Curtin University

Work done over the Neutral Beams CRP using the CCC approach

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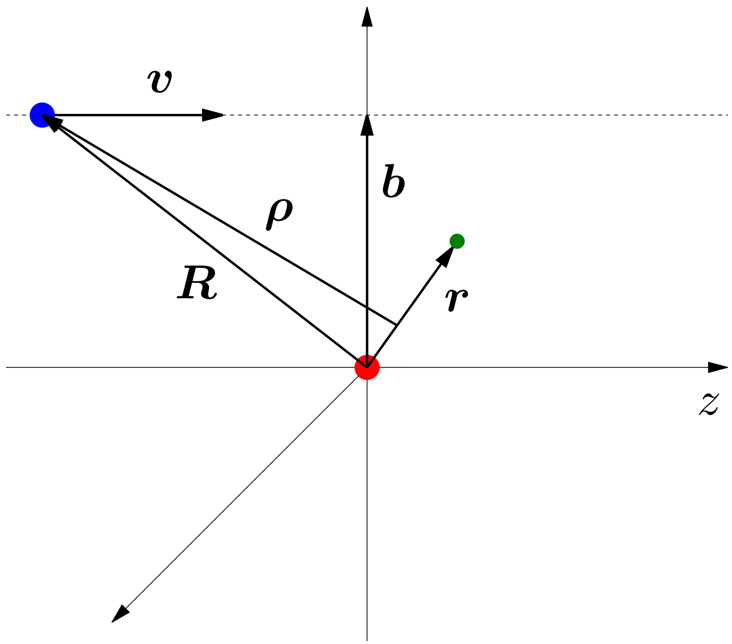
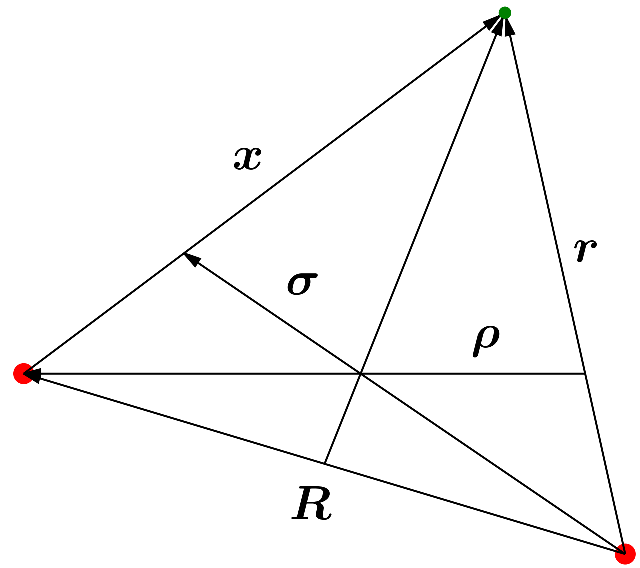
2-centre CCC approach





2 sets of Jacobi coordinates

$$H\Psi_i^+ = E\Psi_i^+$$ this is the total scattering wave function (not electronic)

$$\Psi_i^+ = \sum_{\alpha=1}^{N} F_\alpha(t,\boldsymbol{b}) e^{i\boldsymbol{q}_\alpha\cdot\boldsymbol{\rho}} \psi_\alpha(\boldsymbol{r}) + \sum_{\beta=1}^{M} G_\beta(t,\boldsymbol{b}) e^{i\boldsymbol{q}_\beta\cdot\boldsymbol{\sigma}} \psi_\beta(\boldsymbol{x})$$

A new ansatz that doesn't require so-called electron translation factors (ETF)

2-centre CCC approach

$$\begin{cases} i\dot{F}_{\alpha'} + i\sum_{\beta=1}^{M} \dot{G}_\beta \tilde{K}_{\alpha'\beta} = \sum_{\alpha=1}^{N} F_\alpha D_{\alpha'\alpha} + \sum_{\beta=1}^{M} G_\beta \tilde{Q}_{\alpha'\beta} \\ i\sum_{\alpha=1}^{N} \dot{F}_\alpha K_{\beta'\alpha} + i\dot{G}_{\beta'} = \sum_{\alpha=1}^{N} F_\alpha Q_{\beta'\alpha} + \sum_{\beta=1}^{M} G_\beta \tilde{D}_{\beta'\beta} \end{cases}$$

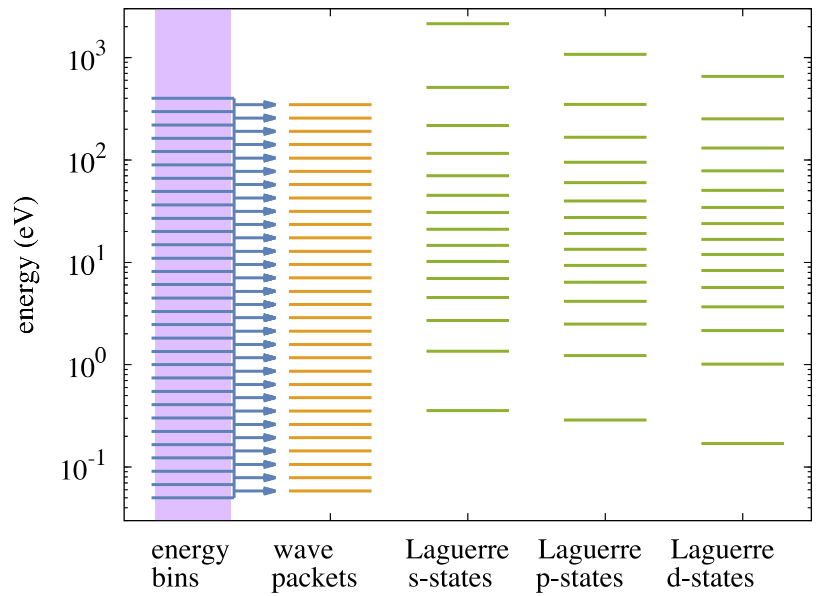
Probability amplitudes

$$A_\alpha^{\mathrm{DS}}(\boldsymbol{b}) = F_\alpha(+\infty, \boldsymbol{b}) - \delta_{\alpha i}$$

$$A_\beta^{\mathrm{EC}}(\boldsymbol{b}) = G_\beta(+\infty, \boldsymbol{b})$$

Direct scattering (DS): elastic scattering or target excitation including continuum
Electron capture (EC): this could be capture to bound state or continuum (ECC)

