Ionization, total and state selective charge exchange cross sections in fusion related collision systems

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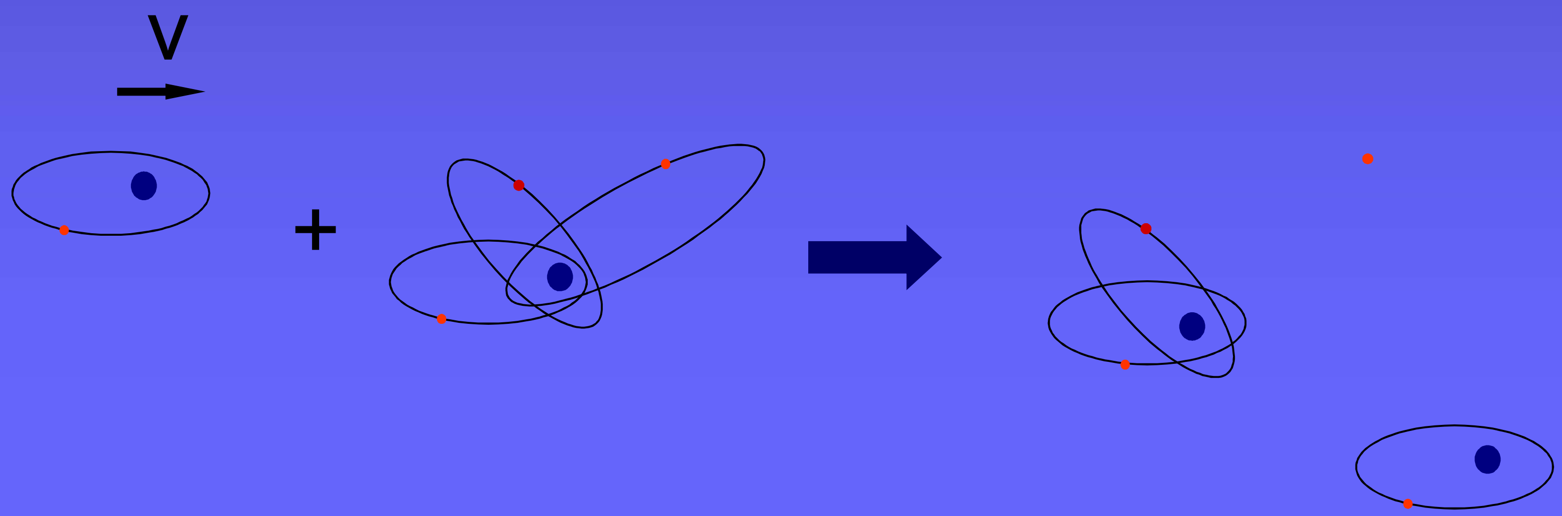
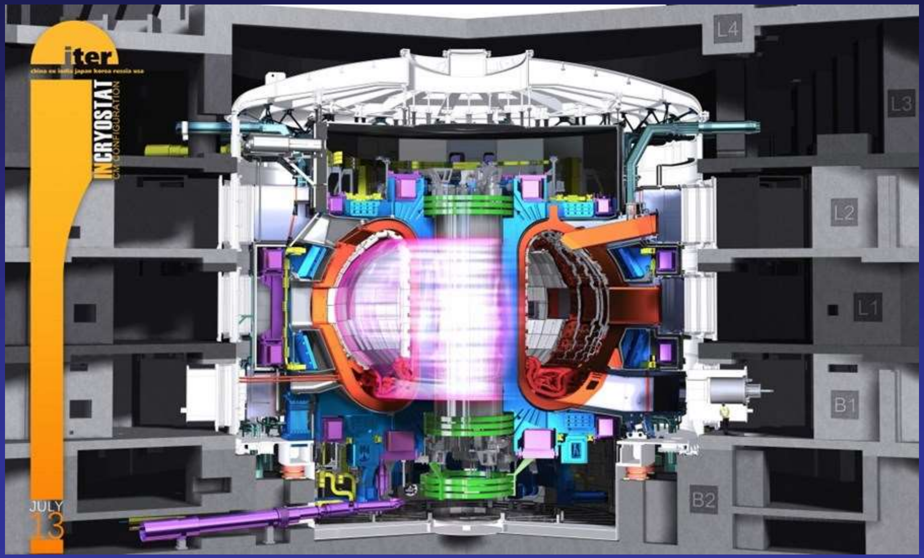
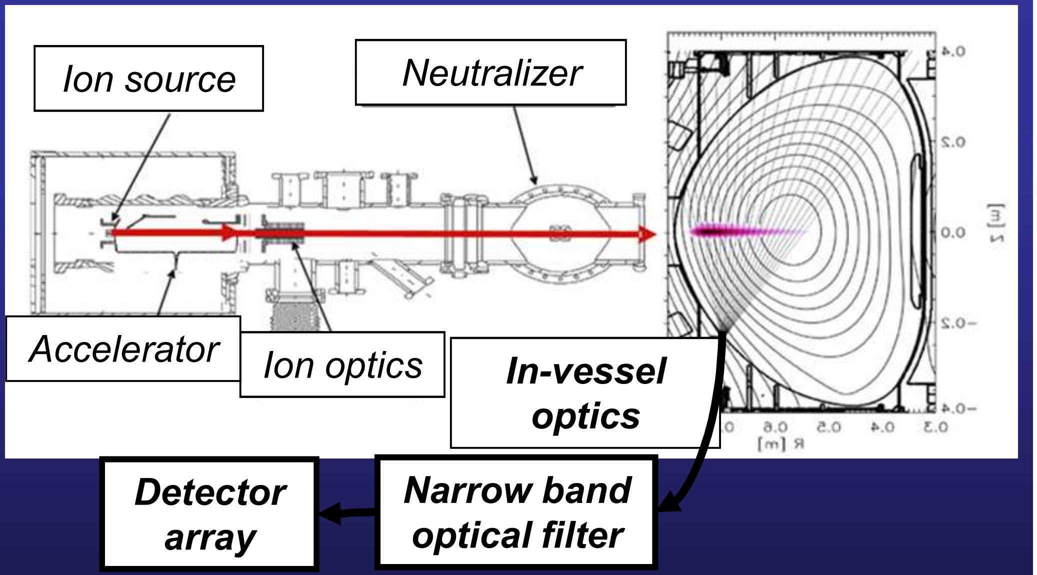


The aim



BES diagnostics

- **Active** plasma diagnostics procedure
- Use of H-type of atoms such as D,Li,Na. (which posses **one valence electron**)
  - Heating beams (H, D)
  - Diagnostic beams (Li, Na)
- Purpose: **density** and **fluctuation** meas.
  - Fluct. timescale: 10 – 200kHz
  - Fluct. spatial scale: 1 – 4 cm



