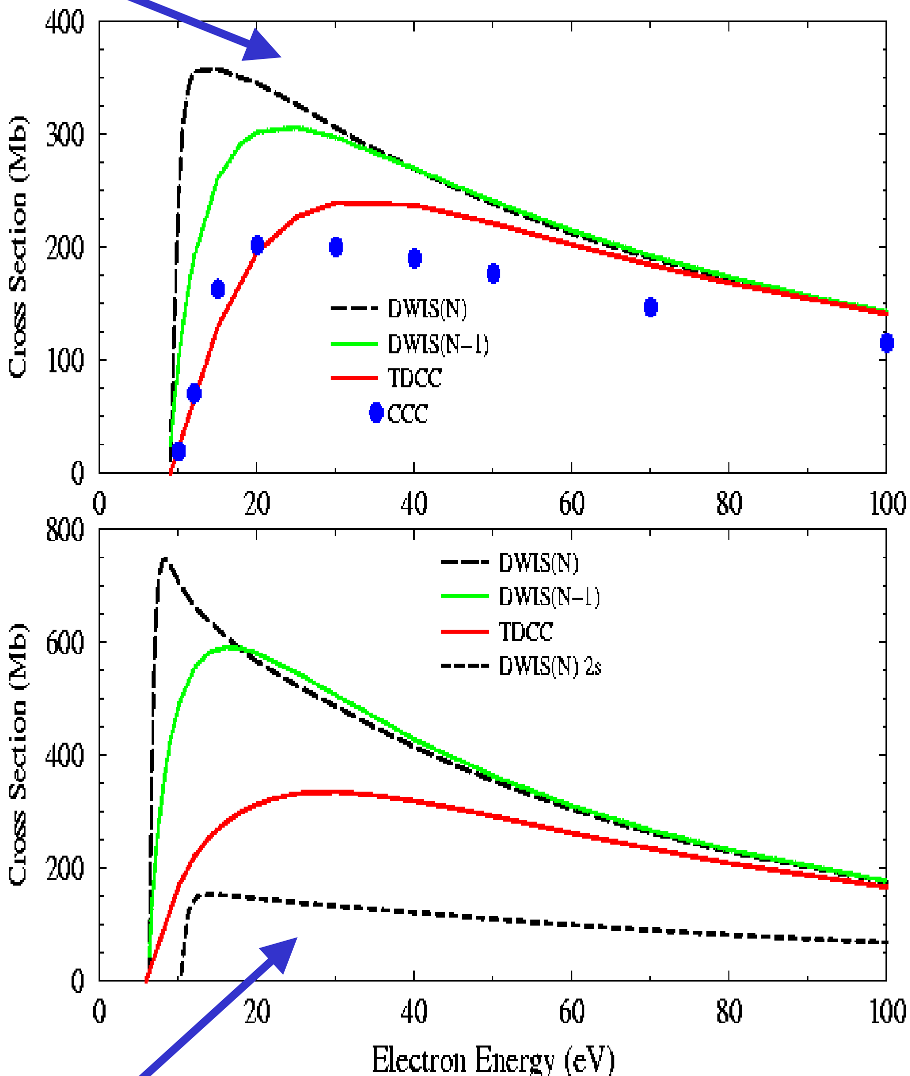
Li (2p)

- Demonstrated importance of treating the three-body Coulomb problem using non-perturbative methods
- Large differences with perturbative calculations on the order of 50 – 100 % in ionization cross section

J. Colgan, M. S. Pindzola, D. M. Mitnik, D. C. Griffin, and I. Bray, Phys. Rev. Lett. (2001)

Electron-impact ionization of Be

Be($1s^2 2s^2$)



Be($1s^2 2s2p$)

- Red line: TDCC
- Green line: DWIS(N)
- Black line: DWIS(N-1)
- Blue circles: CCC

- Large differences near ionization threshold and cross section peak between the perturbative and nonperturbative calculations
- No experimental measurements with which to compare for either configuration

J. Colgan, S. D. Loch, M. S. Pindzola, C. P. Ballance, and D. C. Griffin, Phys. Rev. A (2003)

Dielectronic Recombination

•Project well underway to calculate dielectronic recombination rate coefficients for complete isoelectronic sequences

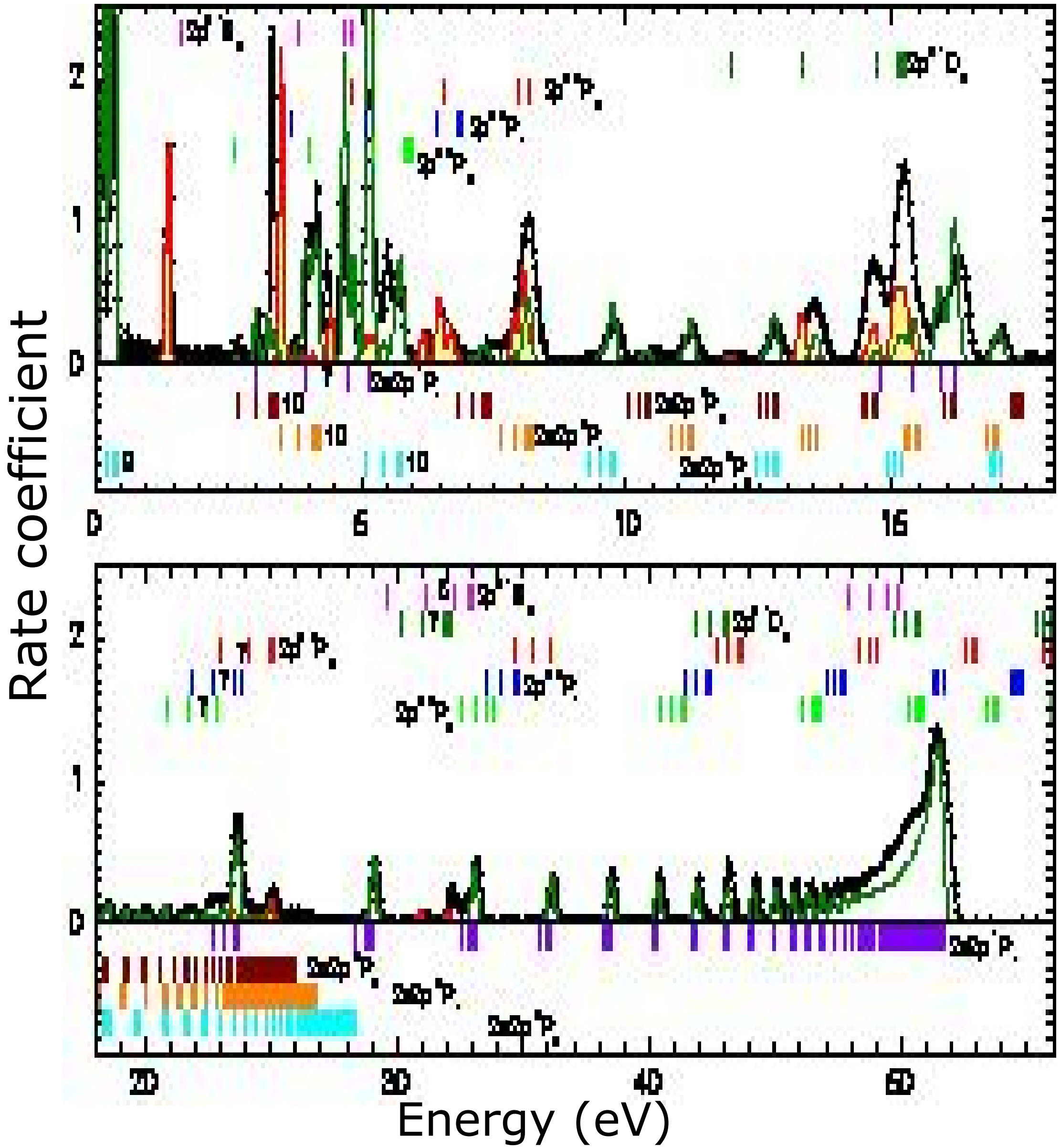
•Currently completed H-like through Be-like sequence

•Moving onto second row of periodic table

•Theoretical approach most accurate at high temperatures where recombination project is focused towards fusion plasma applications

•***Theory & Methodology:*** ***Badnell et al, A&A (2003)***
•***H-like ions:*** ***Badnell et al, A&A (2003)***
•***He-like ions:*** ***Badnell et al, A&A (2003)***
•***Li-like ions:*** ***Colgan, Pindzola, and Badnell, A&A (2003)***
•***Be-like ions:*** ***Colgan, Pindzola, Whiteford, and Badnell, A&A (2003)***

