# Electron capture and excitation in H+ collisions with Li+ and Sn

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# Outline

- Computational Method: TC-AOCC
- Cross section results for:
- p+ Li+(1s^2), Li+(1s2s), Sn (… 5p^2)

- Research Team:
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- Dr. Natasha Markovska

# Computational method: TC-AOCC

- Two-center expansion basis: (centers A and B)

$$\Psi(\vec{r},t)=\sum_{i}^{N}a_i(t)\tilde{\phi}_i^{A}(\vec{r},t)+\sum_{j}^{M}b_j(t)\tilde{\phi}_j^{B}(\vec{r},t)$$

$$\tilde{\phi}_{i,j}(\vec{r},t)=\phi_{i,j}(\vec{r})\xi_{ETF}(r,t;v)$$

$$\phi_{nlm}(\vec{r})=\sum_{k}c_{nk}\chi_{klm}(\vec{r})$$

$$\{\chi_{klm}(\vec{r})\}:\ suitable\ basis\ (STO,GTO.,\ldots)$$

# Coupled Equations (C.E.)

$$(H - i\frac{\partial}{\partial t})\Psi(\vec{r},t) = 0$$

$$H = -\frac{1}{2}\Delta_{\vec{r}} + V_A(r_A) + V_B(r_B)$$

$$i(\dot{A} + S\dot{B}) = HA + KB$$

$$i(\dot{B} + S^*\dot{A}) = \bar{K}A + \bar{H}B$$

$$H = [H_{ii}],\ \bar{H} = [\mathrm{H}_{jj}],\ K = [\mathrm{H}_{ij}],\ \bar{K} = [\mathrm{H}_{ji}]$$

# Solution of C.E. and cross sections

- Classical motion of nuclei
- (straightline trajectory; IPM)
- Initial conditions (A-target, B-projectile):

CX and Exc. $a_i(-\infty) = \delta_{1i}, \quad b_j(-\infty) = 0$

$$\sigma_{ex,i} = 2\pi \int_0^\infty \left| a_i(+\infty) \right|^2 bdb$$

$$\sigma_{cx,\mathrm{j}} = 2\pi \int_0^\infty \left| b_j(+\infty) \right|^2 bdb$$

# Collision systems and processes

- State-selective (*nl*-) electron capture and excitation cross section calculations
- Completed for: p –Li+, p -Sn
  (with IAPCM, Beijing): p-Be+, Be3+ -Li
- In progress: p-Sn+, He2+ - Li+
- Planned: He+ - Sn+, He+ - Li, Li+; He+ - Be+
- CX and Exc states: with $n \leq 4$
- Energy range: 1- 300keV/u

# Results for p +Li+(1s^2)/Li+(1s2s)

## Model potentials:

$$V_{s,t}(r) = -\frac{2}{r} - \frac{1}{r}\left(Z_1 + Z_2 r\right) e^{-Z_3 r}$$

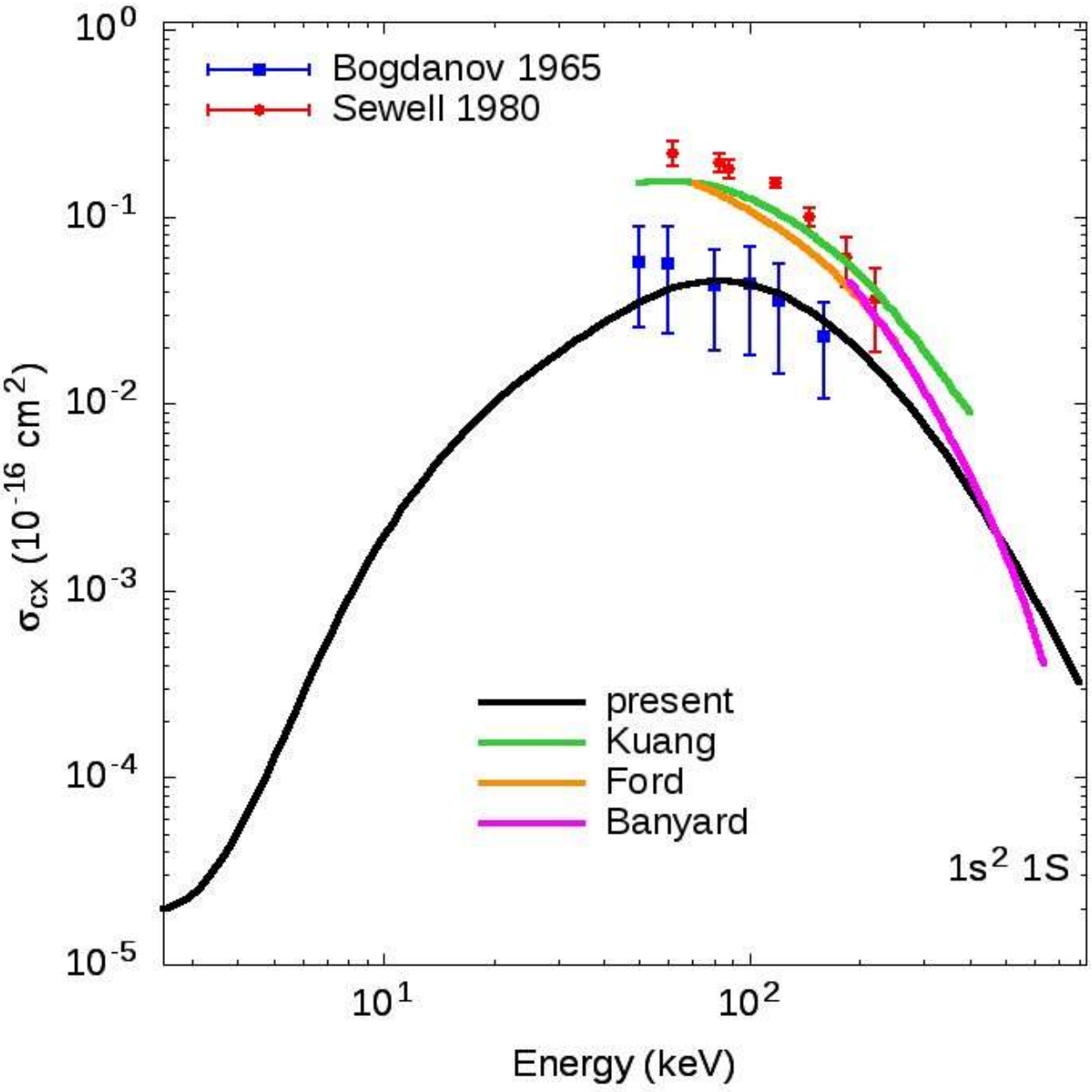
$$\text{sin}\,glet: Z_1 = 0.76294,\ Z_2 = 2.140135,\ Z_3 = 5.091085$$

$$triplet:\ Z_1 = 1.20962,\ Z_2 = 1.91843,\ Z_3 = 3.70290$$

Accuracy of excited state energies: 2%

Expansion basis: all states with n ≤ 7 on both centers

# Cross sections from Li+(1s^2) initial state




## *Total capture*

*Theory* :

