Recommended Excitation Cross Sections in X^{q+} + H(1s) collisions of interest for CXRS.

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Overview

- Motivation
- Methods
  - Semi-classical Molecular OEDMs
  - Semi-classical 1CAO-Bessel
  - Classical CTMC
- Excitation Cross sections: $\left\{ \begin{array}{lll} \text{Li}^{3+} & + & \text{H(1s)} \\ \text{Ne}^{10+} & + & \text{H(1s)} \\ \text{Ar}^{18+} & + & \text{H(1s)} \end{array} \right.$
- Scaling Laws
- Conclusions

Motivation

Charge eXchange Recombination Spectroscopy (CXRS) is relevant diagnostic tool in tokamak plasmas:

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Concentration and Temperature of the impurities:

Spectral analysis: $I^{\mathrm{CX}} = \int q_{eff}^{\mathrm{CX}} n_I n_B ds$

- q_{eff}^{CX} is the CR effective coefficient
- n_I and n_B are the impurity and beam densities

Presence of the excited atoms H(n=2) in the beam ?

$$\Downarrow$$

Excitation cross sections

Scope.

To complete the cross section data bases for:

$$\mathrm{A^{q+} + H(1s) \quad \rightarrow \quad A^{q+} + H(}n'l'm'\mathrm{)} \quad \text{excitation}$$

with $\mathrm{A^{q+} : Li^{3+}, Ne^{10+}, Ar^{18+}}$

Li $\rightarrow$ Coating the first wall

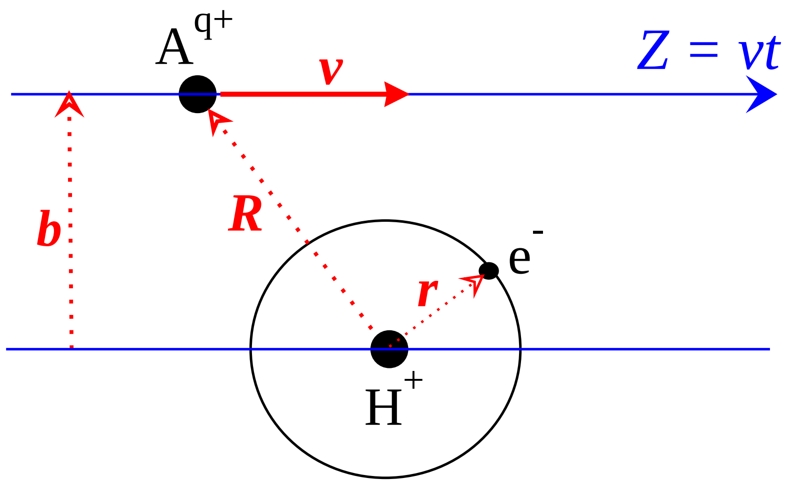
Ne, Ar $\rightarrow$ Found in the plasma divertors

in the broad low-intermediate-high energy domain:

1 keV/amu $< E <$ 1000 keV/amu

Semi-classical approximation.

Impact parameter approximation: $\boldsymbol{R}(t) = \boldsymbol{b} + \boldsymbol{v}\, t$



($E > 250$ eV/amu)

We must solve the *eikonal equation*:

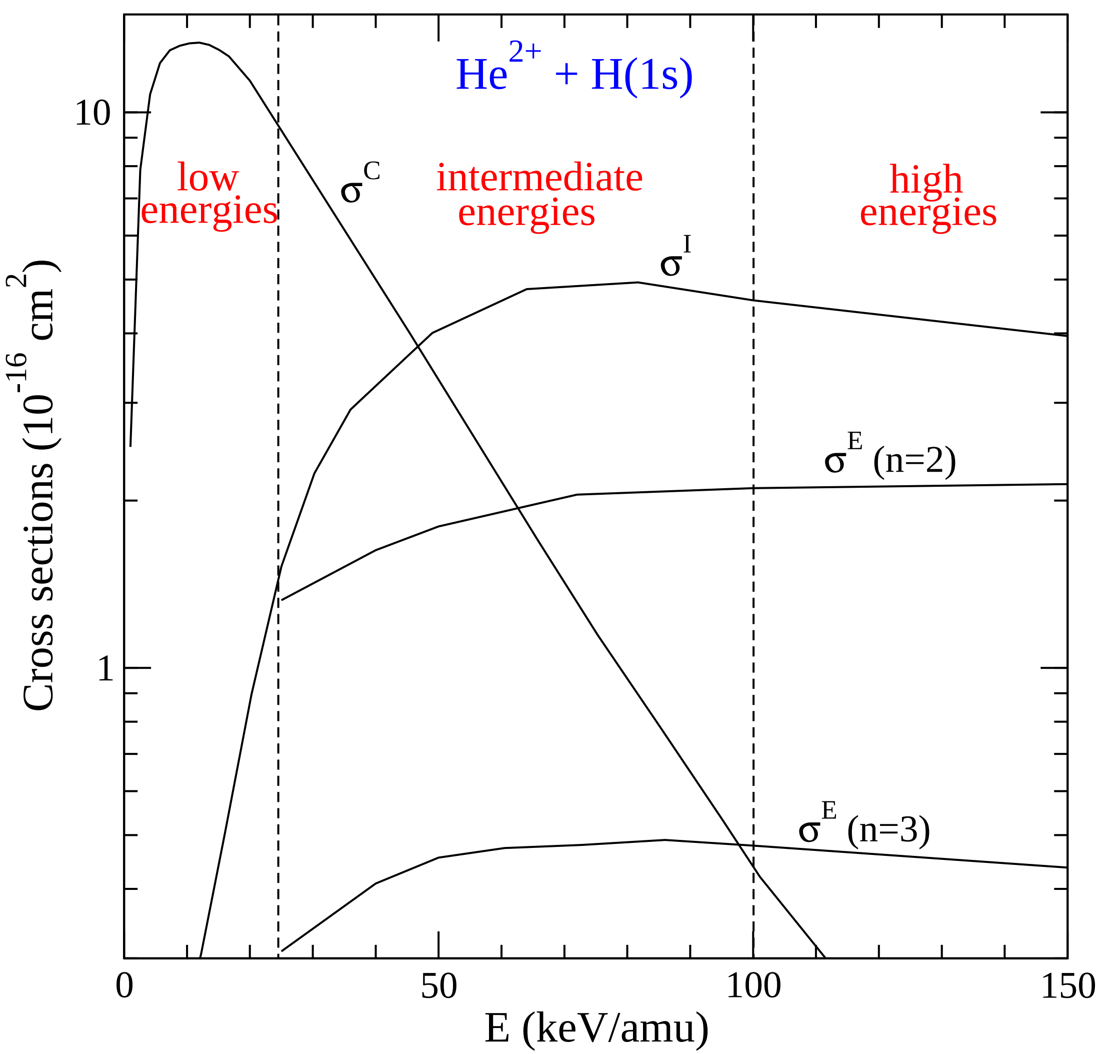
$$\left[H_{el} - \mathrm{i}\frac{\partial}{\partial t}\right] \Psi(\boldsymbol{r}, v, b, t) = 0$$

$$H_{el}(\boldsymbol{r}, \boldsymbol{R}) = -\frac{1}{2}\nabla^2_{\boldsymbol{r}} - \frac{Z_A}{r_A} - \frac{Z_H}{r_H}$$

$$\Downarrow$$

Close Coupling methods

Difficulty of a broad energy domain



Methods employed

We have employed 3 different methods:

- Molecular OEDMs
  - Reproduces the molecularization of the electronic cloud
  - Low impact velocities
- Atomic 1CAO-Bessel
  - Close-coupling expansion on the target
  - Intermediate-high impact velocities
- Classical Trajectory MonteCarlo (CTMC)
  - Separate description of ionization, exciation and capture processes
  - Intermediate impact velocities

Merging the data obtained from the three independent calculations

$$\Downarrow$$

Recommended Excitation Cross Sections

Molecular treatment.

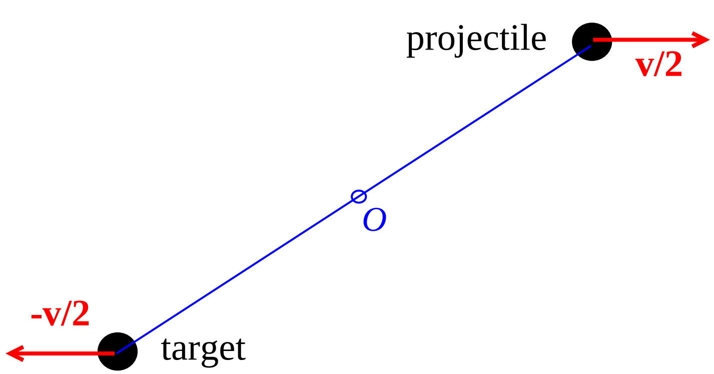
$$\Psi(\boldsymbol{r},t) = \sum_j a_j(t)\chi_j(\boldsymbol{r},R)\mathrm{e}^{\mathrm{i}U(\boldsymbol{r},R)}\exp\left[-\mathrm{i}\int^t E_j^{cc}(t')\mathrm{d}t'\right]$$

where:

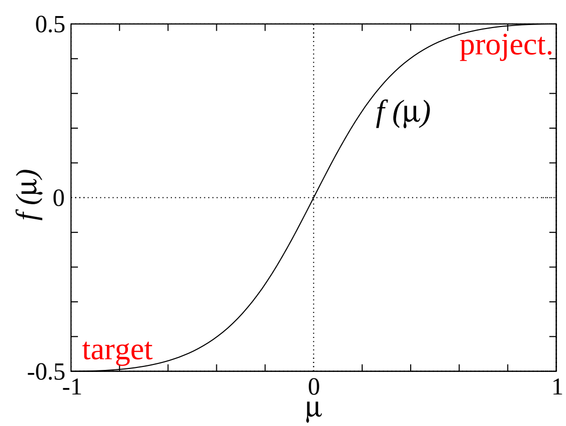
$$H_{el}(\boldsymbol{r},R)\chi_j = E_j^{cc}(R)\chi_j(\boldsymbol{r},R)$$

$E_j^{cc} \rightarrow$ electronic molecular energy for the state j

$U(\boldsymbol{r},R) = f(\boldsymbol{r},R)\boldsymbol{v}\cdot\boldsymbol{r} - \frac{1}{2}f^2(\boldsymbol{r},R)v^2t \rightarrow$ Common Translation Factor



$\Rightarrow$



Limitation of Molecular treatment.

All the molecular orbitals are assyptotically correlated to:

- e^- attached to the projectile $\Rightarrow$ (capture)
- e^- attached to the target $\Rightarrow$ (excitation / elastic)

What happens with **ionization**?

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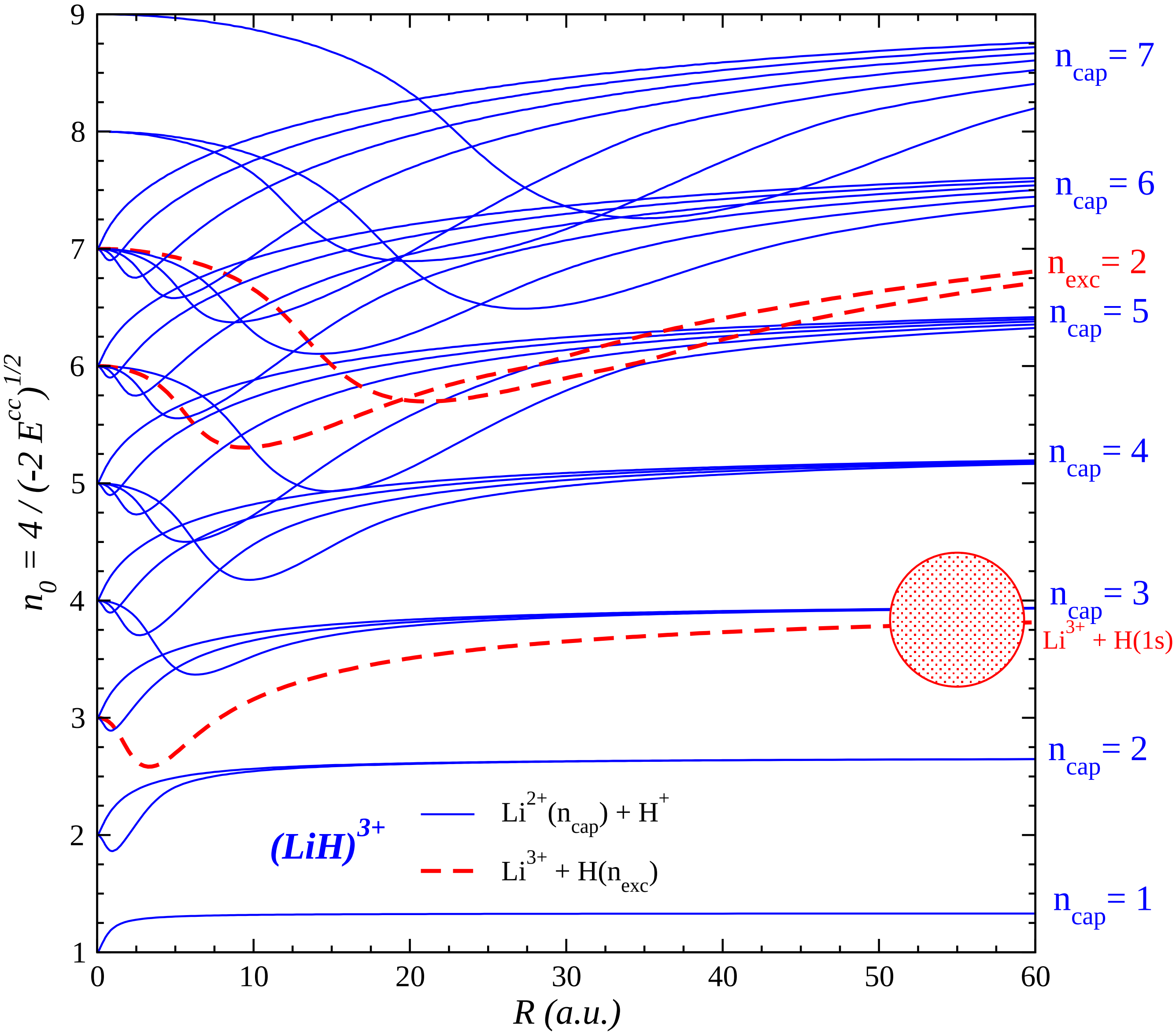
Described by **diffuse** molecular orbitals $\Rightarrow n \uparrow\uparrow$

$$\Downarrow$$

Contamination of the most energetic levels by ionization.