Dielectronic Recombination of Cl^{13+}



Dielectronic recombination rate coefficients for Be-like Cl^{13+}

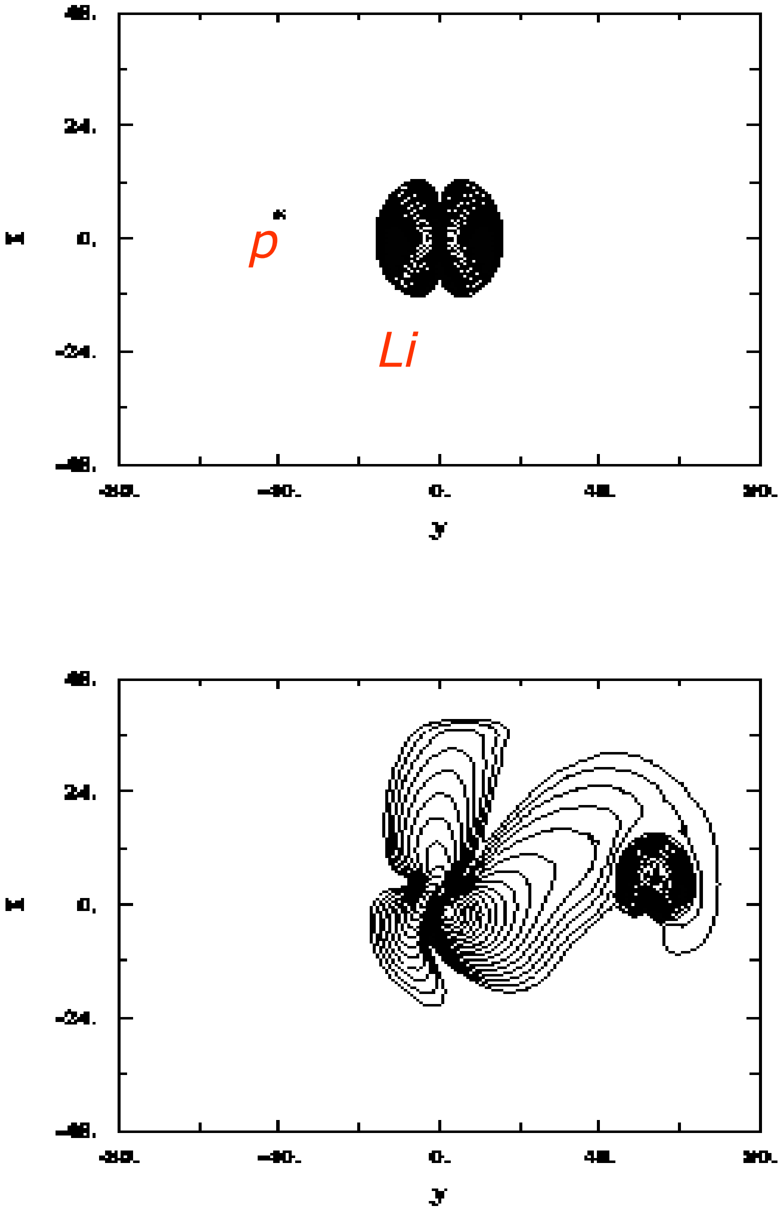
Comparisons of our theoretical calculations with experiment of Heidelberg group at the TSR

Experimental confirmation of DR project results

Trielectronic recombination (core excitation of two electrons) observed for the first time

Schnell et al. Phys. Rev. Lett. (2003)

Ion-Atom Collisions



Time-dependent evolution of electronic wave function during p + Li collision

Large scale calculations have established benchmarks by which to judge and evaluate other calculations and experiments, have lead to significant revisions of accepted results

p + H: Kolakowska, et al, Phys. Rev. A (1998)

p + H: Schultz, et al., Phys. Rev. Lett. (1999)

p + Li: Pindzola, Phys. Rev. A (1999)

p + Li:* Pindzola, Phys. Rev. A (2002)

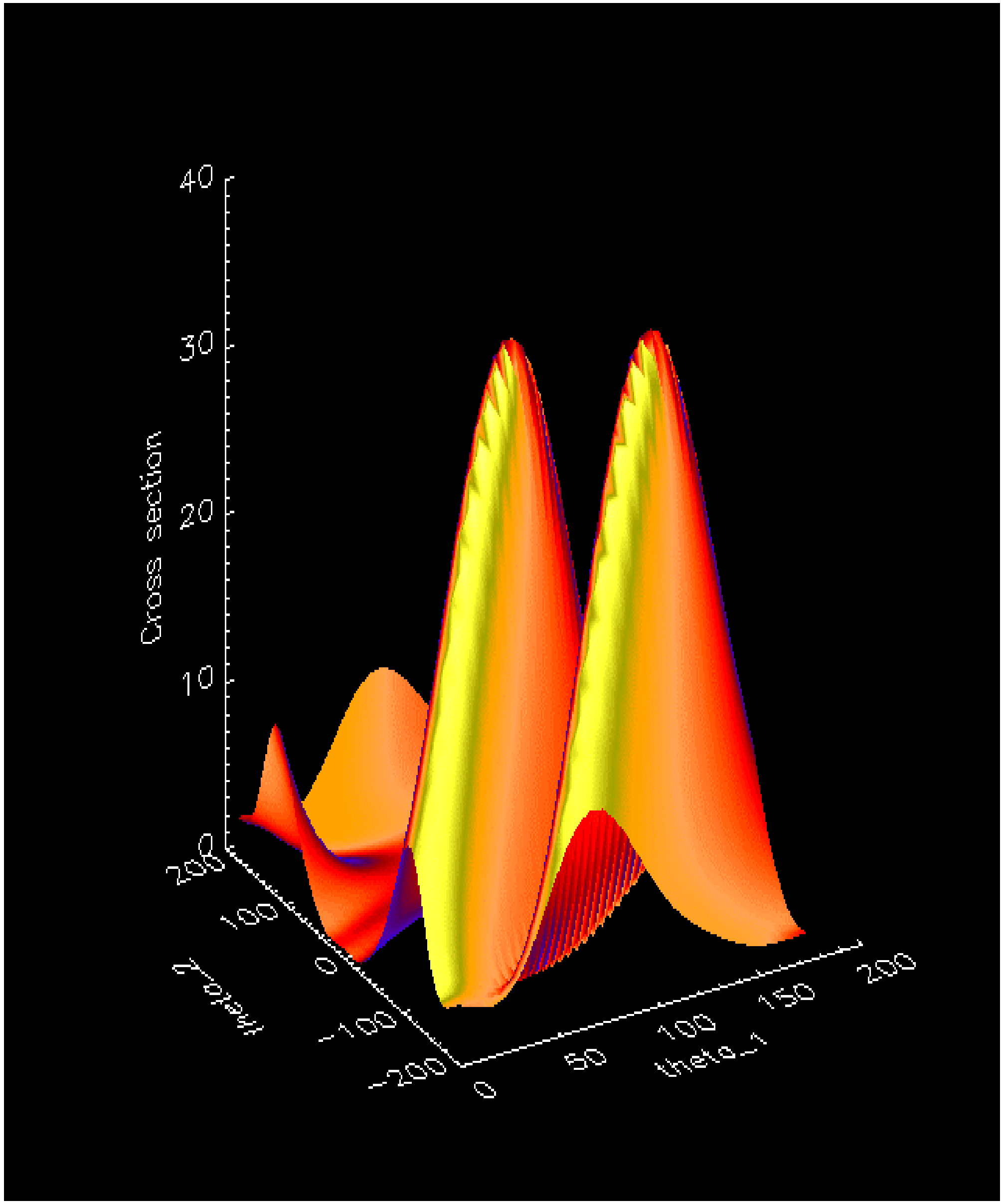
α + H: Pindzola, Minami, and Schultz, Phys. Rev. A (2003)

Currently working on:

Be^{4+}, C^{6+} + H total and state-selective charge transfer

p + H in ExB fields with the goal of reaction and population control*

Double photoionization of helium



- **$(\gamma,2e)$ He:** Colgan, Pindzola, and Robicheaux, J. Phys. B (2001)
- **$(\gamma,2e)$ He:** Colgan and Pindzola, Phys. Rev. A (2002)
- **$(\gamma,2e)$ Be:** Colgan and Pindzola, Phys. Rev. A (2002)
- **$(2\gamma,2e)$ He:** Colgan and Pindzola, Phys. Rev. Lett. (2002)
- **$(\gamma,2e)$ He*:** Colgan and Pindzola, Phys. Rev. A (2003)

Triple differential cross section at equal energy sharing between the ejected electrons