Wave-packet continuum discretisation



$$\phi_{nl}(r) = \frac{1}{\sqrt{w_n}} \int_{k_{n-1}}^{k_n} dk U_l(k,r)$$

Coulomb wave

For n^{th} bin the wave packet is at

$$\epsilon_n = (k_n^2 + k_n k_{n-1} + k_{n-1}^2)/6$$

Advantages of WPs:

- Flexible density and distribution
- WPs aligned for different ℓ
- Overlap with Coulomb wave is simple

$$\langle \psi^-_{\boldsymbol{\kappa}} | \psi_f^{\mathrm{WP}} \rangle = \sqrt{\frac{2}{\pi}} (-i)^l e^{i\sigma_l} b_{nl}(\kappa) Y_{lm}(\hat{\boldsymbol{\kappa}})$$

$$b_{nl}(\kappa) = \int_0^\infty dr U_l(\kappa, r) \phi_{nl}(r) = \frac{1}{\sqrt{w_n}}$$

p – He collisions (4-body problem)

$$\Psi = \sum_{\alpha=1}^{N} F_\alpha(t,\boldsymbol{b})\psi_\alpha^{\mathrm{He}}(\boldsymbol{r}_1,\boldsymbol{r}_2)e^{i\boldsymbol{q}_\alpha\cdot\boldsymbol{\rho}}$$

$$+\frac{1}{\sqrt{2}}\sum_{\beta=1}^{M} G_\beta(t,\boldsymbol{b})\left[\psi_\beta^{\mathrm{H}}(\boldsymbol{x}_1)\psi_{1s}^{\mathrm{He}^+}(\boldsymbol{r}_2)e^{i\boldsymbol{q}_{1\beta}\cdot\boldsymbol{\sigma}_1}+\psi_\beta^{\mathrm{H}}(\boldsymbol{x}_2)\psi_{1s}^{\mathrm{He}^+}(\boldsymbol{r}_1)e^{i\boldsymbol{q}_{2\beta}\cdot\boldsymbol{\sigma}_2}\right]$$

Target structure (3-body problem) in the CI-FC approximation

$$\psi_\alpha^{\mathrm{He}}(\boldsymbol{r_1},\boldsymbol{r_2}) = \psi_\alpha(\boldsymbol{r_1})\psi_{1s}(\boldsymbol{r_2})+\psi_\alpha(\boldsymbol{r_2})\psi_{1s}(\boldsymbol{r_1})$$

$$H_T\psi_\alpha^{\mathrm{He}}(\boldsymbol{r}_1,\boldsymbol{r}_2) = E_\alpha\psi_\alpha^{\mathrm{He}}(\boldsymbol{r}_1,\boldsymbol{r}_2)$$

This gives

- Negative-energy discrete states and
- Positive-energy continuum solution (non-normalisable wave function)

The continuum solution is used to generate WP

Integrated cross sections

$$\sigma_f = 2\pi \int_0^\infty db\; b|A_f(b)|^2, \quad f = \alpha, \beta$$

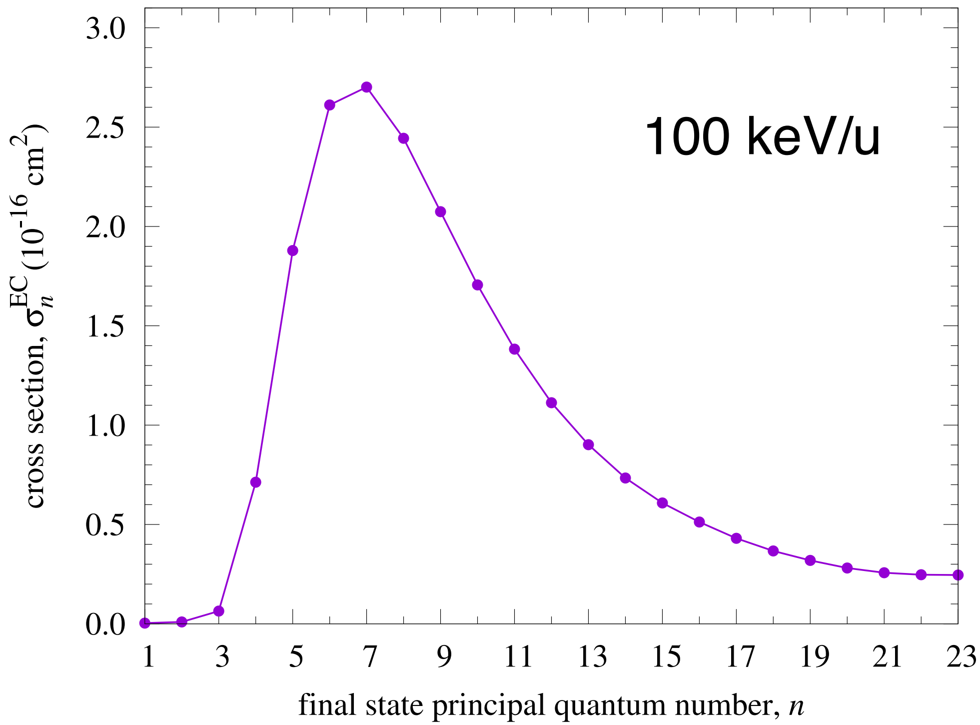
$$\sigma_{\mathrm{TECS}} = \sum_{\beta \in [\epsilon_\beta < 0]}^{M} \sigma_\beta^{\mathrm{EC}}$$