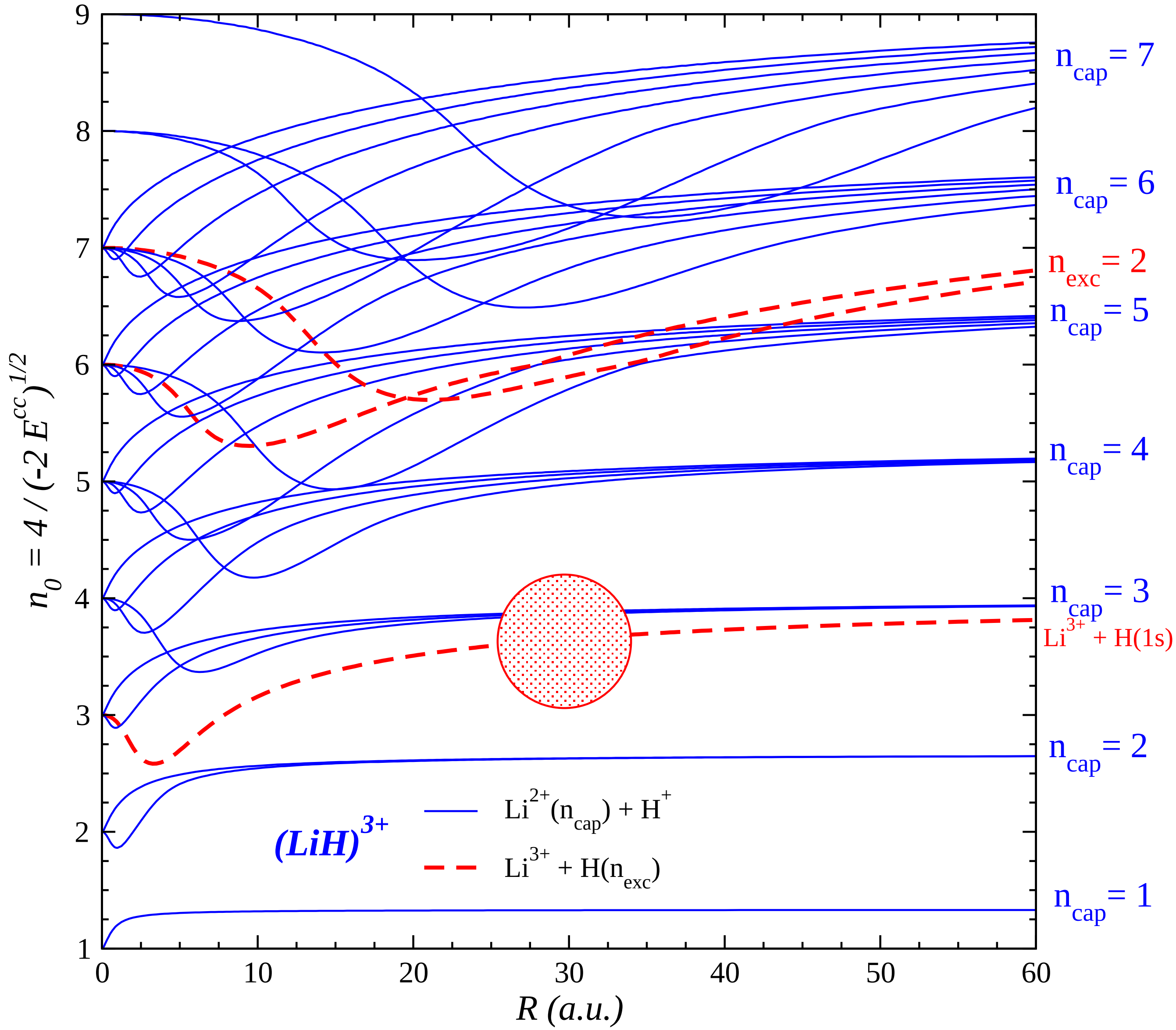
Molecular energy correlation diagram

Qualitative picture of the collisional dynamics



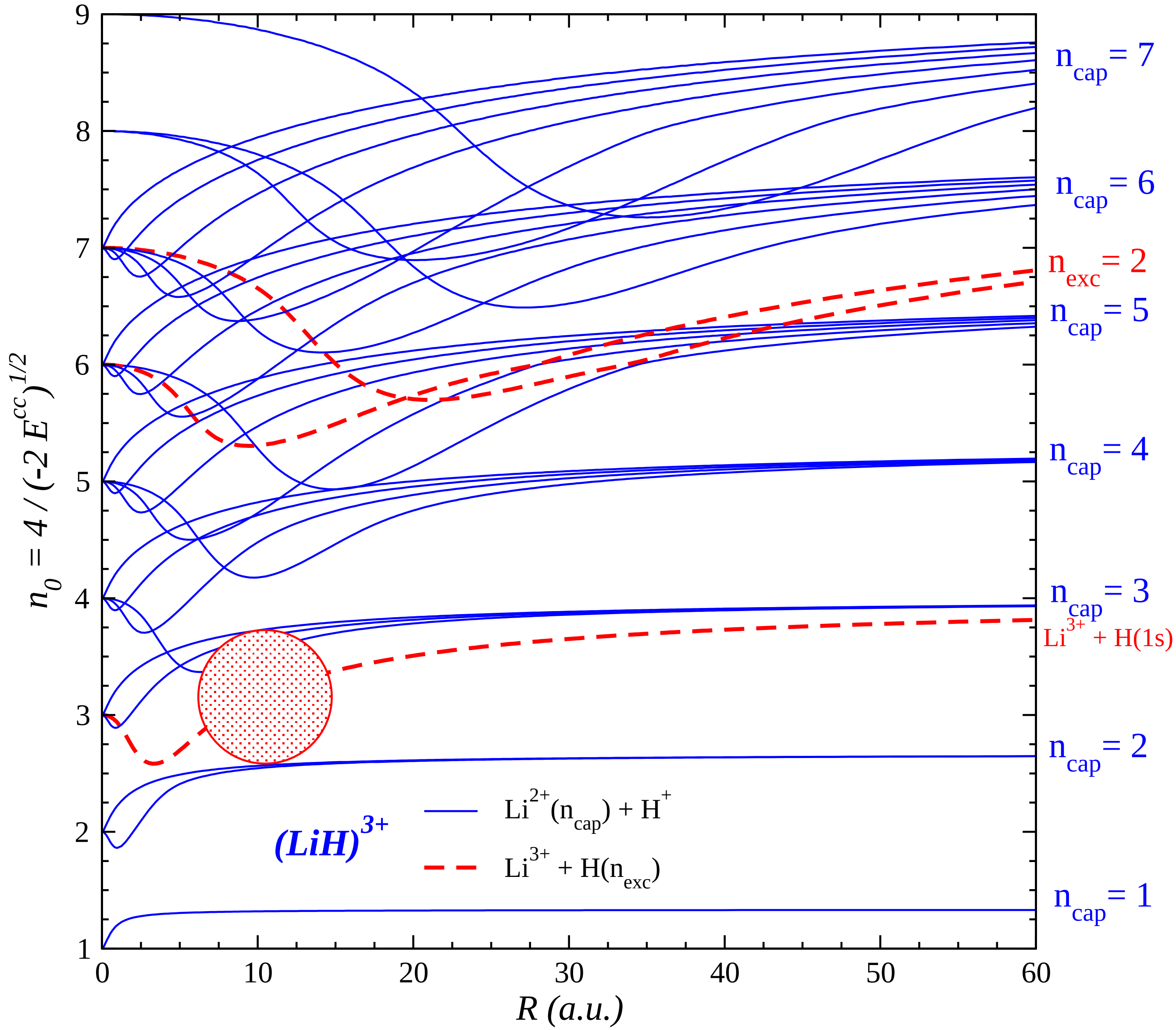
Molecular energy correlation diagram

Qualitative picture of the collisional dynamics



Molecular energy correlation diagram

Qualitative picture of the collisional dynamics



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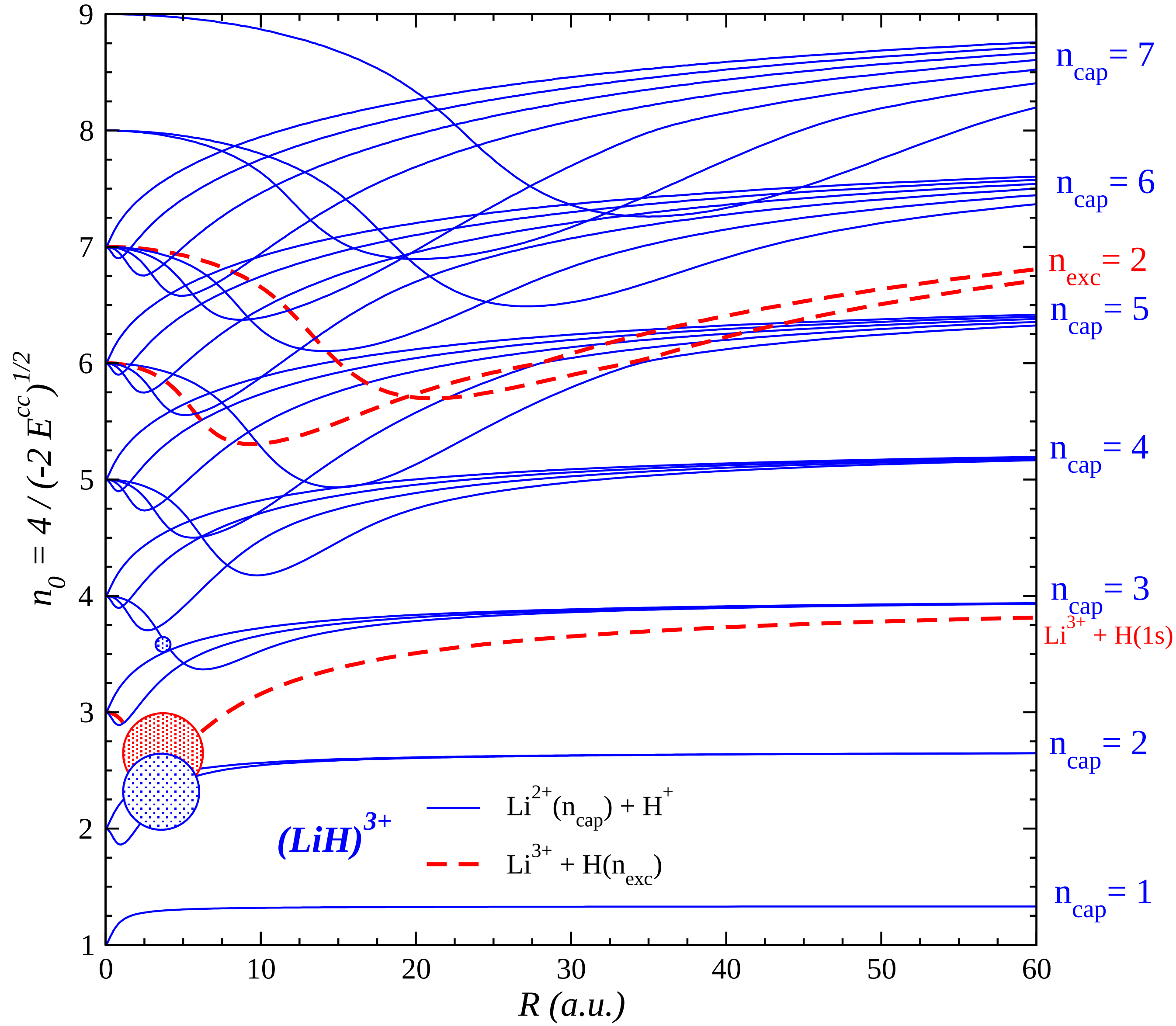

Molecular energy correlation diagram

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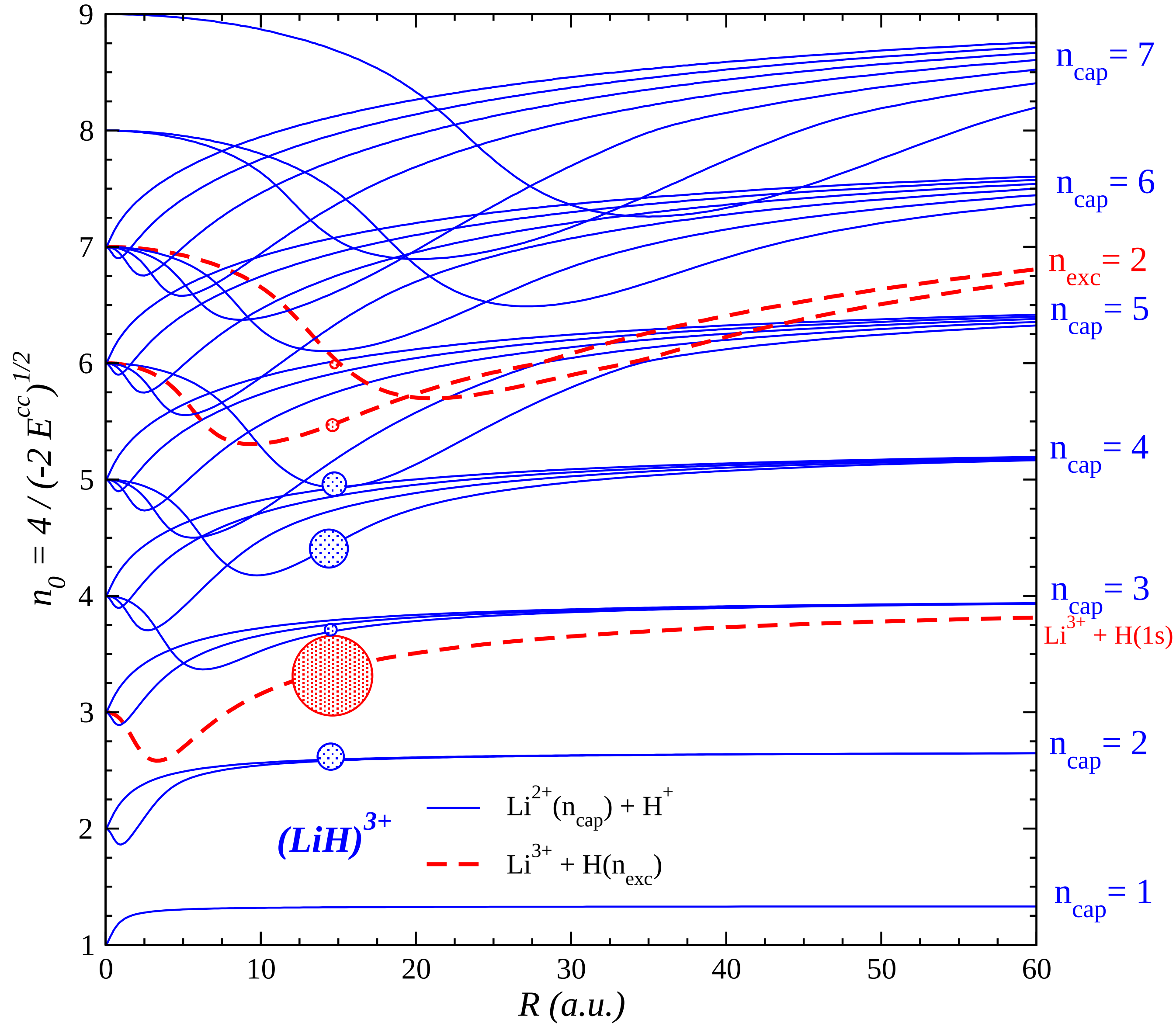
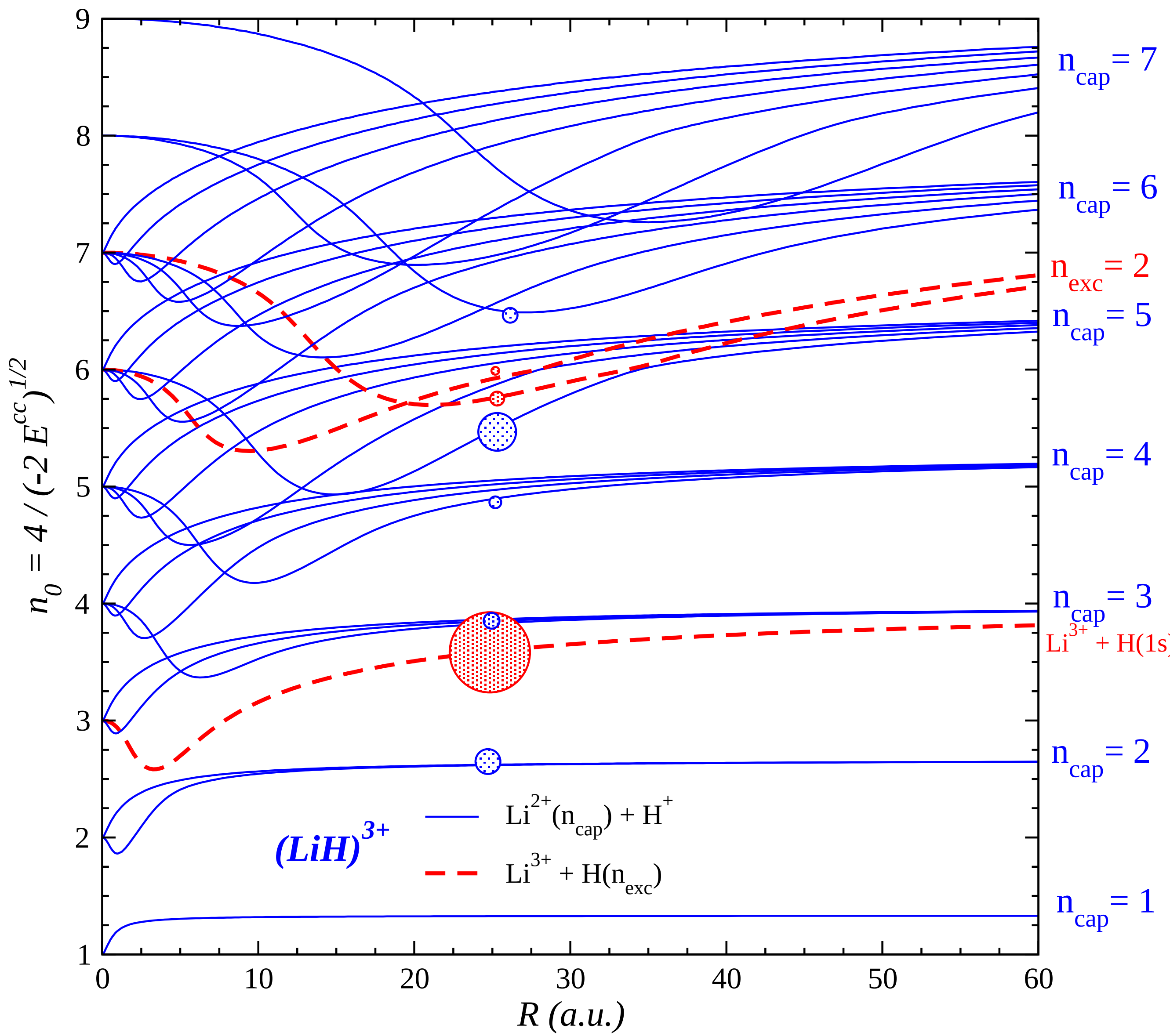