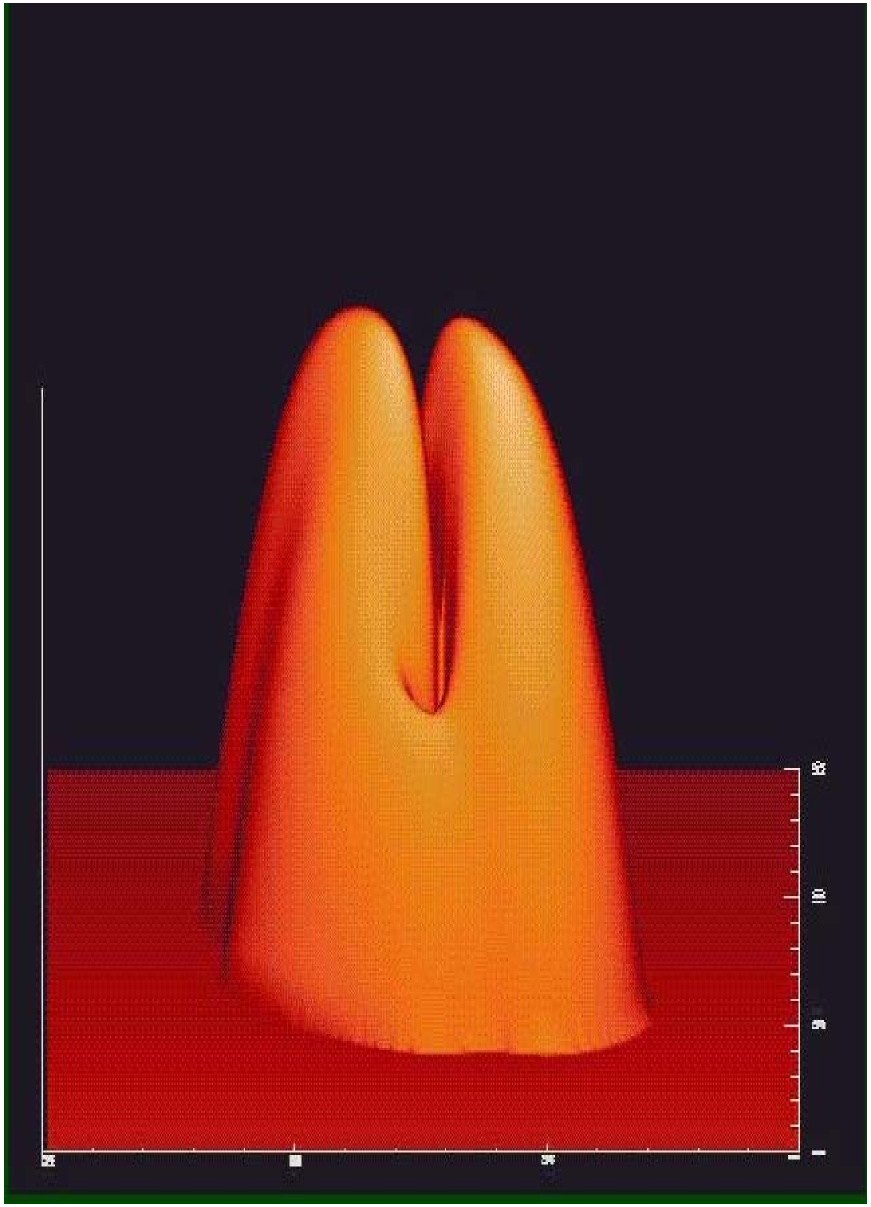
Mode excitation of a BEC soliton state

•Feder, Pindzola, Collins, Schneider, Clark, Phys. Rev. A (2000)

•Denschlag et al, Science (2000)

•Pindzola and Texier, J. Phys. B (2003)

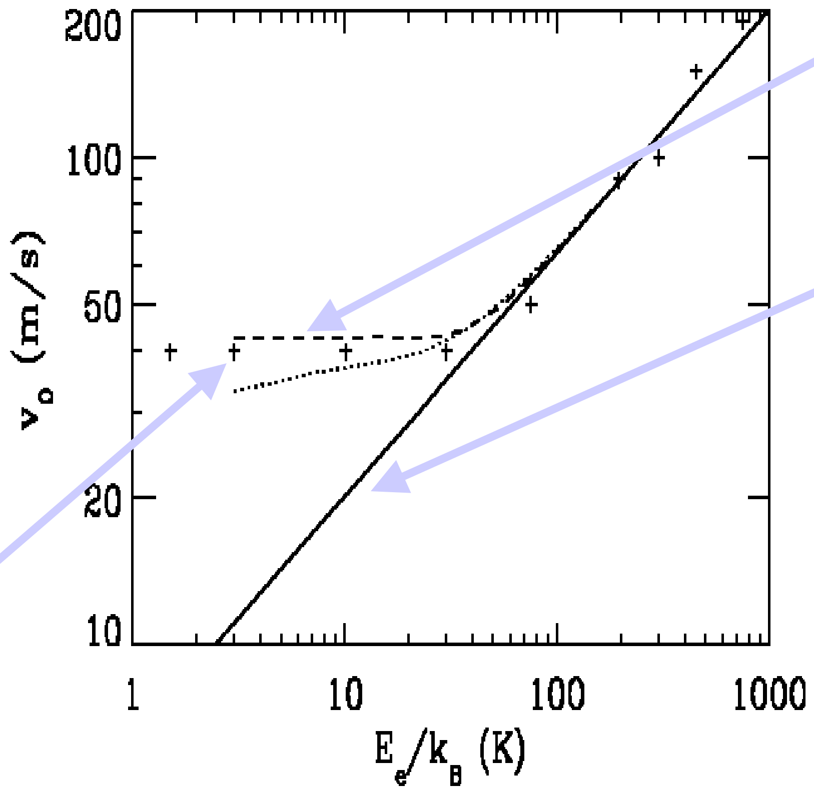
•Currently working on BEC's in wave-guides in collaboration with the MIT group of Pritchard and Ketterle



Density plot of a sodium condensate in a soliton state undergoing mode excitation

Simulations of ultra-cold plasmas

Inclusion of electron - Rydberg atom scattering and three-body recombination is necessary to properly simulate the expansion of an ultra-cold plasma



With new effects

Without new effects

Asymptotic expansion velocity

Experiment

Initial average ion energy

•Robicheaux and Hanson, Phys. Rev. Lett. (2002)

•Robicheaux and Hanson, Phys. Plasmas (2003)

Science Applications

1. **Li beam diagnostics at General Atomic's DIIID**
   - **Rate data: Physica Scripta (2003), modeling comparisons: Phys. Rev. E (2003)**
2. **Be wall studies at PISCES-B experiment at UCSD**
   - **Rate data to be published in Physica Scripta**
3. **He beam diagnostic at University of Wisconsin**
4. **PPPL, GA Beam penetration modeling**
5. **GA Charge Exchange Recombination Spectroscopy**
6. **Kr diagnostics at Tore-Supra**
   - **Kr^{q+} (PRA 2002)**
7. **W, Hf wall erosion studies at JET**
8. **X-ray spectra from Chandra and XMM-Newton**
   - **Fe^{20+} (JPB 2001), Fe^{21+} (JPB 2001), Fe^{23+} (JPB 2002), …**
9. **Early universe isotope abundances**
   - **He (PRA 2002), Li (PRA 2003)**
10. **Hypernovae spectra**
    - **Fe^{3+} (JPB 2003)**

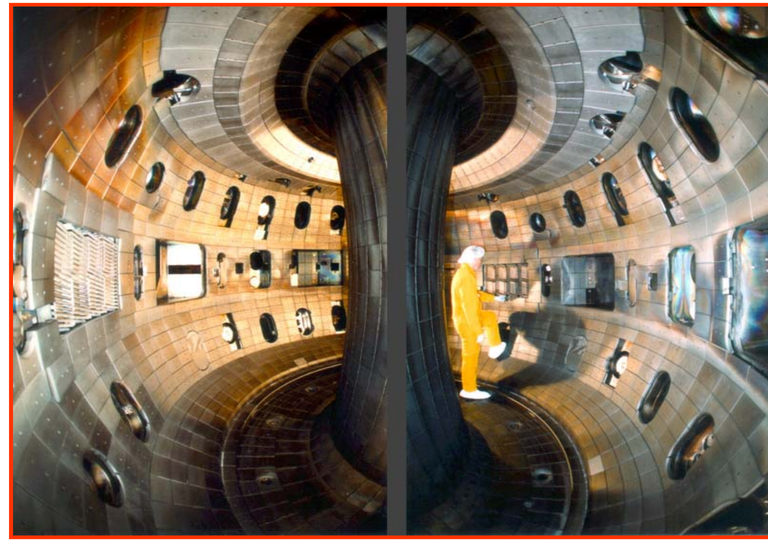
Electron-impact ionization data for fusion plasmas

