Update on CX calculations from UAM

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Collisions studied

We have considered the following projectiles colliding with H atoms:

- Ne^{10+}, $\mathrm{Ar}^{18+,\,17+,\,16+}$ (rare gases are added in the plasma edge).
- B^{5+} (can be formed due to the boronization of the first wall).
- Li^{+} (Li is used to coat the first wall).

Energy range ≈ 10 eV/amu -1000 keV/amu.

We have applied three methods:

1. Quantal treatment
2. Semiclassical approach with a molecular basis.
3. Eikonal CTMC

Collisions studied

We have considered H^+ + H_2O collisions.

Energy range $\approx 25 - 5000$ keV/amu.

Method : Eikonal CTMC

Organization.

1. Description of the methods.
2. Previous results:
   - $Ar^{16+,17+,18+}$ + H(1s) collisions. (J. Phys. B, 39, L91 (2006))
   - B^{5+} + H(1s) collisions. (Plasma Phys. Control. Fusion 48, 1585 (2006))
3. H^{+}+ Li and Li^{+}+H collisions
4. H^{+}+H_2O collisions (Physical Review A 76, 040701(R) (2007))
5. Summary

Quantal treatment.

- At low energies, the Schrödinger equation:

(1) $$H\Psi^{\mathrm{Q}}(\boldsymbol{r},\boldsymbol{R};J,\mathcal{E})=\mathcal{E}\Psi^{\mathrm{Q}}(\boldsymbol{r},\boldsymbol{R};J,\mathcal{E})$$

where $H=-\frac{1}{2\mu}\nabla_R^2+H_{\mathrm{el}}$ is the non-relativistic Hamiltonian for the collision system and $\mathcal{E}$ is the center of mass energy and μ the nuclear reduced mass.

- Ψ is expanded in terms of molecular wavefunctions:

(2) $$\Psi^{\mathrm{Q}}(\boldsymbol{r},\boldsymbol{\xi};J,\mathcal{E})=\sum_k F_k(\xi,J,\mathcal{E})\phi(\boldsymbol{r},\boldsymbol{\xi};J,\mathcal{E})$$

- The cross sections are given by:

(3) $$\sigma^k(\mathcal{E})=\frac{2\pi}{k_i^2}\sum_J(2J+1)\left|\delta_{ik}-S_{ik}(J,\mathcal{E})\right|^2$$

Semiclassical treatment.

- **Impact parameter approximation:**
  - Nuclear rectilinear trajectories $\boldsymbol{R} = \boldsymbol{b} + \boldsymbol{v}t$
  - Semiclassical equation

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

- **Molecular expansion:**

$$\Psi(\boldsymbol{r}, t; v, b) = \exp\left[{\rm i}U(\boldsymbol{r}, t)\right] \sum_k a_k(t; v, b) \boldsymbol{\chi_k}(\boldsymbol{r}, R) e^{-{\rm i}\int_0^t E_k(t')dt'}$$

  - $\boldsymbol{\chi_k}(\boldsymbol{r}, R)$ are molecular orbitals.
  - $\exp({\rm i}U)$ is a Common Translation Factor.

Semiclassical treatment.

Total cross sections:

$$\sigma_{nlm}^{\mathrm{A,H}}(v) = 2\pi \int |a_{nlm}^{\mathrm{A,H}}(v, b, t \to \infty)|^2 b\mathrm{d}b = 2\pi \int P_{nlm}^{\mathrm{A,H}}(v, b) b\mathrm{d}b$$

Pseudostates can be introduced to evaluate ionization cross sections and to extend the method to high energies

IP-CTMC methods

- Impact parameter approximation: $\boldsymbol{R} = \boldsymbol{b} + \boldsymbol{v}t$
- Classical distribution function $\rho(\boldsymbol{r}, \boldsymbol{p}, t)$, solution of the Liouville's equation:

$$\frac{\partial \rho}{\partial t} = -[\rho, H]$$

Taking

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

leads to the Hamilton's equations

$$\dot{\boldsymbol{r}}_j = \frac{\partial H}{\partial \boldsymbol{p}_j};\ \dot{\boldsymbol{p}}_j = -\frac{\partial H}{\partial \boldsymbol{r}_j}$$

Initial distribution.