Molecular energy correlation diagram

Qualitative picture of the collisional dynamics



Molecular energy correlation diagram

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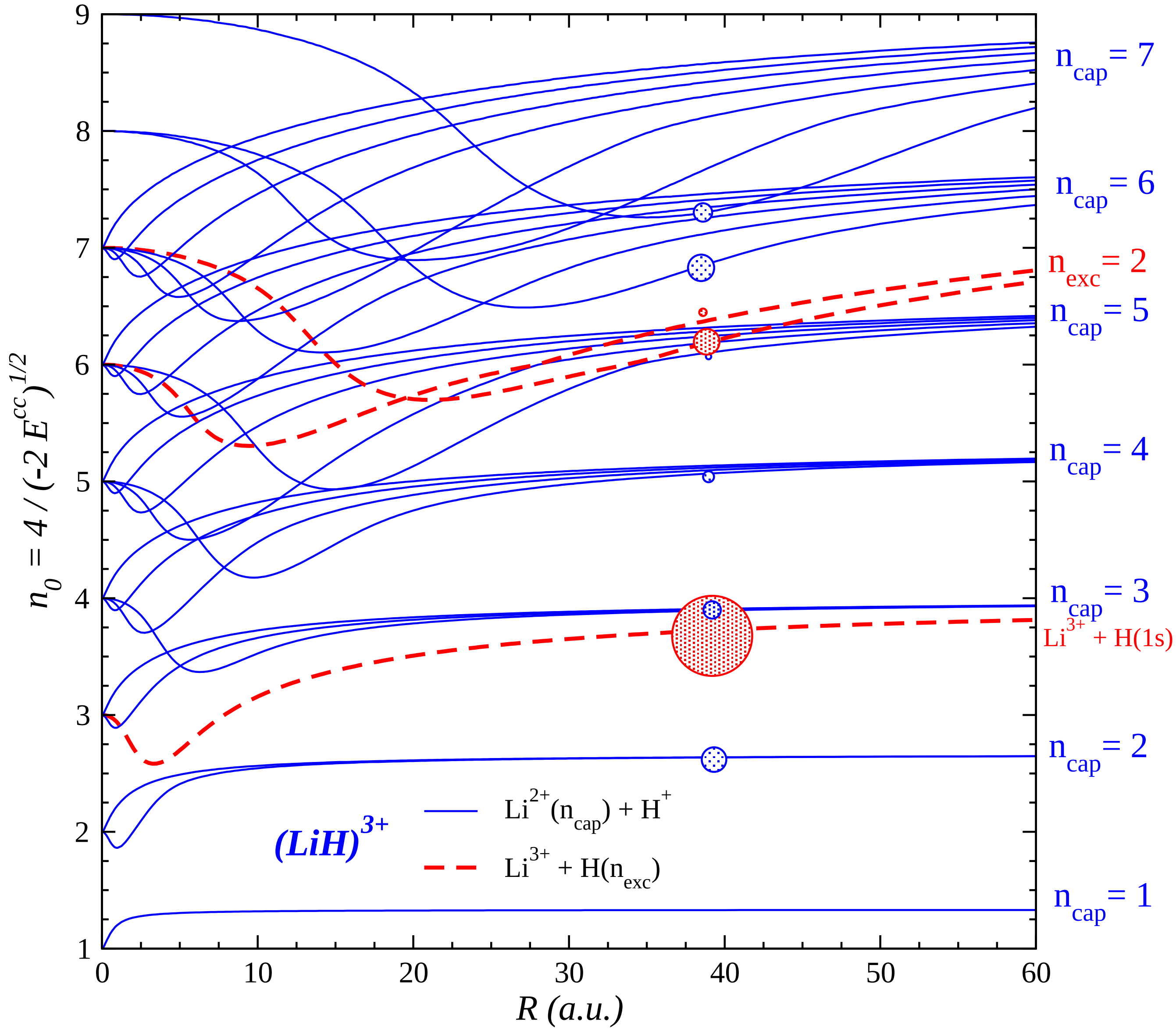
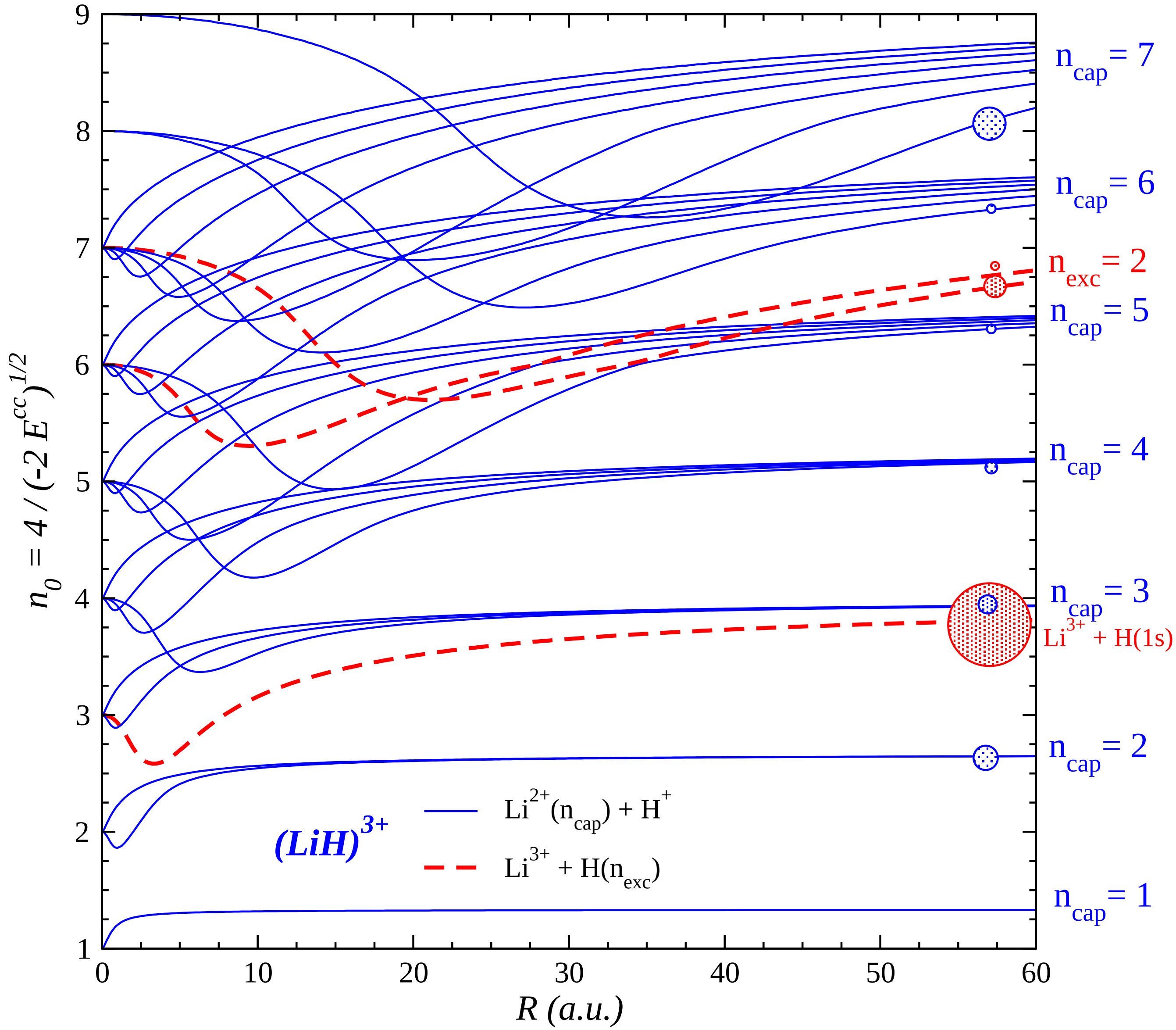


Molecular energy correlation diagram

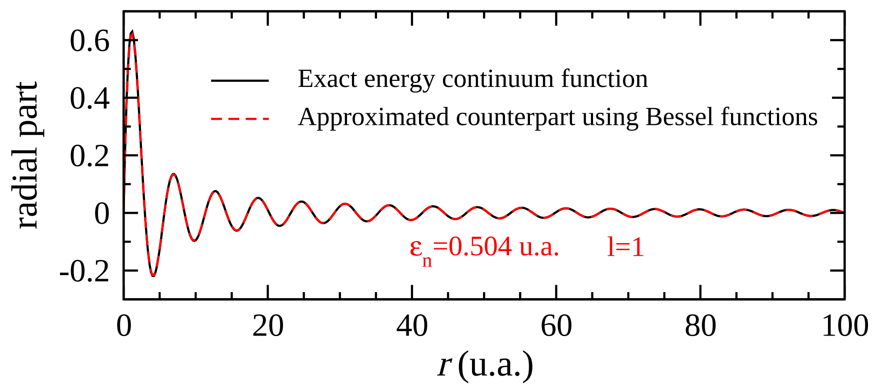
Qualitative picture of the collisional dynamics



Single-centre expansion at high v.

$$\Psi(\boldsymbol{r}, v, b, t) = \sum_{\epsilon_n lm} a_{\epsilon_n lm}(v, b, t)\phi_{\epsilon_n lm}(\boldsymbol{r})\mathrm{e}^{-\mathrm{i}\epsilon_n t}$$

$\phi_{\epsilon_n lm}(\boldsymbol{r}) \rightarrow$ eigenfunctions obtained by diagonalization of the target Hamiltonian h_H in a basis of *confined* spherical Bessel functions $j_l(kr)$:



$$\epsilon_n = \langle \phi_{\epsilon_n lm} | h_H | \phi_{\epsilon_n lm} \rangle \quad \begin{cases} \epsilon_n < 0 \ \mathit{excitation} \\ \epsilon_n > 0 \ \mathit{ionization, capture} \end{cases}$$

Implicit description of the **capture** flux by the ionization states !!!

Classical CTMC method.