- Program initiated to completely revise atomic collisional data for lithium

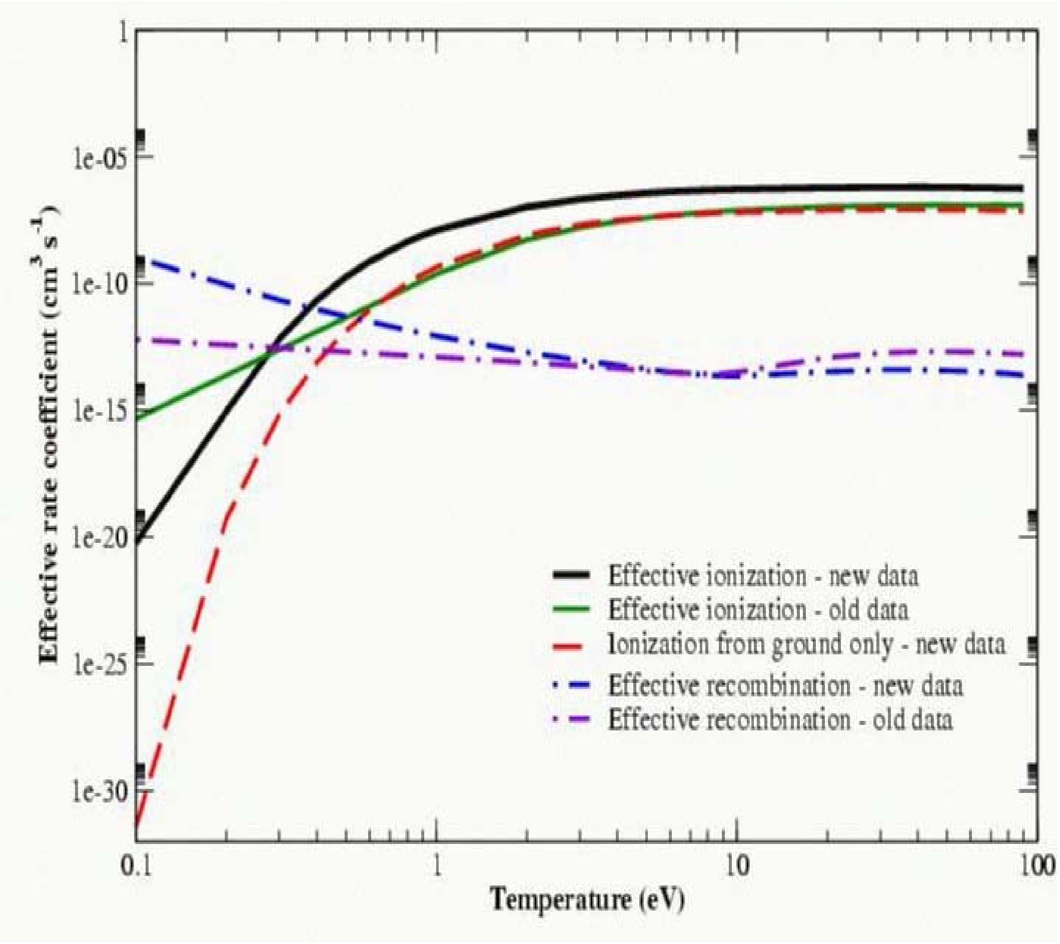
- Calculations have been used to perform modeling in support of plasma edge diagnostics made by Todd Evan's group at ***DIIID***

- Accurate atomic data essential for collisional radiative modeling to be meaningful

- Plasma modeling calculations also improve edge diagnostics at ***JET***



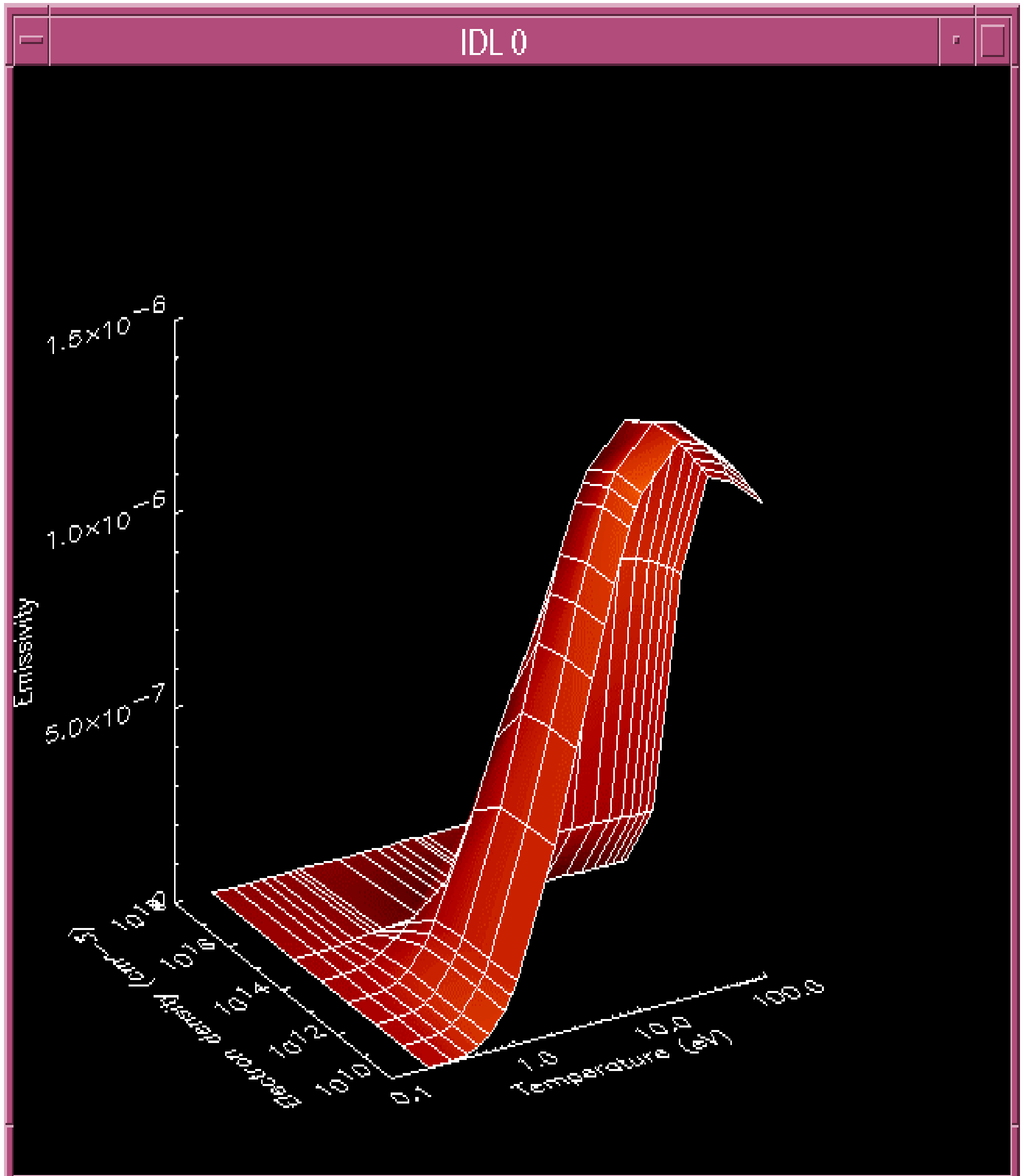
Effective ionization rates for Li



Effective ionization rate for Li at an electron density of 10^{14} cm^{-3} as a function of electron temperature

- New data for excitation, ionization, and recombination has been incorporated into an ADAS plasma modeling calculation
- Also available at CFADC database
- Very large differences compared to model using older atomic data (log scale!)
- Significant increase in the accuracy of the plasma modeling for lithium
- ***Loch et al, Physica Scripta, (2003)***