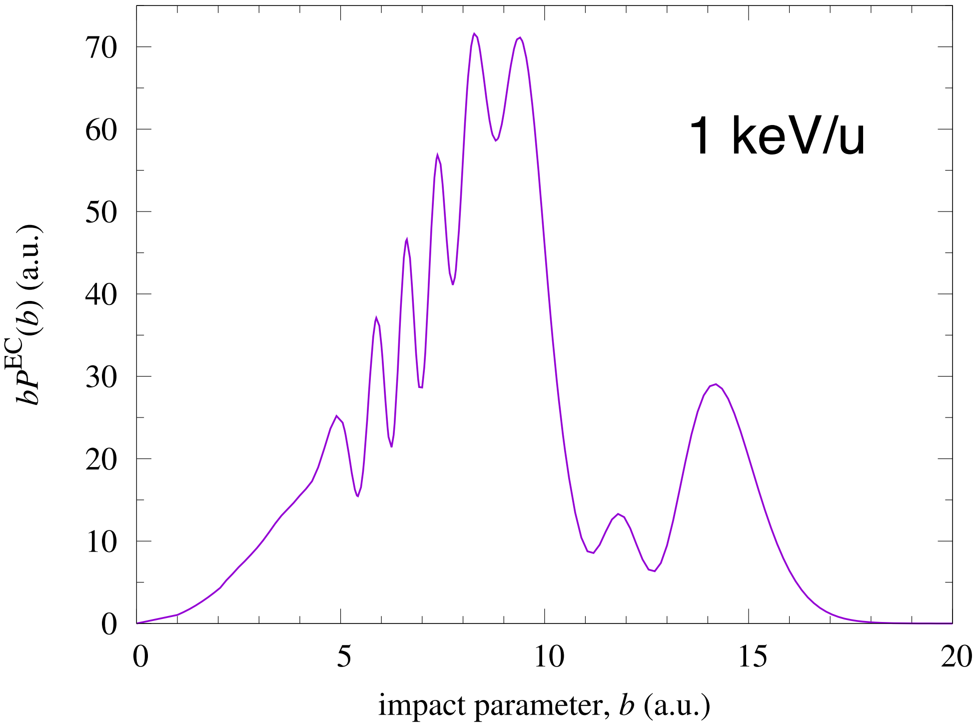
$$\sigma_{\mathrm{TICS}} = \sum_{\alpha \in [\epsilon_\alpha > 0]}^{N} \sigma_\alpha^{\mathrm{DS}} + \sum_{\beta \in [\epsilon_\beta > 0]}^{M} \sigma_\beta^{\mathrm{EC}}$$

- We increase *N* and *M* until the results converge not only for the total electron capture cross section (TECS) and total ionisation cross section (TICS) but also for most important state-selective cross sections
- Use GPU-based supercomputers

- Calculated: p, He^{2+}, Be^{4+}, C^{6+}, Ne^{10+} on H
  p on He, Li, Na, K and H_2

Electron capture and ionisation in Ne^{10+} - H(1s)