- Electronic motion described by a classical distribution function:

$$\rho(\boldsymbol{r},\boldsymbol{p},t) = \frac{1}{N}\sum_{j=1}^{N}\delta\left(\boldsymbol{r}-\boldsymbol{r}_j(t)\right)\delta\left(\boldsymbol{p}-\boldsymbol{p}_j(t)\right)$$

$\downarrow$

Liouville equation:

$$\frac{\partial\rho}{\partial t} = -\left[\rho, H_{el}\right] = -\frac{\partial\rho}{\partial\boldsymbol{r}}\cdot\frac{\partial H_{el}}{\partial\boldsymbol{p}} + \frac{\partial\rho}{\partial\boldsymbol{p}}\cdot\frac{\partial H_{el}}{\partial\boldsymbol{r}}$$

obtaining the **Hamilton equations**:

$$\left.\begin{aligned}\dot{\boldsymbol{r}}_j(t) &= \frac{\partial H}{\partial\boldsymbol{p}_j(t)}\\ \dot{\boldsymbol{p}}_j(t) &= -\frac{\partial H}{\partial\boldsymbol{r}_j(t)}\end{aligned}\right\}$$

- Energy criterion is applied at $t = 500 a.u./v$

$E_H < 0 \rightarrow$ Excitation $E_A < 0 \rightarrow$ Capture $E_H > 0, E_A > 0 \rightarrow$ Ionization

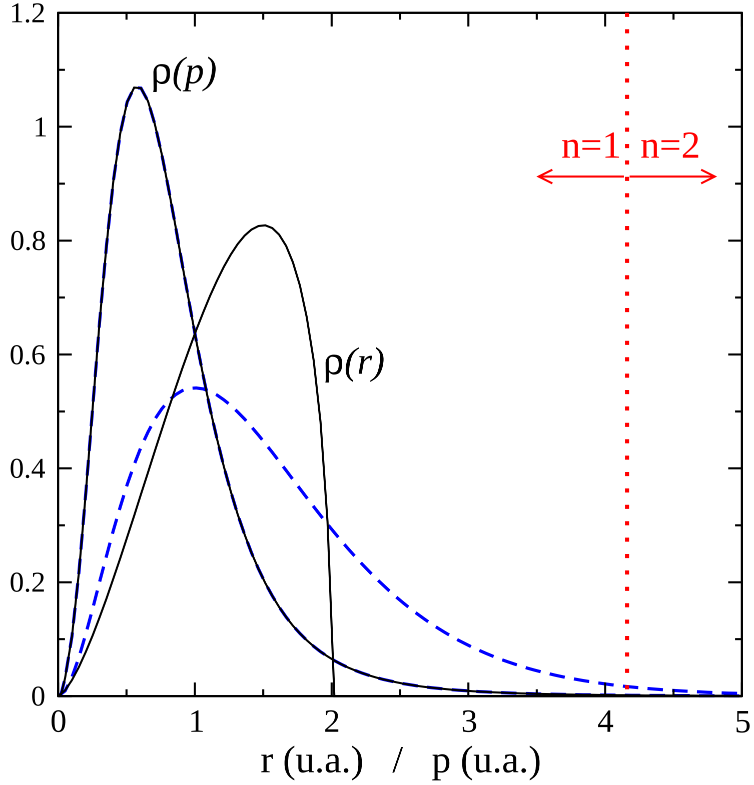
- Binning method of *Becker and MacKellar* $\longrightarrow (n,l)$

$$n(n-1/2)(n-1) \le n_c^3 < n(n+1/2)(n+1) \qquad n_c = \frac{Z_H}{\sqrt{-2E_H}}$$

$$l \le L_c < (l+1) \qquad L_c = (n/n_c)(\boldsymbol{r}\times\boldsymbol{p})$$

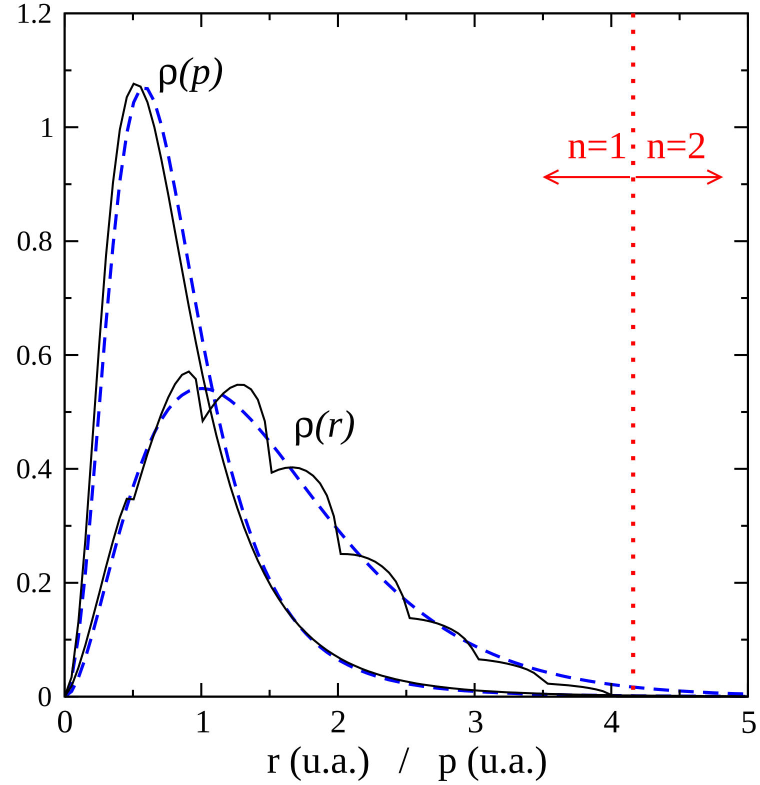
CTMC initial distribution.

- Microcanonical distribution:



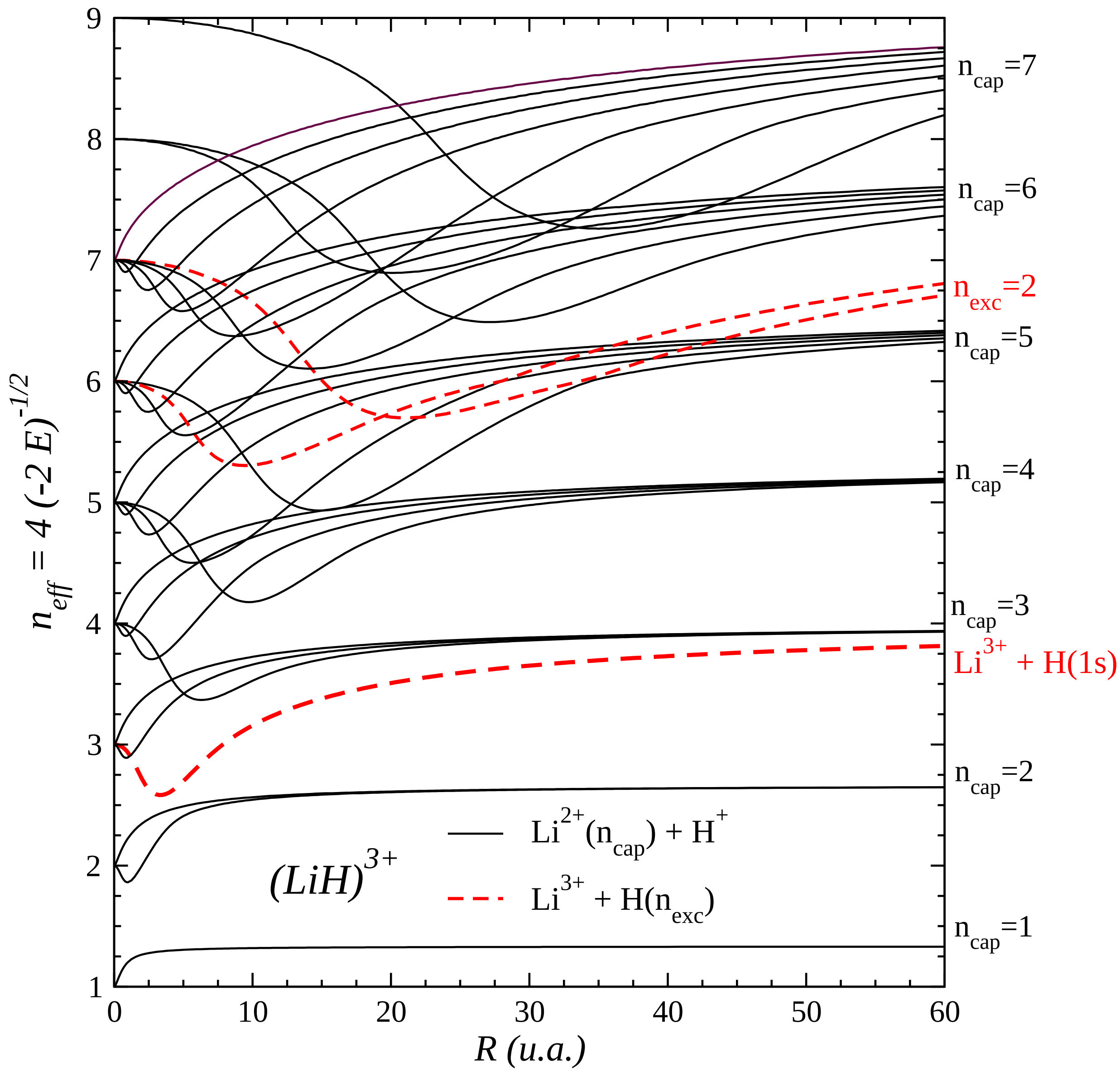
$$\rho^m(\boldsymbol{r},\boldsymbol{p};E_0) = \frac{1}{8\pi^3}\delta\left(\frac{p^2}{2} - \frac{1}{r} - E_0\right)$$

- Hydrogenic distribution:



$$\rho(\boldsymbol{r},\boldsymbol{p}) = \sum_{j=1}^{8} w_j \rho^m(\boldsymbol{r},\boldsymbol{p};E_j)$$

$(\text{Li H})^{3+}$ energy correlation diagram.

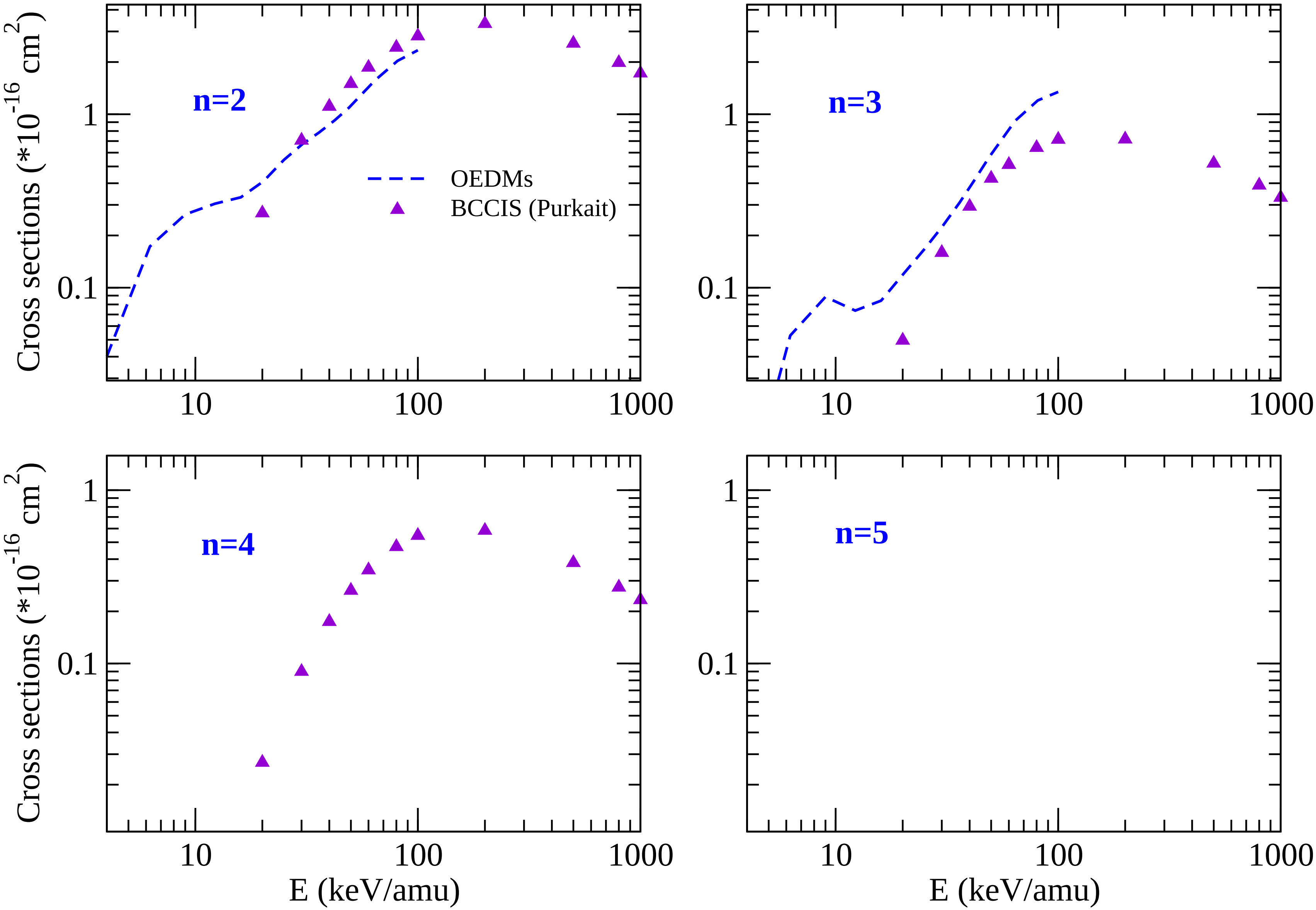


175 OEDMs:

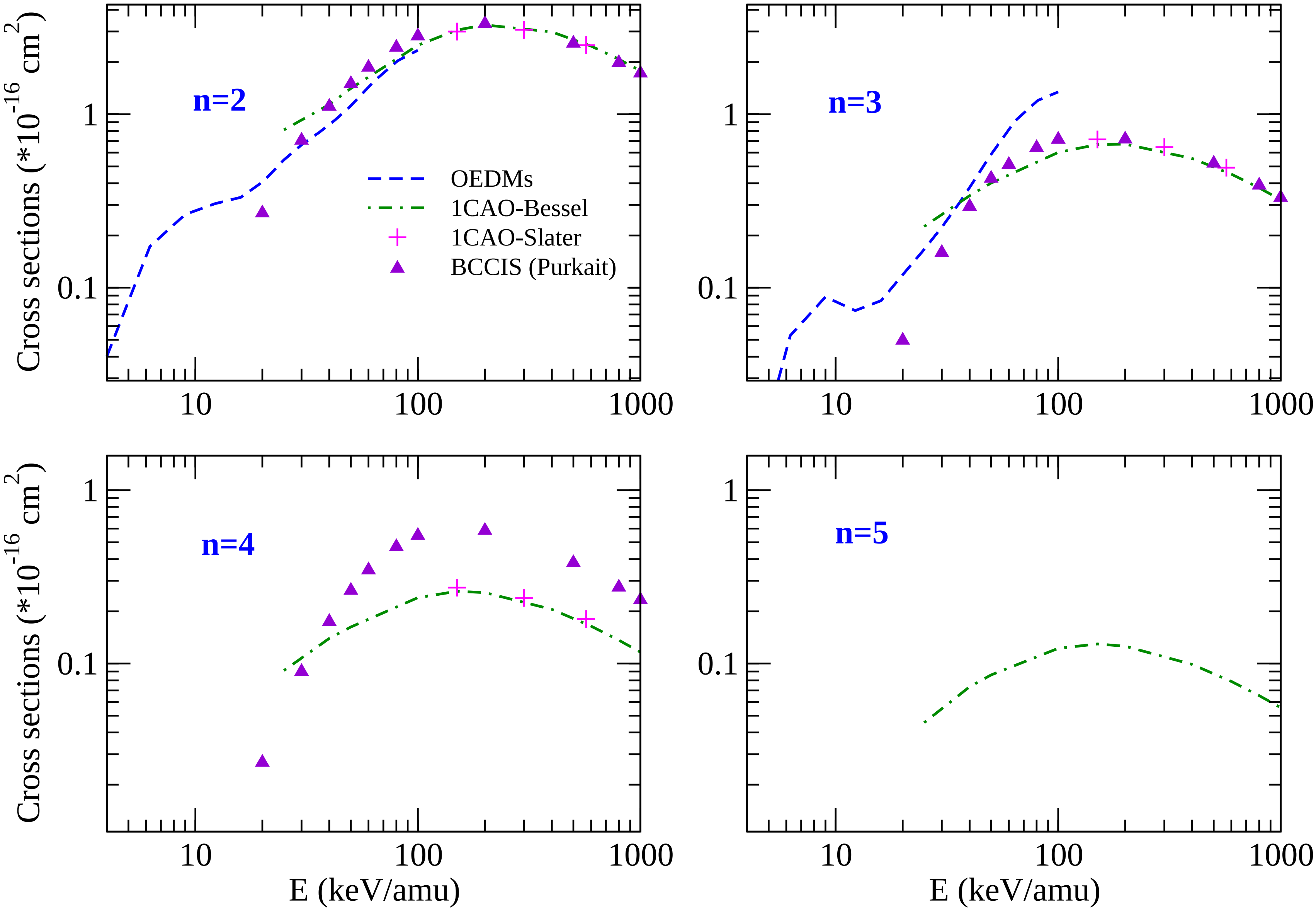
capture n =1–9 (all m)

excitation $n' = 2, 3$ (all m)

Li^{3+}+H(1s) $\rightarrow$ Li^{3+}+H(n) cross sections.