Li emissivity coefficients

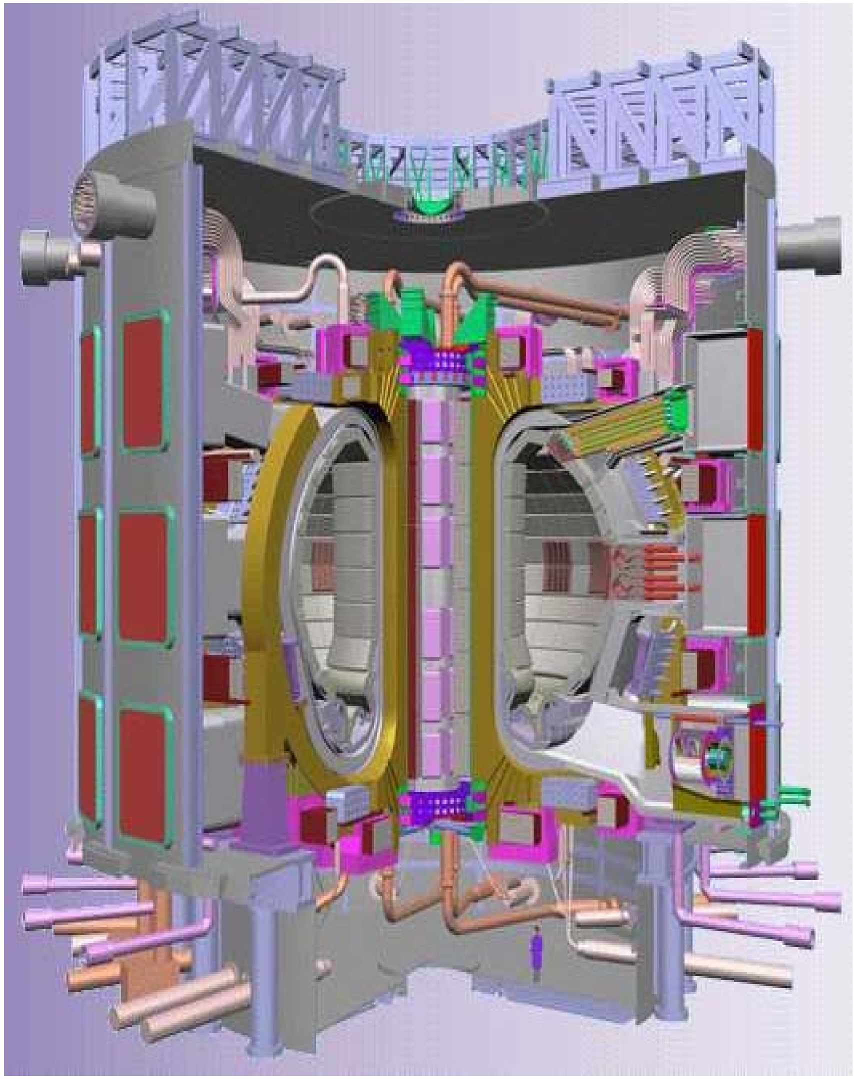


- Emissivity coefficients as a function of electron temperature and density
- Obtained from ADAS modeling calculation
- Data such as this is used in a wide range of fusion plasma edge diagnostics
- Also comparing these and similar plasma characteristics with modeling calculations made using Los Alamos set of computer codes
- ***Loch, Fontes, et al, Phys. Rev. E, (2003)***

Collisional Data for modeling plasmas

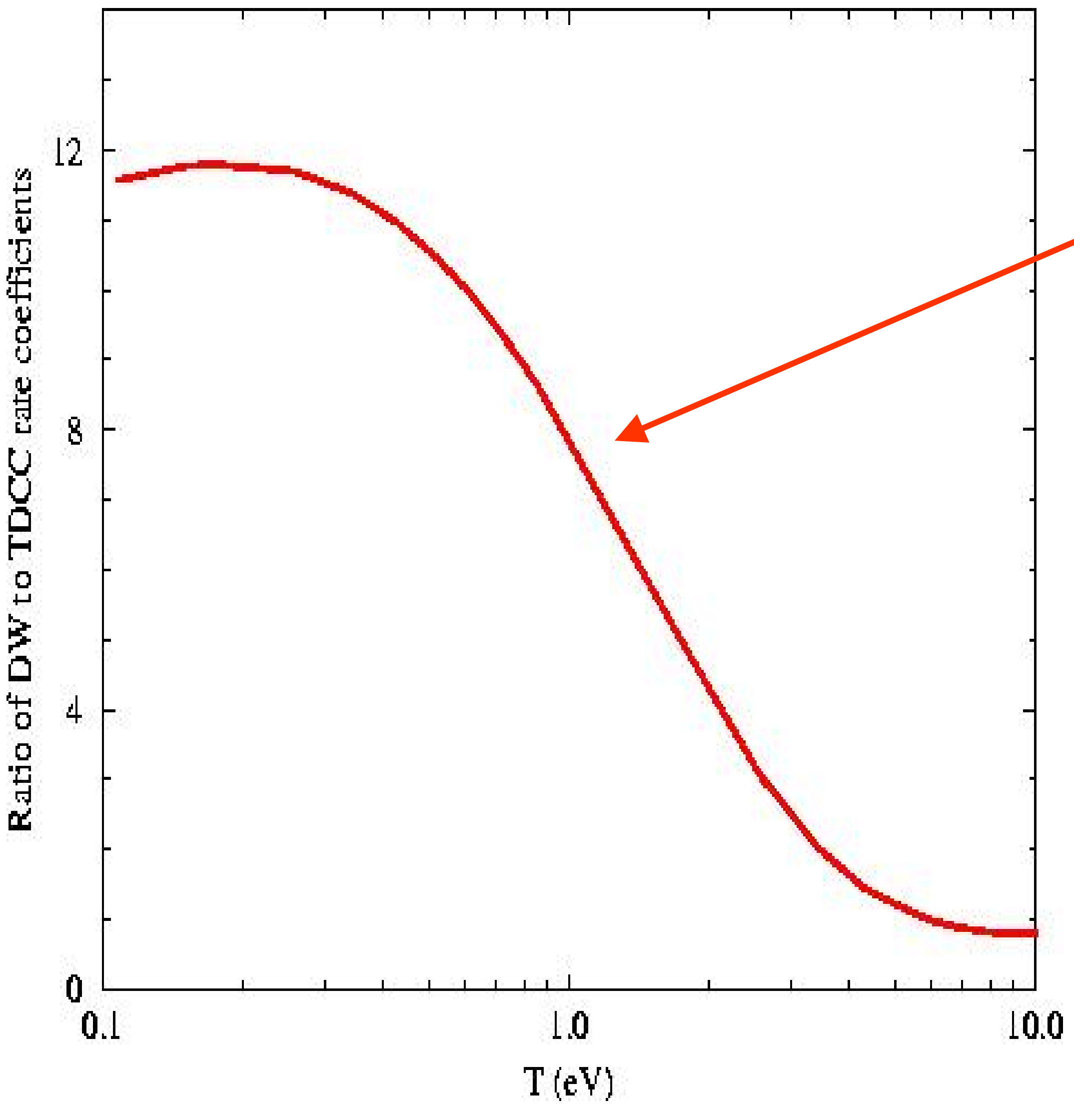
- ITER may use Be as a plasma wall component – our calculations made in support of the ITER fusion development program of Alberto Loarte (MPI – Garching)

- Collisional Radiative modeling also made for the PISCES-B fusion device which will use Be as a potential plasma-facing wall component – in collaboration with Russ Doerner's group at UCSD