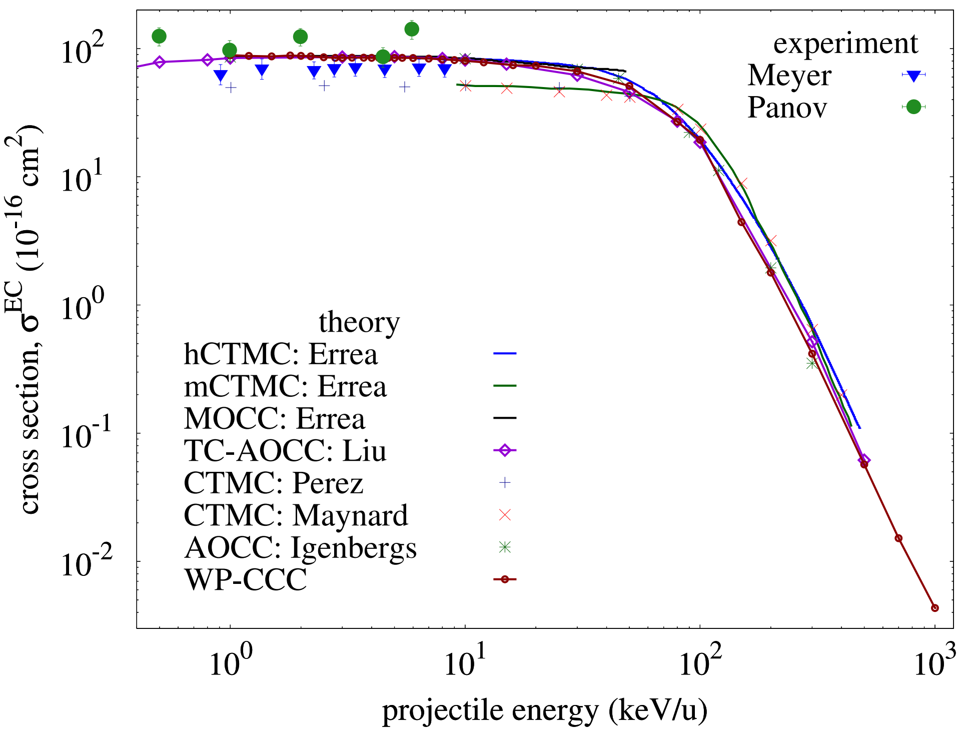


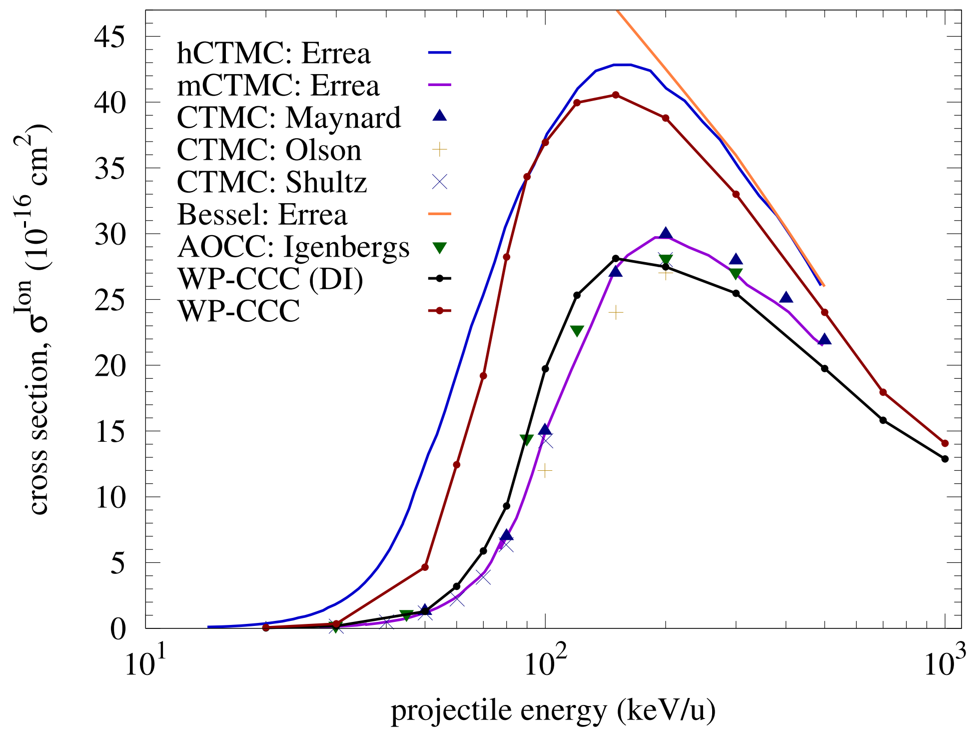


Energy range considered: 1 keV/u to 2 MeV/u.
The results have converged within a few % over the entire energy range.
Usually, for low Z ions $n_{\max} \approx Z$, but for HCI we find $n_{\max} > Z$

At 100 keV/u we had to go up to $n = 23$ to achieve a few % convergence.
The number of WP states was $N_c = 15$ and $\ell_{\max} = 9$.

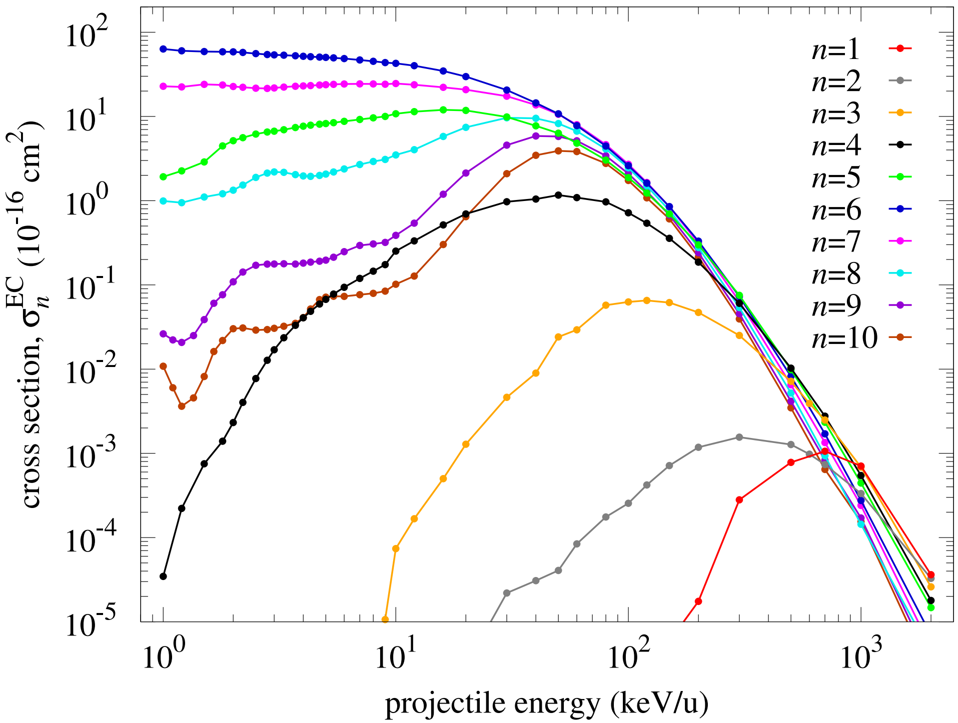
Total capture and ionisation in Ne^{10+} - H(1s)

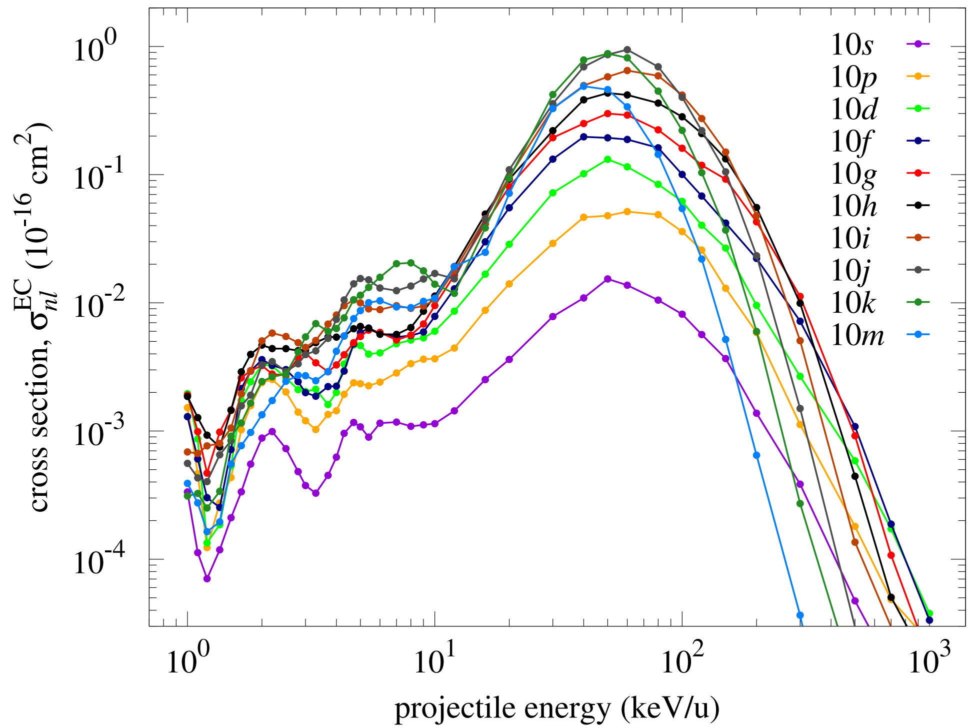




Kotian *et al.* 2022 J. Phys. B 55, 115201

State-selective electron capture in Ne^{10+} - H(1s)