Li^{3+}+H(1s) → Li^{3+}+H(n) cross sections.



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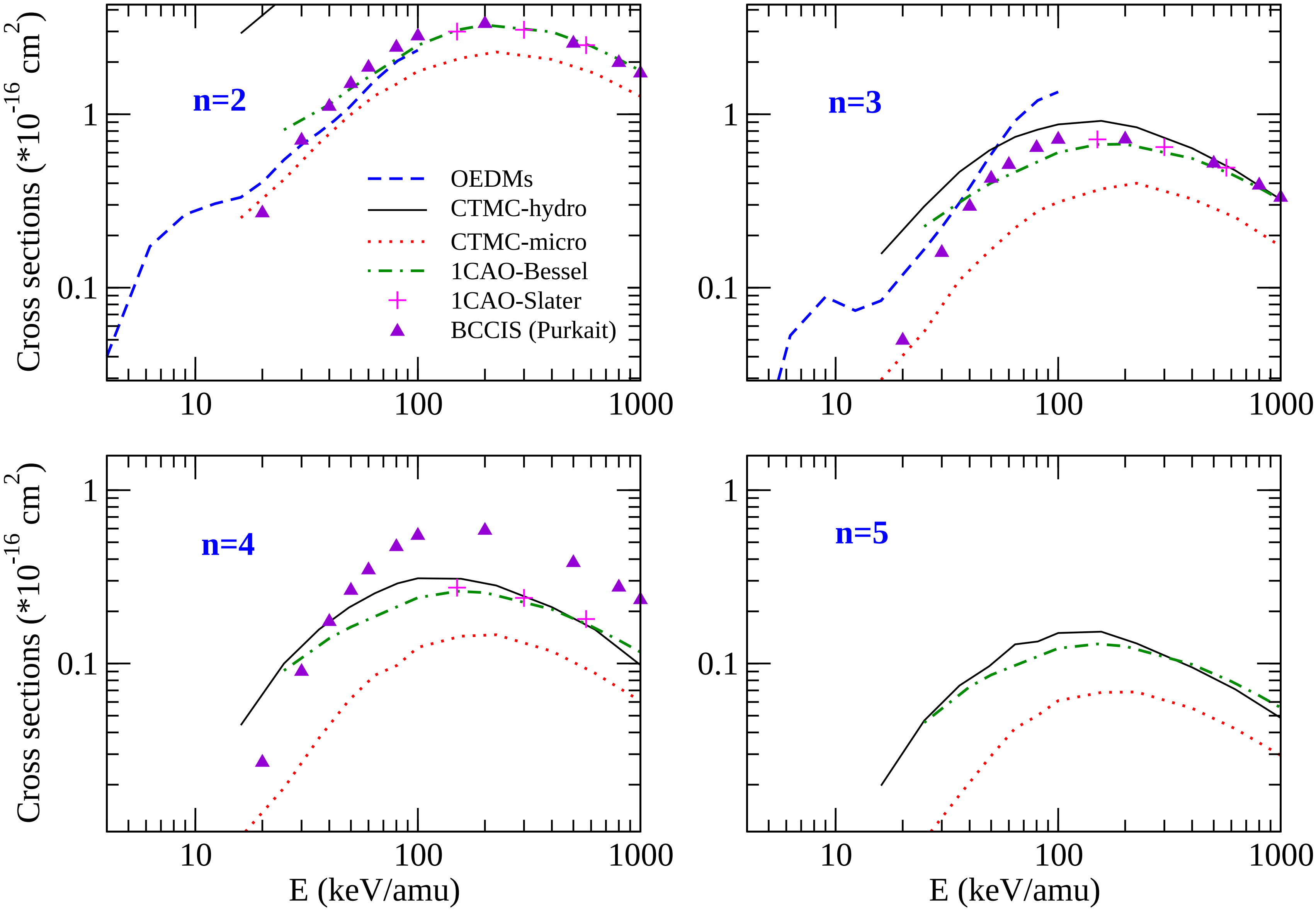
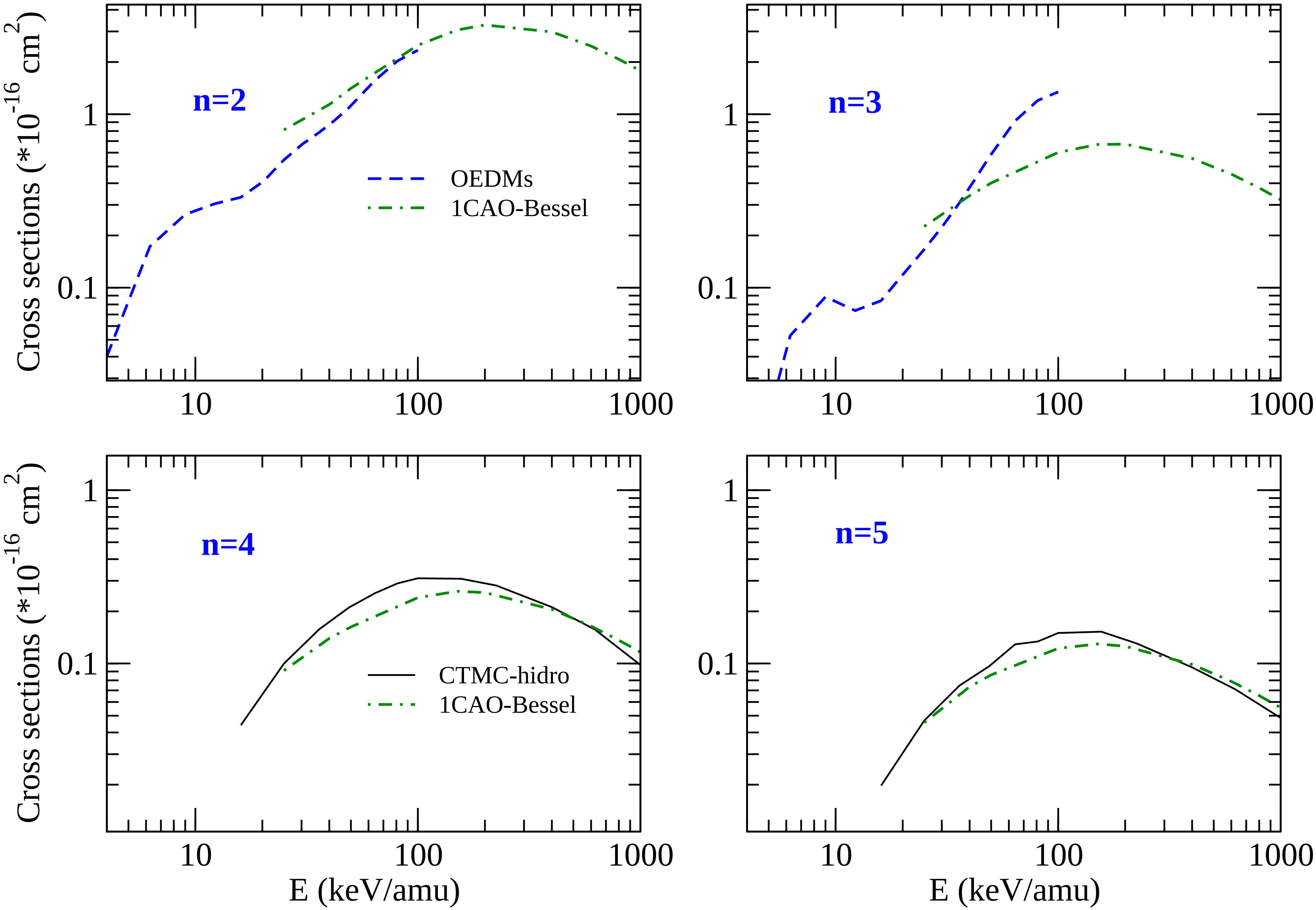
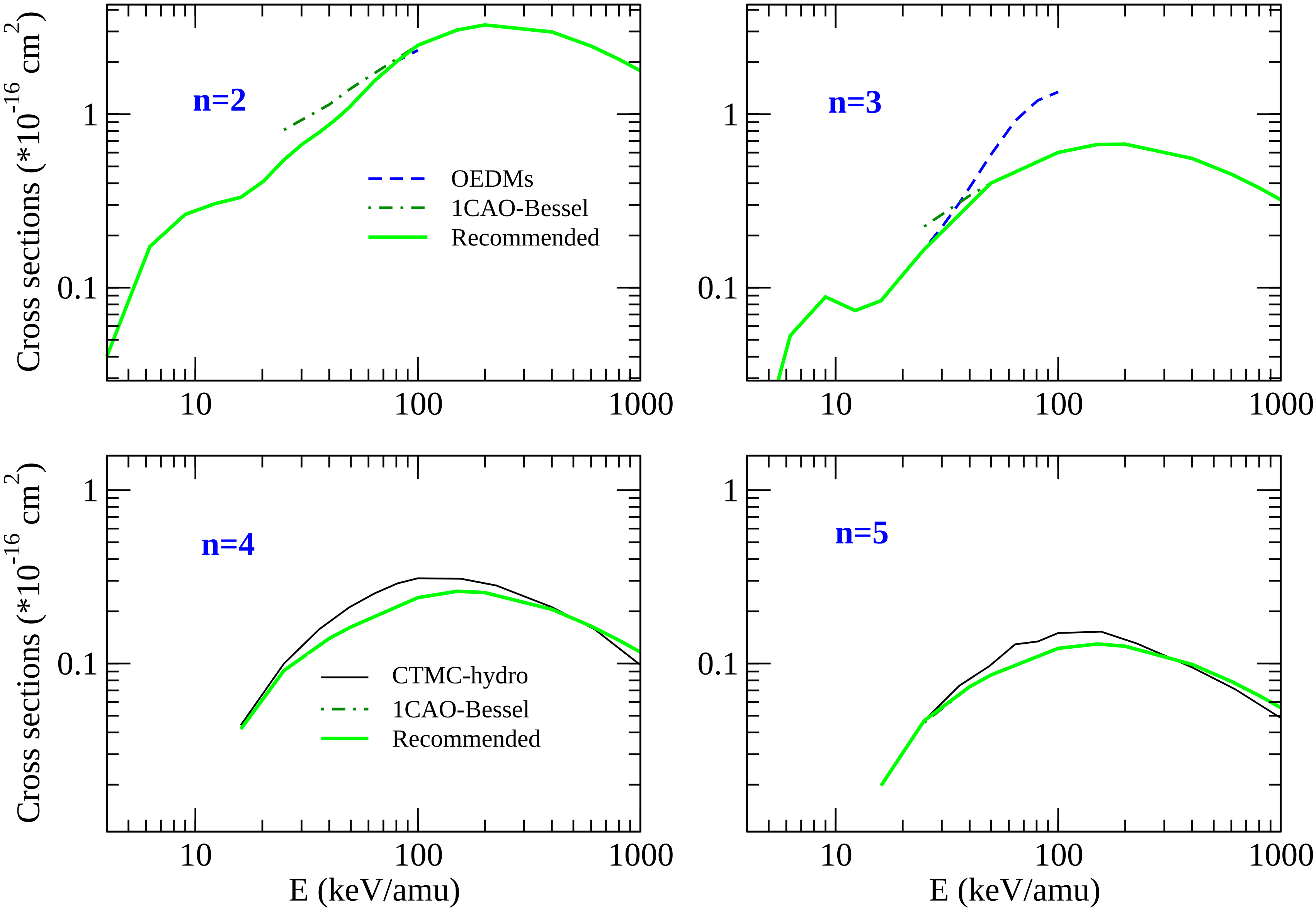


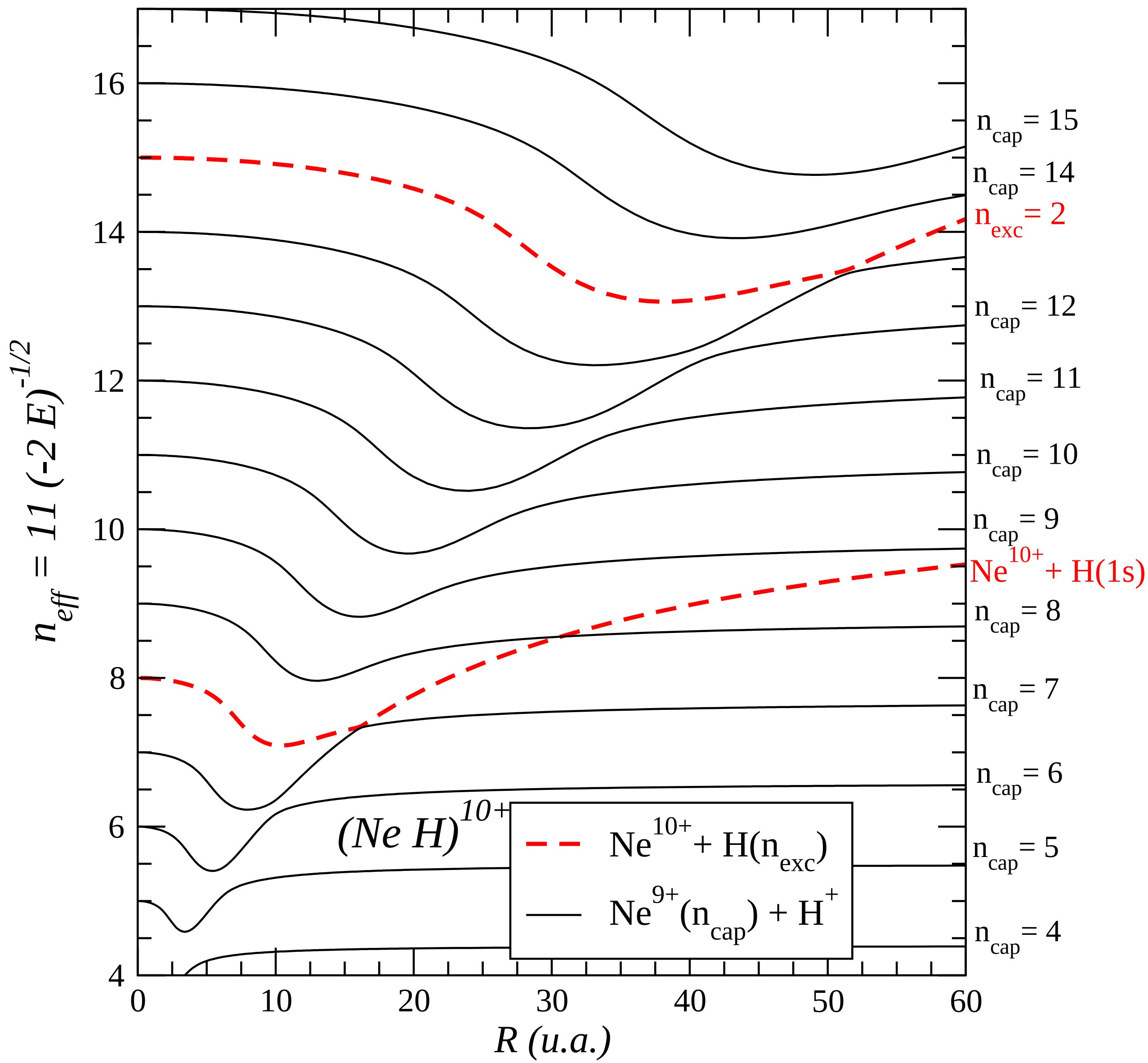
Li^{3+}+H(1s) → Li^{3+}+H(n) cross sections.