*Kuang* : 2 *states*

$(1s-1s;\ Z_{eff}=2.36)$

*Ford* : OHCE

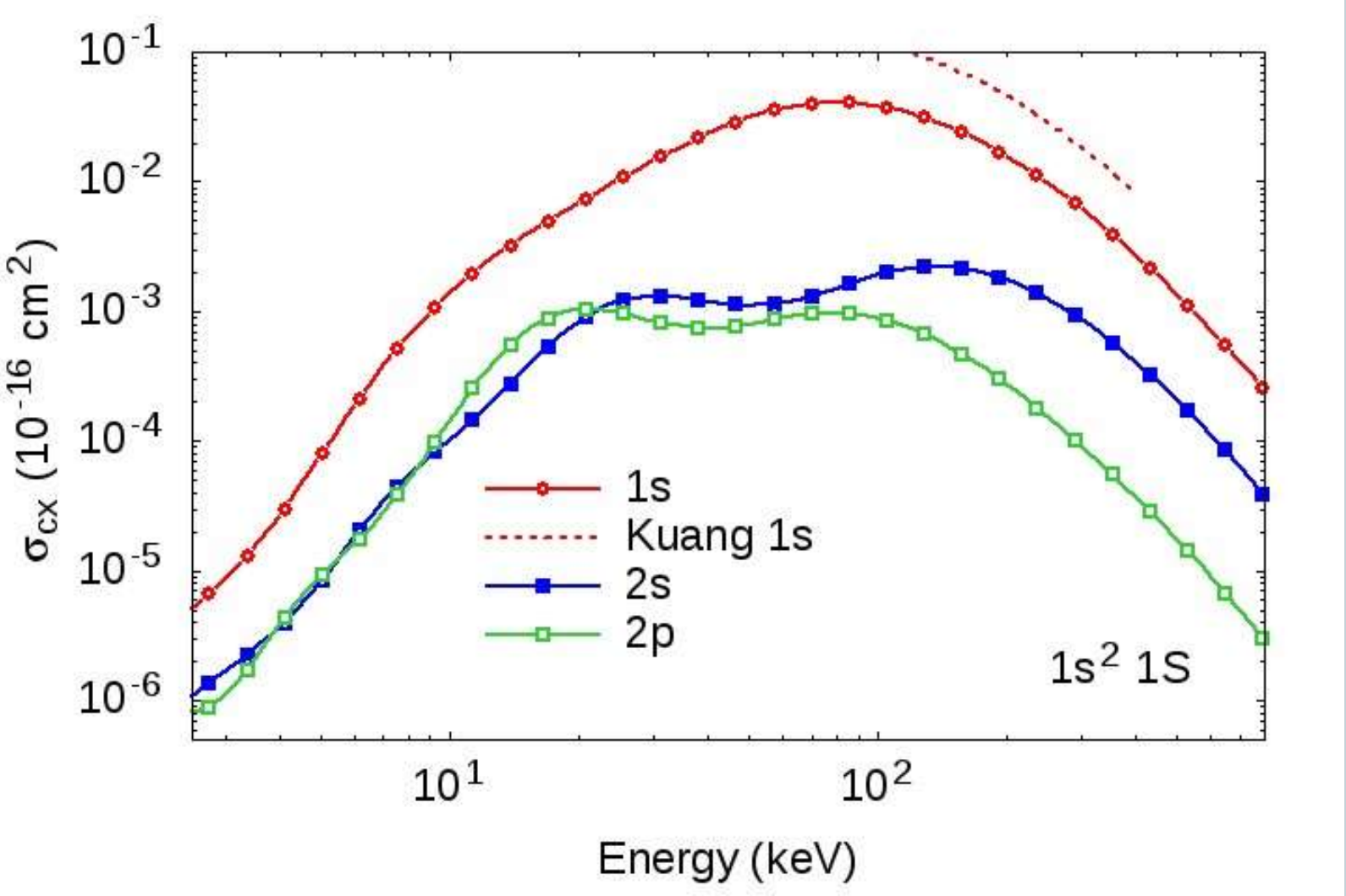
$(H:1s;Li^{+}:18 states)$

Banyard : CDW

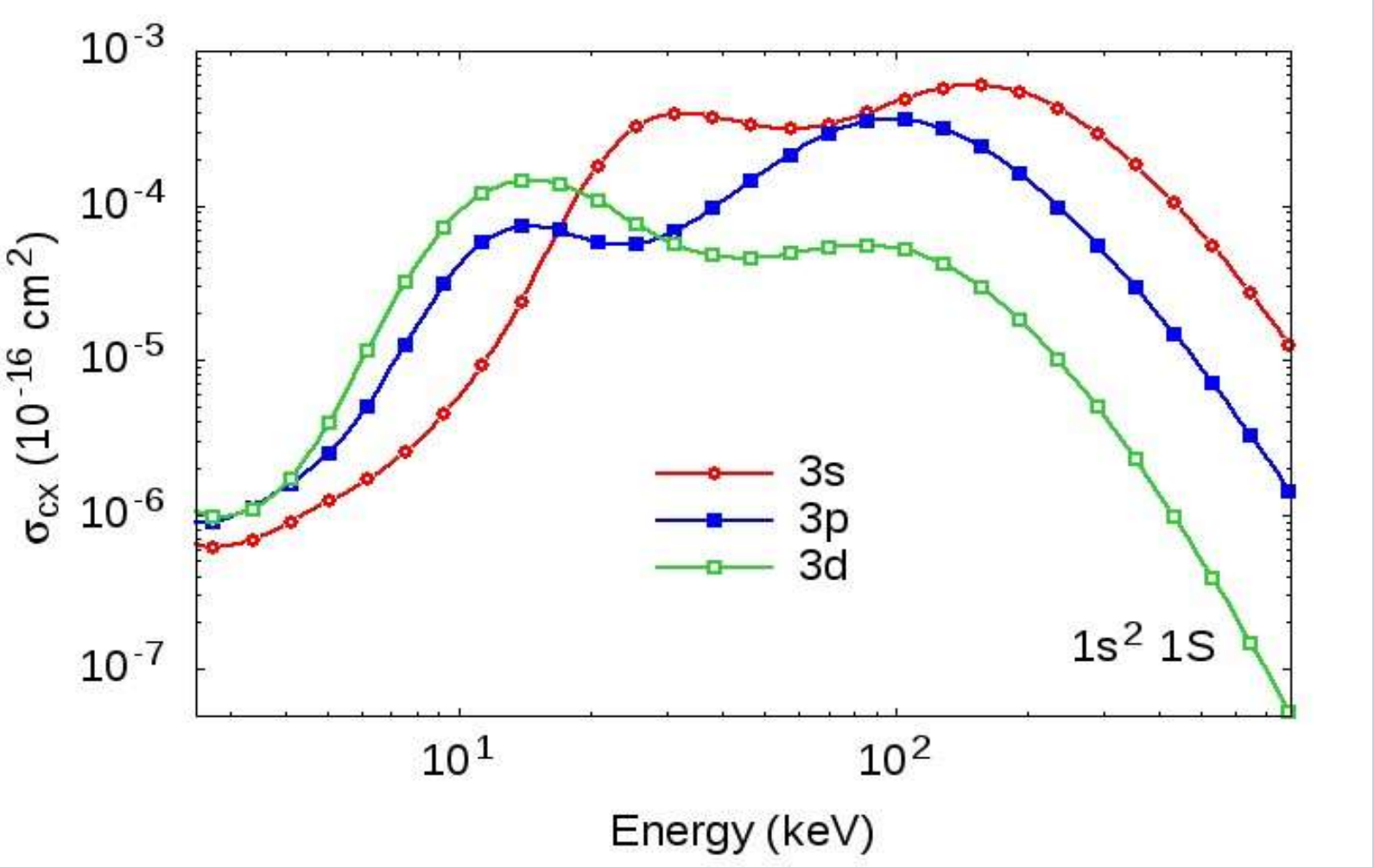
present : *all* $n \le 7$ *states*

*on both H and* $Li^{+}$

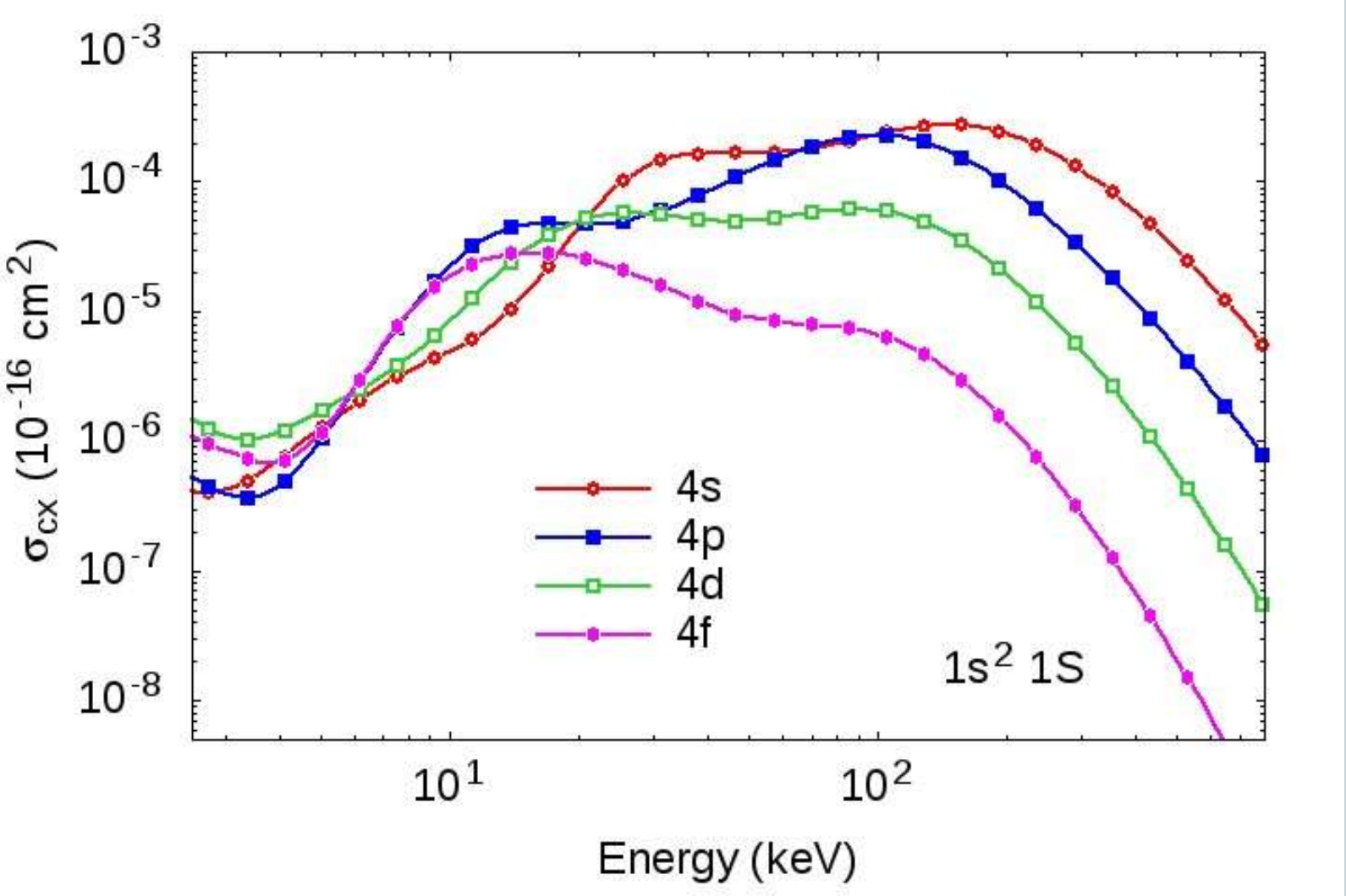
# Capture to 1s, 2s 2p



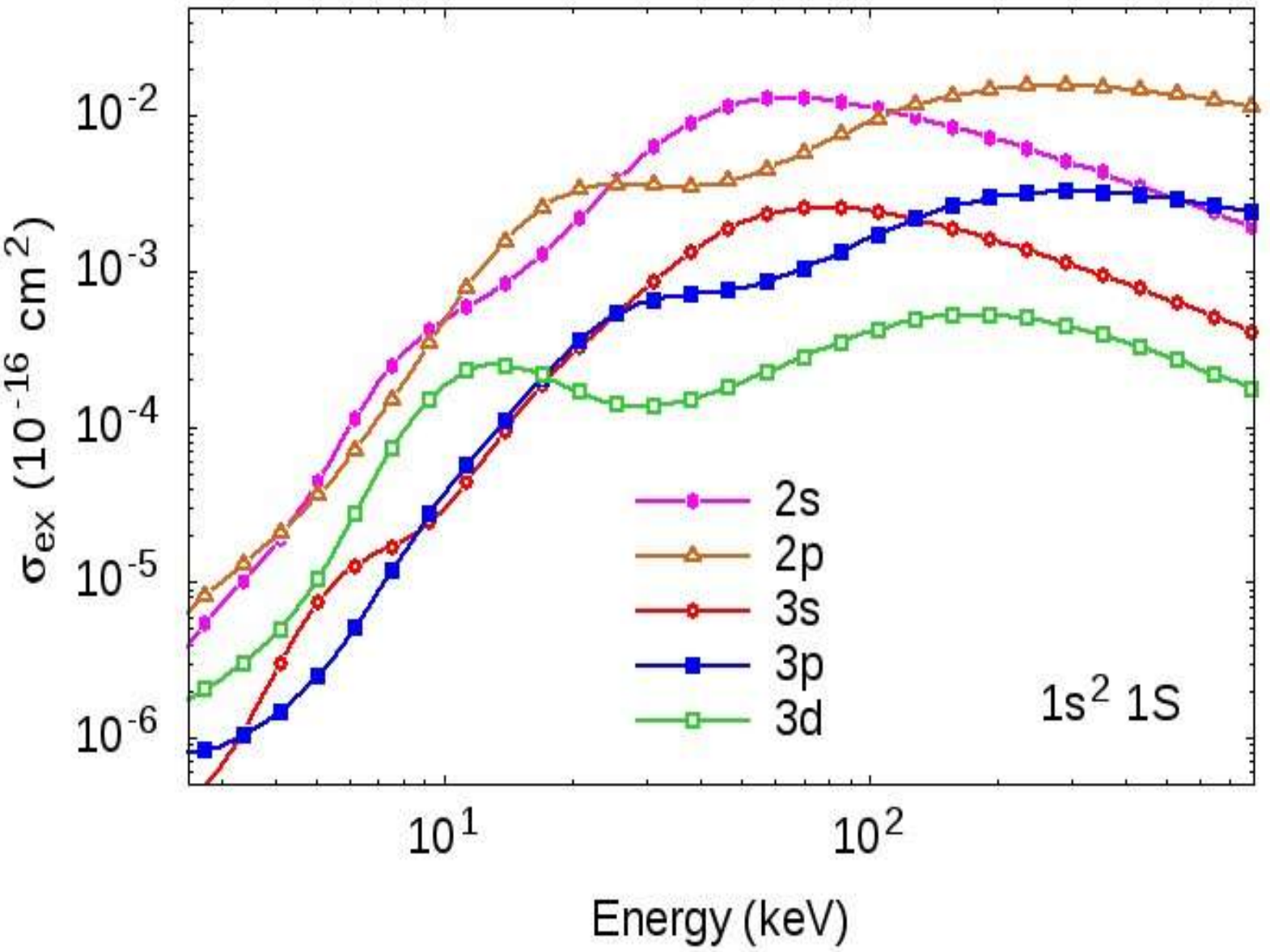
# Capture to 3l states



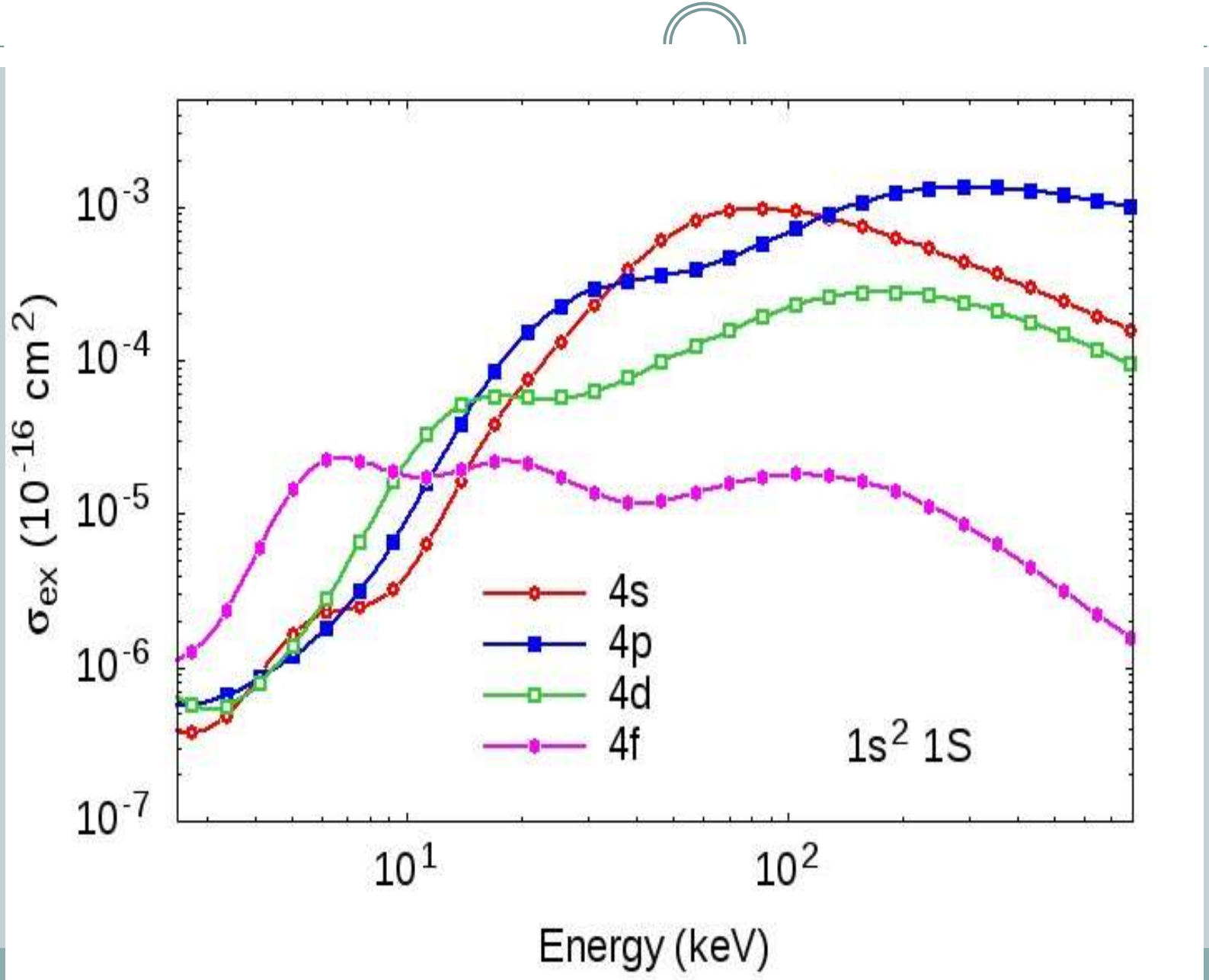
# Capture to 4l states



# Excitation to 2l and 3l states



# Excitation to 4l states



# Dynamics in p+ Li+(1s2s) system

In atomic picture:

Quasi-resonant energy levels (in a.u.) :

Li+ (2s 1S): -0.5411; (2s 3S): -0. 61100

(4s 1S): -0.1298; (4s 3S): -0.13719

(4p 1P): -0.1242; (4p 3P): -0.12850

(4d 1D): -0.1251; (4d 3D): -0.1252

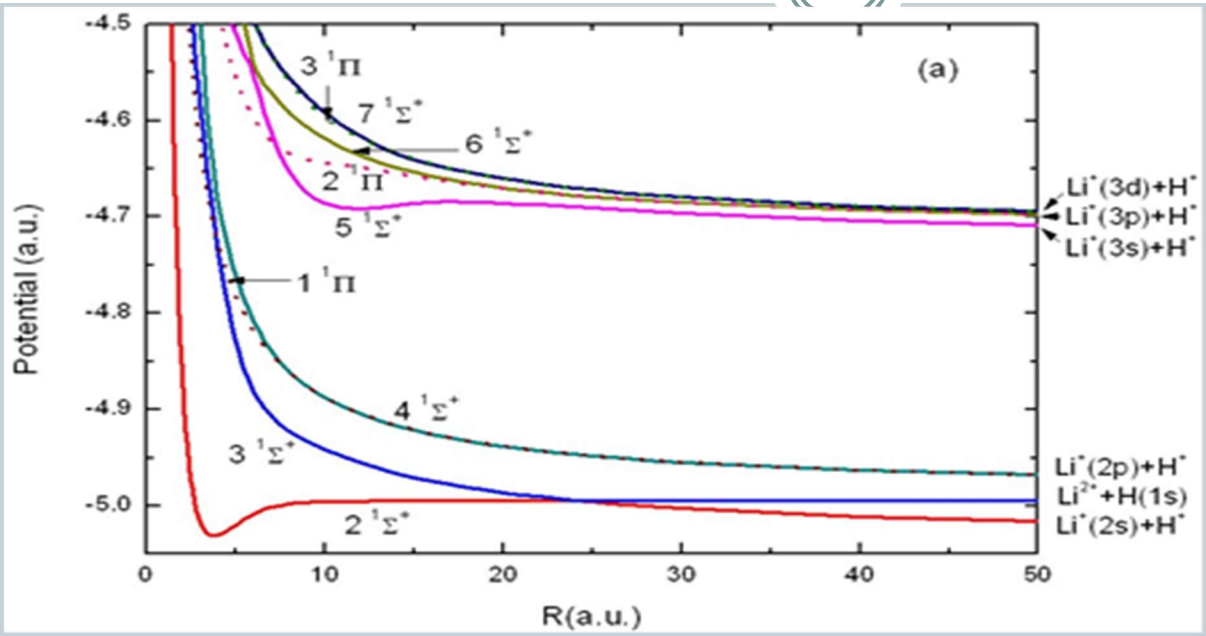
(4f 1F): -0.1251; (4f 3F): -0.1251

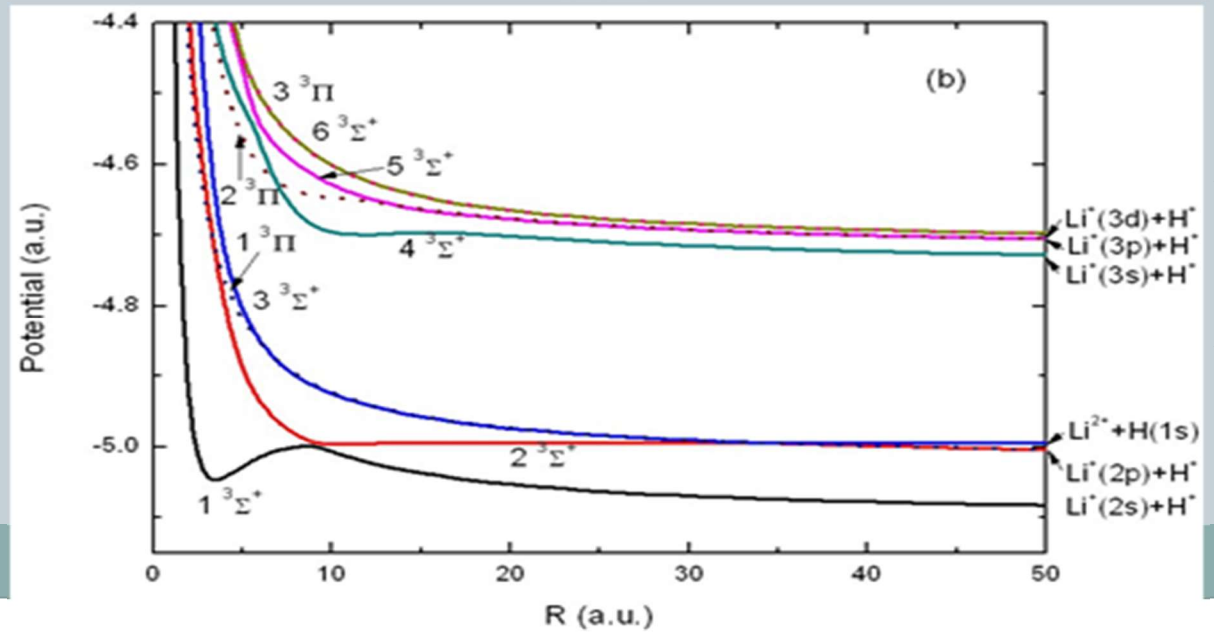
H(1s): -0.500

H(n=2): -0.125

$(e-back-capture)$

# Dynamics in MO picture:




Ref. *L.L.Yan et al.*

*EPJ D* 69, 26 (2015)