Outlook

Basic idea – Classical treatments

Theory

Classical Trajectory Monte Carlo (CTMC) model

Quasi-Classical Trajectory Monte Carlo (QCTMC) model

Results

1. **Data for Atomic Processes of Neutral Beams in Fusion Plasma**

Be^{4+}+ H(1s) collisions

H + H type collisions

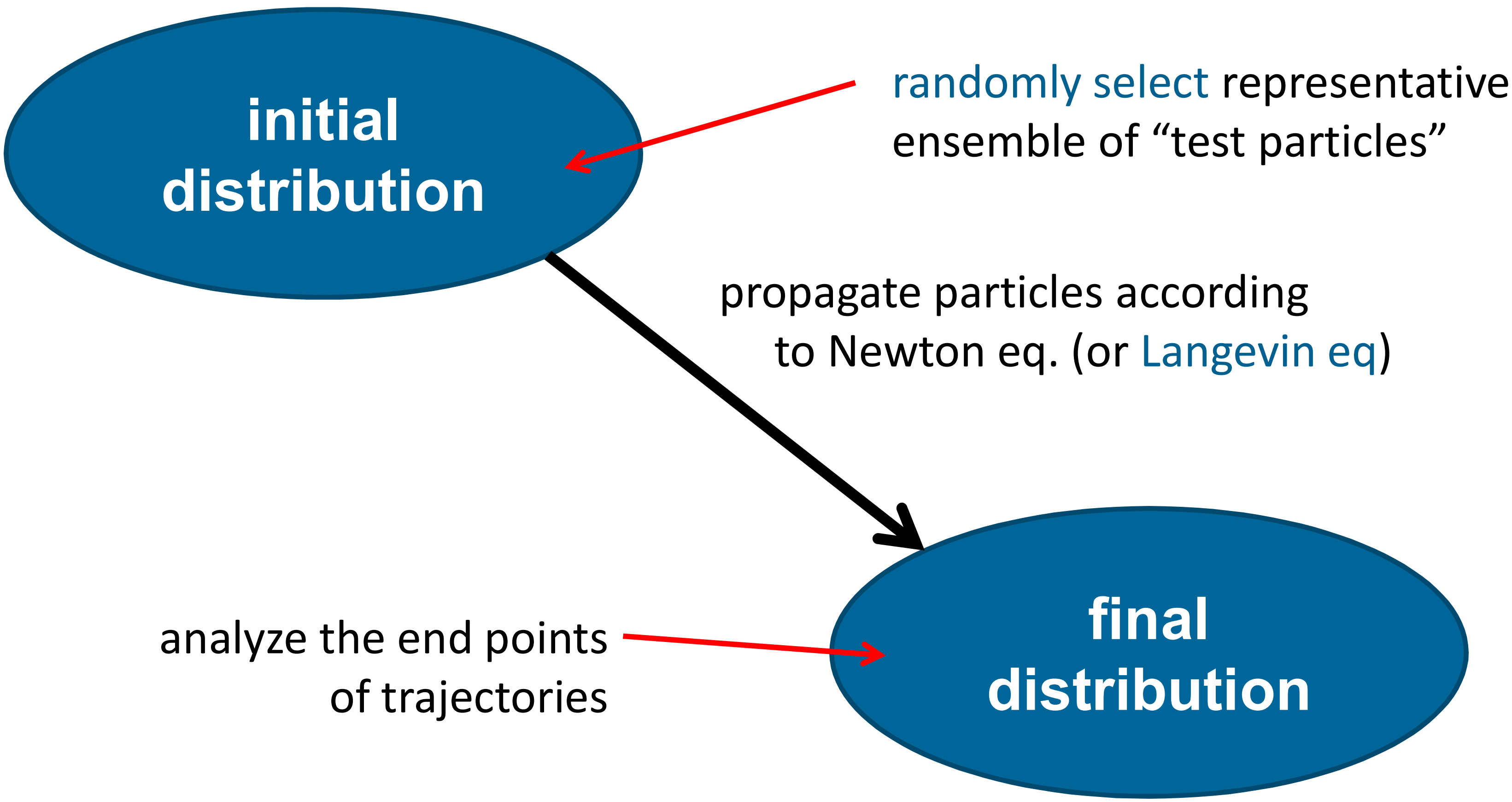
2. Injected Impurities

Li^{+} + He, Li^{+} N

Summary

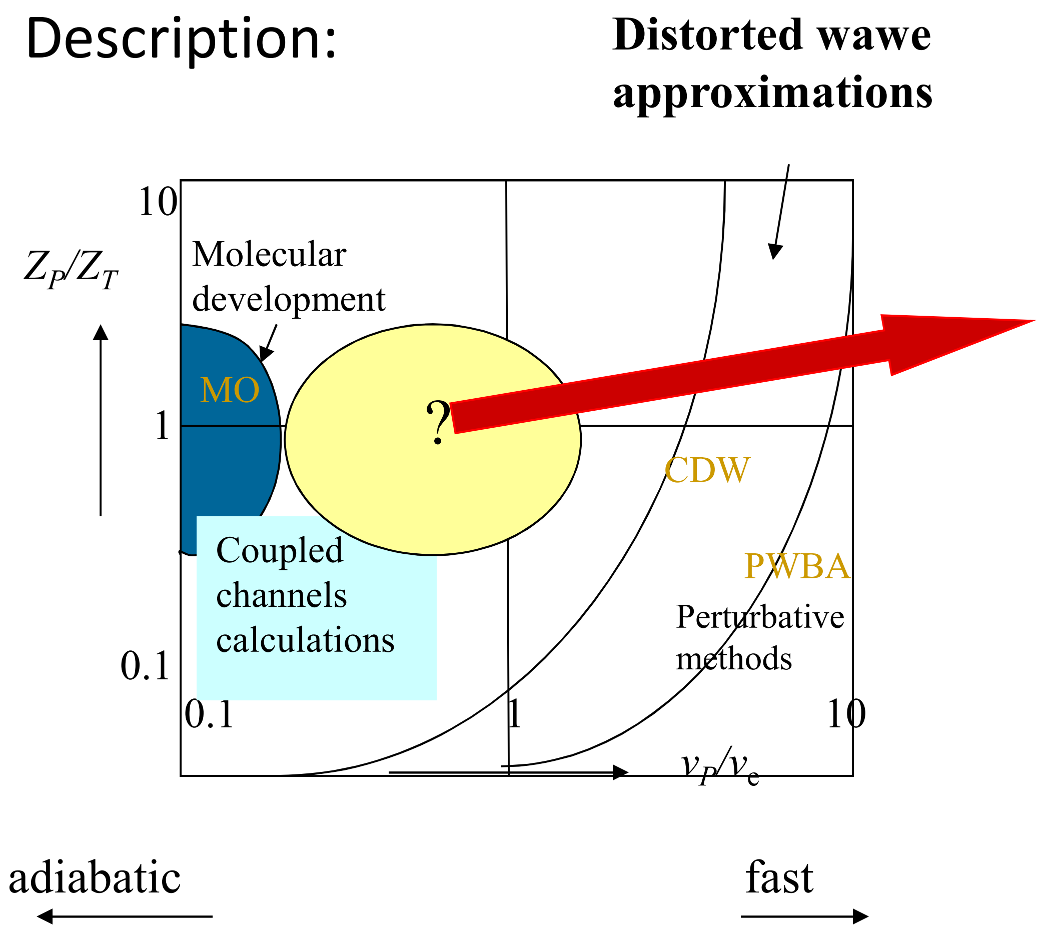
Approximations: CTMC simulations

Flow diagram for a MC simulation:



Ionization in ion-atom collisions

Description:



Non-perturbative models:

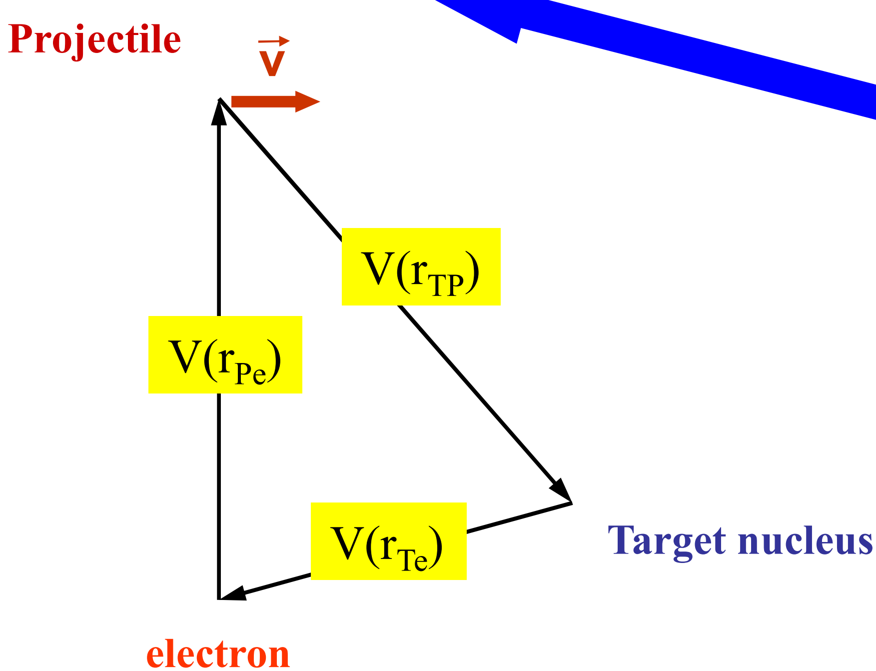
Classical Trajectory Monte Carlo (CTMC) method

3-body CTMC approach

- **Classical nonperturbative method – „theoretical experiment”**
- **Treats the many-body interactions**

Model potential:

$$V(r) = -\frac{(Z-1)\Omega(r)+1}{r}, \quad \text{where} \quad \Omega(r) = \left[Hd(e^{r/d}-1)+1\right]^{-1}$$



Specific for the present work:

-Screened core potentials for both partners (analytic GSZ model pot.)

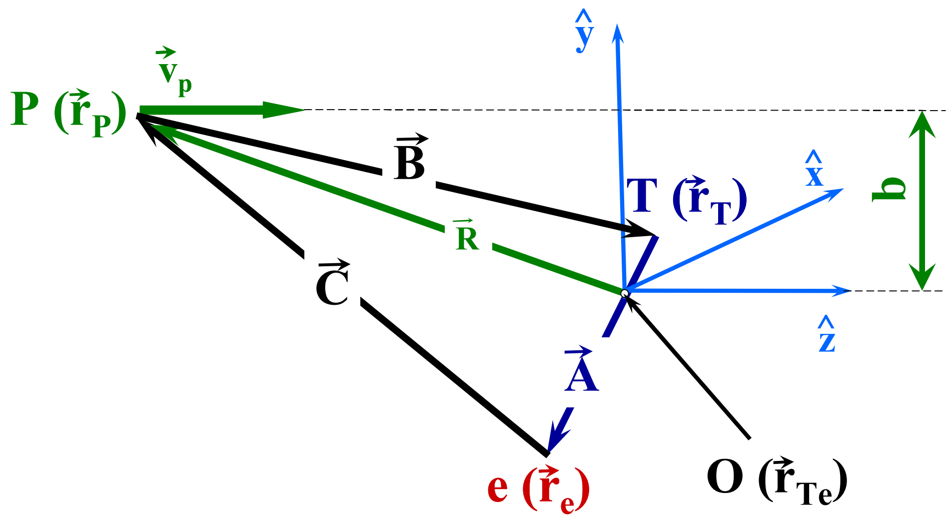
-Strategies for extracting the relevant information

• a three-body balance is bound by E and **p** conservation;

• final-state kinematics does not provide information about the mechanism

CTMC approach

- **Classical nonperturbative method**
  - **„theoretical experiment”**
- **Treats the many-body interactions**



$$L = L_K - L_V$$

$$L_K = \frac{1}{2} m_P \dot{\vec{r}}_P^{\,2} + \frac{1}{2} m_e \dot{\vec{r}}_e^{\,2} + \frac{1}{2} m_T \dot{\vec{r}}_T^{\,2}$$

$$L_V = \frac{Z_P(|\vec{r}_P - \vec{r}_e|)Z_e}{|\vec{r}_P - \vec{r}_e|} + \frac{Z_P(|\vec{r}_P - \vec{r}_T|)Z_T(|\vec{r}_P - \vec{r}_T|)}{|\vec{r}_P - \vec{r}_T|} + \frac{Z_e Z_T(|\vec{r}_e - \vec{r}_T|)}{|\vec{r}_e - \vec{r}_T|}$$

Classical principal number	Classical orbital angular momentum	Classical magnetic angular momentum
$n_c = Z_T Z_e \left(\frac{\mu_{Te}}{2U}\right)^{1/2}$	$l_c = \sqrt{m_e[(x\dot{y} - y\dot{x})^2 + (x\dot{z} - z\dot{x})^2 + (y\dot{z} - z\dot{y})^2]}$	$m_c = m_e(y\dot{z} - z\dot{y})$

$$[(n-1)(n-1/2)n]^{1/3} \le n_c \le [n(n+1/2)(n+1)]^{1/3}$$

$$l \le {}^{n}/_{n_c}\, l_c < l + 1$$

$$(2m-1)/(2l+1) < {}^{m_c}/_{l_c} < (2m+1)/(2l+1)$$

The total cross sections	The statistical uncertainty
$\sigma = \frac{2\pi b_{max}}{T_N} \sum_j b_j^{(i)}$	$\Delta\sigma = \sigma \left(\frac{T_N - T_N^{(i)}}{T_N T_N^{(i)}}\right)^{1/2}$

T_N : Total number of trajectories calculated for impact parameters less than b_{max}

$T_N^{(i)}$: Number of trajectories that satisfy the criteria for a given channel

$b_j^{(i)}$: Actual impact parameter for the trajectory corresponding to the channels.

Classical Limits - extension

Improvement of the classical description of the one electron atomic system by including a model potential in the Hamiltonian of the system mimicking quantum features.

Quasi-Classical Trajectory Monte Carlo (QCTMC) Model

Constraining Heisenberg Potential

$$H_{QCTMC} = T + V_{coul} + V_H$$

$$V_H = \sum_{n=a,b} \sum_{i=1}^{N} f(r_{ni}, p_{ni}; \xi_H, \alpha_H)$$

$$f(r_{\lambda\nu}, p_{\lambda\nu}; \xi, \alpha) = \frac{\xi}{4\alpha r_{\lambda\nu}^2 \mu_{\lambda\nu}} exp\left\{\alpha\left[1 - \left(\frac{r_{\lambda\nu} p_{\lambda\nu}}{\xi}\right)^4\right]\right\}$$

$\alpha_H - \xi_H$

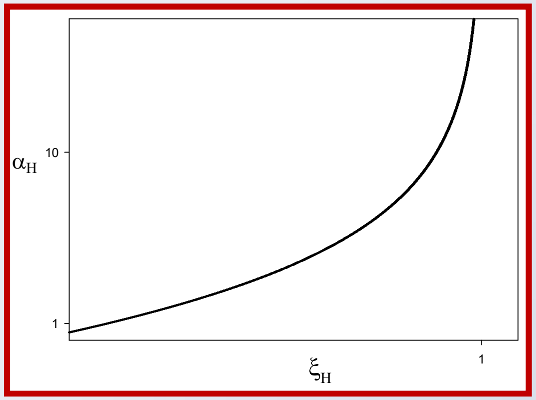
- Hamiltonian of hydrogen atom is defined as follows:

$$H = \frac{p^2}{2} - \frac{1}{r} + \left[\frac{{\xi_H}^2}{4\alpha_H r^2}\right] exp\left\{\alpha_H \left[1 - \left(\frac{rp}{\xi_H}\right)^4\right]\right\}$$

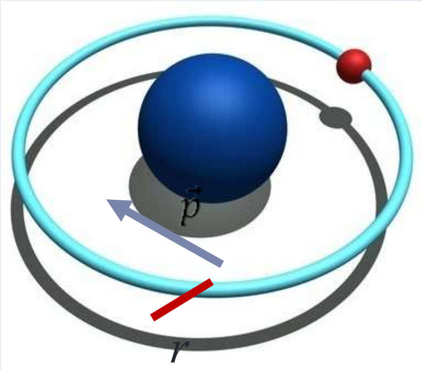
- In the ground or lowest-energy configuration, we requires $\frac{\partial H}{\partial p} = 0$ and $\frac{\partial H}{\partial r} = 0$

$$E = -\frac{1}{2{\xi_H}^2\left(1 + \frac{1}{2\alpha_H}\right)}$$

Electron binding energy = 0.5



Initial conditions for *r* and *p*



❖ In CTMC model, the initial conditions in *r* and *p* :