Improved distributions have been proposed (Hardie and Olson J. Phys. B, 27, 36903 (1983)).

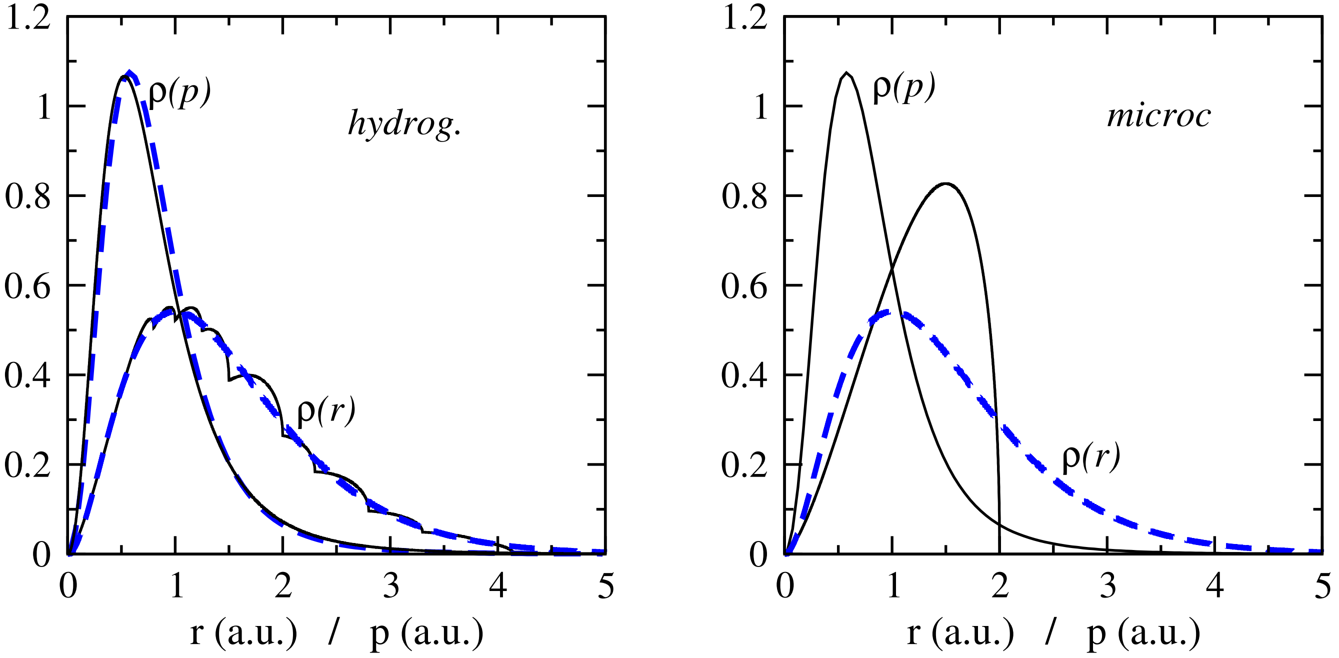
To describe the H(1s) target, we have used a hydrogenic initial distribution, which is a linear combination of 10 microcanonical distributions:

$$\rho(\boldsymbol{r},\boldsymbol{p}) = \sum_{j=1}^{10} w_j \rho^m(\boldsymbol{r},\boldsymbol{p},E_j)$$

Initial distribution.

Comparison between the classical initial distributions: microcanonical ($E = -0.5 a.u.$) and hydrogenic, which is a linear combination of 10 microcanonical distributions:

$$\rho(\boldsymbol{r}, \boldsymbol{p}) = \sum_{j=1}^{10} w_j \rho^m(\boldsymbol{r}, \boldsymbol{p}, E_j)$$



Classical distributions for H(1s) compared to the quantal ones.