$Li^{2+} + H(1s)$ *collision*

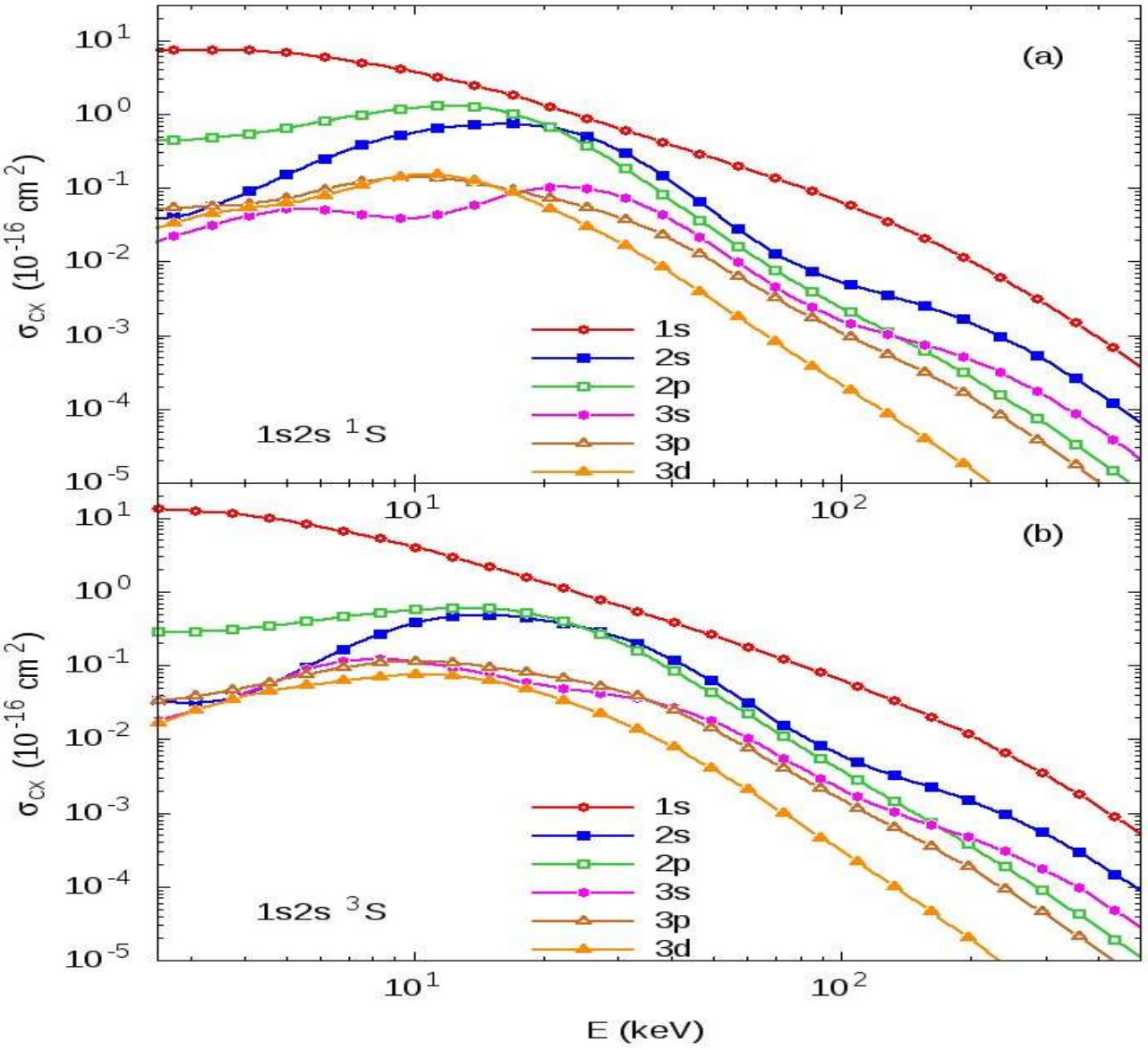
*Avoided curve – crossings:*

$R_x^s \approx 24a_0$

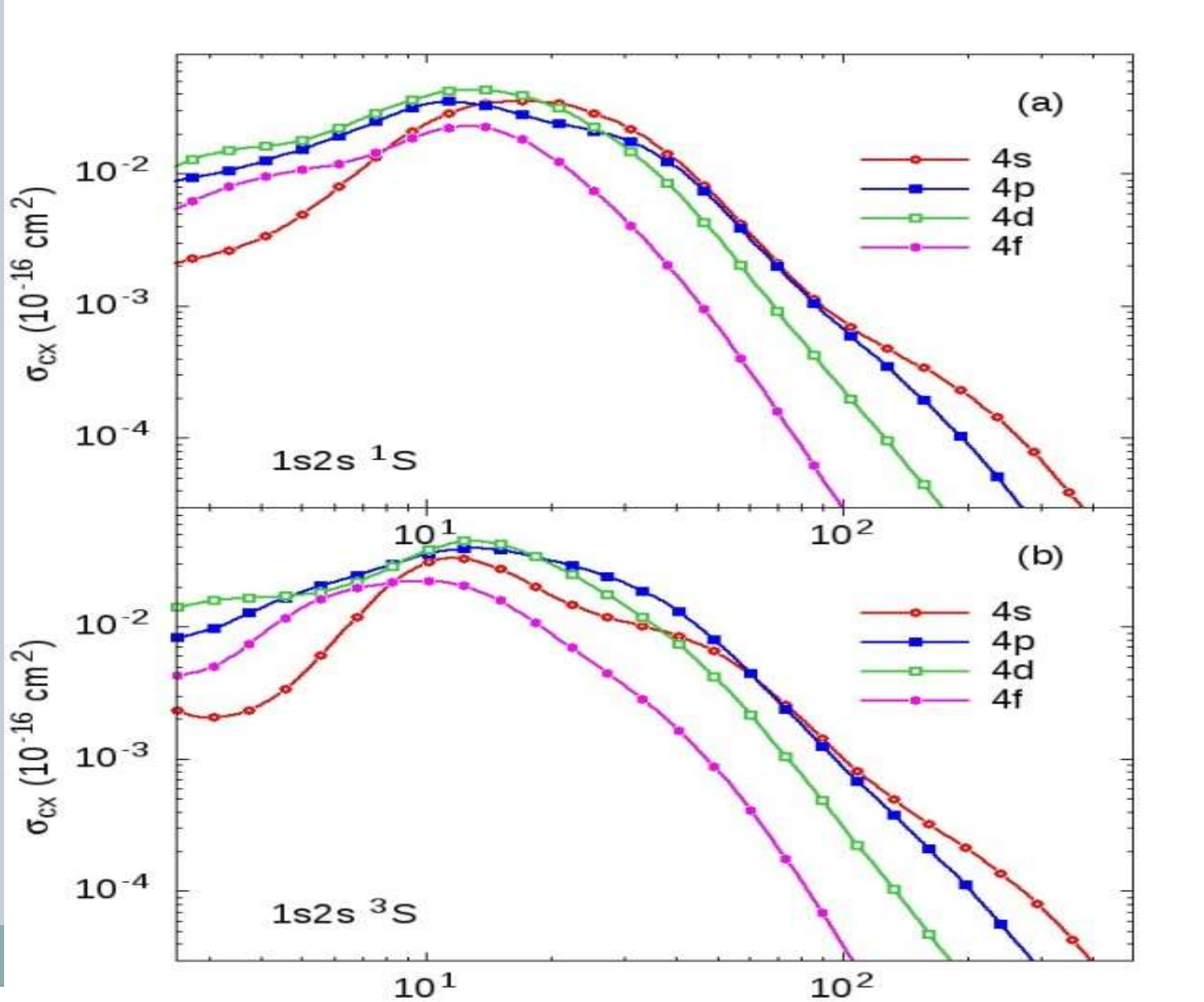
$R_x^t \approx 9a_0$

# Li+(1s2s^1,3S) initial states

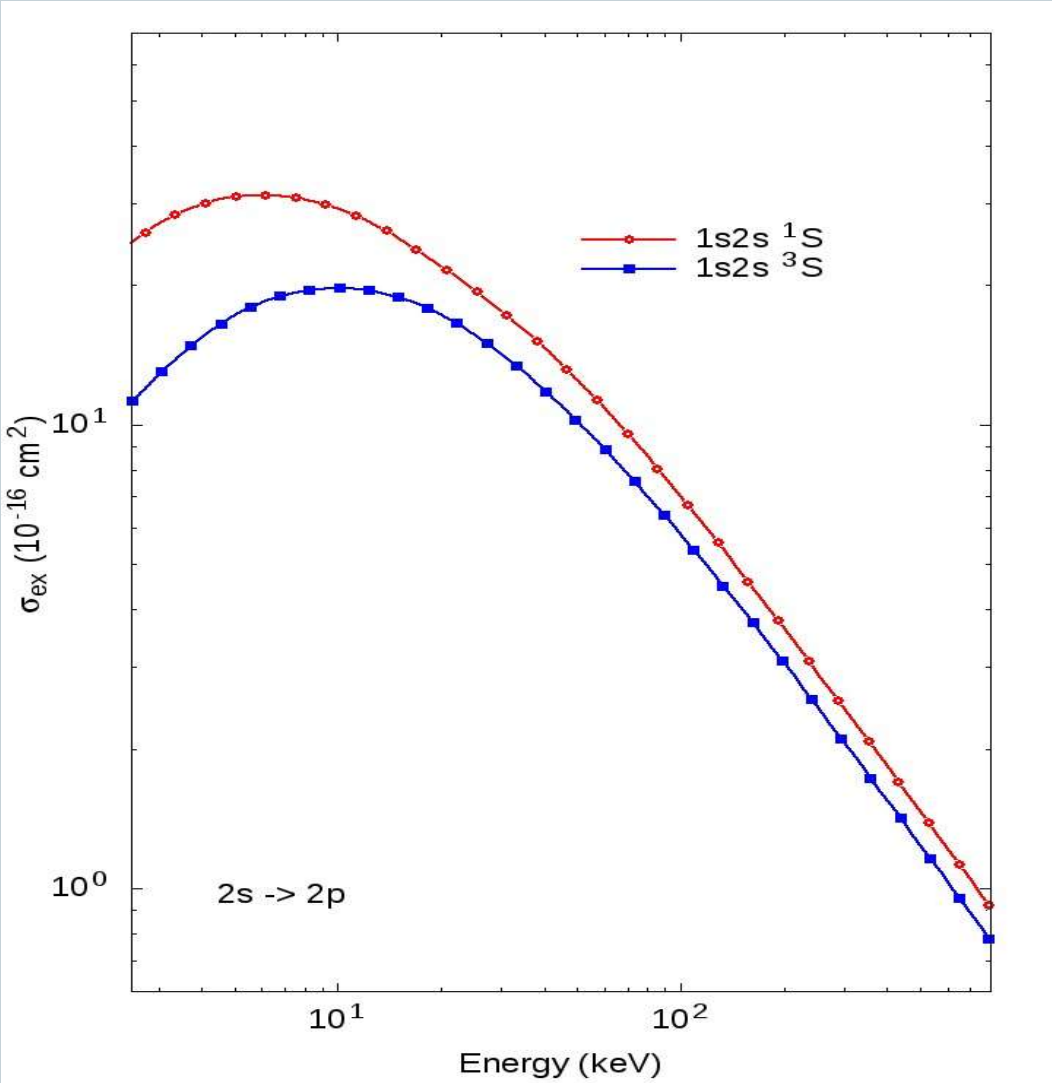
## Capture to 1s, 2l and 3l states



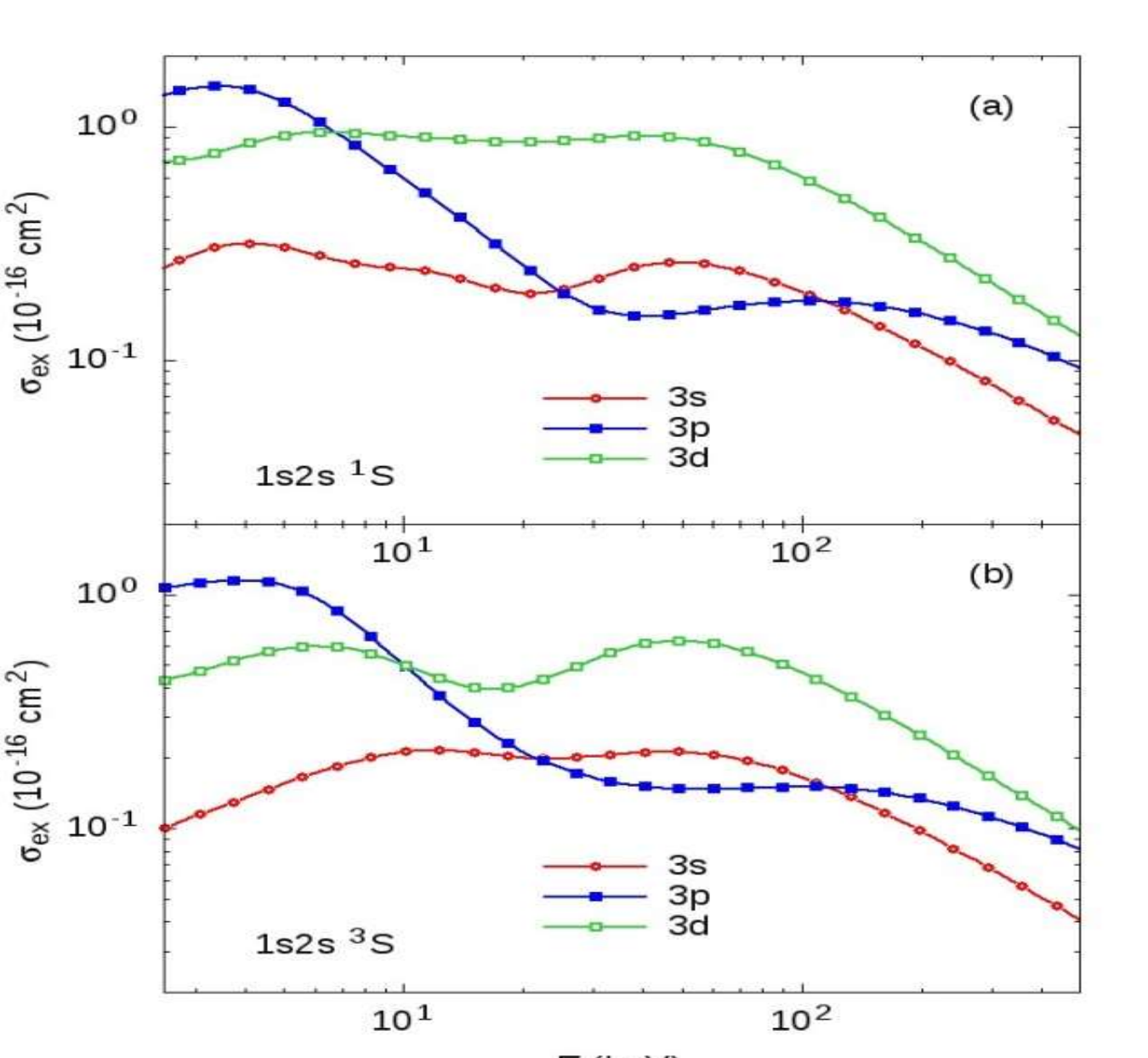
# Capture to 4l states



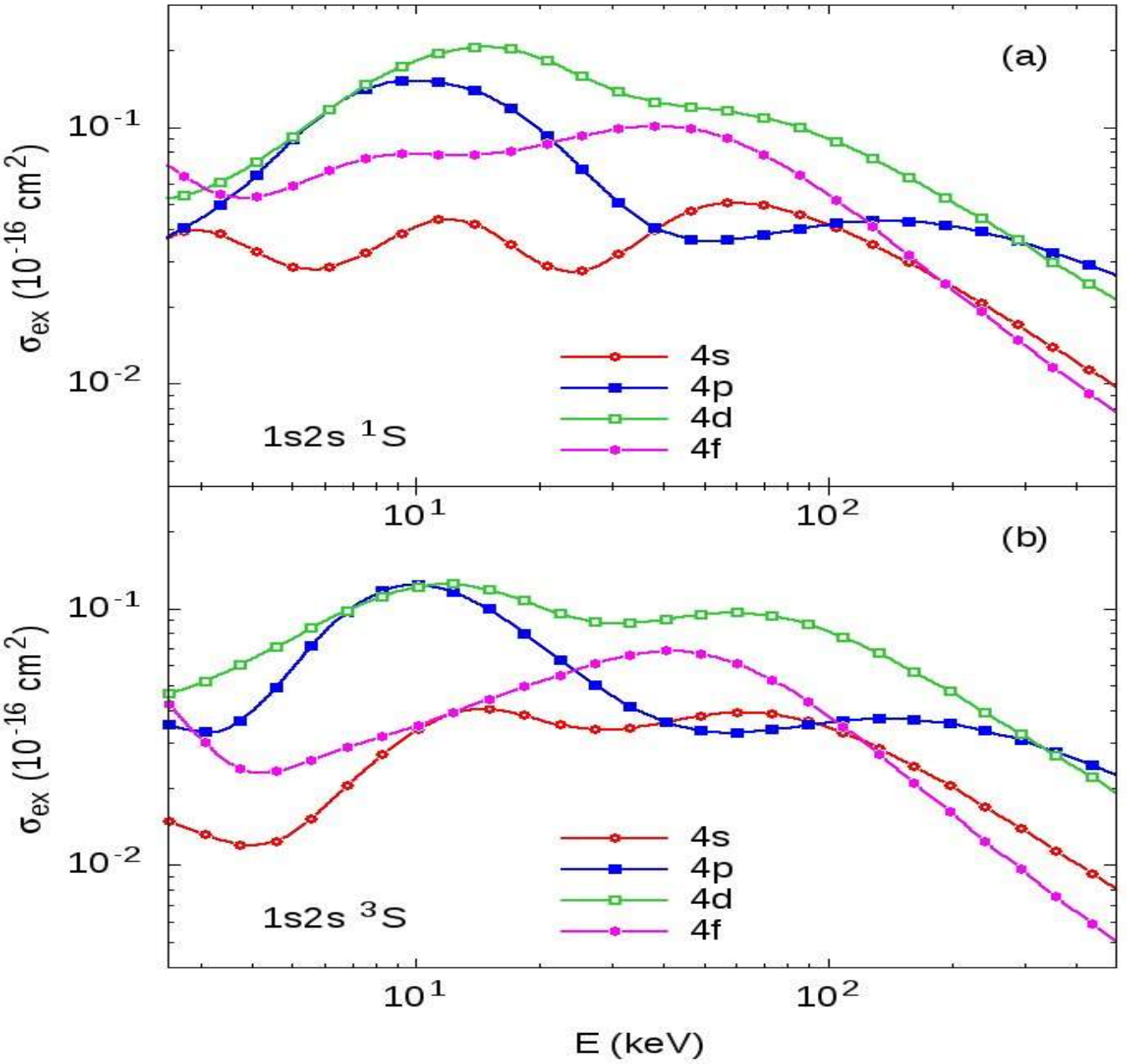
# 2s→2p excitation



# Excitation to 3l states



# Excitation to 4l states



# Cross sections for p + Sn collisions

Sn ground state: ....4d^10 5s^25p^2 |3P_0-2;

- Model potentials for e- Sn+: |1S_0; |1D_2

$$V_{s,t}(r) = -\frac{1}{r}\left[Z_0 + (Z_1 + Z_2 r)\right]\exp(-Z_3 r)$$

$$\text{sin}\,glet: Z_0 = 0.714,\ Z_1 = 6.454,\ Z_2 = 4.418,\ Z_3 = 0.473$$

$$triplet: Z_0 = 1.084,\ Z_1 = 6.4134,\ Z_2 = 5.739,\ Z_3 = 0.567$$

$$Accuracy:\ \ better\ than\ 7\%$$

# Expansion basis sets:

- On Sn: lowest 9 states with lowest J-values;
- On H: all states with $n \leq 8$
- Convergence of results: within 5%