ITER

Be data applications



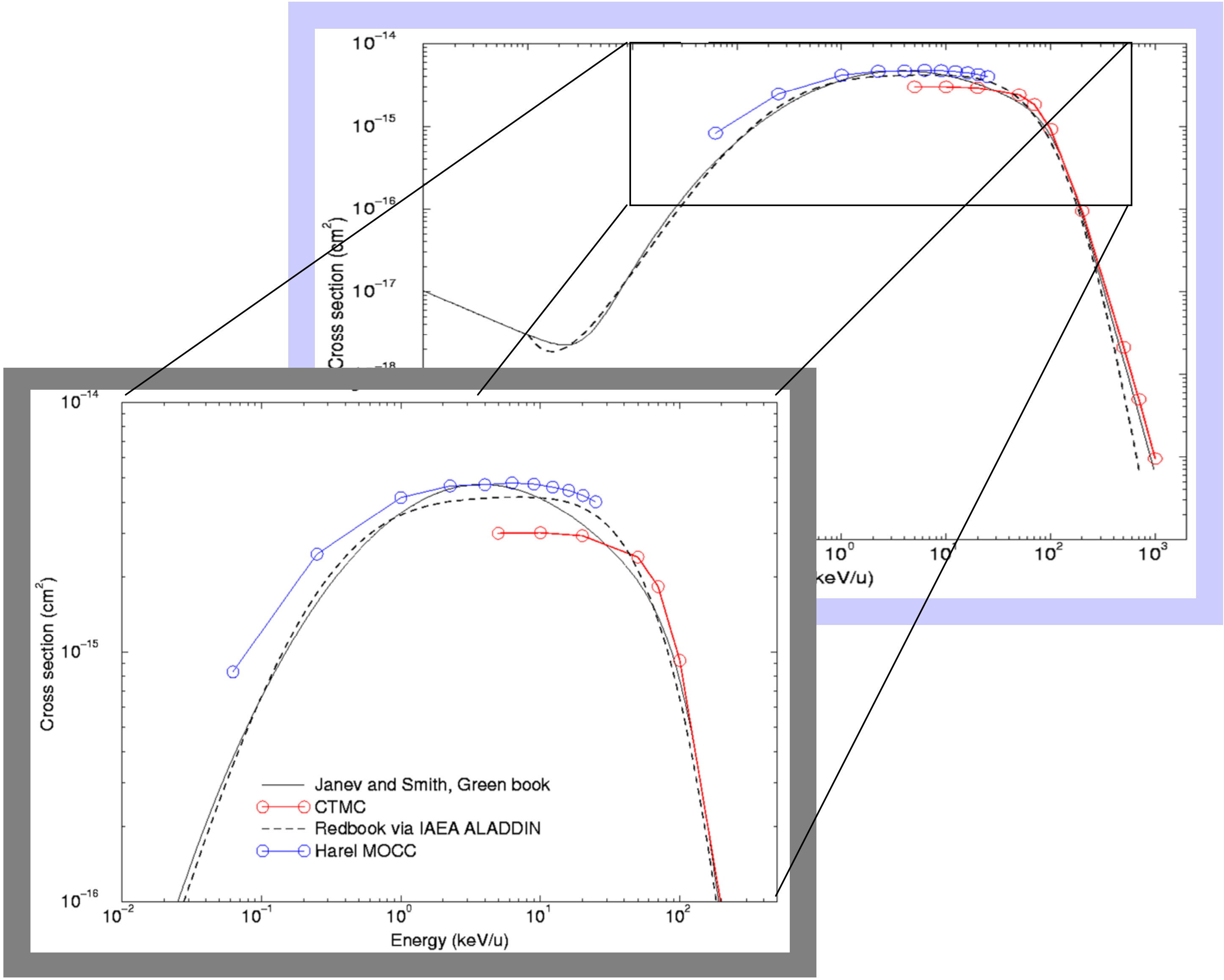
Ratio of ionization rate coefficients for Be

Large difference between typically employed DW calculations and new TDCC results show as much as a factor of 10 difference in the rate coefficient

Revision of TRANSP and ONETWO collision data

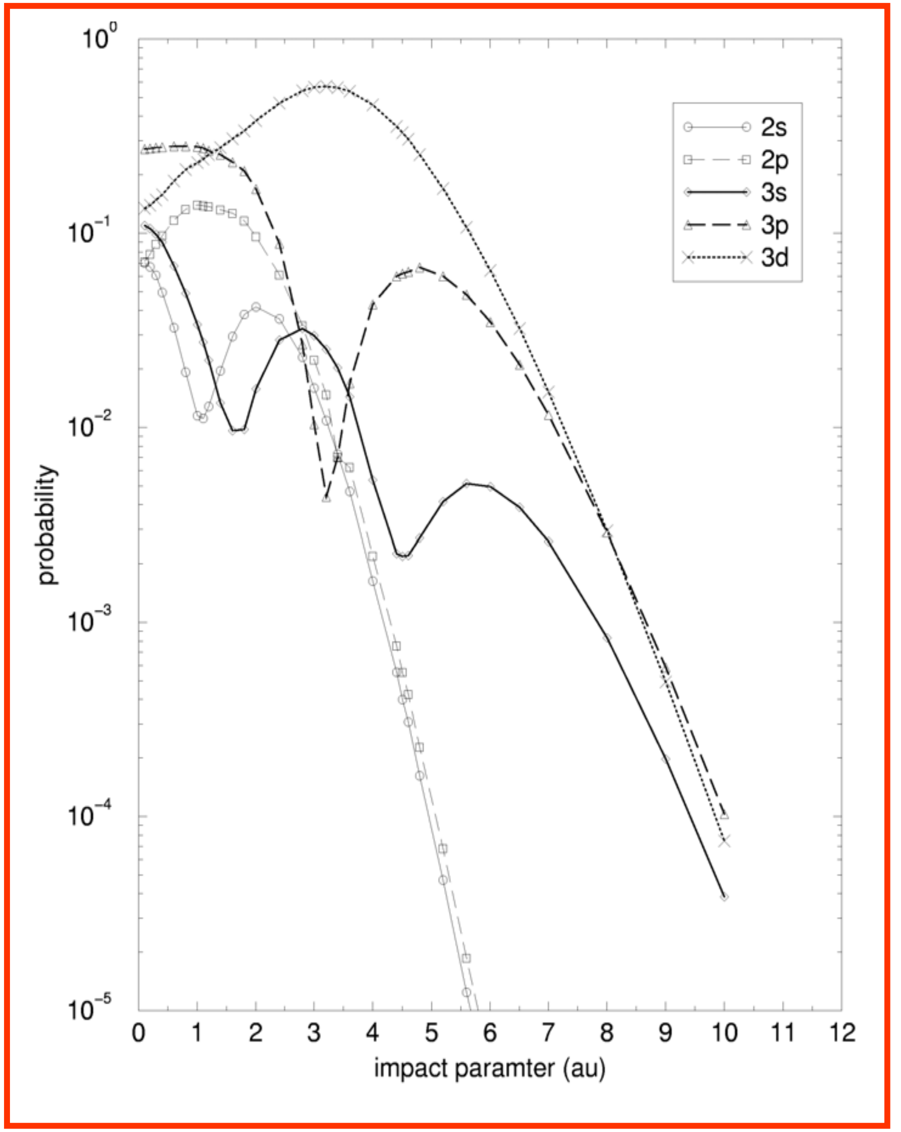
- Data needed to update the inelastic, heavy-particle collision database used by TRANSP (PPPL, McCune) and ONETWO (GA, Murakami) for neutral beam deposition, transport modeling
  - Priorities include charge transfer, ionization/excitation of light impurity ions (C^{6+}, O^{8+}, Be^{4+}) between 10 eV and 150 keV colliding with hydrogen
  - Next phase, excited hydrogen targets, other light impurities, helium
  - Synergy with charge exchange recombination spectroscopy data production

Status of recommended charge transfer cross section for C^{6+} + H



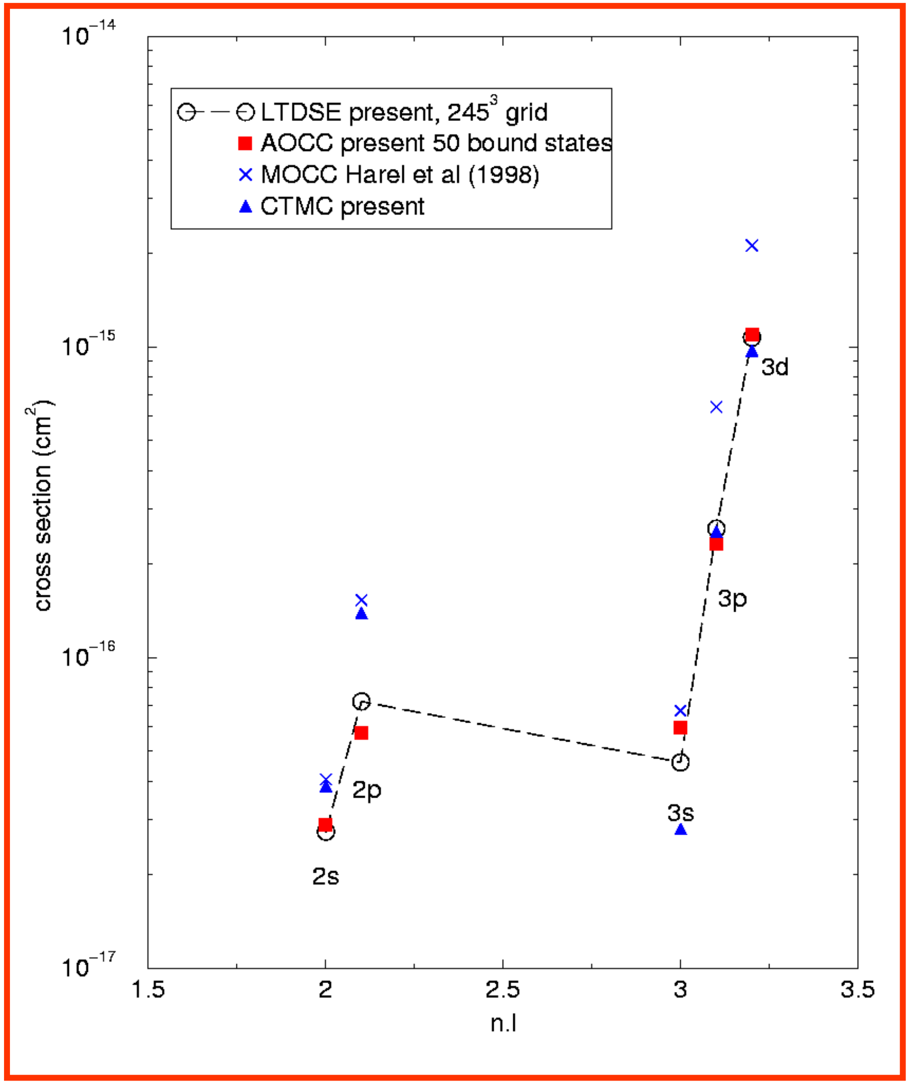
LTDSE calculations to address charge transfer data needs