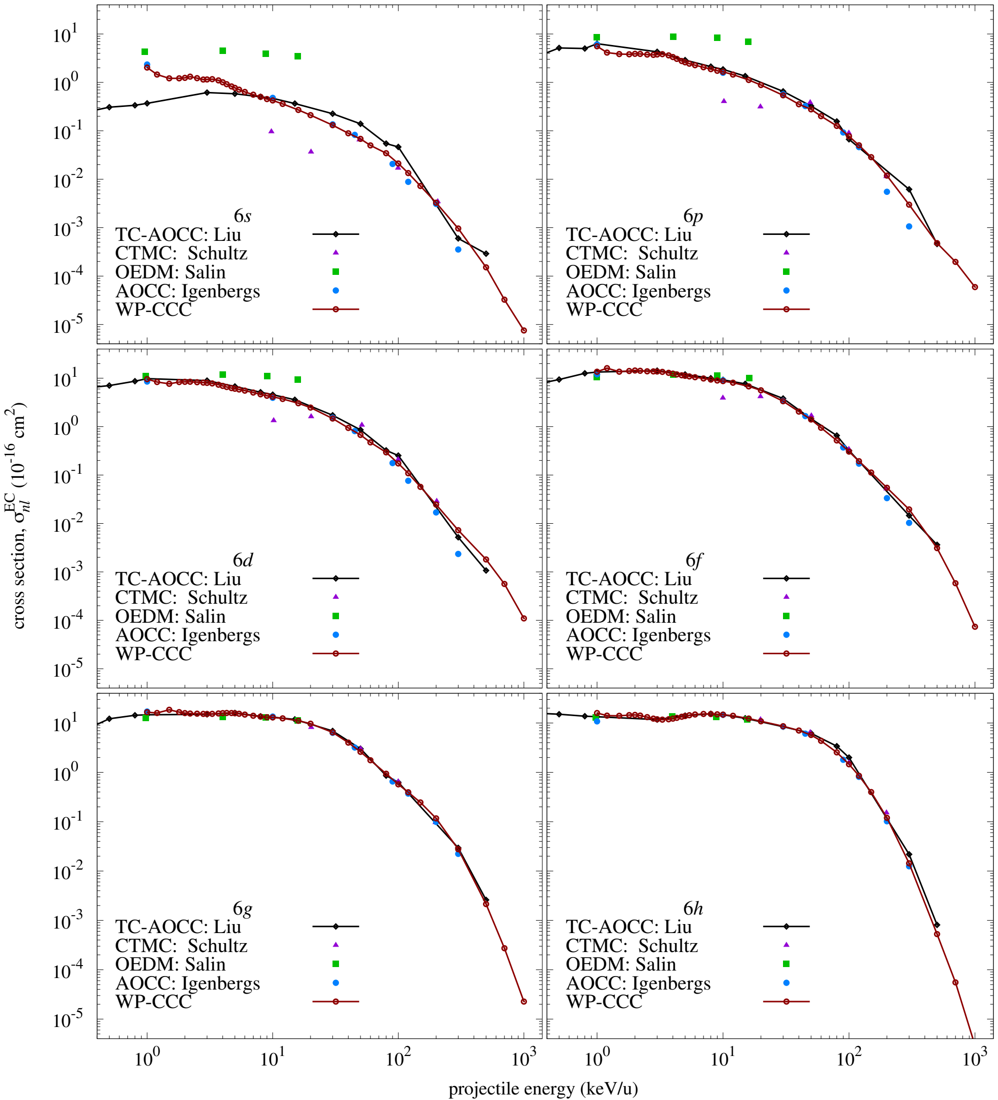


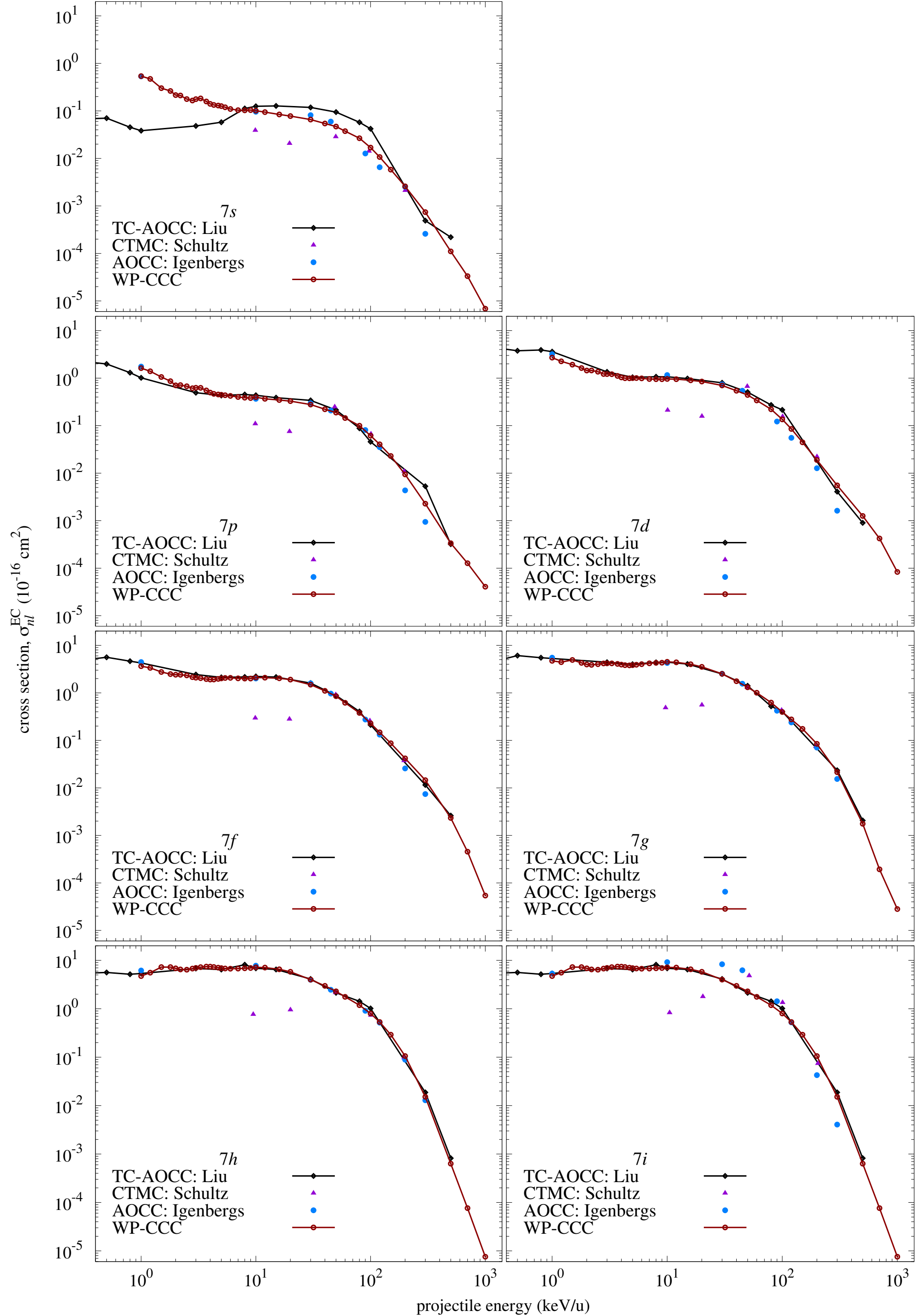
Oscillations in the 10ℓ partial cross sections. Only in non-resonant transitions. See Schultz et al., PRL 78, 2720 (1997).