A microcanonical ensemble characterizes the initial state of the target constrained to an initial binding energy of the given shell:

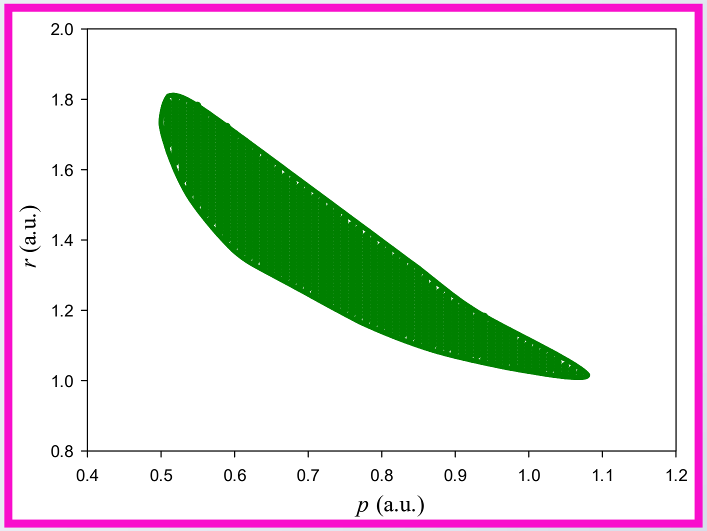
$$\rho_{E_0}(\vec{A},\dot{\vec{A}}) = K_1\delta(E_0 - E) = \delta\left(E_0 - \frac{1}{2}\mu_{Te}\dot{\vec{A}}^2 - V(A)\right)$$

$$r_0 = \left|\frac{Z_e Z_T}{2E_b}\right| \qquad p_0 = \sqrt{2|E_b|\mu_{te}}$$

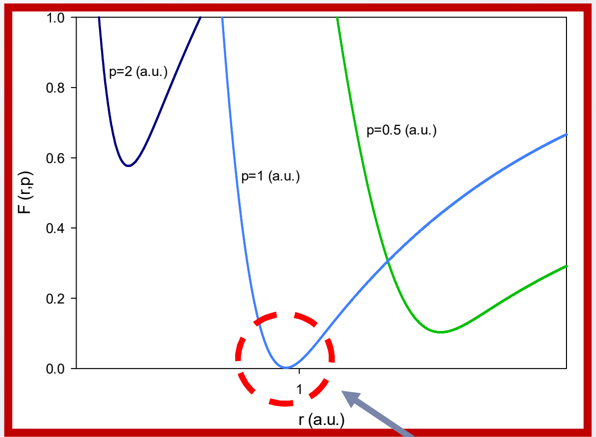
❖ In QCTMC model, we considered two conditions that *r* and *p* have to satisfy them as follows:

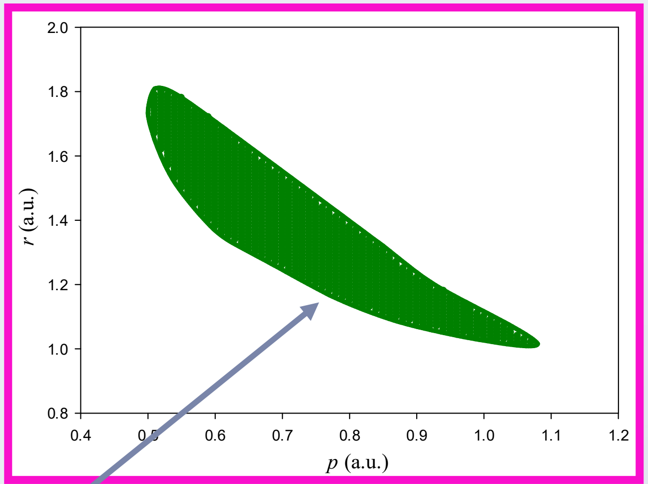
$$\frac{|Z_e Z_T|}{2r} + f_H(r,p) < 0.5$$

$$\frac{p^2}{2\mu_{Te}} - \frac{1}{r} + f_H(r,p) \approx -0.5$$



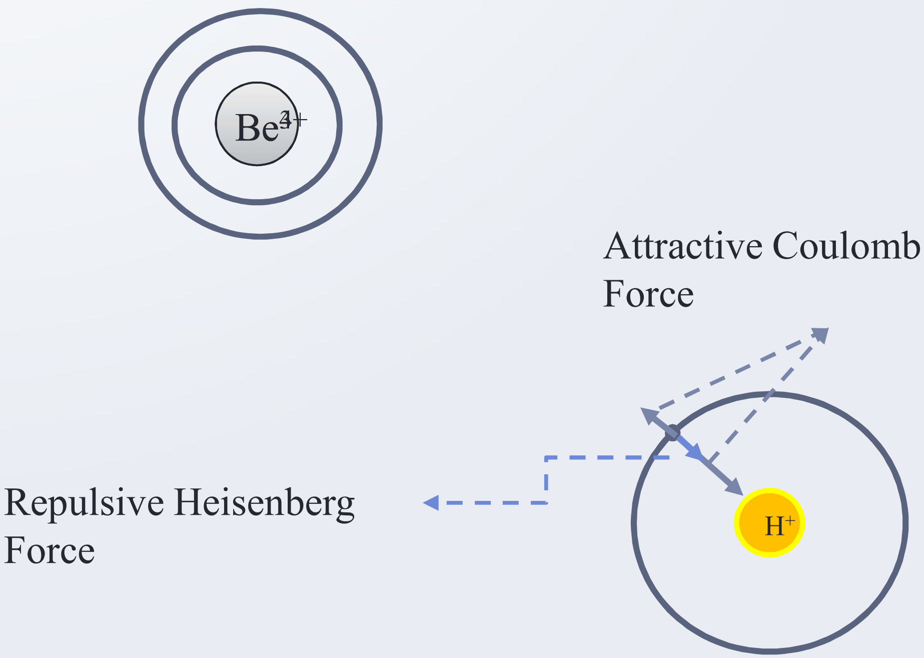
$$F(r,p) = \frac{p^2}{2\mu_{Te}} - \frac{1}{r} + f_H(r,p) + 0.5$$