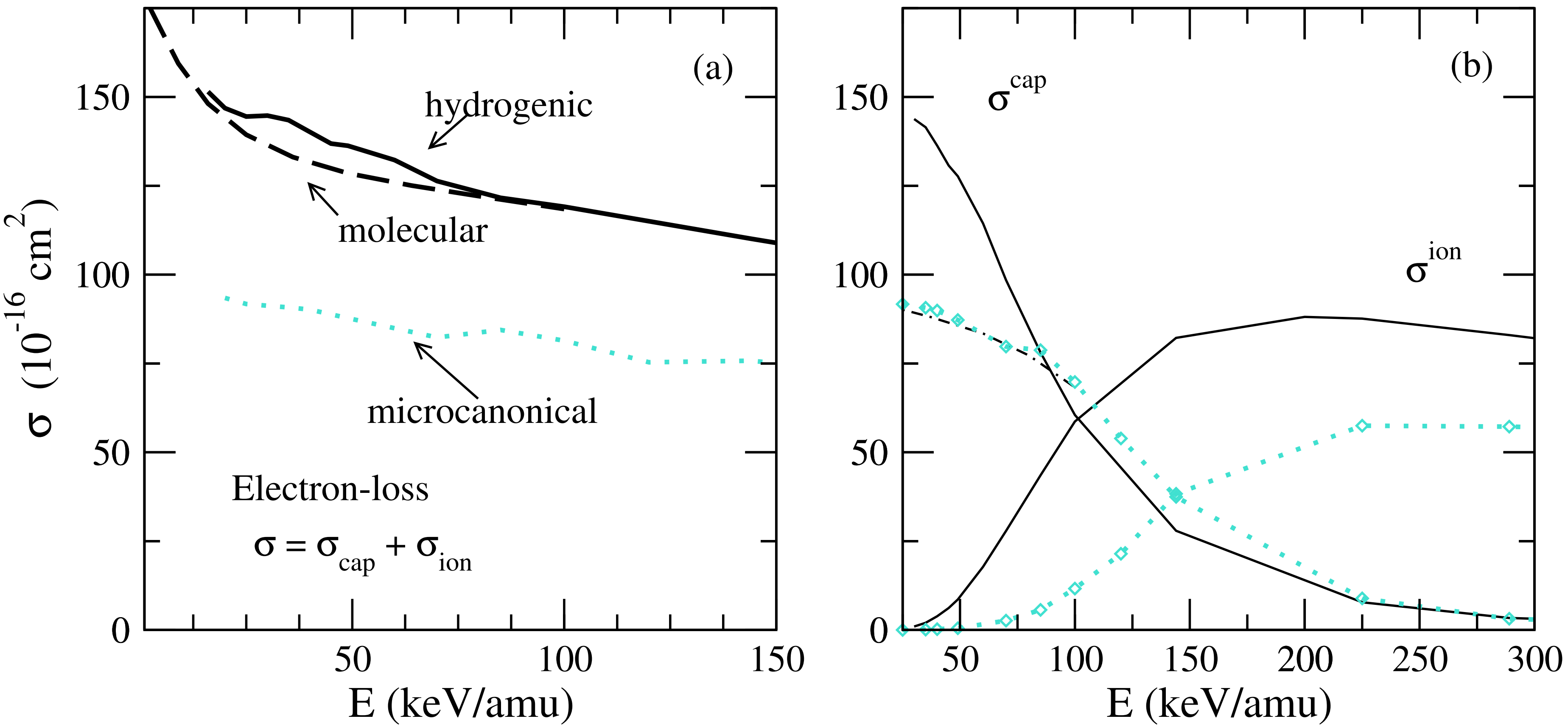
Final states.