Li^{3+}+H(1s) → Li^{3+}+H(n) cross sections.



$(Ne\ H)^{10+}$ energy correlation diagram.

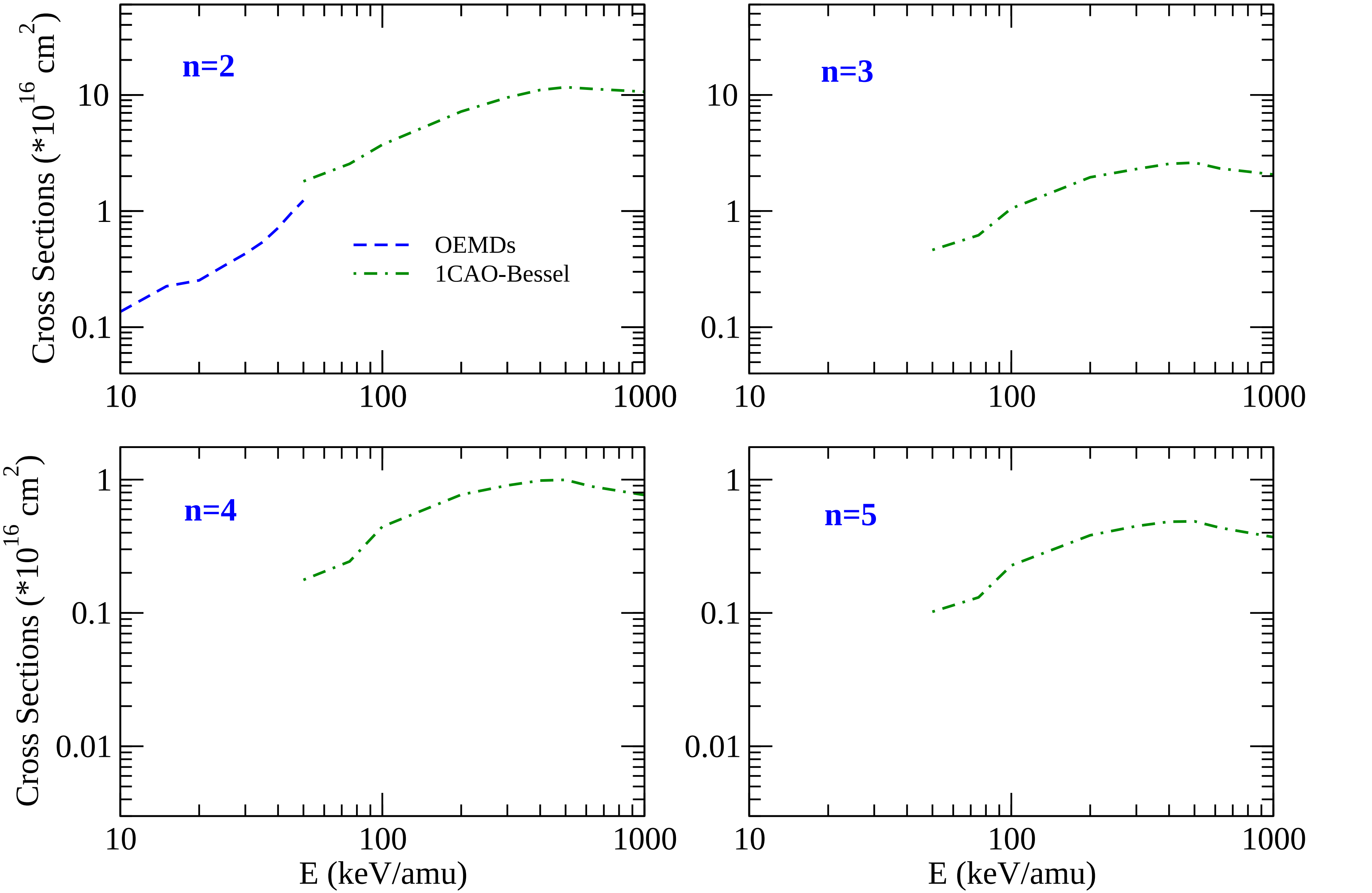


310 OEDMs:

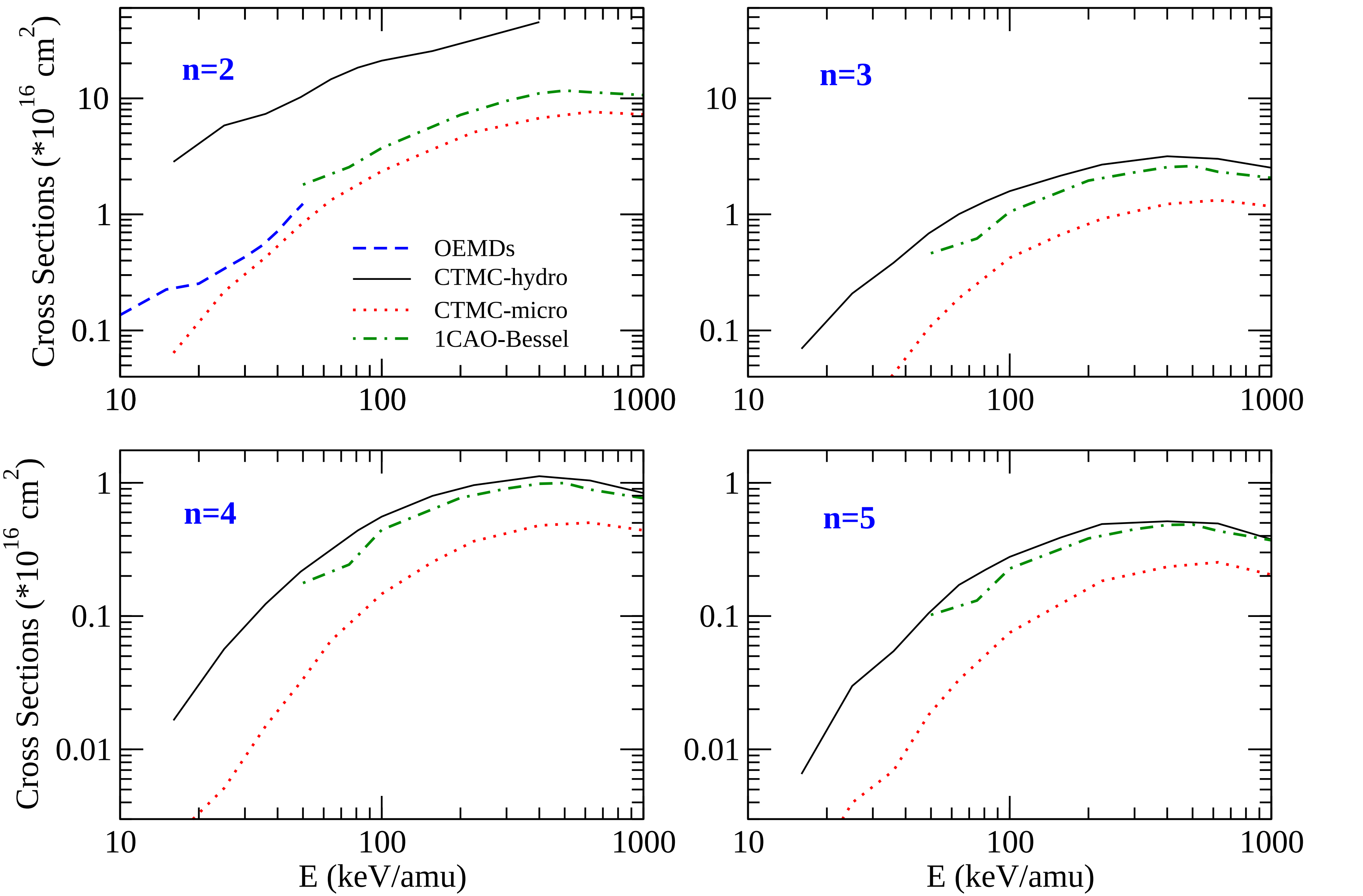
capture n =4–15 ($m = 0, 1, 2$)

excitation $n' = 2$ (all m)

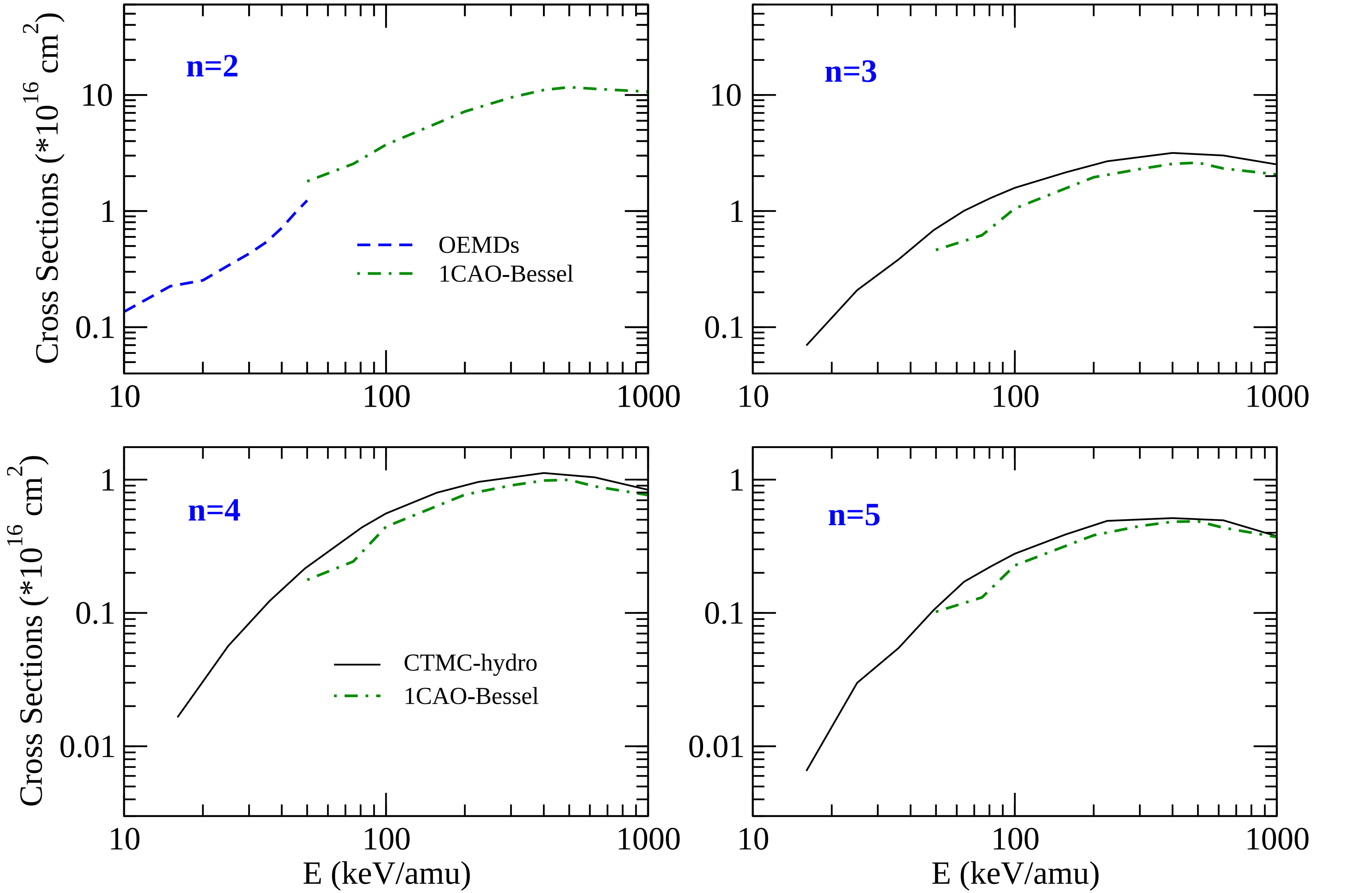
Ne^{10+}+H(1s) → Ne^{10+}+H(n) cross sections.



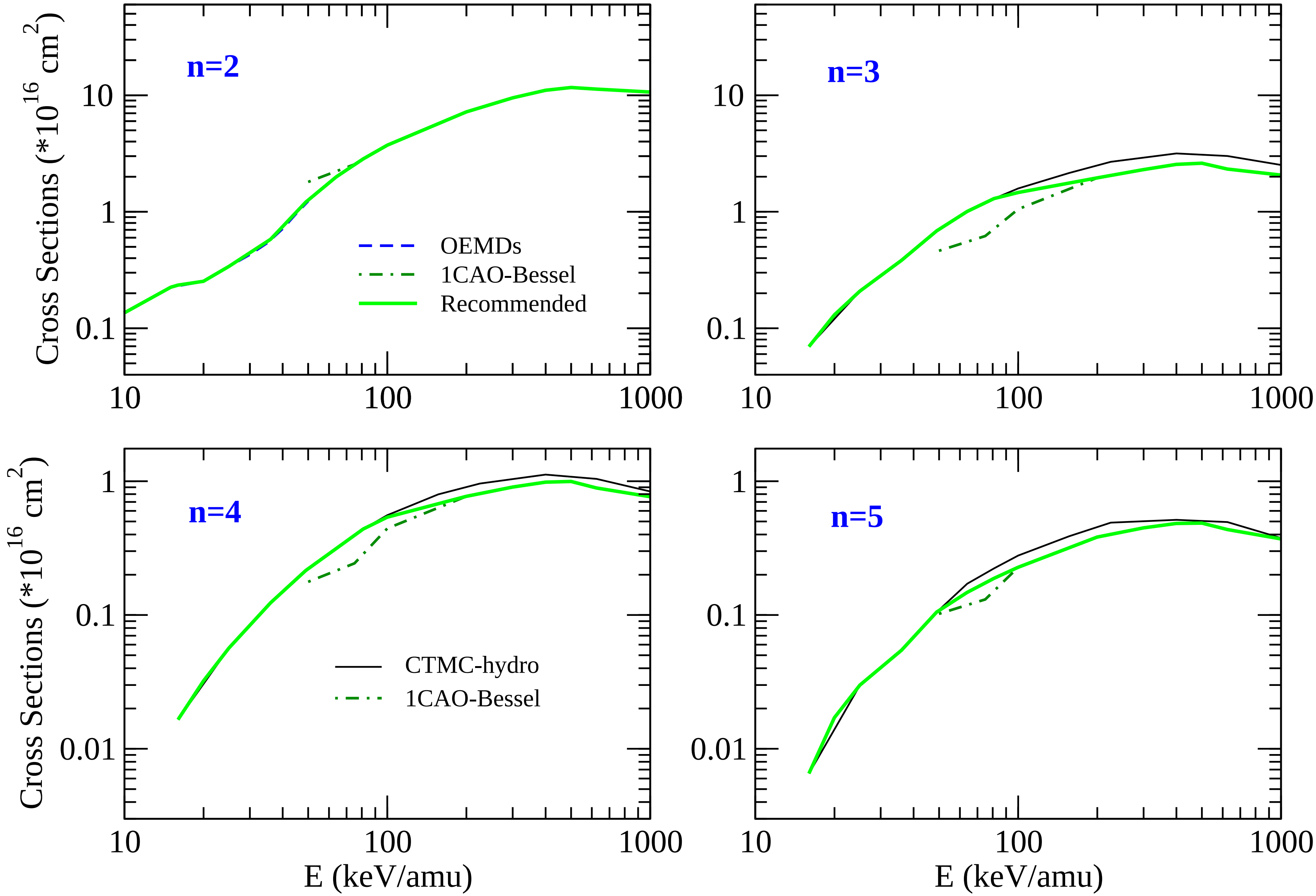
Ne^{10+}+H(1s) → Ne^{10+}+H(n) cross sections.