- Asymmetric nuclear charges necessitate larger grids with high-order methods, 245^3 and 512^3 Fourier collocation – ORNL Cheetah IBM SP4
- First case Be^{4+} + H, H(2s)
- Impurity charge exchange database project, ions + H, H(2s)

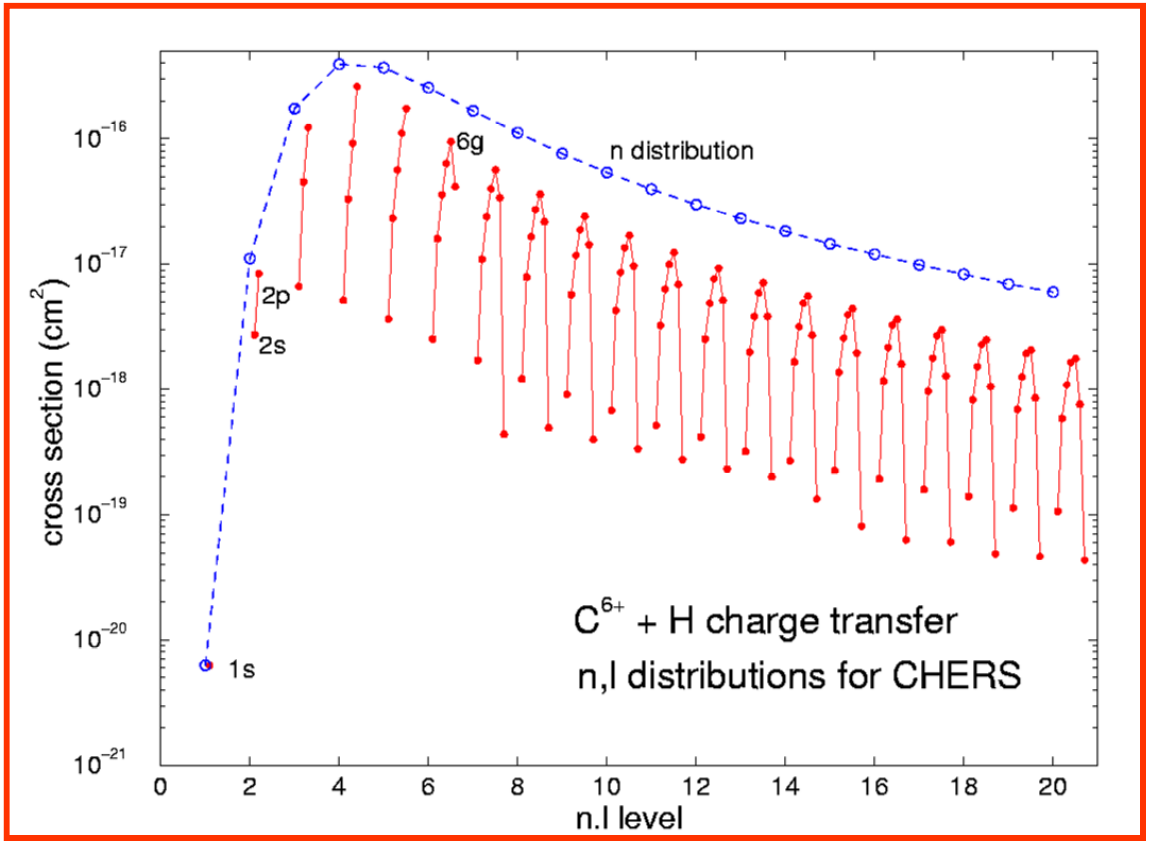


LTDSE results for Be^{4+} + H charge transfer

- State-selective charge transfer results are providing stringent test of other theories
- First results show significant deviations from best existing calculations
- State-selective results will benefit spectroscopy diagnostics

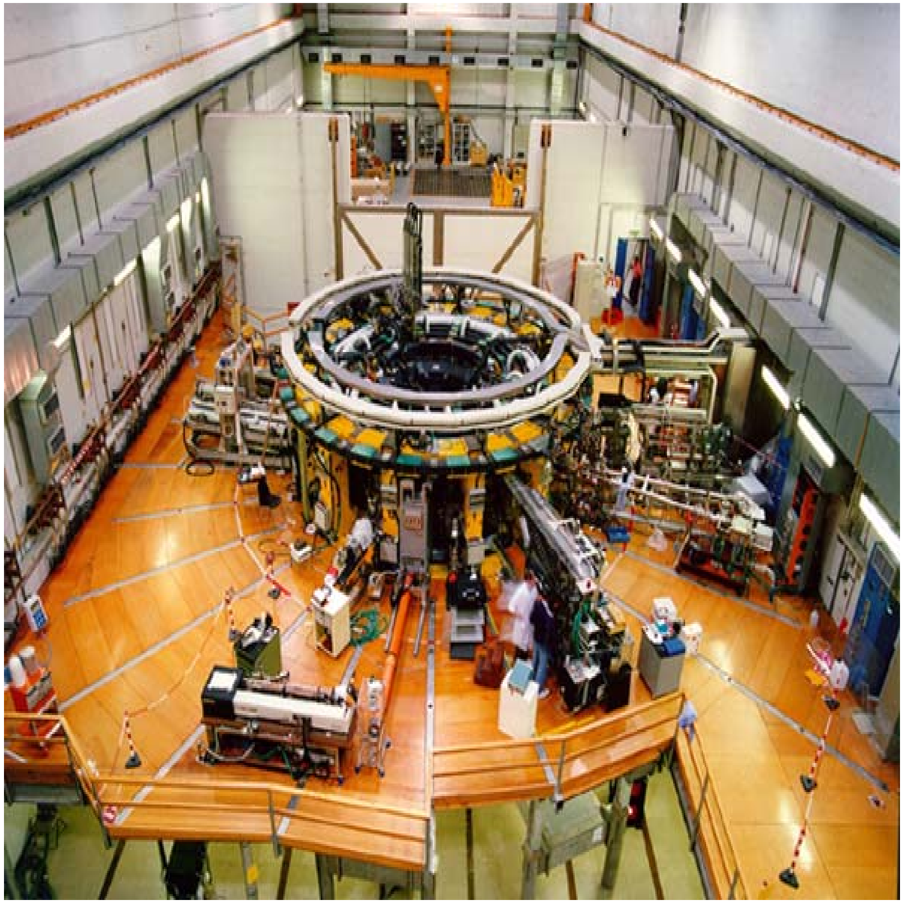


New results relevant to CHERS



- For highly charged ions of great importance to diagnostics (e.g. C^{6+}), optical transitions are detected between relatively high-lying n-levels
- MPP computer have enabled half-billion trajectory simulations to produce new results pertaining to GA diagnostics
- C, O, N, Ne, …, data will be generated for H and H^*

Heavy species plasma studies



Reverse field pinch plasma device (RFX) at Padova, Italy

- Plasma transport models study heavy species impurity transport studies
- Our calculations generated collisional rate coefficients for all ion stages of krypton
- Work has impacted plasma modeling of Mario Mattioli and coworkers at the CEA, Cadarache, France

Computational Aspects

1. **NERSC support by Ng and Lamoureux on memory access by lattice codes – Winter 2001/02**

2. **Fourier transform method by Robicheaux and Colgan for lattice codes – Spring 2002**

3. **Comparison study of TDSE1 and TDSE2 codes by Minami – Summer 2002**

4. **Variable mesh studies by Pindzola and Witthoeft – Fall 2002**

5. **Propagator studies by Robicheaux and Pindzola for lattice codes – Winter 2002/03**

6. **Comparisons of ADAS and Los Alamos plasma modeling codes by Loch and Fontes – Spring 2003**

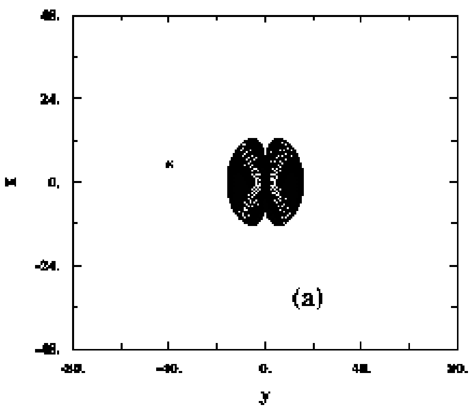
7. **ORNL PERC evalution of R-matrix and LTDSE codes – Summer 2003**