Kotian *et al.* 2022 J. Phys. B 55, 115201

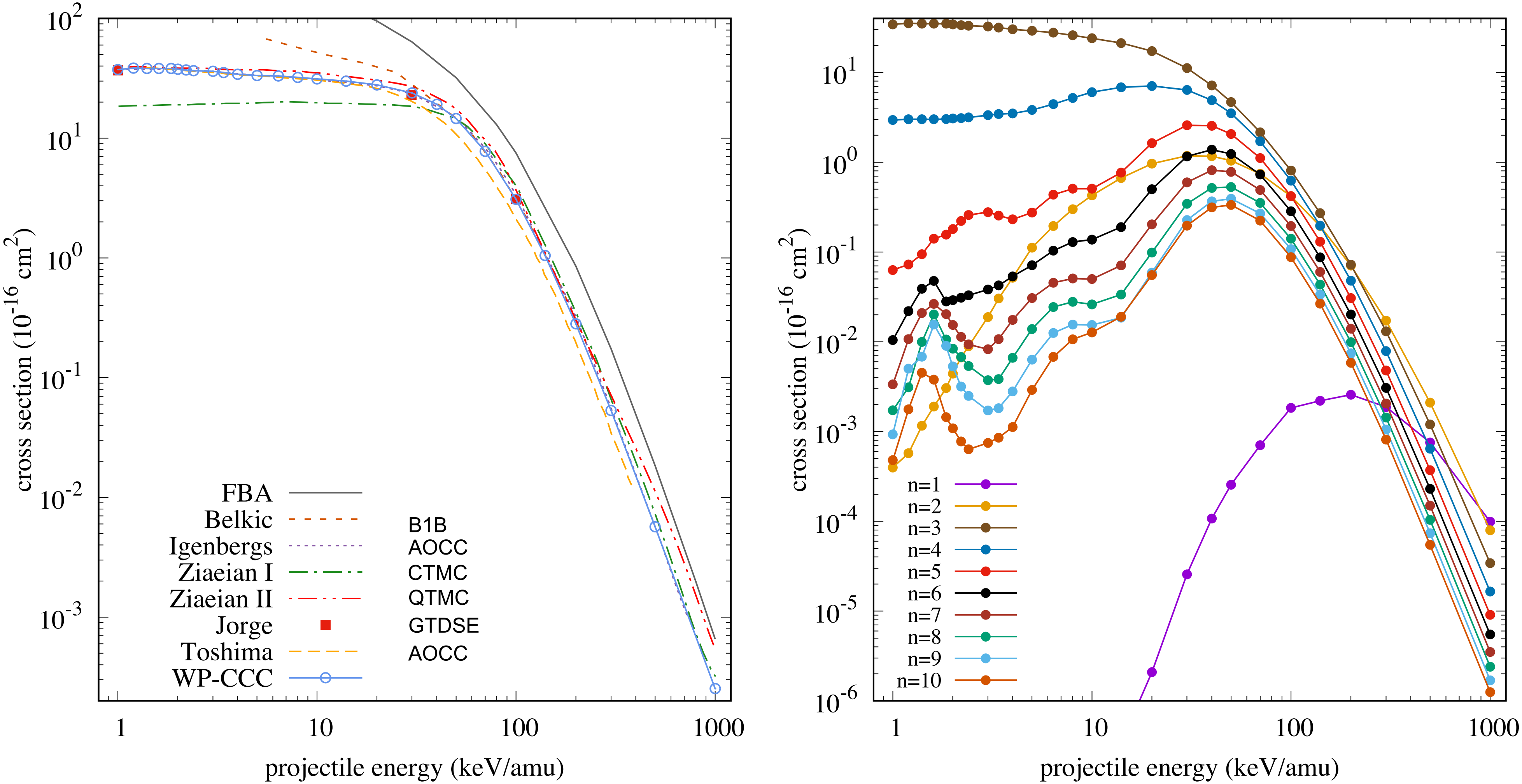
Ne^{10+} - H(1s) → $Ne^{9+}(n\ell)$ - H^+