We have employed the binning method of Becker and McKellar (J. Phys. B, 17, 3923 (1984))

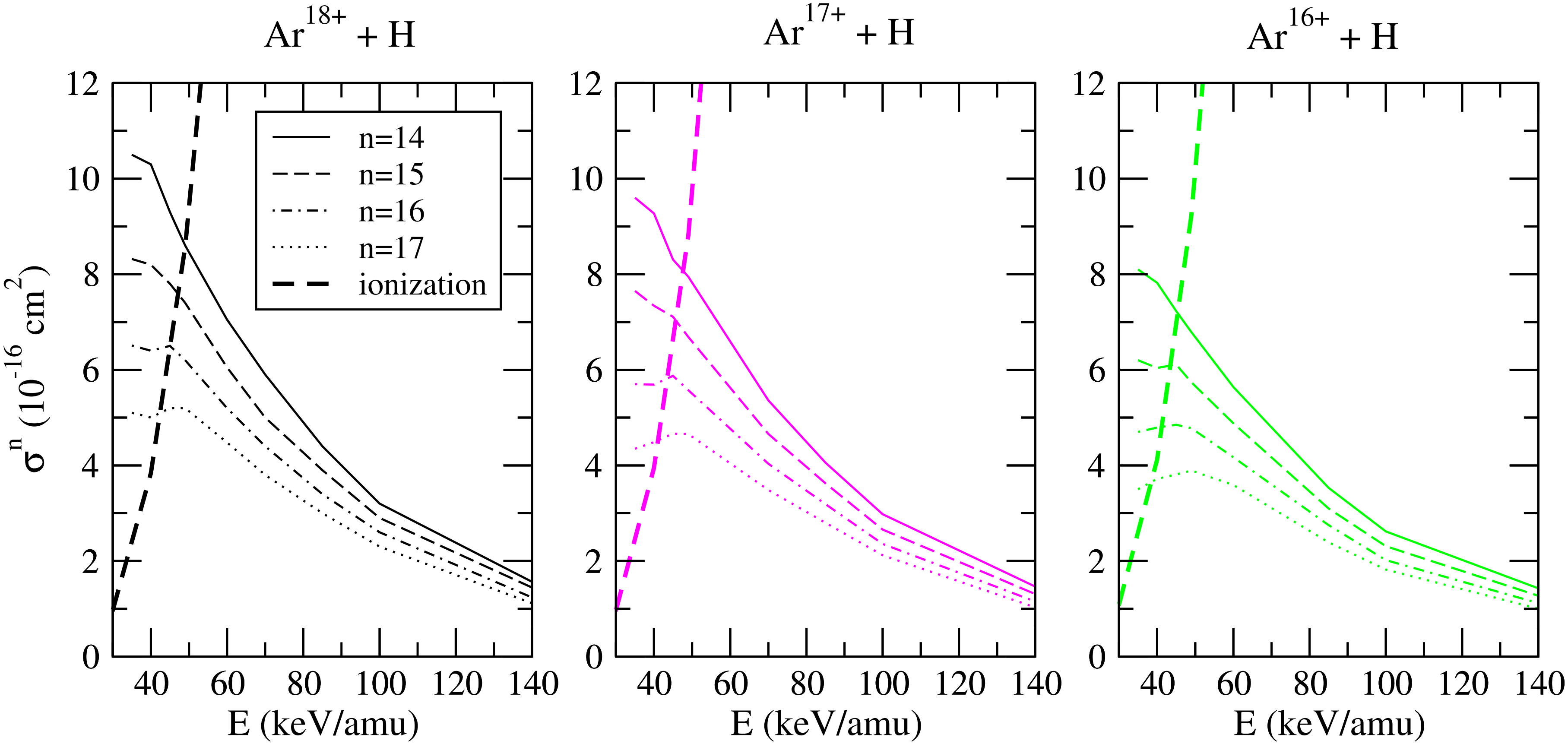
$$\left[\left(n-\frac{1}{2}\right)(n-1)n\right]^{1/3} < \quad n_c \quad \leq \left[n\left(n+\frac{1}{2}\right)(n+1)\right]^{1/3}$$