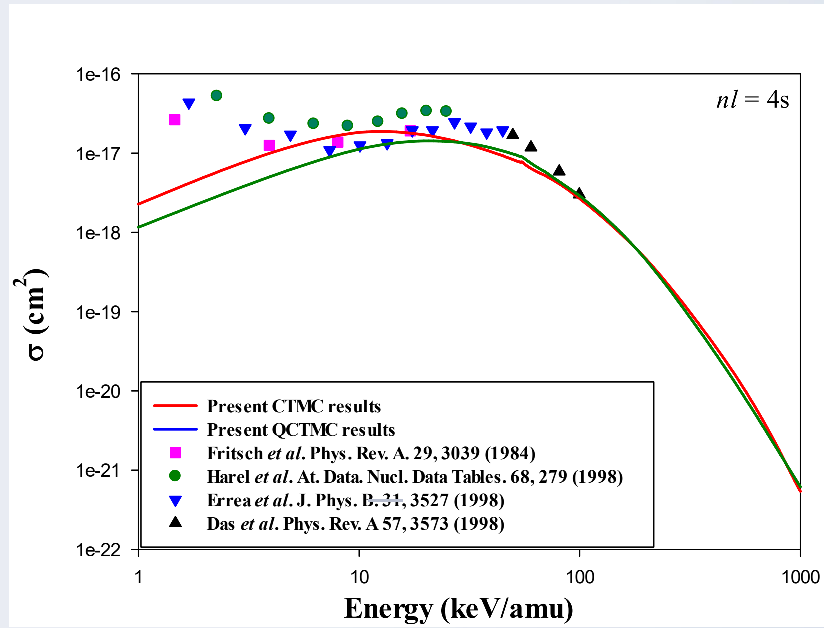




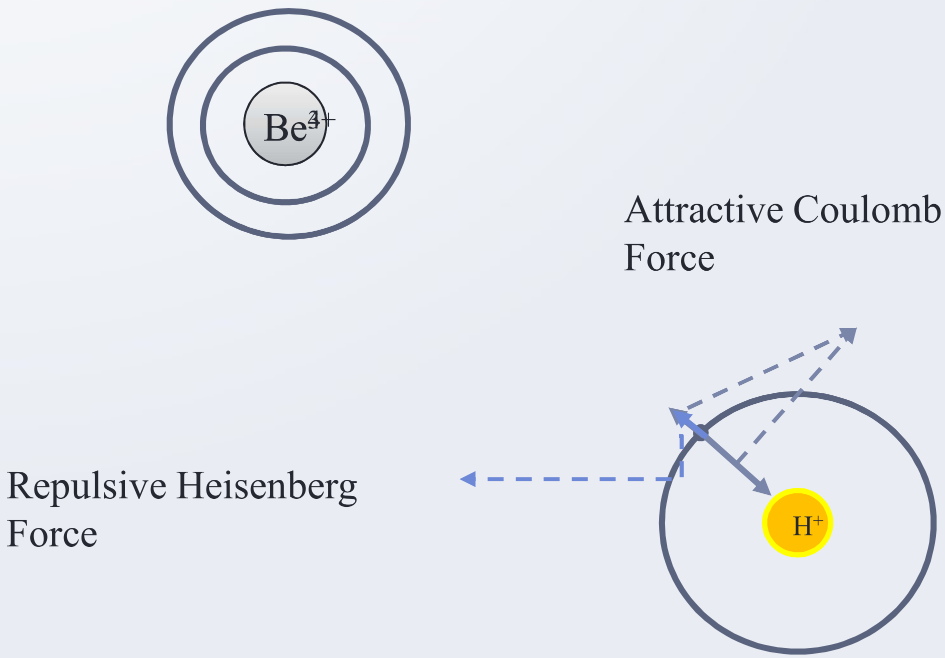
QCTMC initial conditions

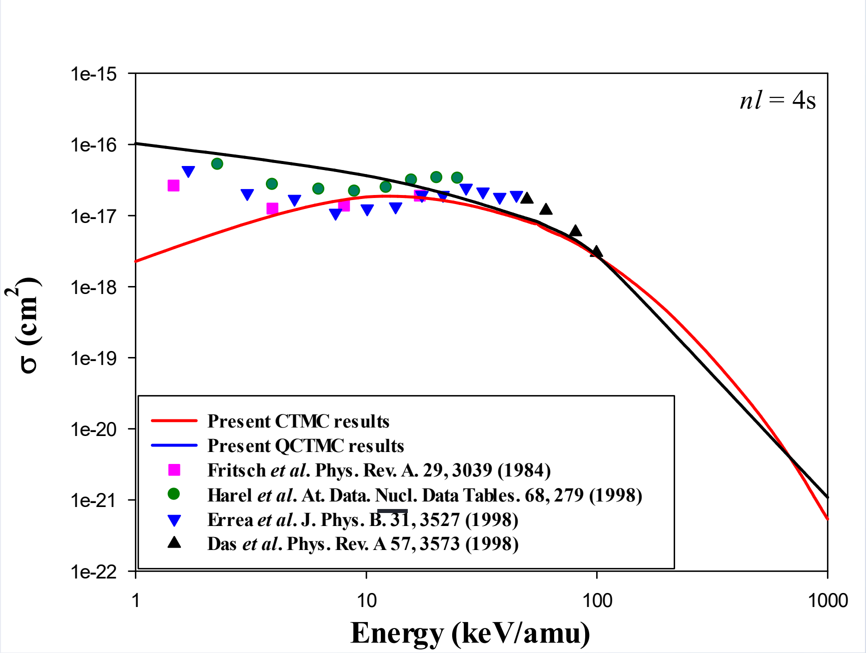
Projectile-centered Scheme



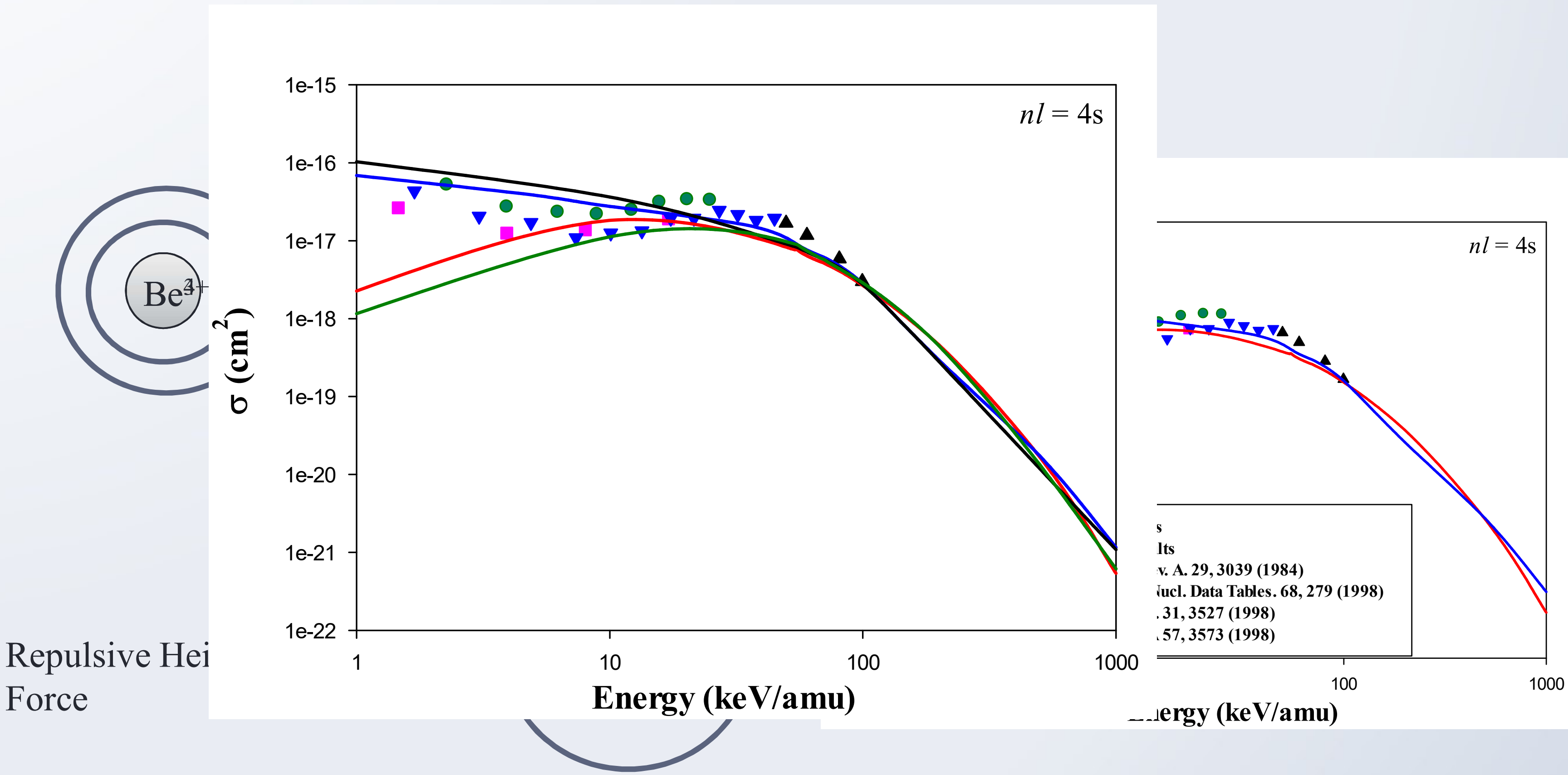


Target-centered scheme





Combined one; i.e. ,target and projectile-centered scheme



Finding Best Combination of α , ξ

Interaction between H^+ and Hydrogen atom

Total Electron Capture
$H^+ + H(1s) \rightarrow H + H^+$

QCTMC ($\alpha_H = 3$, $\xi_H = 0.9258$)

QCTMC ($\alpha_H = 3.5$, $\xi_H = 0.9354$)

QCTMC ($\alpha_H = 4$, $\xi_H = 0.9428$)

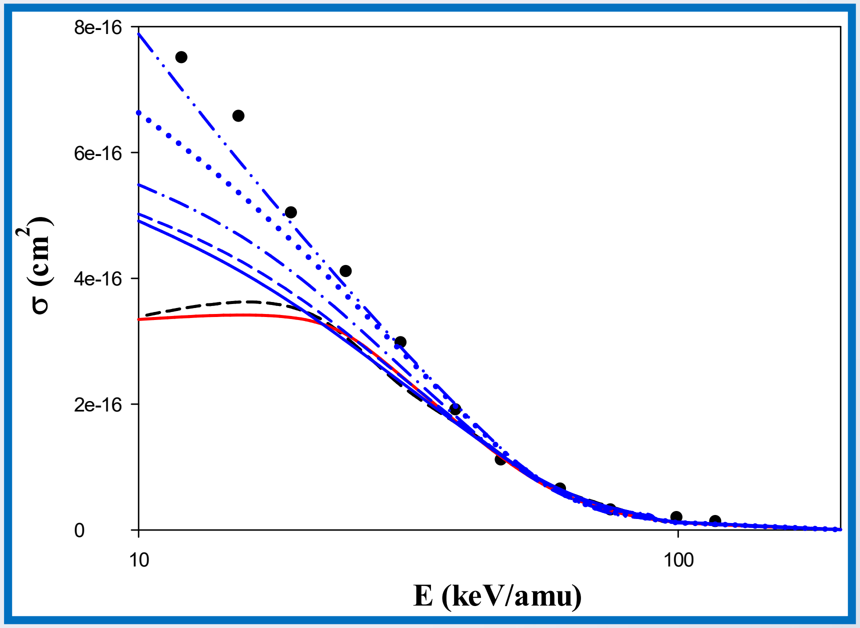
QCTMC ($\alpha_H = 4.5$, $\xi_H = 0.9486$)

QCTMC ($\alpha_H = 5$, $\xi_H = 0.9534$)

CTMC

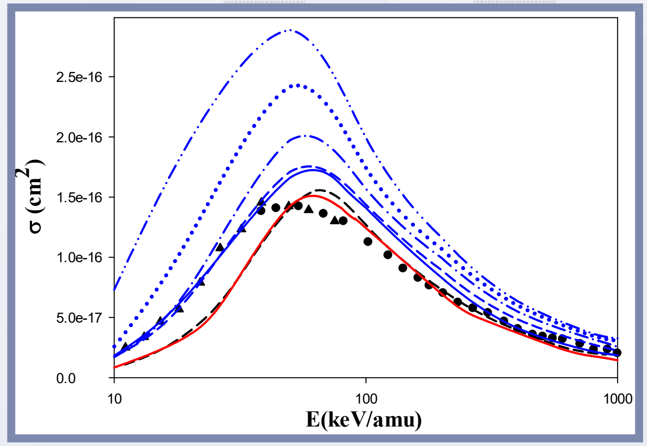
QTMC-EB

Exp: McClure



Ionization

$H^+ + H(1s) \rightarrow H^+ + H^+ + e^-$

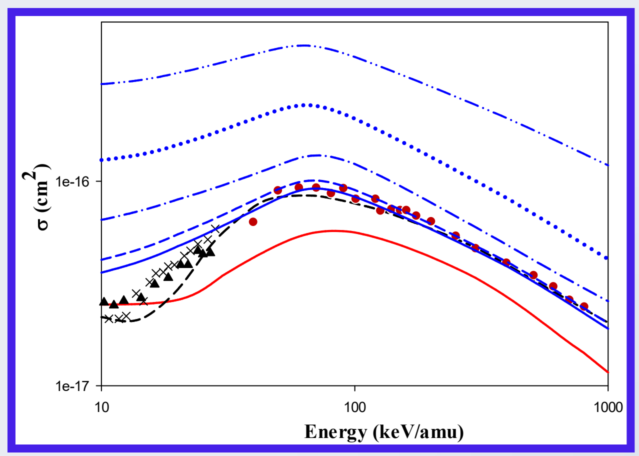


- QCTMC ($\alpha_H = 3$, $\xi_H = 0.9258$)
- QCTMC ($\alpha_H = 3.5$, $\xi_H = 0.9354$)
- QCTMC ($\alpha_H = 4$, $\xi_H = 0.9428$)
- QCTMC ($\alpha_H = 4.5$, $\xi_H = 0.9486$)
- QCTMC ($\alpha_H = 5$, $\xi_H = 0.9534$)
- CTMC
- QTMC-EB

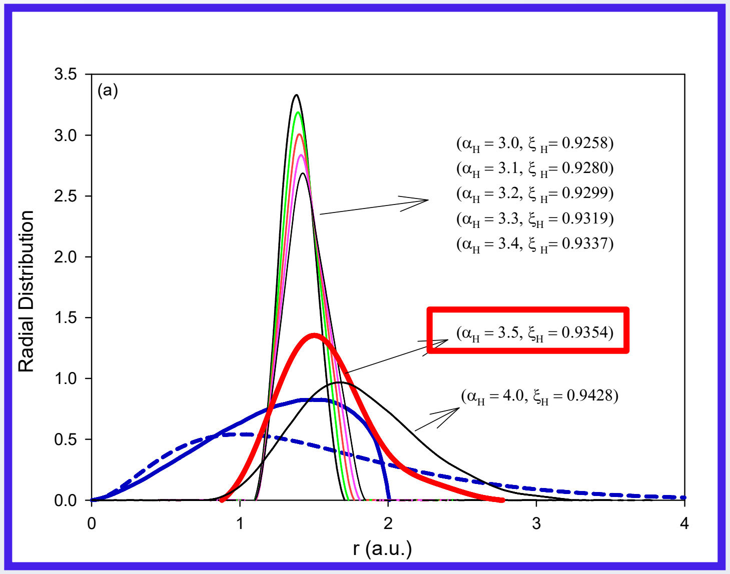
- ● Exp: Shah and Gilbody
- ▲ Exp: Shah and Eliot
- ● Exp: Detleffsen
- ▲ Exp: Morgan
- ✖ Exp: Kondov