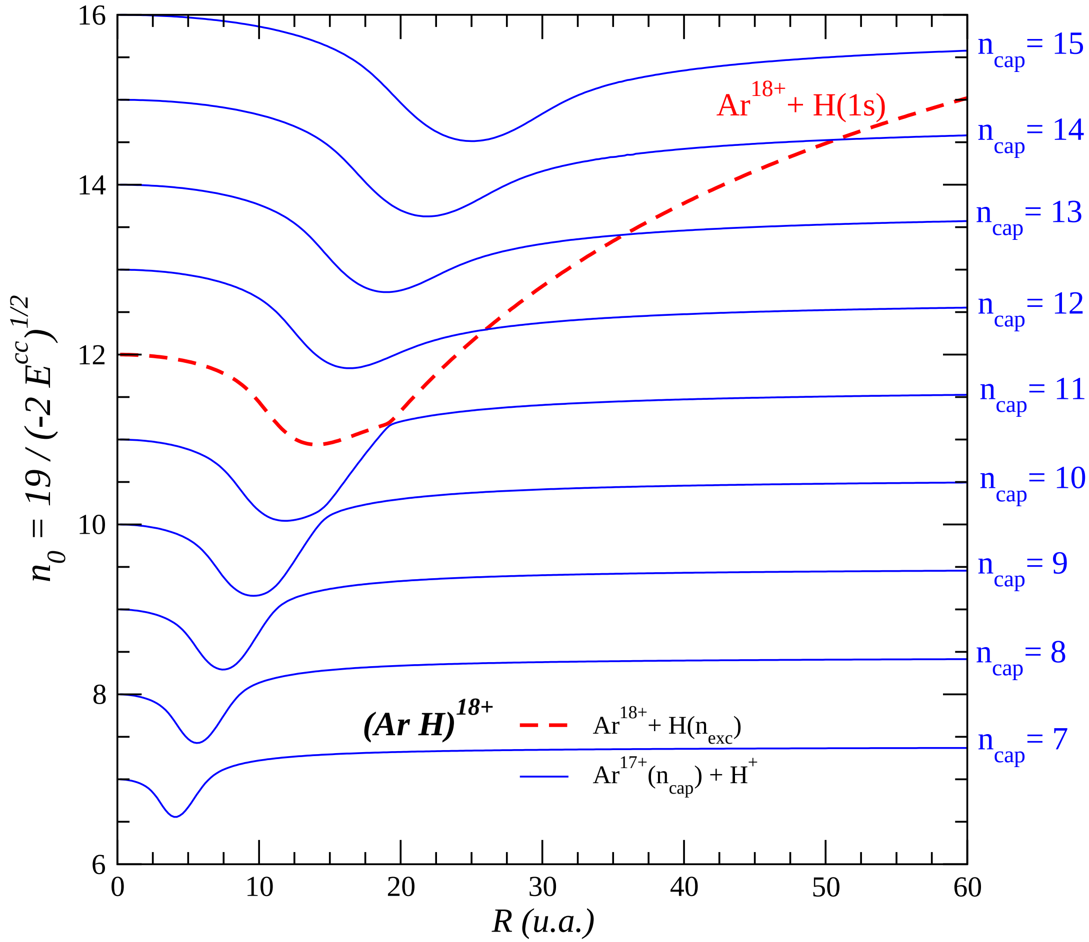
Ne^{10+}+H(1s) → Ne^{10+}+H(n) cross sections.



Ne^{10+}+H(1s) → Ne^{10+}+H(n) cross sections.



$(\mathrm{Ar\ H})^{18+}$ energy correlation diagram.



271 OEDMs:

capture n =7–15 ($m = 0, 1, 2$)

Since $Z_A >> Z_H$

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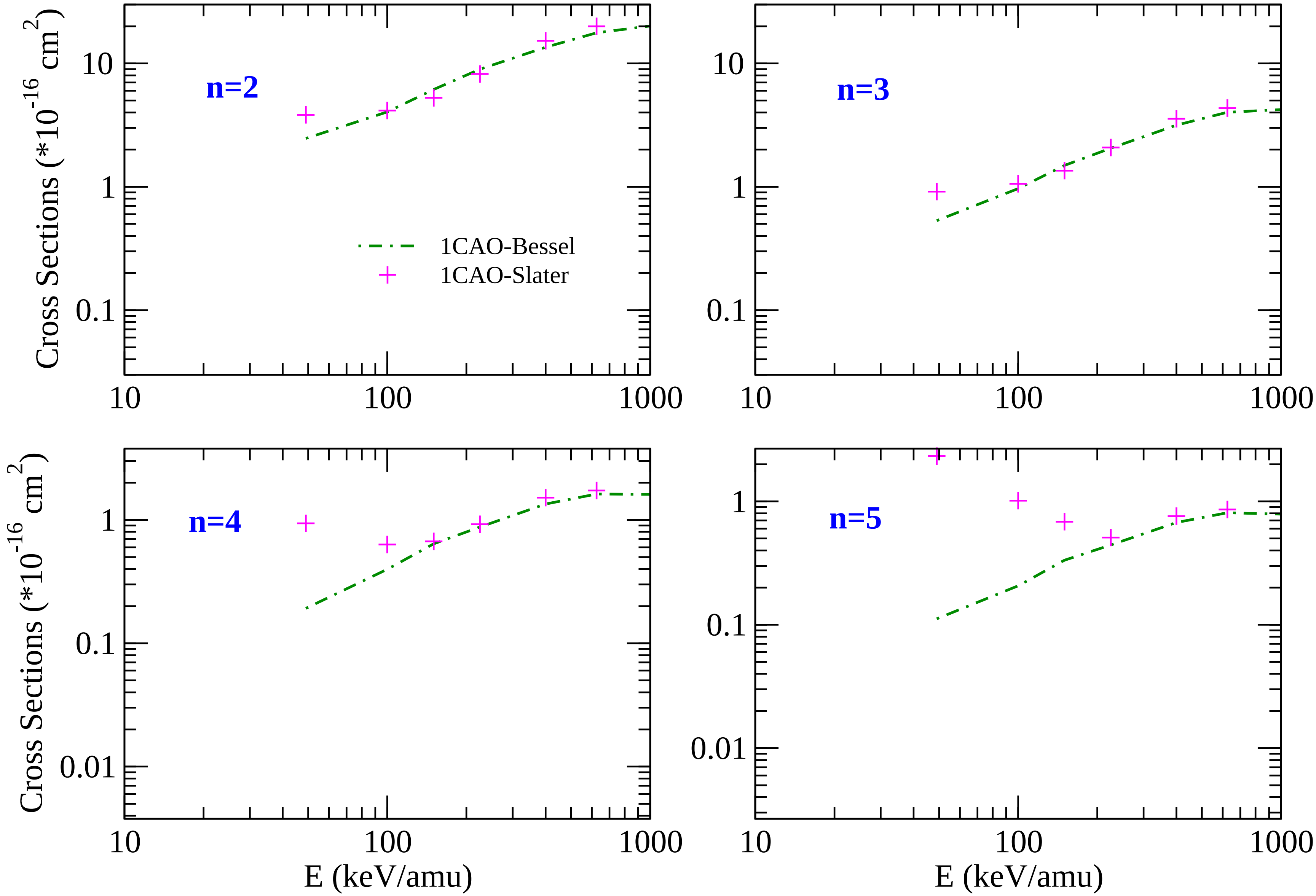
Density of capture states $\gg$ excitation states

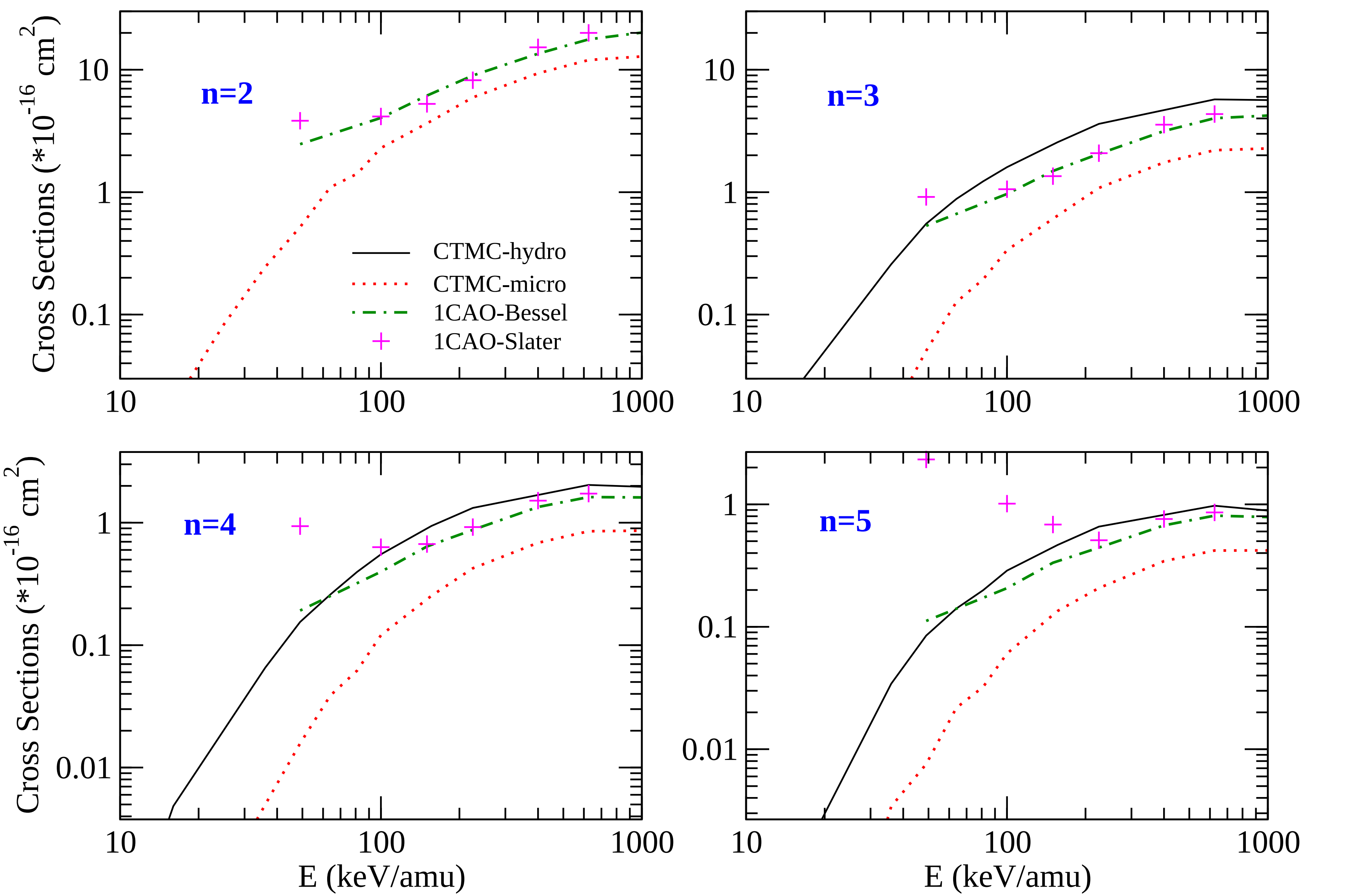
$\Downarrow$

Cannot include excitation !!

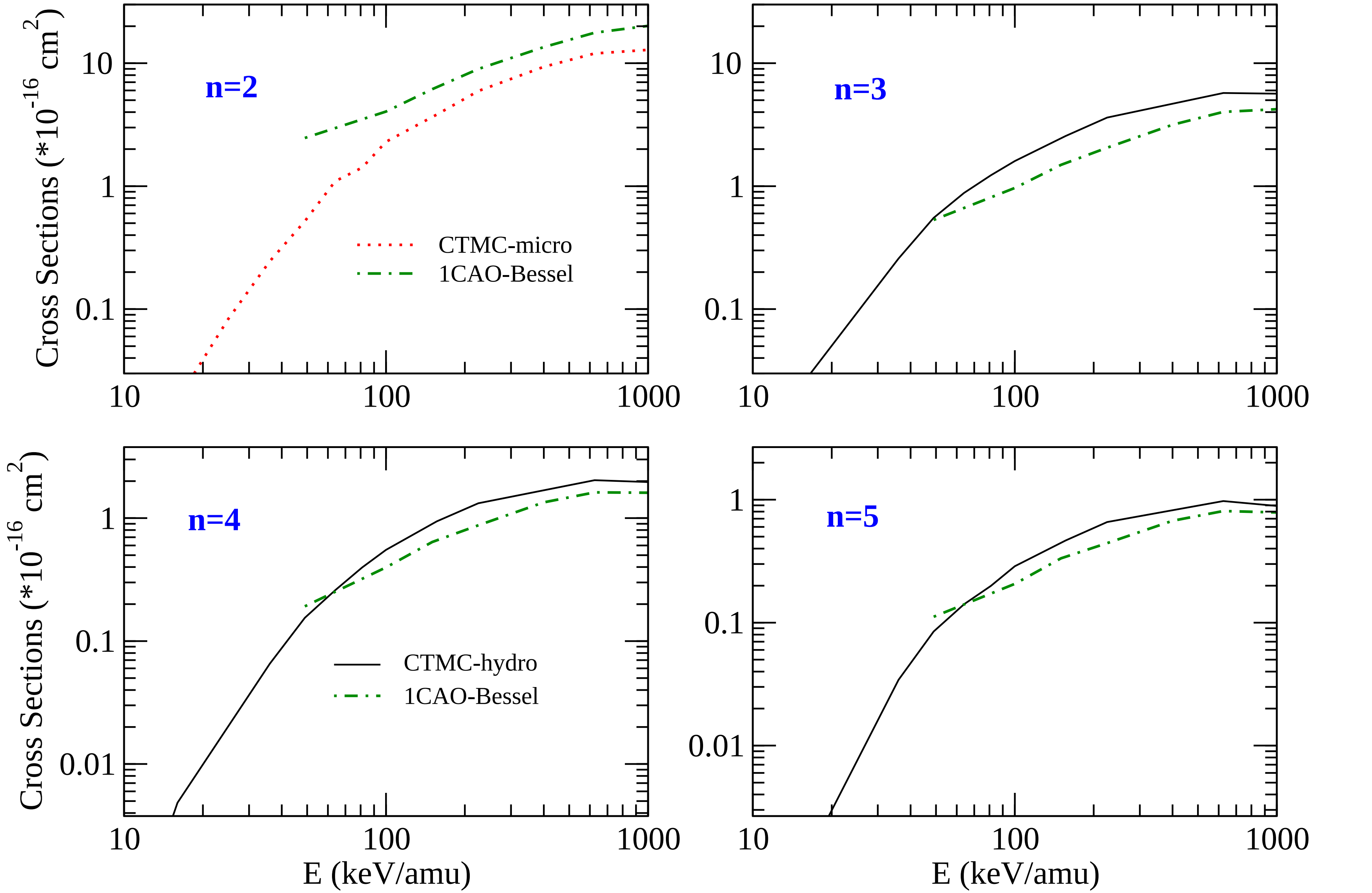
Ar^{18+}+H(1s) → Ar^{18+}+H(n) cross sections.