$$l < \quad \frac{n}{n_c}\, l_c \quad \leq l+1$$

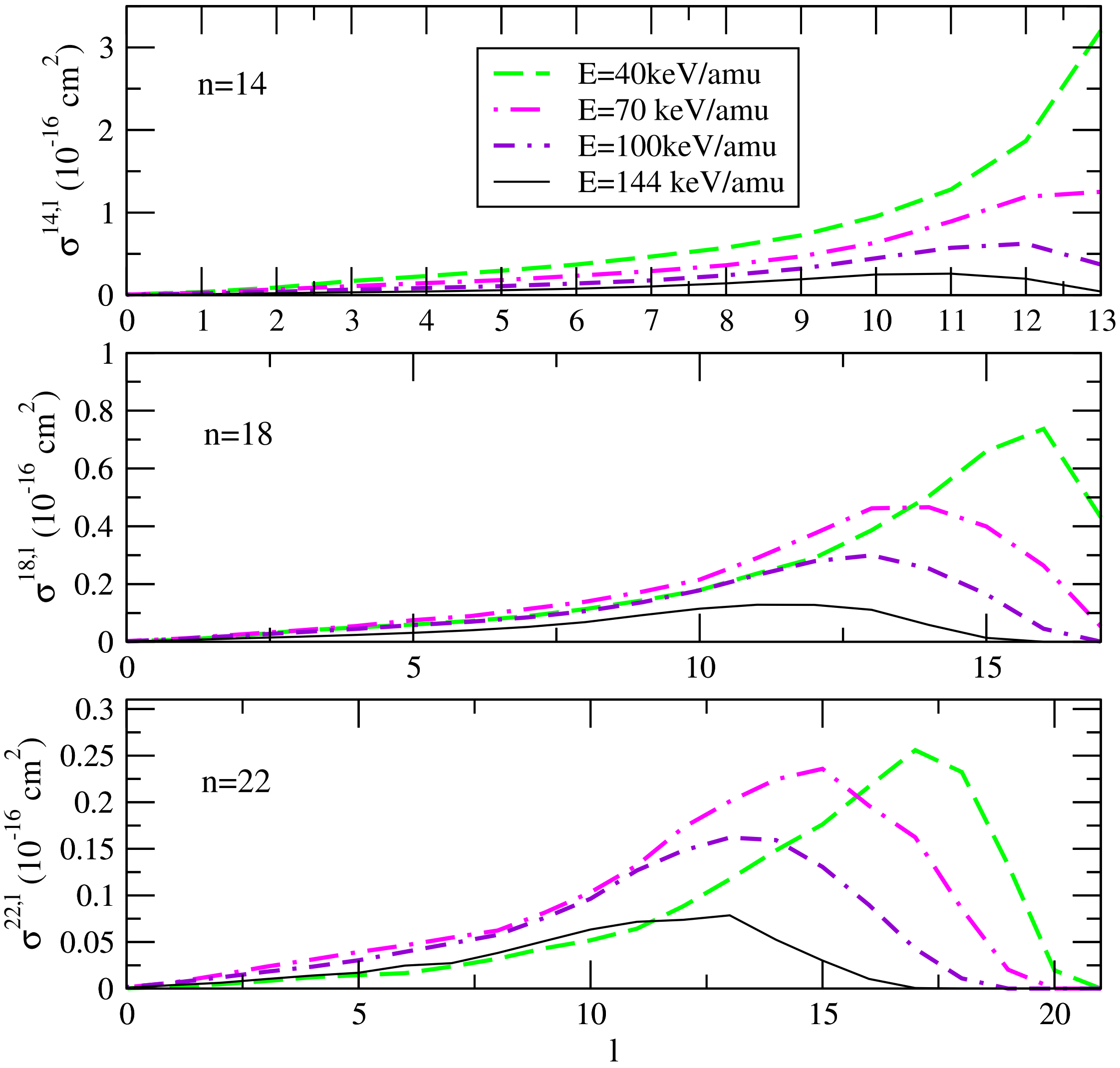
Ar^{18+} + H(1s) collisions.