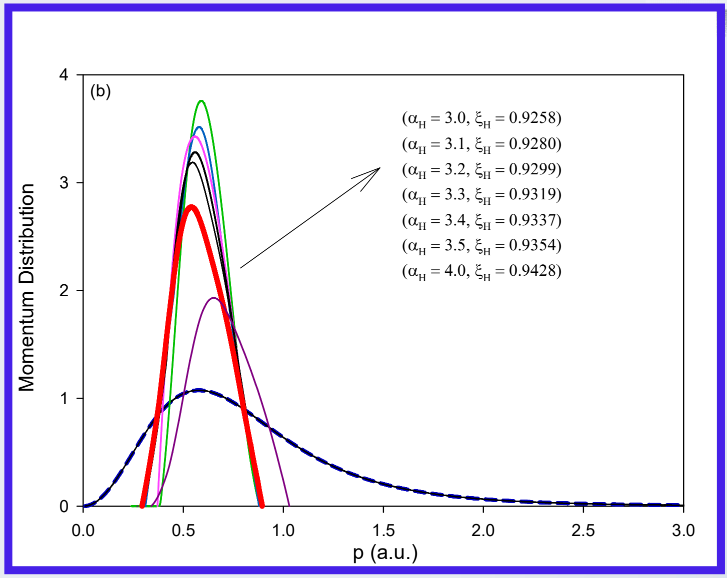
Excitation

$H^+ + H(1s) \rightarrow H^+ + H(2p)^*$



QCTMC Radial & Momentum Distribution





—— CTMC Distribution

- - - Quantum Distribution

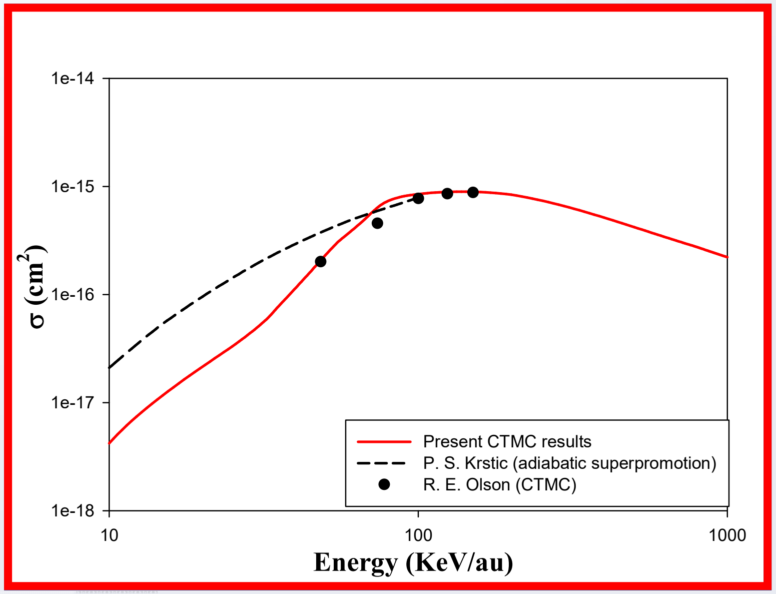
Data for Atomic Processes of Neutral Beams in Fusion Plasma

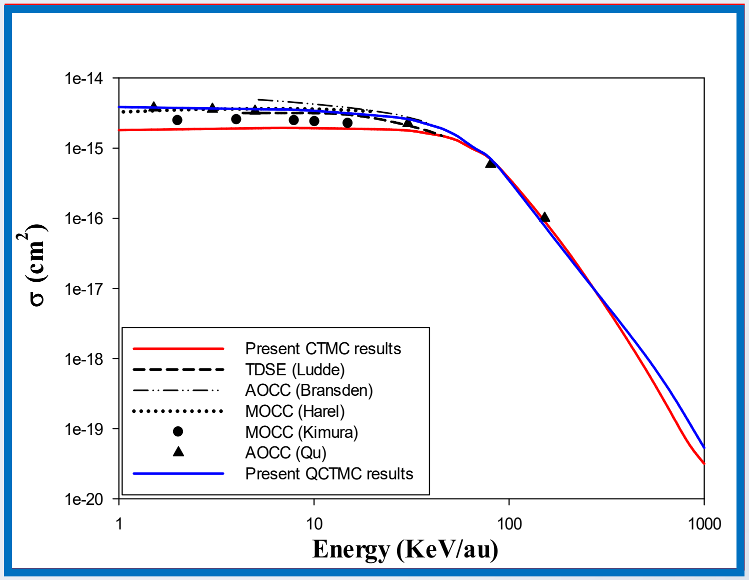
Ionization

$Be^{4+} + H(1s) \rightarrow Be^{4+} + H^{+} + e^{-}$

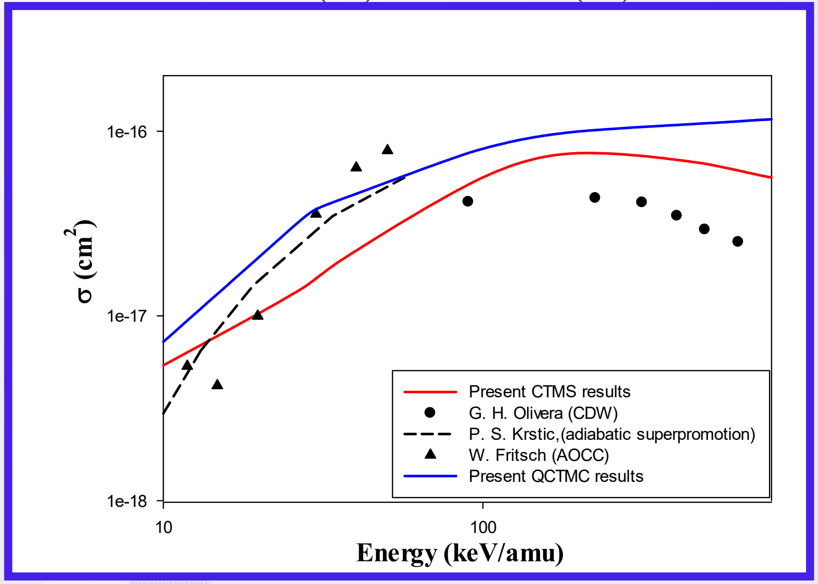
Total Electron Capture

$Be^{4+} + H(1s) \rightarrow Be^{3+}(nl) + H^{+}$

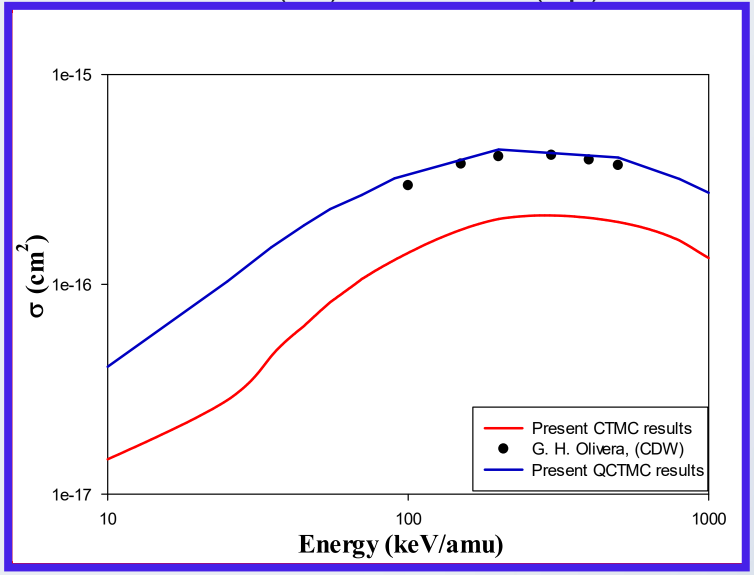




Excitation
$Be^{4+} + H(1s) \rightarrow Be^{4+} + H(2s)^*$



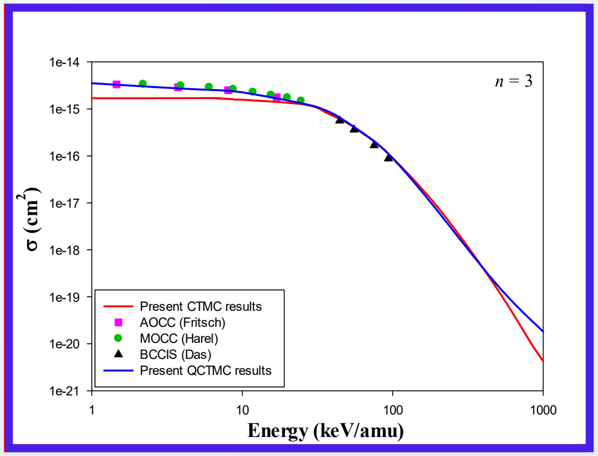
Excitation
$Be^{4+} + H(1s) \rightarrow Be^{4+} + H(2p)^*$

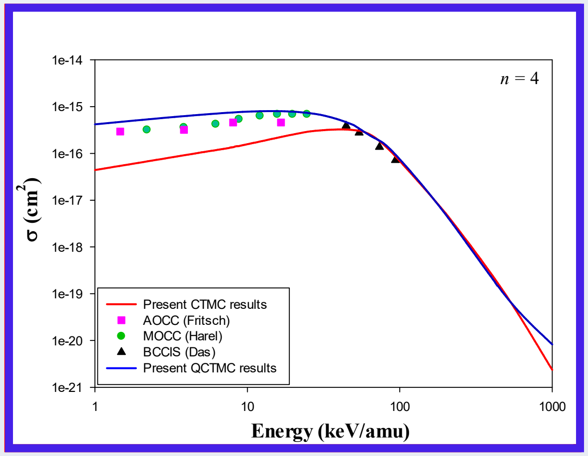


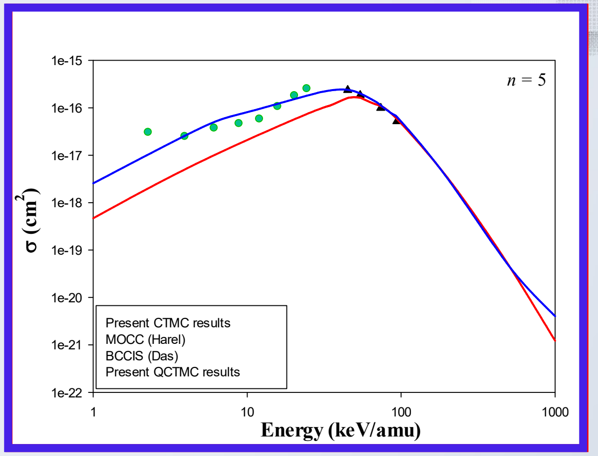
Electron capture cross sections into n = 3, 4, 5, 6, 8, 10 and nl = 3l, 4l, 5l states of the projectile in Be^{4+} + H(1s) using CTMC and QCTMC models.