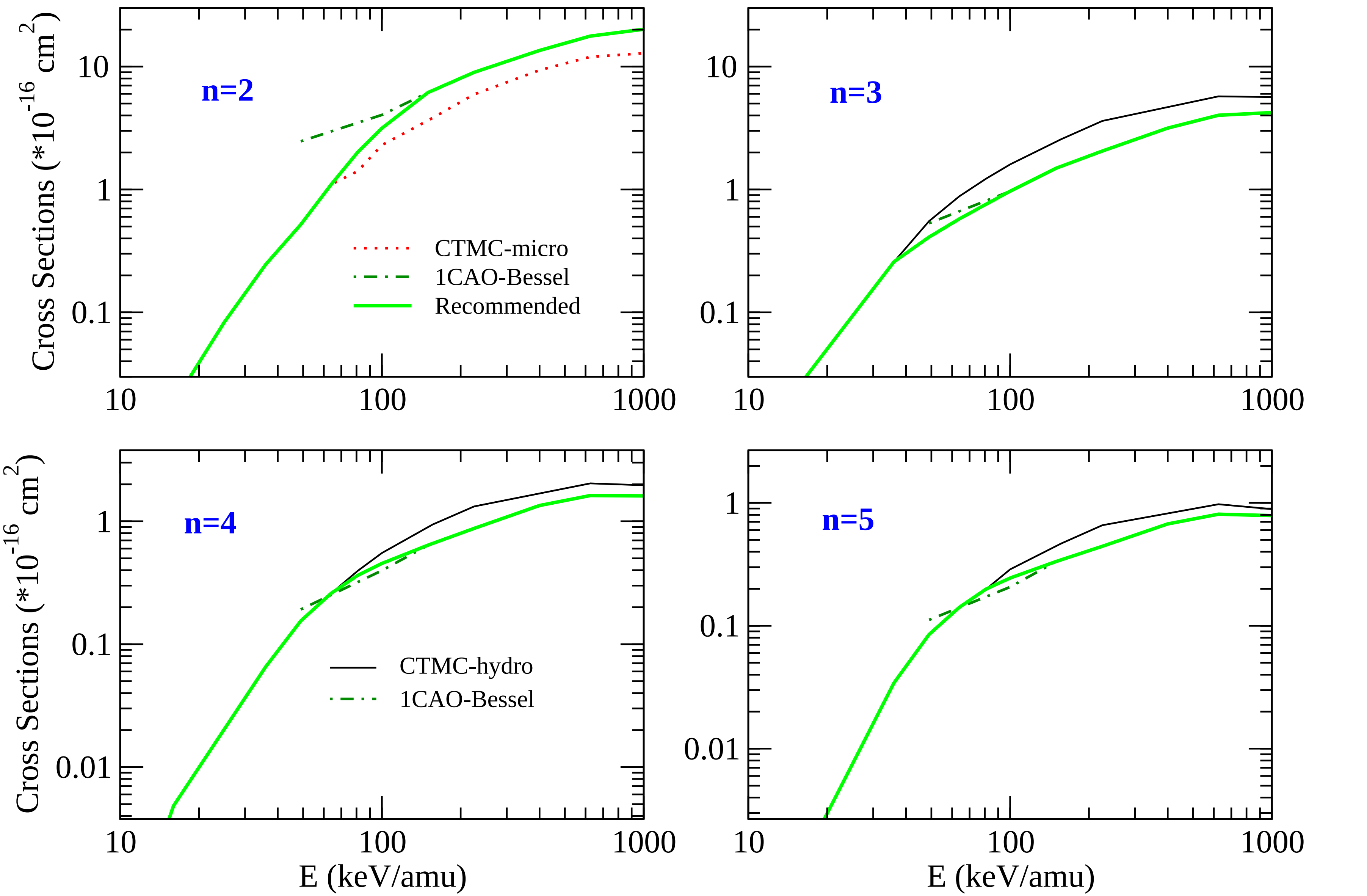
Ar^{18+}+H(1s) → Ar^{18+}+H(n) cross sections.



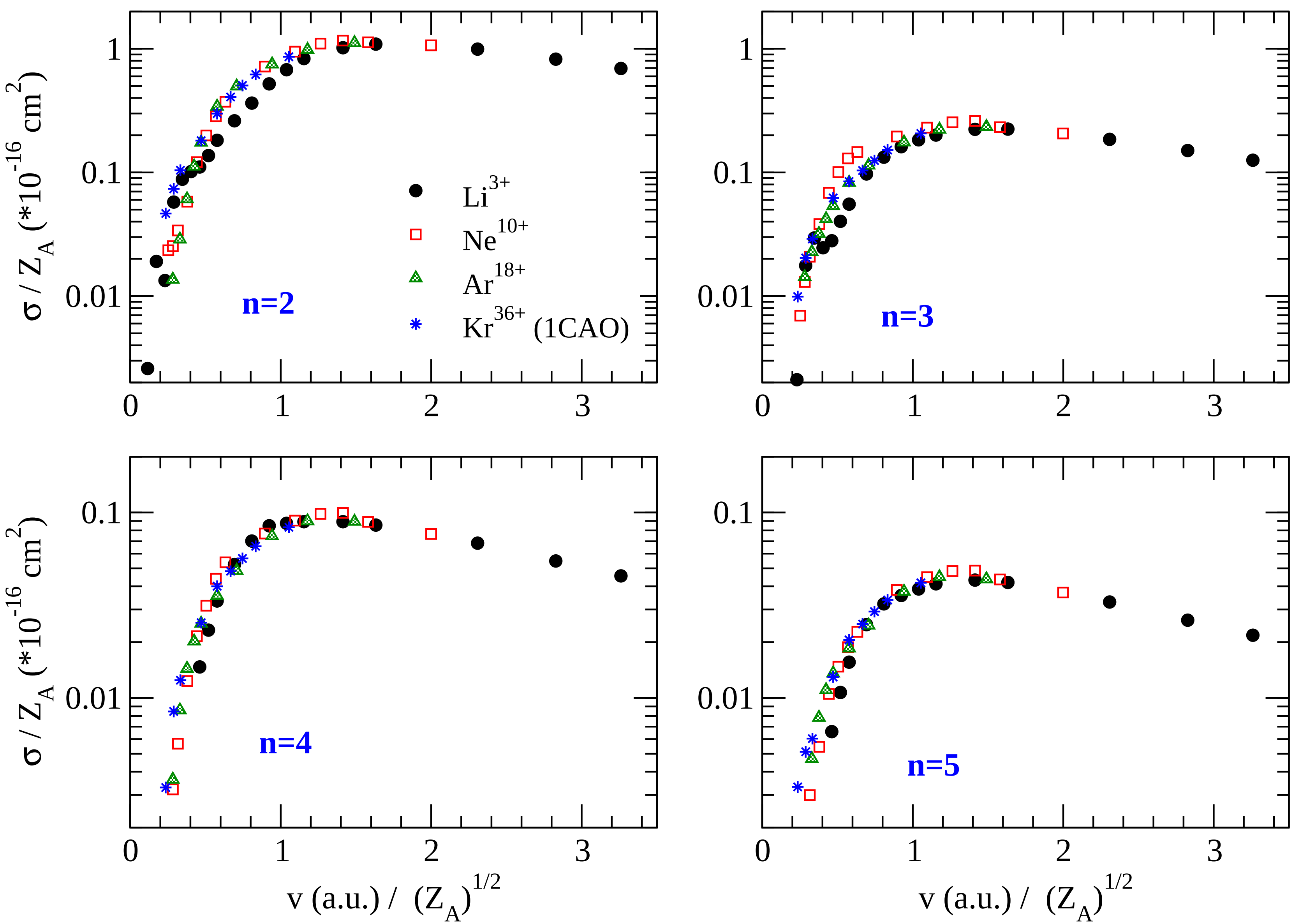
Ar^{18+}+H(1s) $\rightarrow$ Ar^{18+}+H(n) cross sections.



Ar^{18+}+H(1s) → Ar^{18+}+H(n) cross sections.

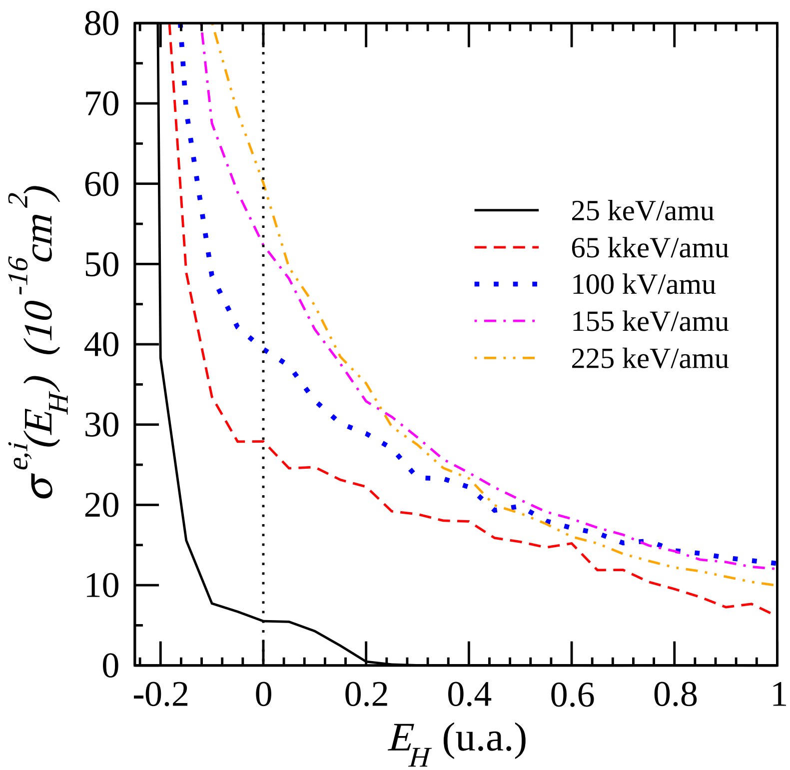


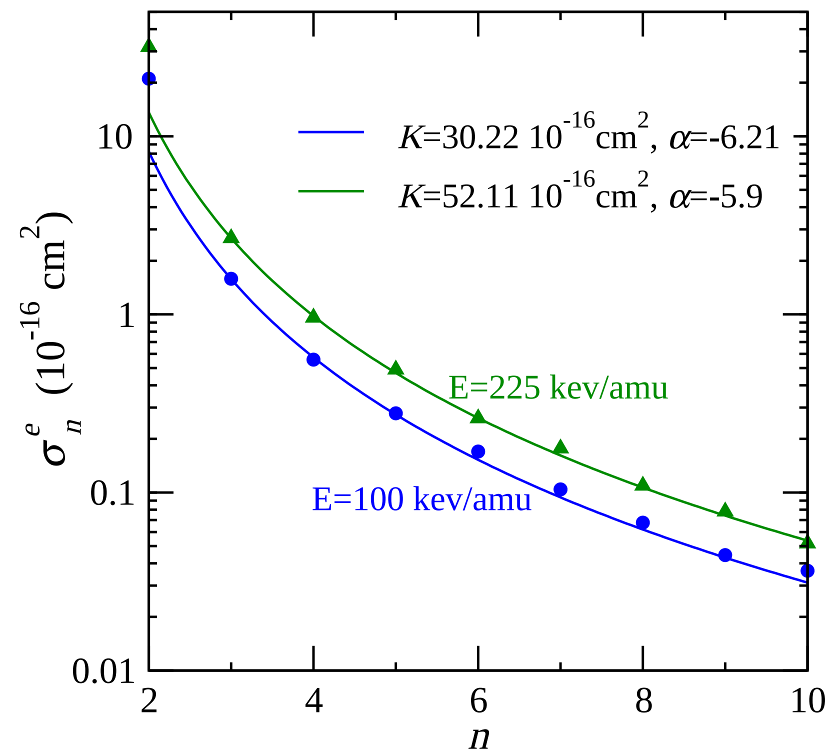
Scaling laws as function of Z_A : $\sigma/Z_A\,(E/Z_A)$



CTMC scaling law as a function of n

Continuity Excitation vs ionization.





$$\sigma_n^e(v) = \frac{Z_H^2}{n^3}\sigma_{E_H}^e(v) \quad \longrightarrow \quad \sigma_{E_H}^e \approx K(v)\exp\left[\alpha(v)E_H\right]$$

$$\boxed{\sigma_n^e \approx K(v) Z_H^2 n^{-3} \exp\left[\alpha(v) Z_H^2/2n^2\right]}$$

Conclusions.

- We provide **recommended n-partial excitation cross sections** for:
  Li^{3+}, Ne^{10+}, Ar^{18+} + H(1s)
- 3 methods employed: OEDMs, 1CAO, CTMC.
- OEDM restricted to **low energies**
  Only for low n' (ionization flux is implicit)
- 1CAO for **intermediate-high** impact energies
  At low v, capture flux might contaminate excitation
- CMTC-hydrogenic method at **intermediate** energies.
  Unable to reproduce quantum interferences
  Problem for excitation to $n' = 2$ ($\longrightarrow$ microcanonical)
- Reasonable **scaling laws** $\sigma(E/Z_A)/Z_A$
- Extrapolation rule for CTMC concerning σ^n (valid from $n' \geq 3$)

Acknowledgements

This work was partially supported by ADAS-EU

- *Teoría de Colisiones Atómicas y Moleculares (TCAM), UAM Madrid:*
  - Luis Méndez
  - Luis Errea
  - Clara Illescas
  - Ismanuel Rabadán
  - Antonio Macías
  - Alba Jorge
- *Centre Lasers Intenses et Applications (CELIA), Bordeaux:*
  - Bernard Pons
- *ADAS-EU:*
  - Francisco Guzmán

Ne^{10+}+H(1s) $\rightarrow$ Ne^{10+}+H(nl) cross sections.