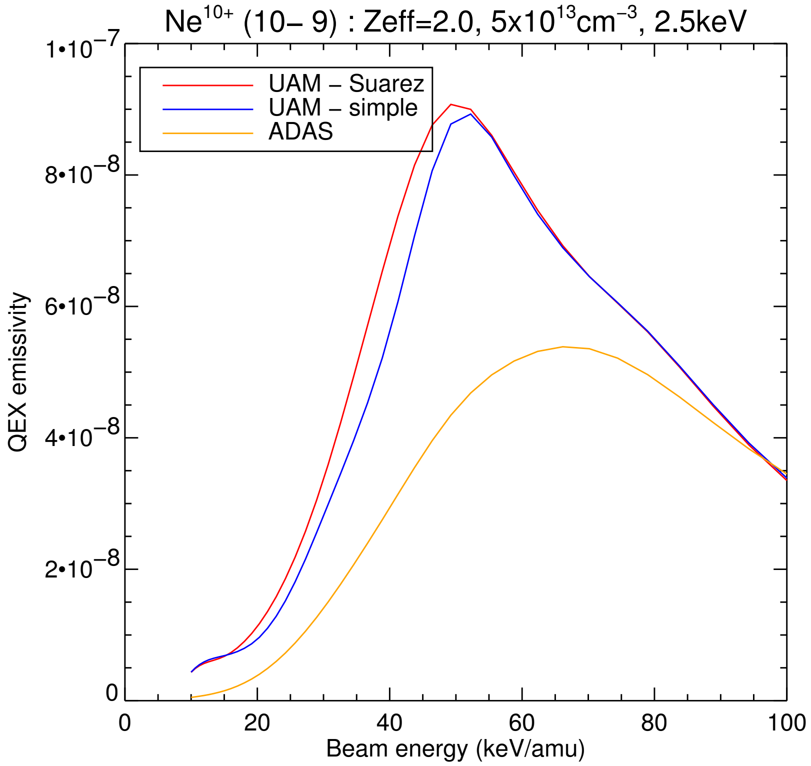
Ar^{q+} + H(1s) collisions.

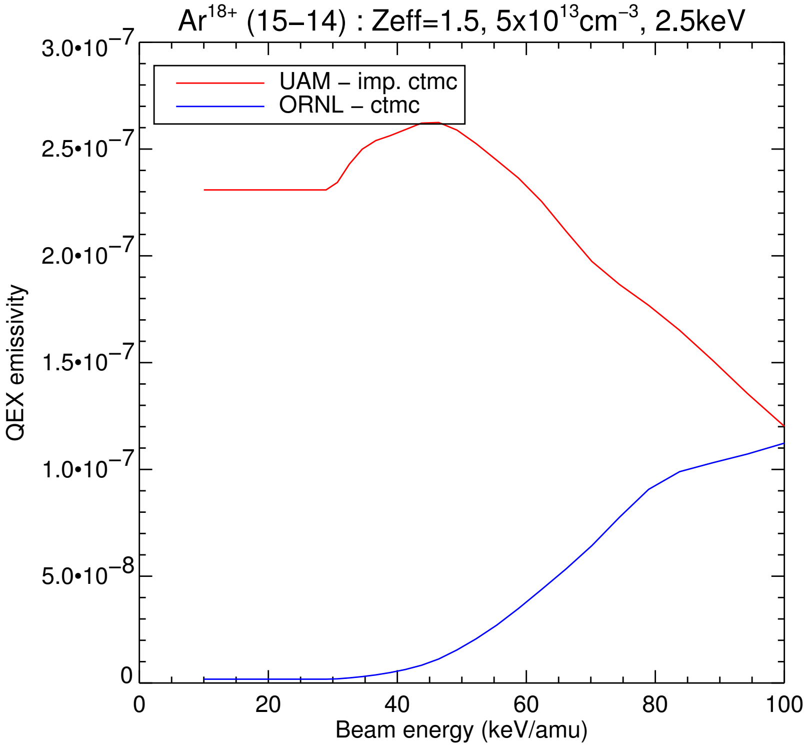


Ar^{18+} + H(1s) collisions.