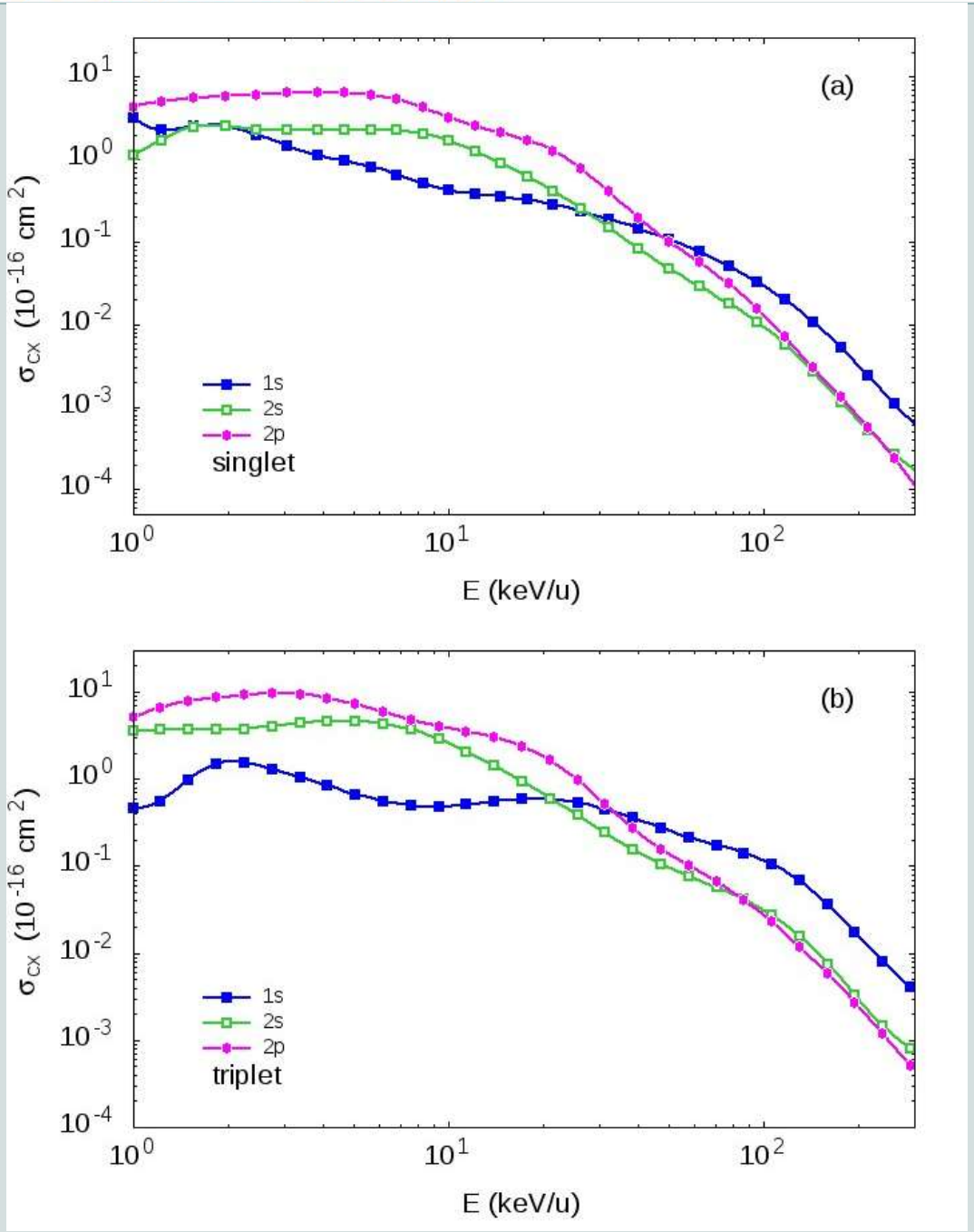
# Energy levels of lowest Sn states

| singlets | Sn | triplets | Sn | n of H | H(n) |
|---|---|---|---|---|---|
| **5p5p** | -0.26401 | **5p5p** | -0.26988 | n=1 | -0.5000 |
| **5p6s** | -0.09192 | **5p6s** | -0.11055 | n=2 | -0.125 |
| **5p6p** | -0.05015 | **5p6p** | -0.06710 | n=3 | -0.0556 |
| **5p5d** | -0.04637 | **5p5d** | -0.06249 | n=4 | -0.03125 |
| **5p7s** | -0.02973 | **5p7s** | -0.05019 | n=5 | -0.0200 |
| **5p5f** | -0.0203 | **5p7p** | -0.03107 | n=6 | -0.01389 |
| **5p6d** | -0.01523 | **5p6d** | -0.03071 | n=7 | -0.01020 |
| **5p6f** | -0.01412 | **5p8s** | -0.02876 | n=8 | -0.00781 |
| **5f7f** | -0.01034 | **5p8p** | -0.02217 | n=9 | -0.00617 |

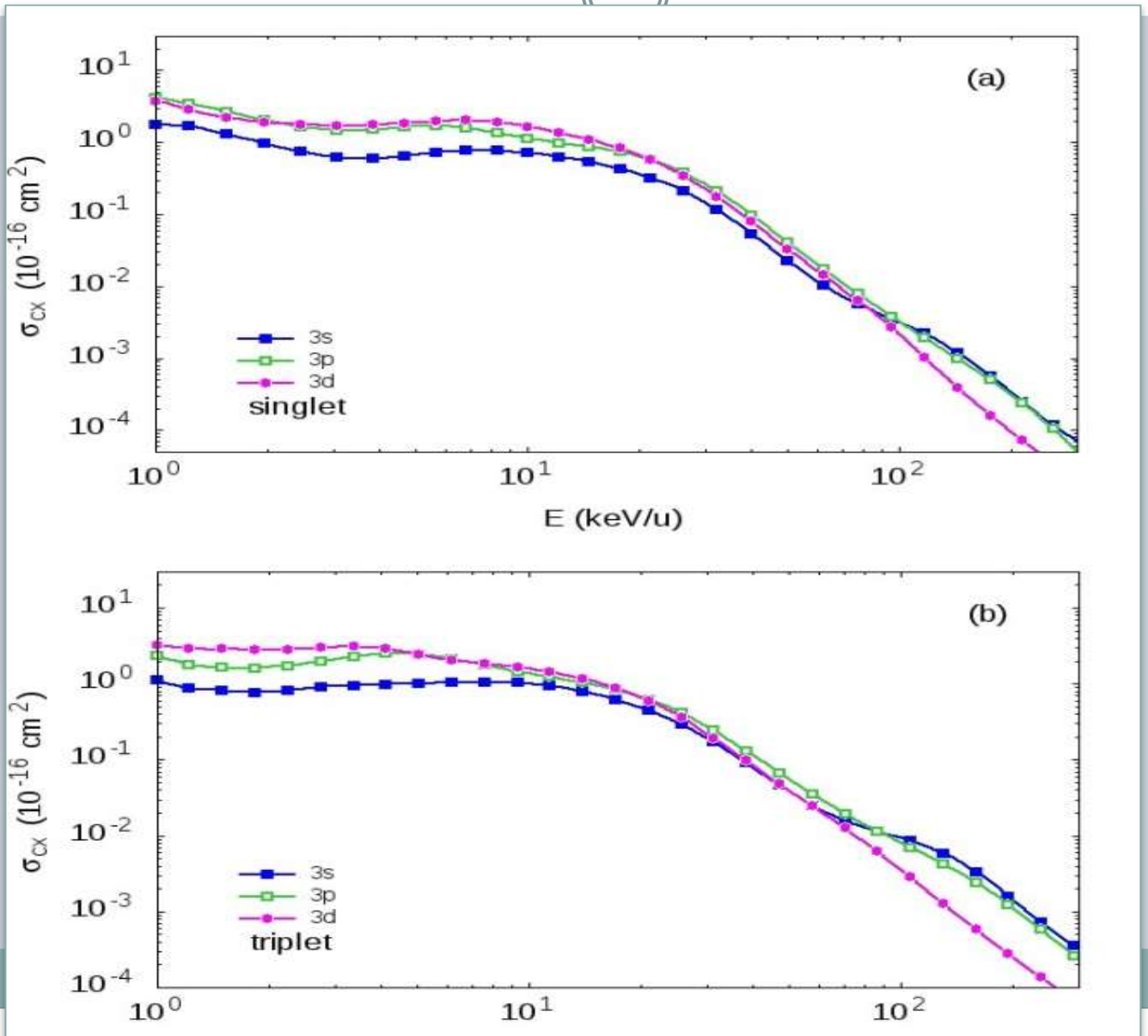
$$Quasi-resonant\ Sn(nl)-H(n)\ energy\ levels$$