Our results deviate from TC-AOCC by Liu *et al* for 6ℓ, 7ℓ, 8ℓ below 5 keV



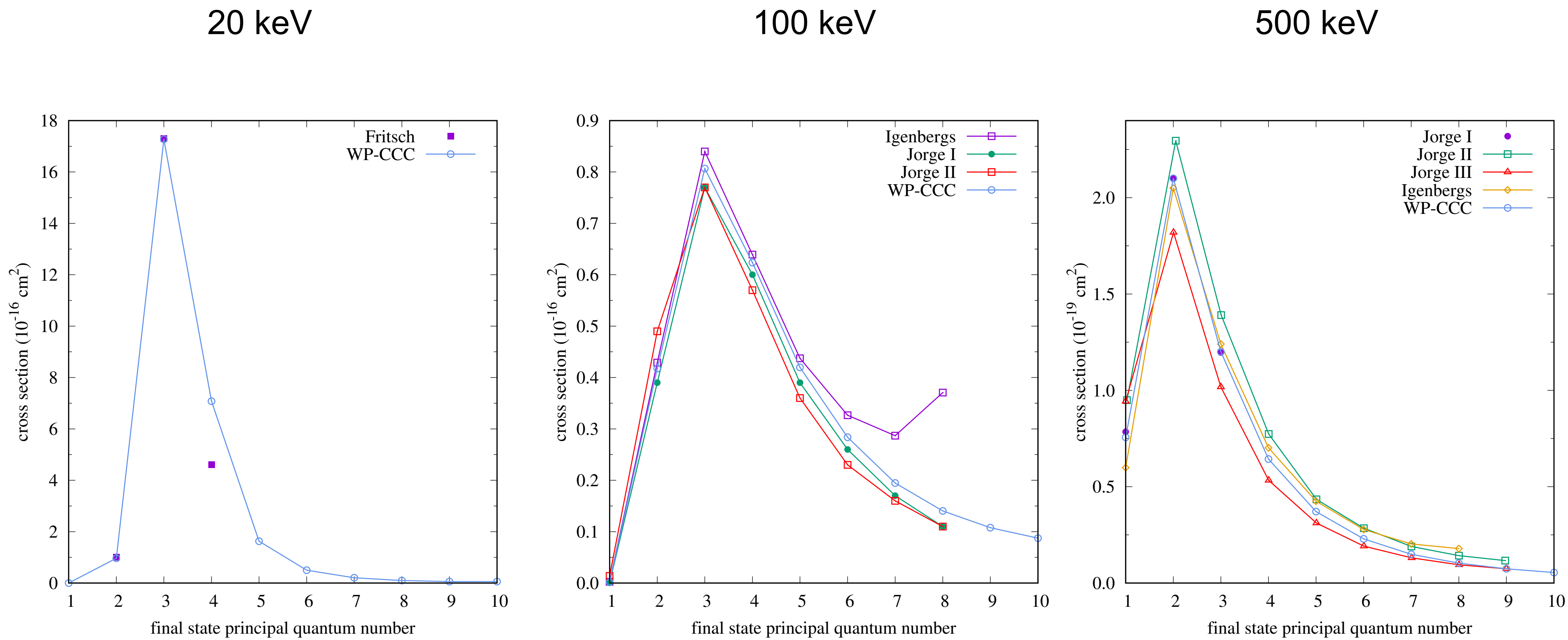


Total and state-selective capture in Be^{4+} - H(1s)



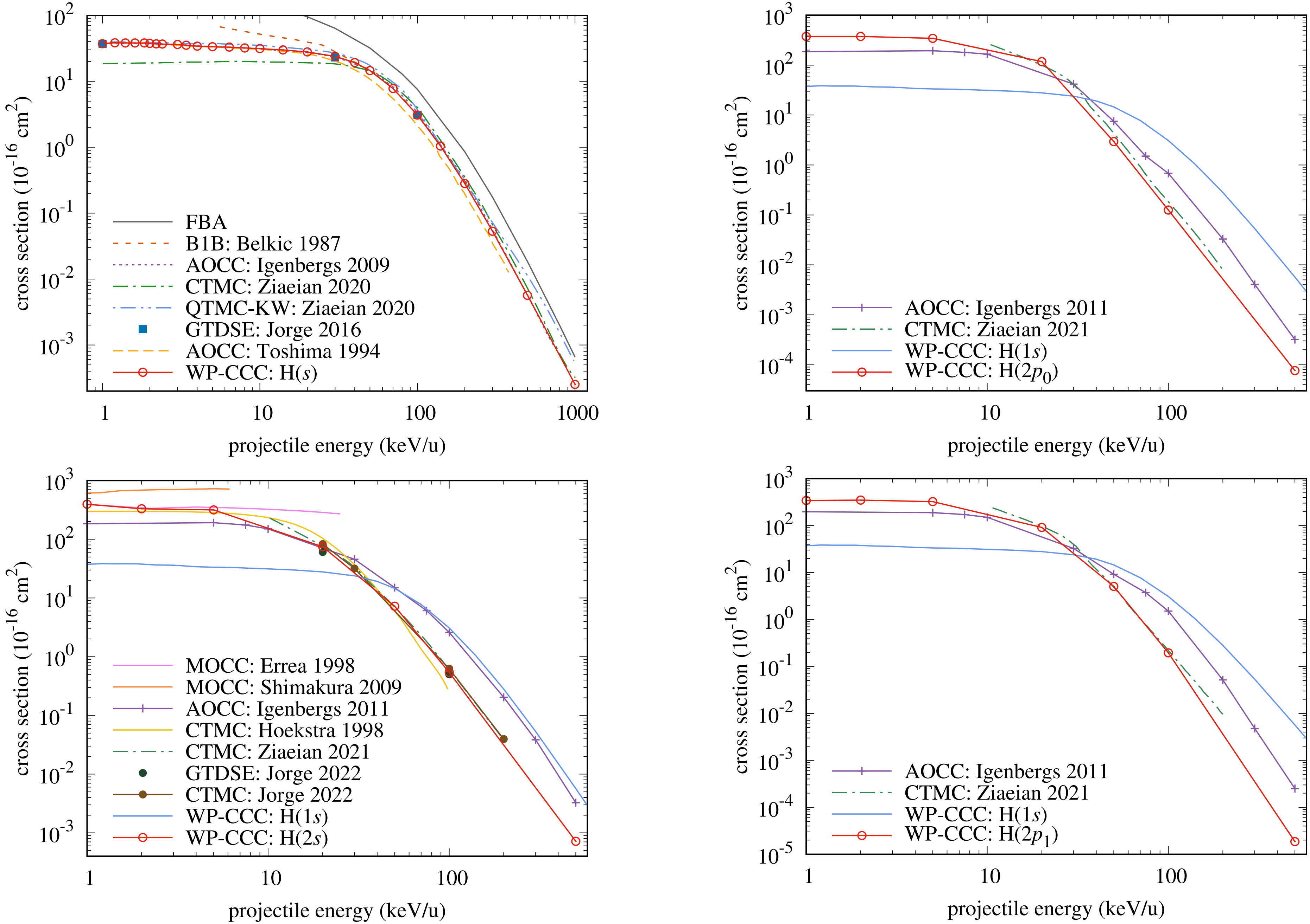
Be^{4+} - H(1s): Antonio et al 2021 J. Phys. B 54, 175201