State-selective Electron Capture

$Be^{4+} + H(1s) \rightarrow Be^{3+}(n) + H^{+}$

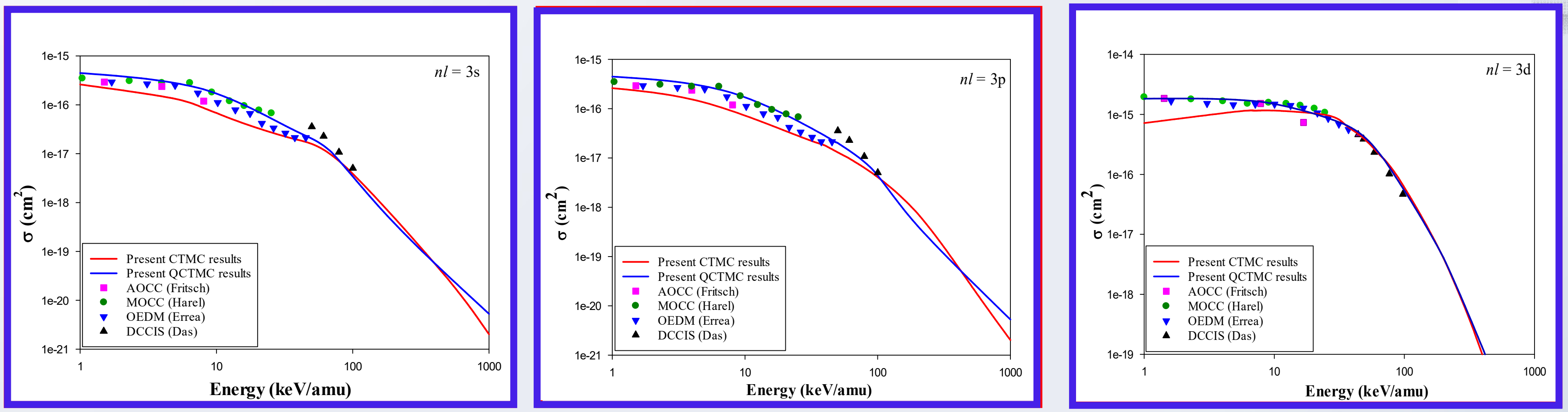






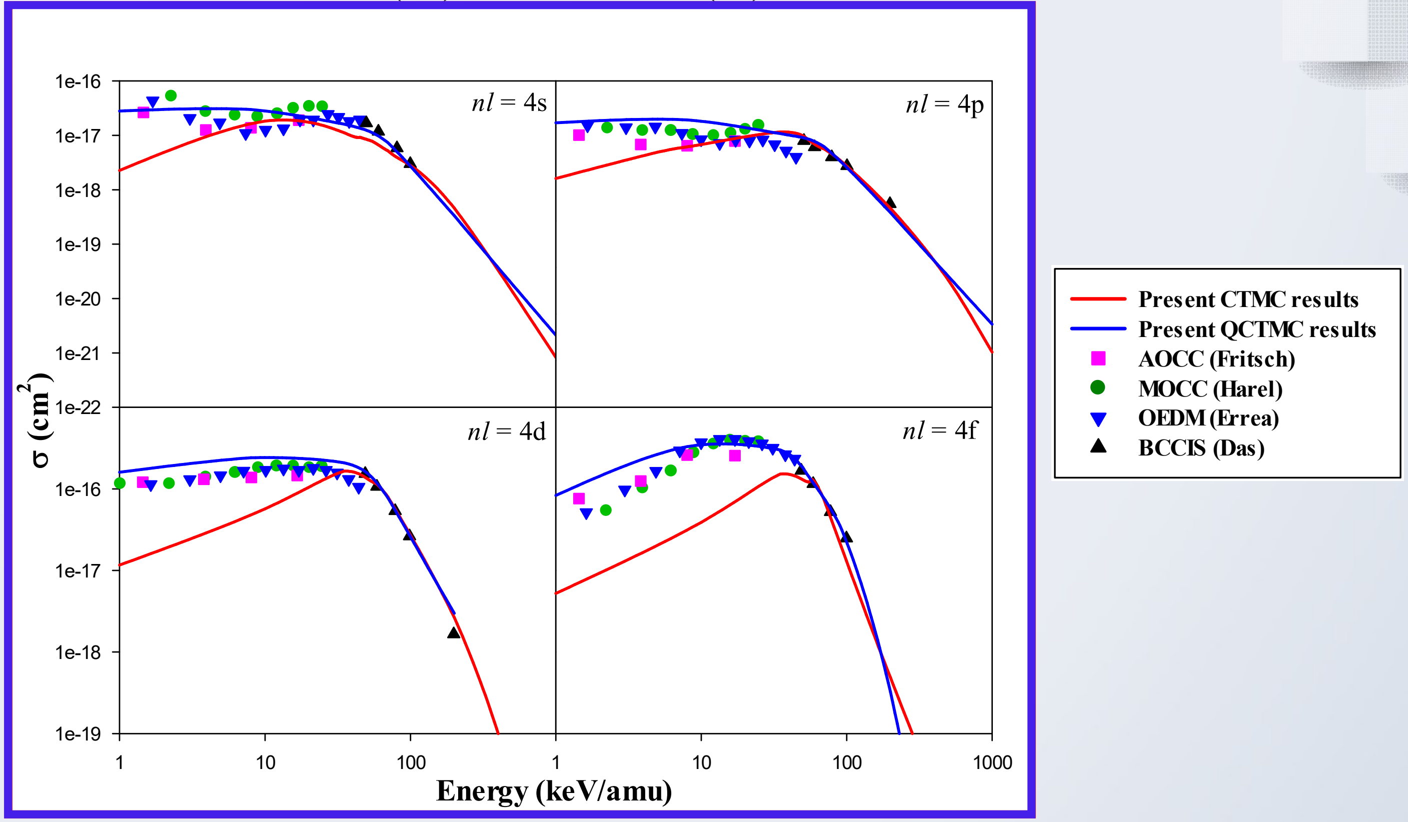
State-selective Electron Capture

$Be^{4+} + H(1s) \rightarrow Be^{3+}(3l) + H^{+}$

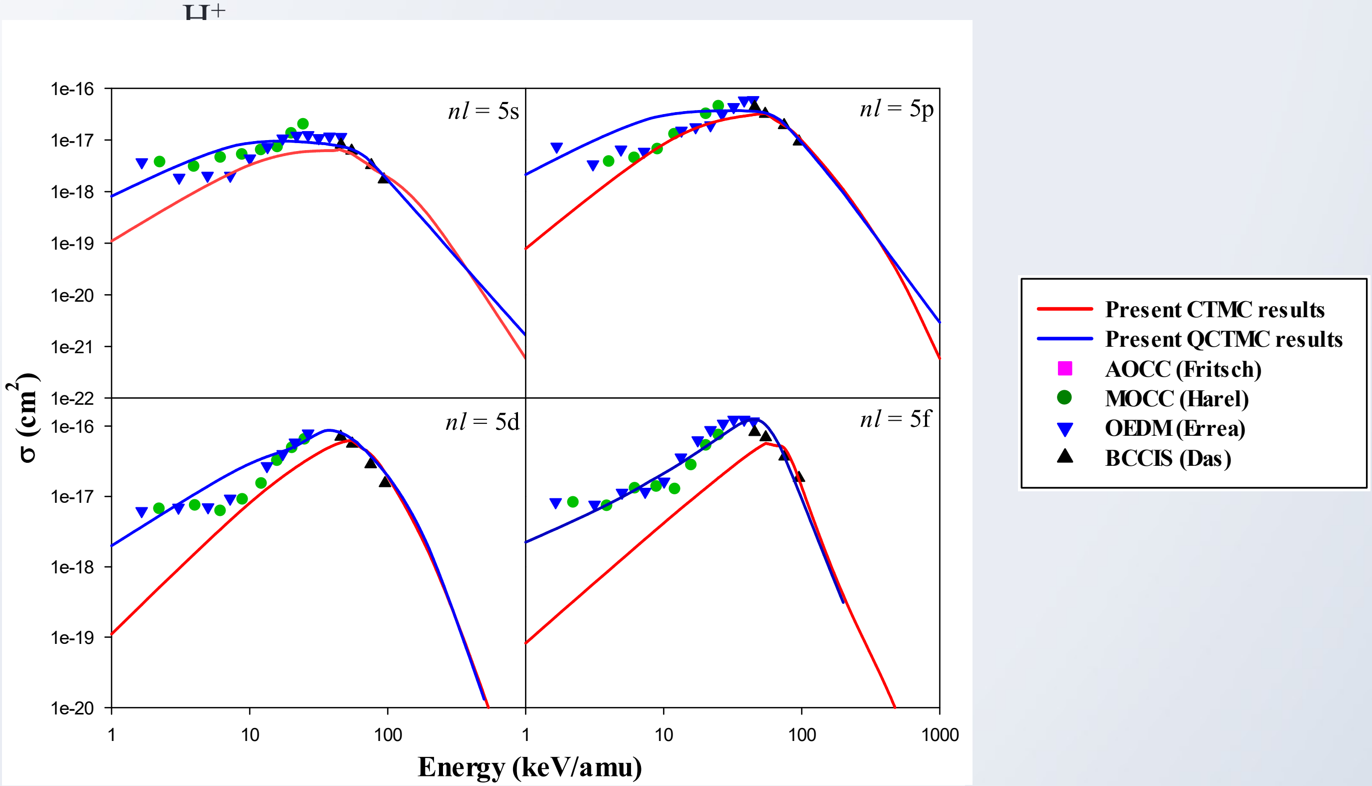


State-selective Electron Capture

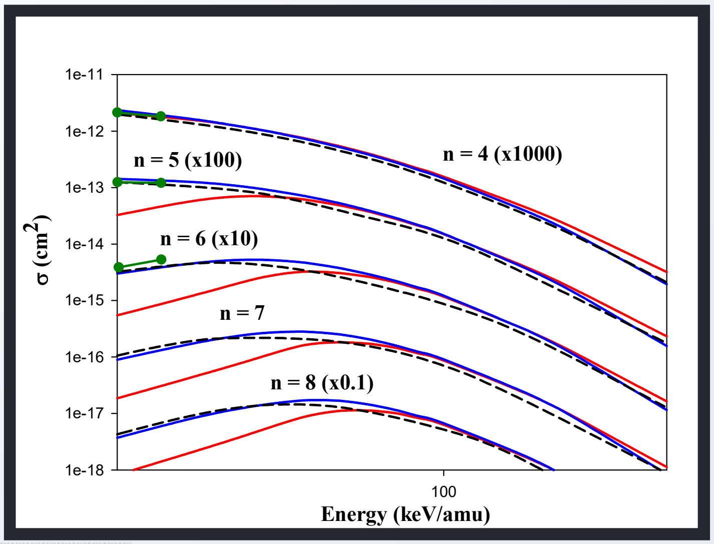
$Be^{4+} + H(1s) \rightarrow Be^{3+}(4l) + H^{+}$



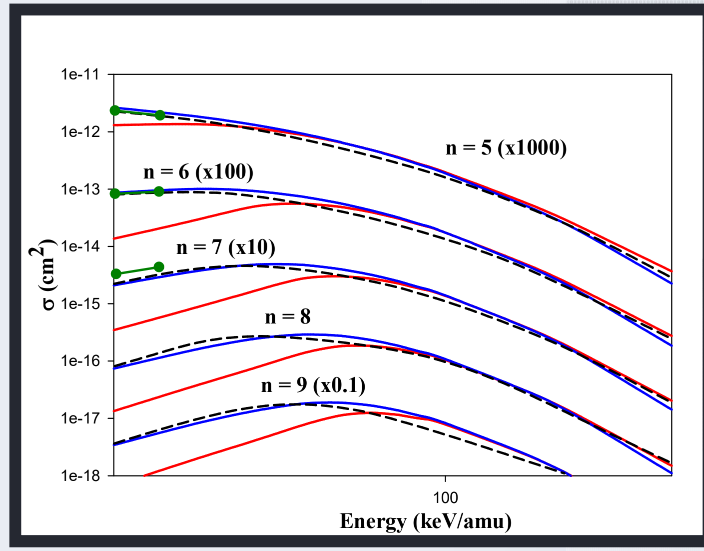
Be^{4+}+ H(1s) → $Be^{3+}(5l)$ + H^+



$C^{6+} + H(1s) \rightarrow C^{5+}(n) + H^{+}$



$N^{7+} + H(1s) \rightarrow N^{6+}(n) + H^{+}$



Present CTMC results
Present QCTMC results
Igenberg et al. J. Phys. B: At. Mol. Opt. Phys. 45, 065203 (2013)
Harel et al. At. Data. Nucl. Data Tables 68, 279 (1998)