# Cross section results

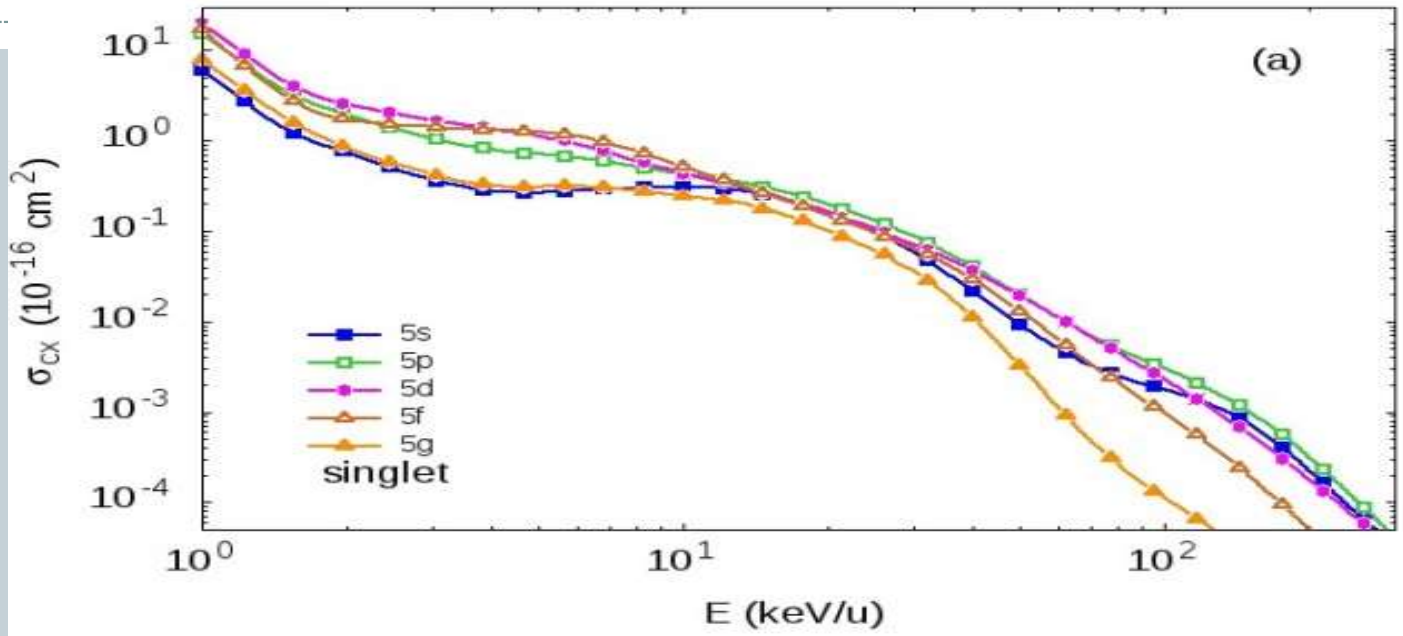
- Capture to 1s, 2s, 2p

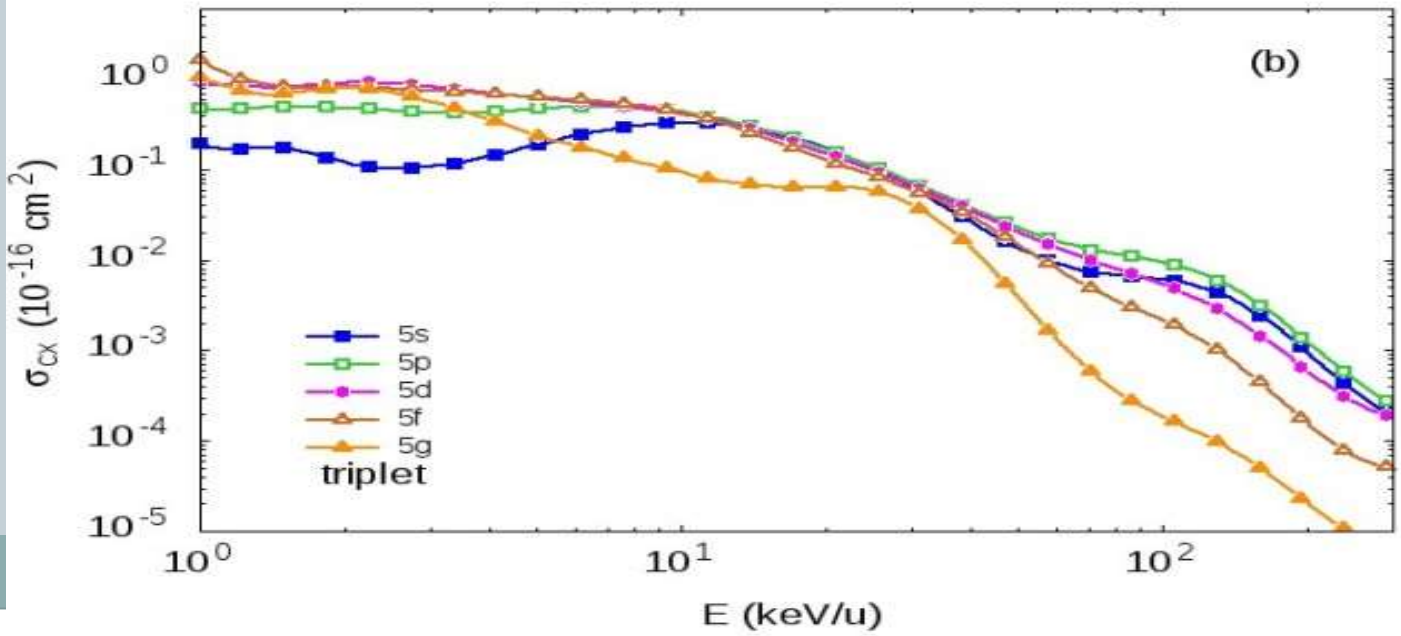


# Capture to 3l

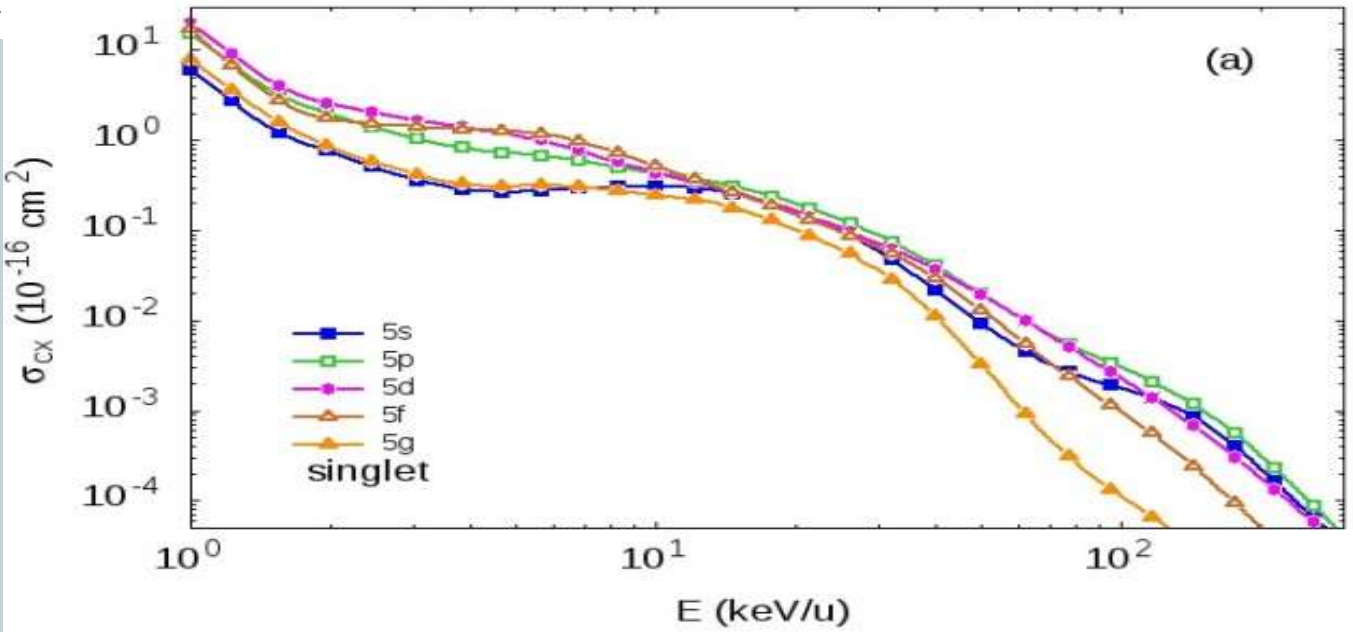


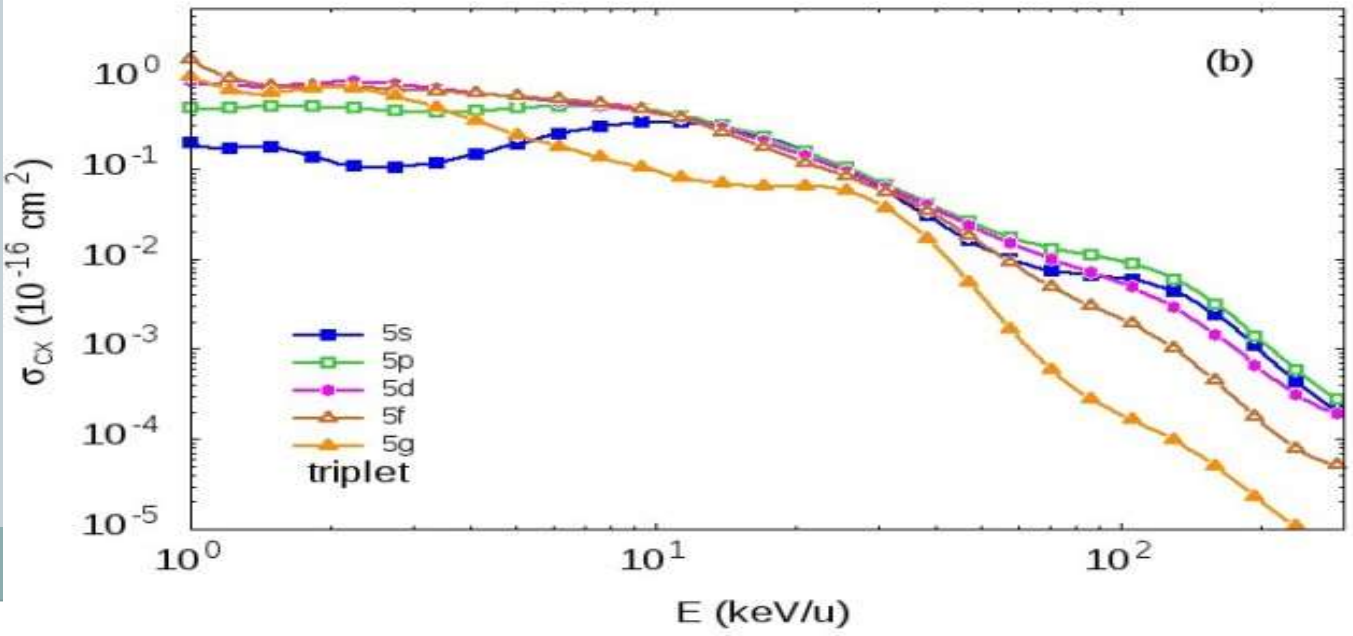
# Capture to 4l



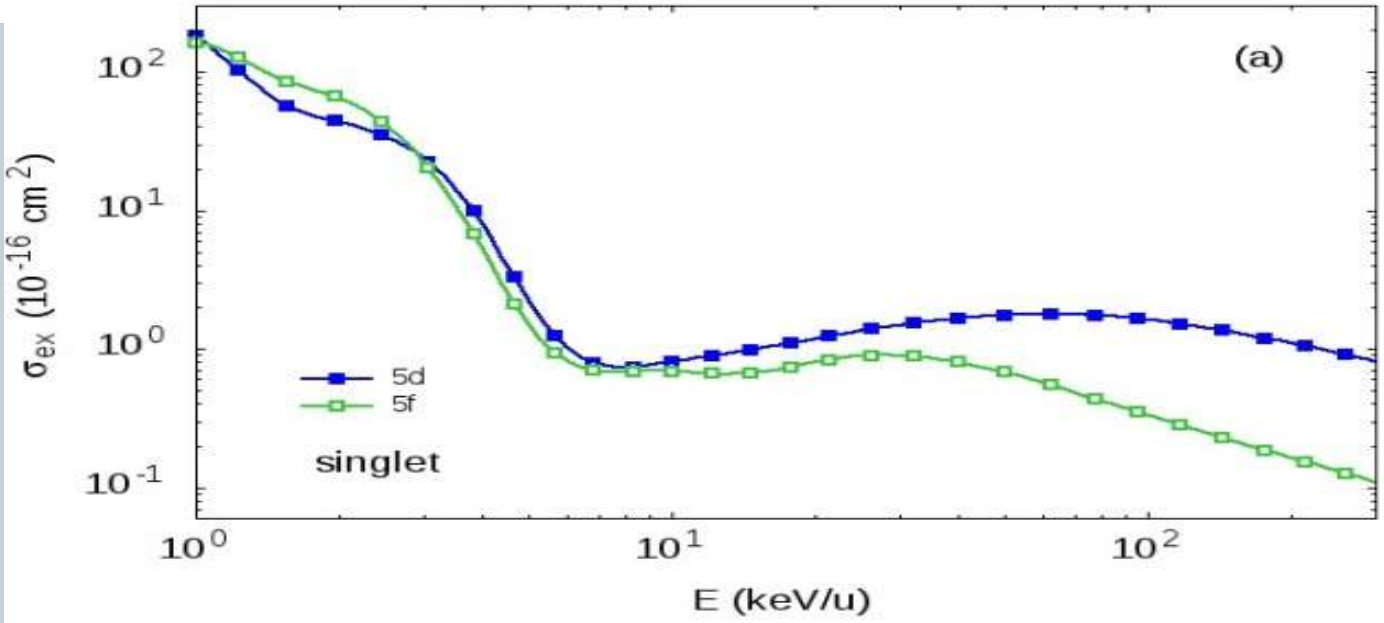



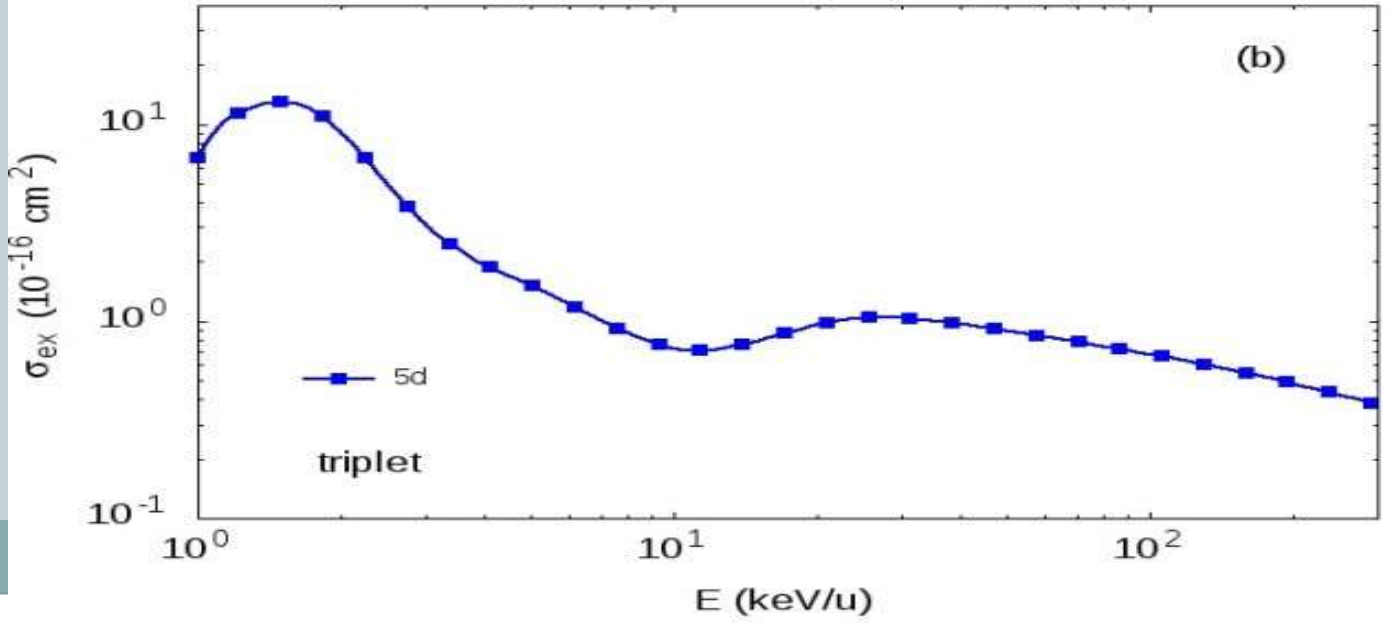
# Capture to 5l



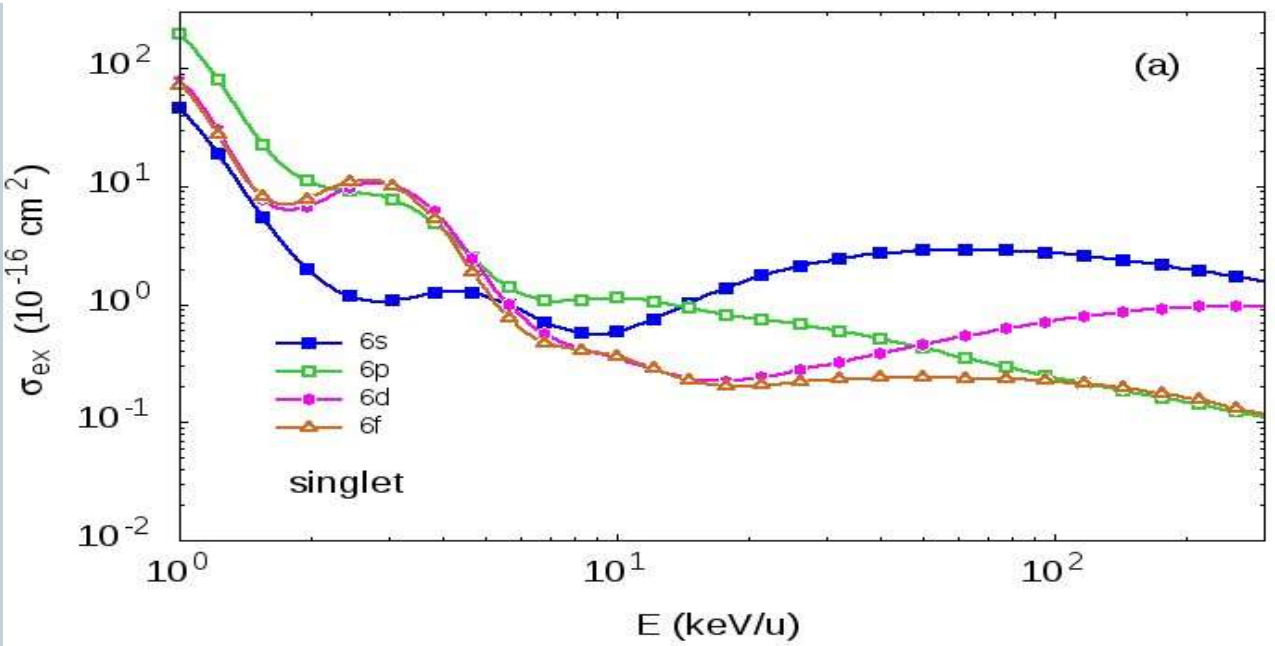