State-selective capture in Be^{4+} - H(1s)

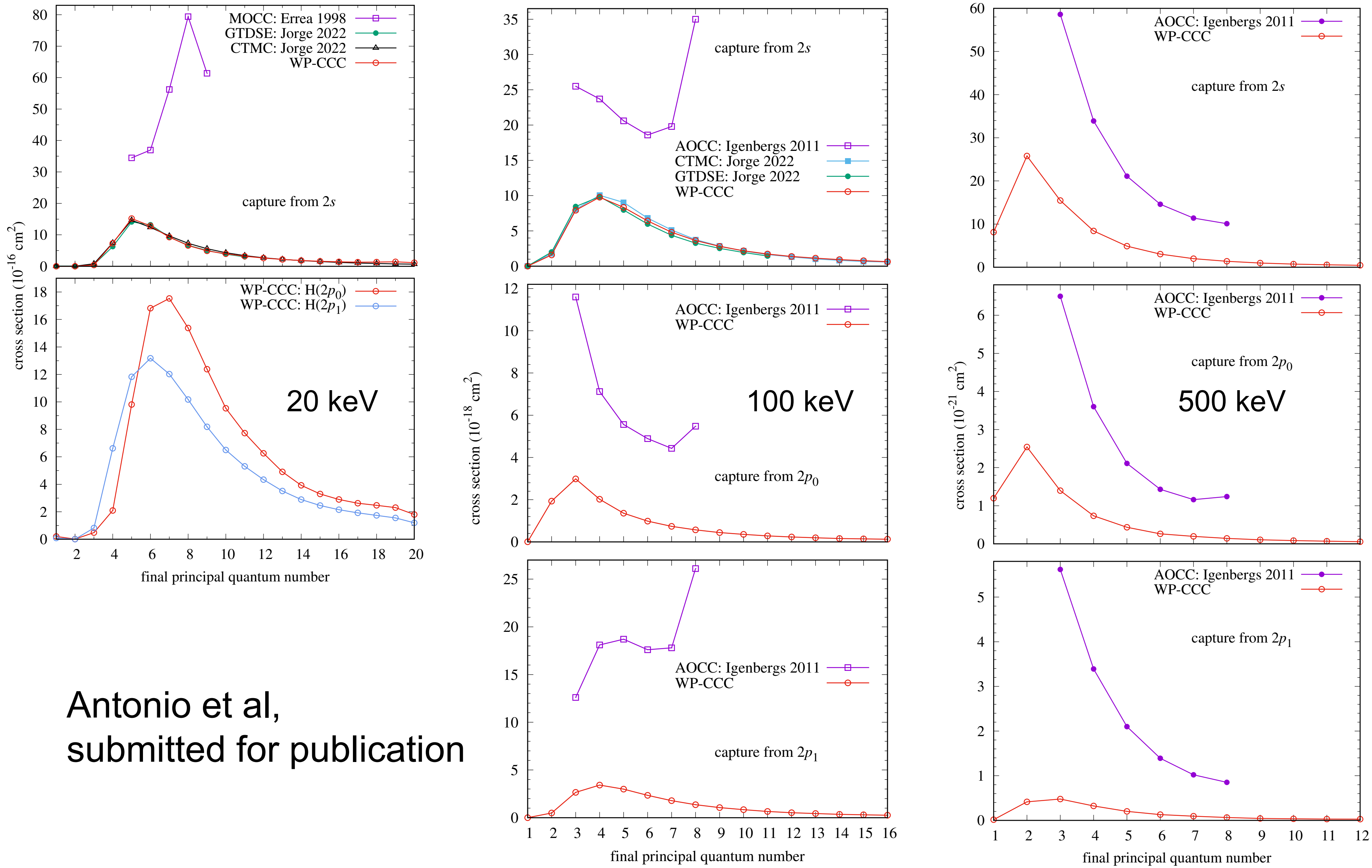


Be^{4+} - H(1s): Antonio et al 2021 J. Phys. B 54, 175201

Total capture in Be^{4+} - H(1s) and Be^{4+} - H(2lm)



Total and state-selective capture in Be^{4+} - H(2lm)



Antonio et al,
submitted for publication

Summary of completed work

- Developed 2-centre CCC approach to ion-atom collisions
- Calculated integrated total and state-selective cross sections for
  - p, He^{2+}, Be^{4+}, C^{6+}, Ne^{10+} - H(1s) collisions
  - p, He^{2+}, Be^{4+}, C^{6+}, Ne^{10+} - H(1s) collisions
  - p, Be^{4+} - H(2s, $2p_0$, $2p_1$) collisions
  - p - He
- Calculated all 3 types of SDCS for ionisation in p-H and p-He collisions

- Developed 1-centre method for 2-centre problems: simple, fast and works well
- Developed E1E method for ion collisions with multielectron targets
  - p - He, Li, Na, K
  - p - H_2
- The E1E results for p-He and p-H_2 agree well with experiment where available

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Thank you for attention!