Two ground-state Hydrogen collision System

QCTMC Result: Projectile Ionization cross section

$$H(1s)_P + H(1s)_T \rightarrow H_P^+ + H(1s)_T + e^-$$

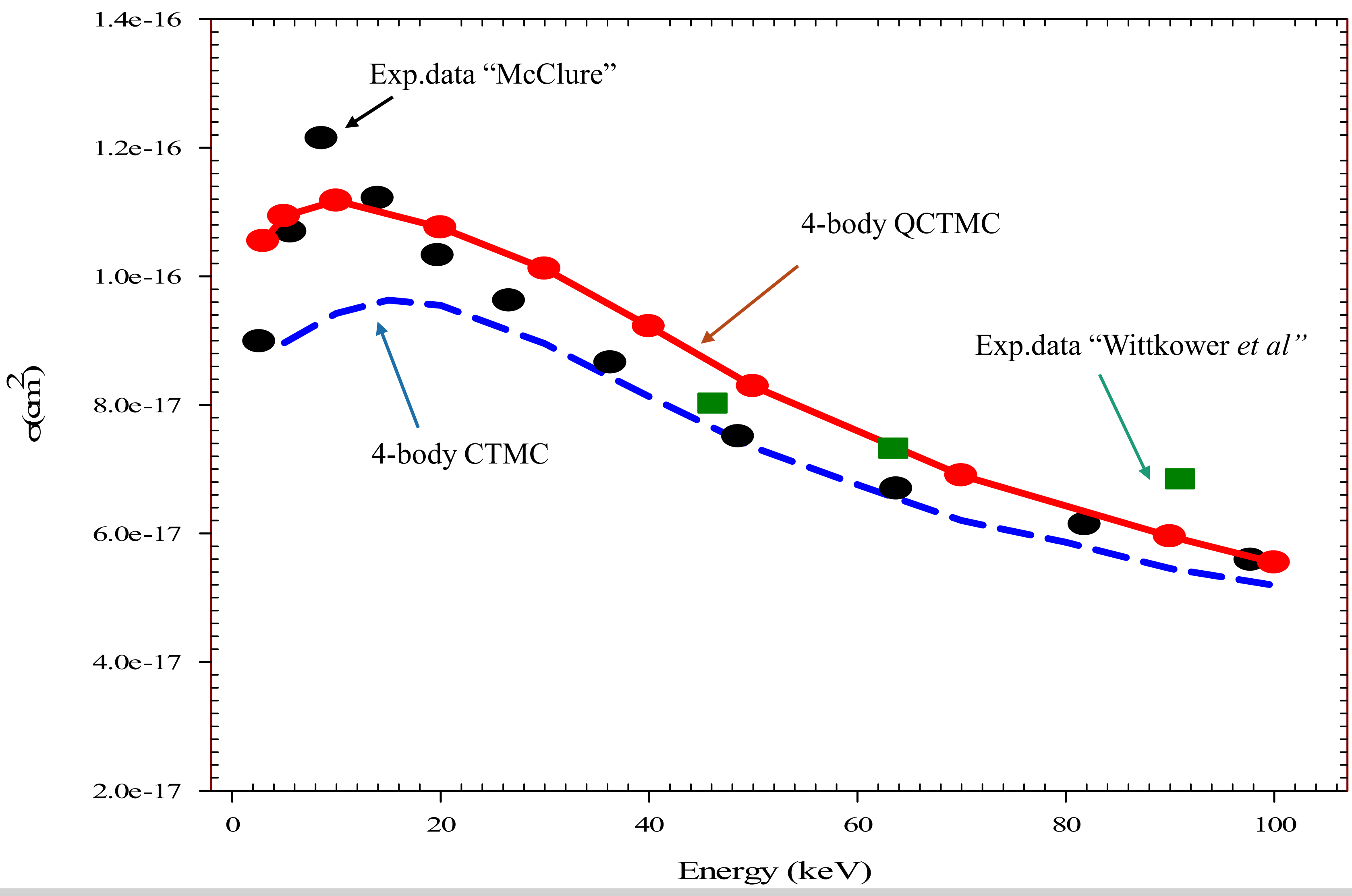
The first possible one the ***direct ionization of the projectile*** channel. This channel originates from a one-step process

$$(H_p^+, e_p^-) + (H_T^+, e_T^-) \rightarrow H_P^+ + (H_T^+, e_T^-) + e_p^-$$

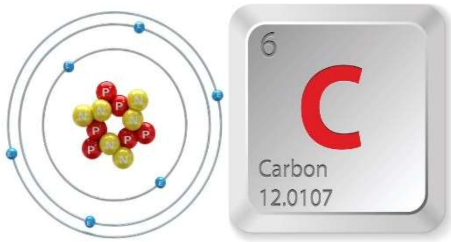
The second possible originates from the multi-electron interaction in a two-step process producing the same final particles.