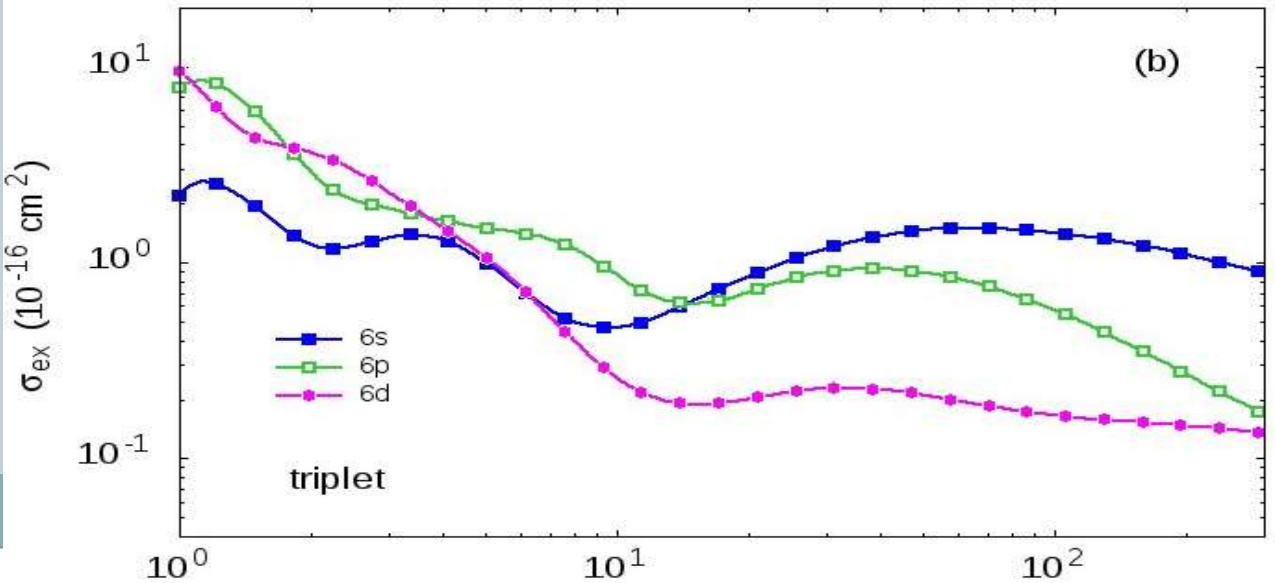
# Excitation to 5d, 5f



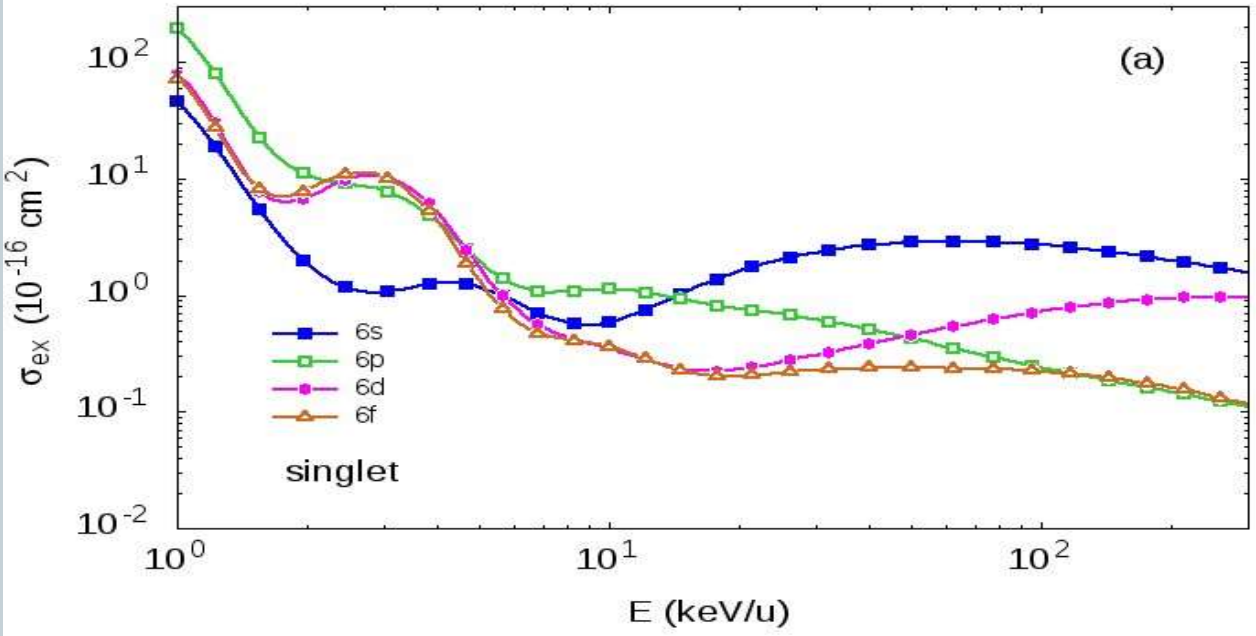



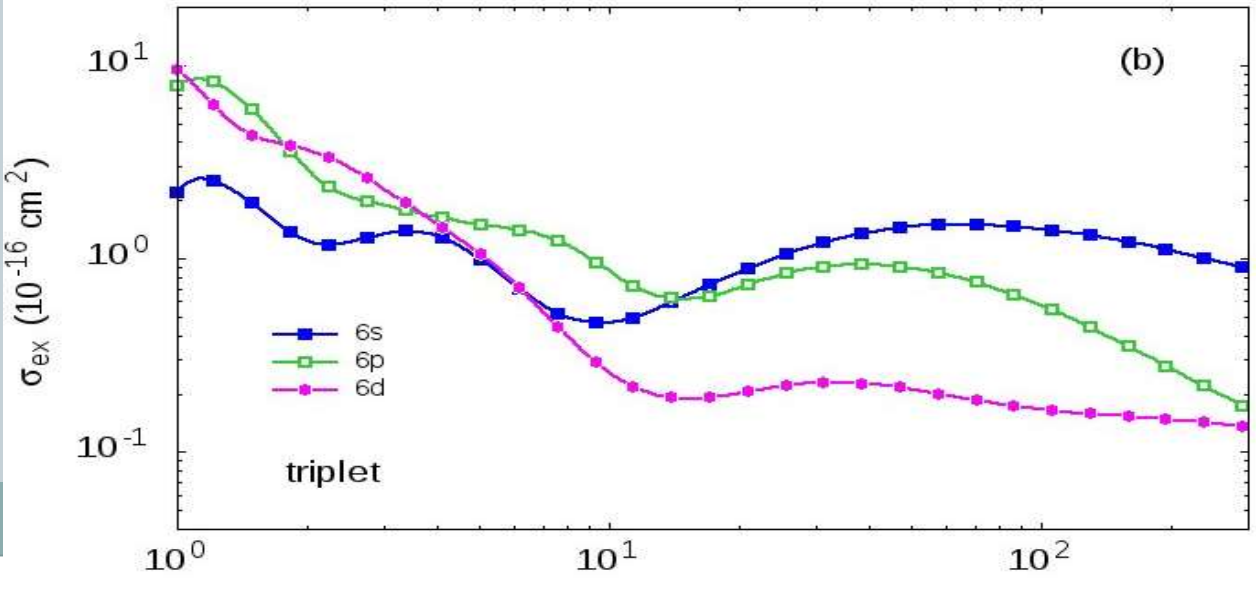
# Excitation to 6l



# Excitation to 7s,7p



# Work in progress and planned

In progress:

$$He^{2+} + Li^{+},\ H^{+} + Sn^{+},\ He^{+} + Sn$$

Planned:

$$He^{+} + Li^{+},\ He^{+} + Sn^{+},\ H^{+} + Ga,\ Ga^{+}$$

- Cross sections and spectral lines
- Collaboration with IAPCM (Beijing)