8. **NERSC support by Schwartz on 3-d visualization for four-body codes – Summer 2003**

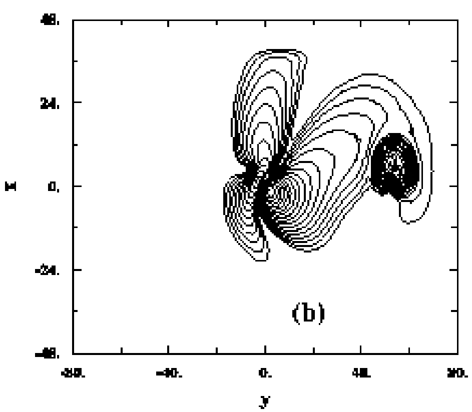
9. **Comparison study of PRMAT1 and PRMAT2 codes by Ballance and McLaughlin – Summer 2003**

LTDSE calculations of proton-lithium excitation

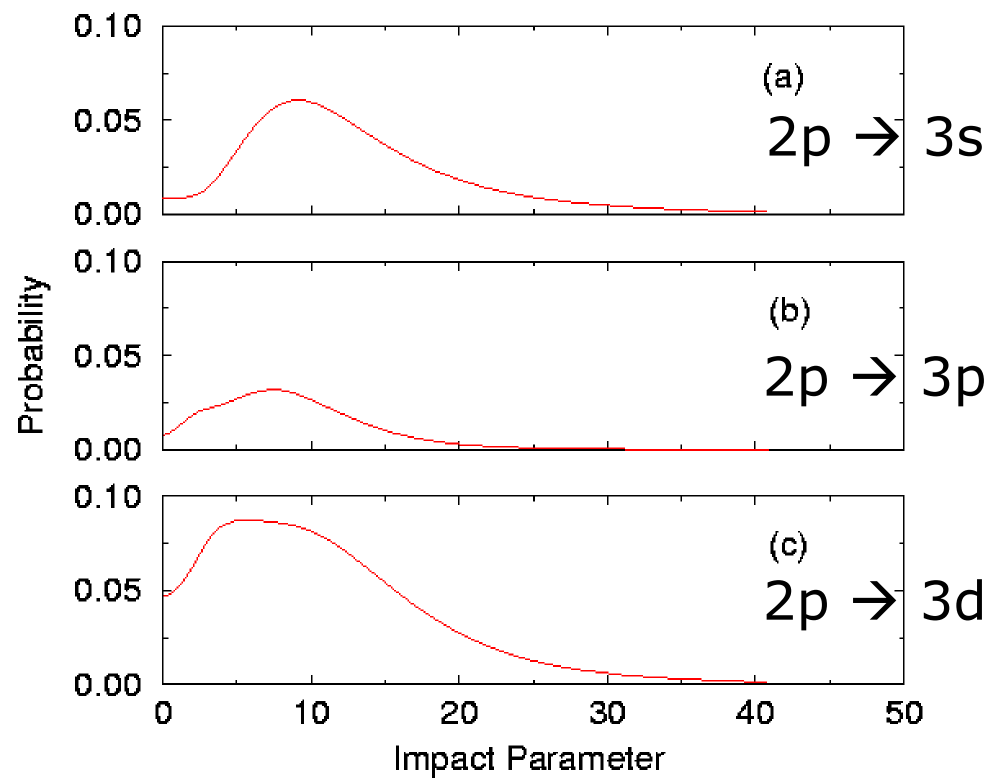
Parallel time-dependent evolution of electronic wavefunction during collision



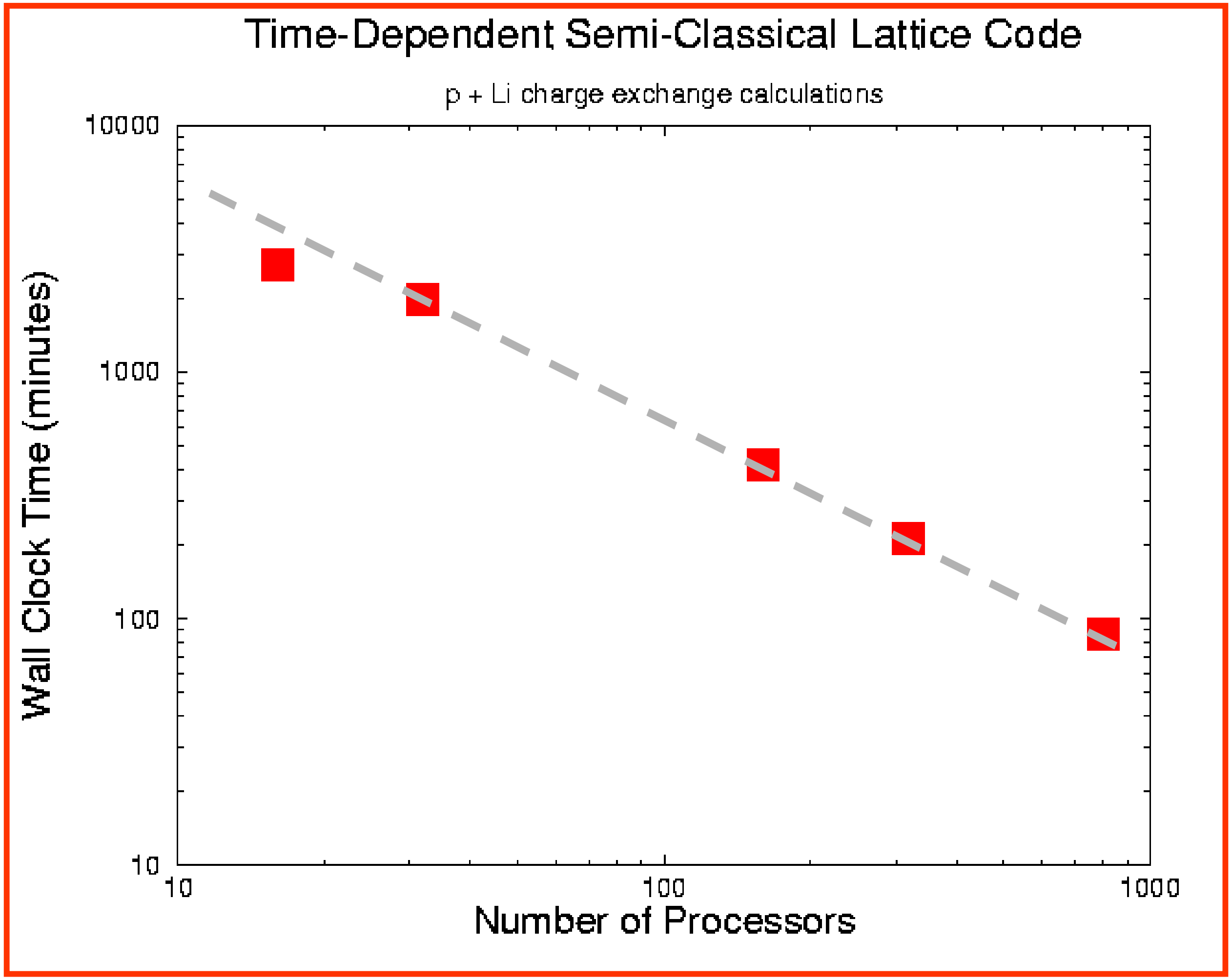
p + Li(2p)



Parallel computation of time evolutions for required impact parameters → cross sections



Scaling of the time-dependent codes on Seaborg



- Calculation of proton Li charge exchange cross sections
- LTDSE finite differences code

Science Education

- **PhD students:**
  - **M. C. Witthoeft (BS Kansas State University)**
  - **T. Topcu (BS Mamara University)**

- **Post-doctoral Fellows:**
  - **J. Colgan (PhD Queen's University, Belfast)**
  - **D. M. Mitnik (PhD Hebrew University)**
  - **S. D. Loch (PhD Strathclyde University)**
  - **C. P. Ballance (PhD Queen's University, Belfast)**
  - **T. Minami (PhD Tokyo University)**

- **Long term visitor: C. Fontes (LANL)**

- **Short term visitors:**
  - **H. P. Summers (Strathclyde University)**
  - **N. R. Badnell (Strathclyde University)**
  - **M. O'Mullane (JET)**
  - **K. Berrington (Sheffield-Hallam University)**
  - **B. M. McLaughlin (Queen's University)**
  - **T. W. Gorczcycz (Western Michigan University)**