$$(H_p^+, e_p^-) + (H_T^+, e_T^-) \rightarrow H_P^+ + (H_T^+, e_p^-) + e_T^-$$

Projectile ionization cross sections



Carbon ions (c^{5+}) with Hydrogen atom collision system



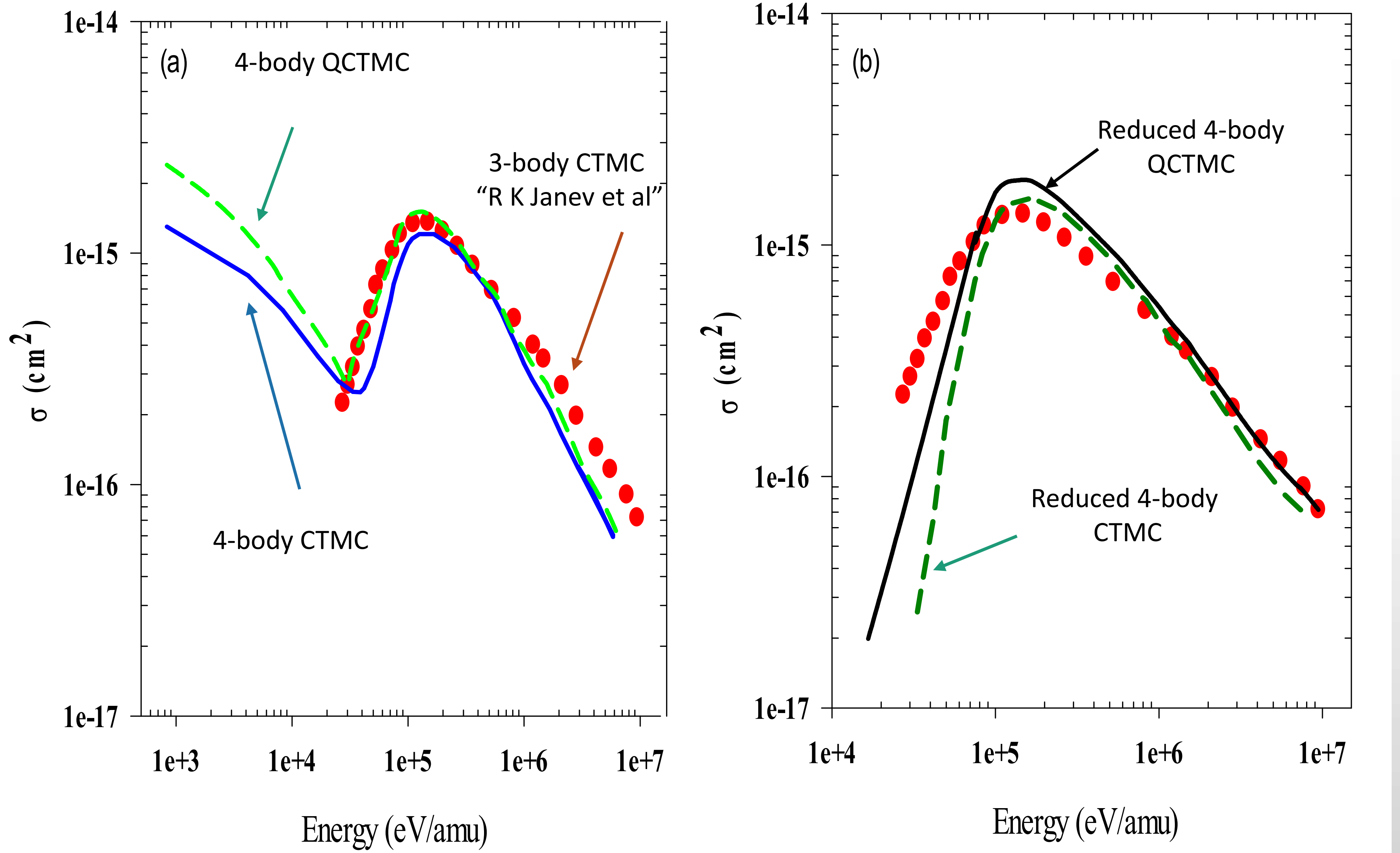
- Target ionization cross section

$$c^{5+} + H \rightarrow c^{5+} + H^{+} + e^{-} \qquad (1)$$

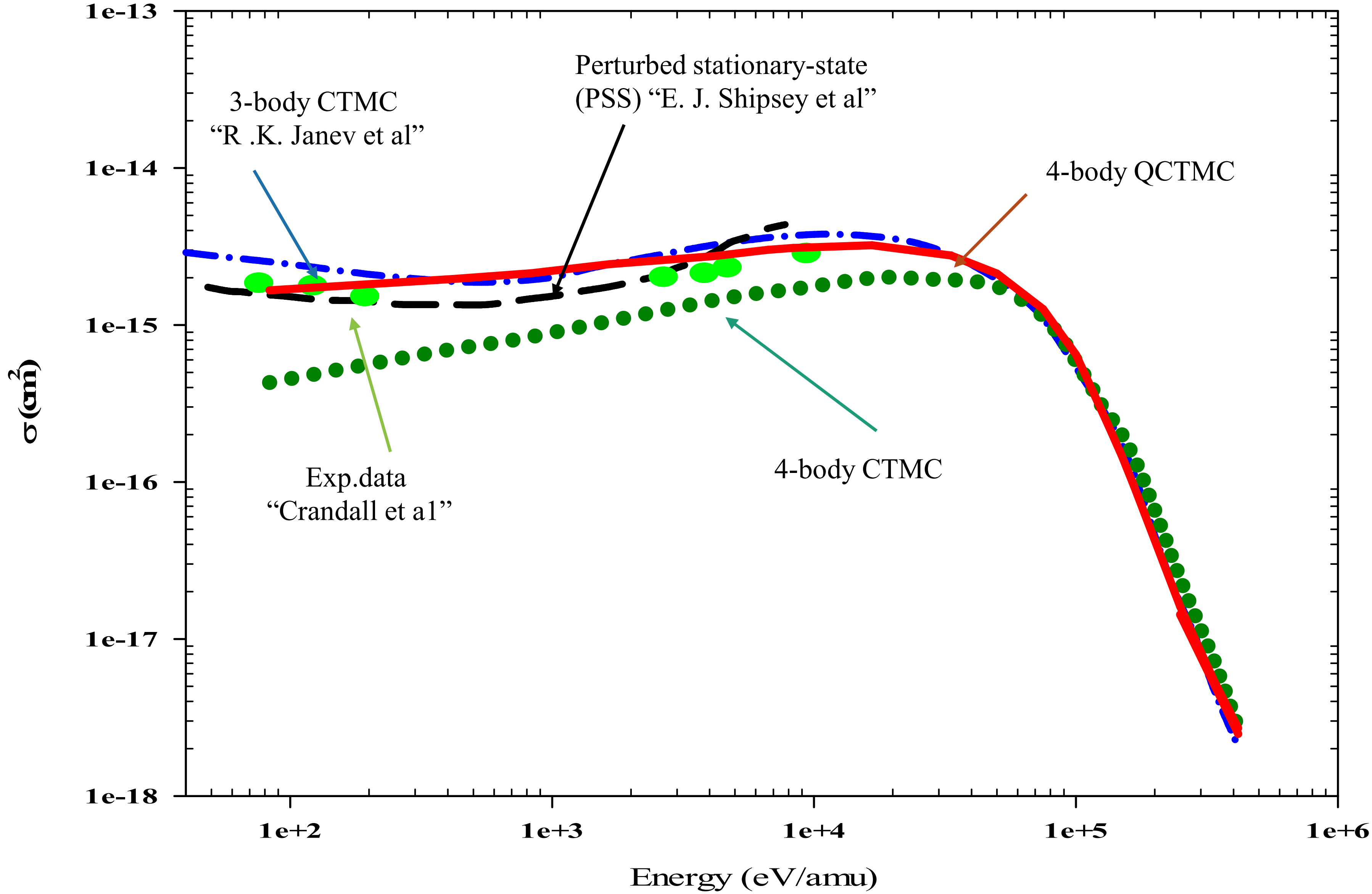
- Electron capture cross section

$$c^{5+} + H \rightarrow c^{4+} + H^{+} \qquad (2)$$

Target Ionization cross-section



Electron Capture Cross-Section of the Projectile



Publications

Be-H

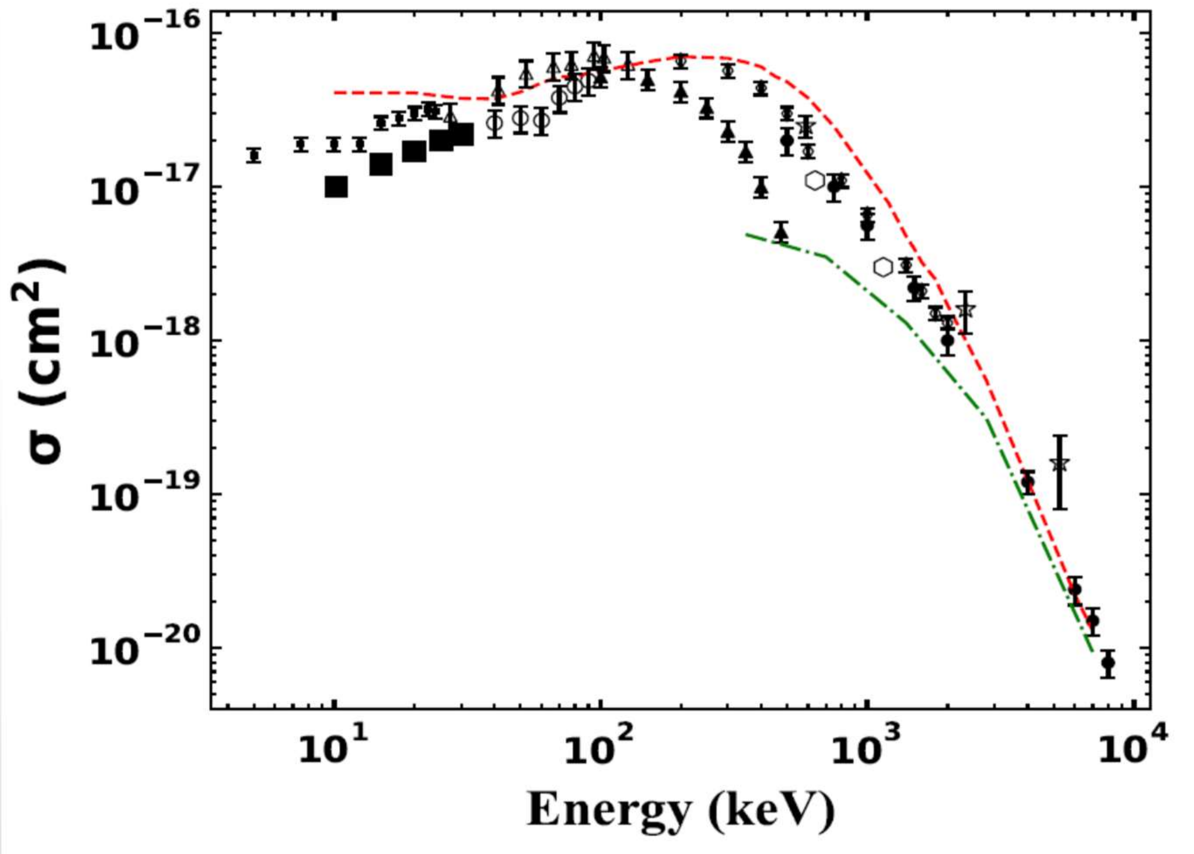
[1] I. Ziaeian and K. Tőkési, Atoms **8** 27 (2020).
[2] I. Ziaeian and K. Tőkési, EPJD J. **75** 138 (2021).
[3] I. Ziaeian and K. Tőkési, Sci. Rep. 20164 (2021).
[4] I. Ziaeian and K. Tőkési, Atoms **10** 90. (2022)
[5] I. Ziaeian and K. Tőkési, , Journal of Physics B: Atomic, Molecular and Optical Physics 55 (2022) 245201.
[6] I. Ziaeian and K. Tőkési, Atomic Data and Nuclear Data Tables **146** 101509 (2022).

H+H type

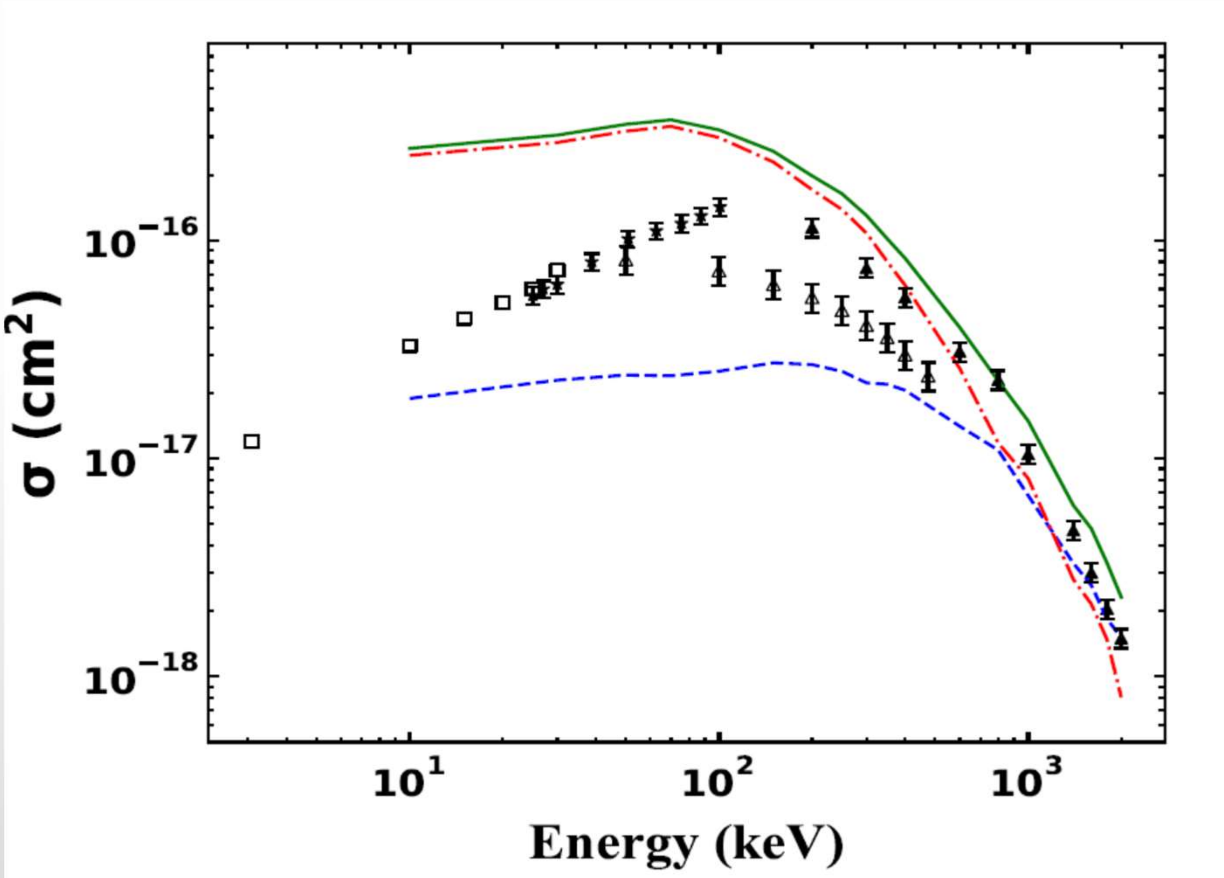
[1] S.J.A. Atawneh and K. Tőkési, Atoms **8** 31 (2020).
[2] S.J.A. Atawneh and K. Tőkési, J. Phys. B: At. Mol. Opt. Phys. **54** 065202 (2021).
[3] S. J. A. Atawneh and K. Tőkési. Nucl. Fusion. **62** 026009 (2021).
[4] S.J.A. Atawneh and K. Tőkési, Atomic Data and Nuclear Data Tables **146** 101513 (2022).
[5] S. J. A. Atawneh and K. Tőkési. Phys. Chem. Chem. Phys. **24** 15280 (2022).

Atomic Data
for Injected Impurities in Fusion Plasmas

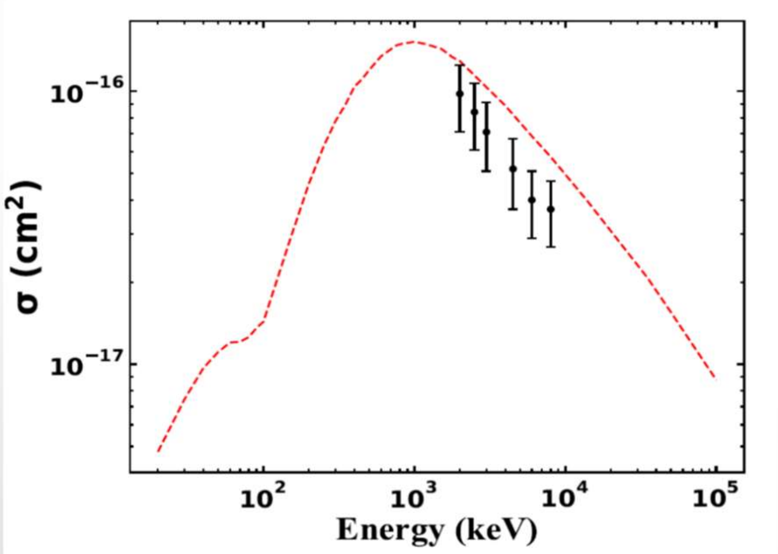
Total cross sections of the single-electron capture from *He*(1*s*) by *Li*+



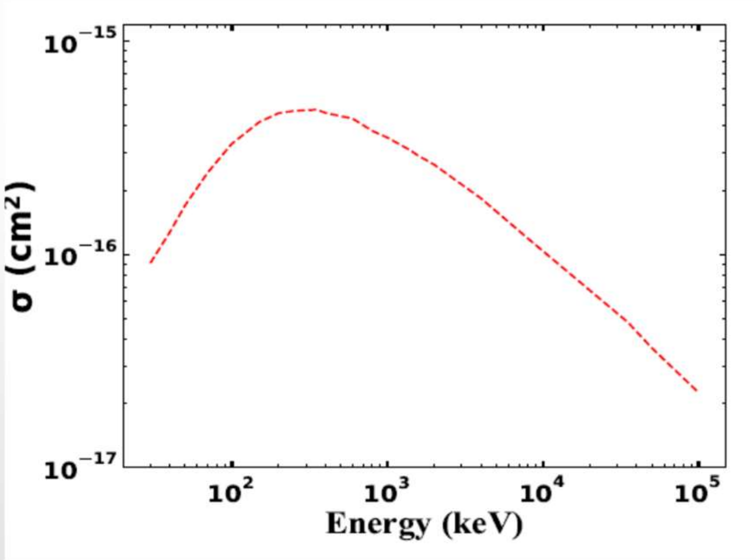
Total cross sections of the single-electron capture from *N*(2*p*) by *Li*+



Total cross sections of the single- electron ionisation from $He(1s)$ by $Li+$



Total cross sections of the single- electron ionisation from N(2p) by $Li+$



Conclusions

- Classical method (CTMC) reproduce different experiments for collisions between charged particles and atoms
- gives accurate cross sections for ionization, capture, excitation
- valid in wide projectile energy range
- can descibe partial cross sections
- QCTMC model, represents one step further towards a better description of the classical atomic collisions. This model with simplicity can time efficiently carry out simulations where maybe the quantum mechanical ones become complicated, therefore, our model should be an alternative way to calculate accurate cross sections and maybe can replace the quantum-mechanical methods.

Thanks for your attention!