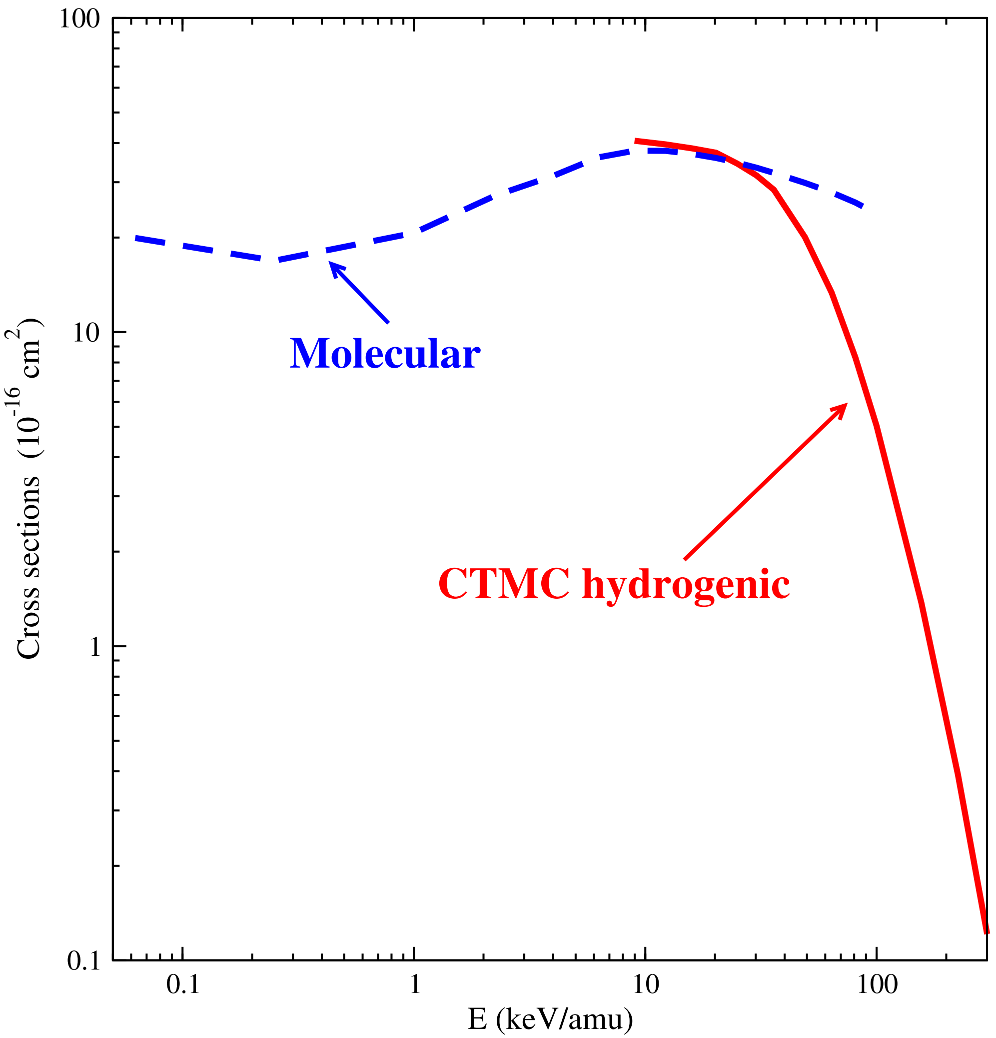
Effective emission coefficients.





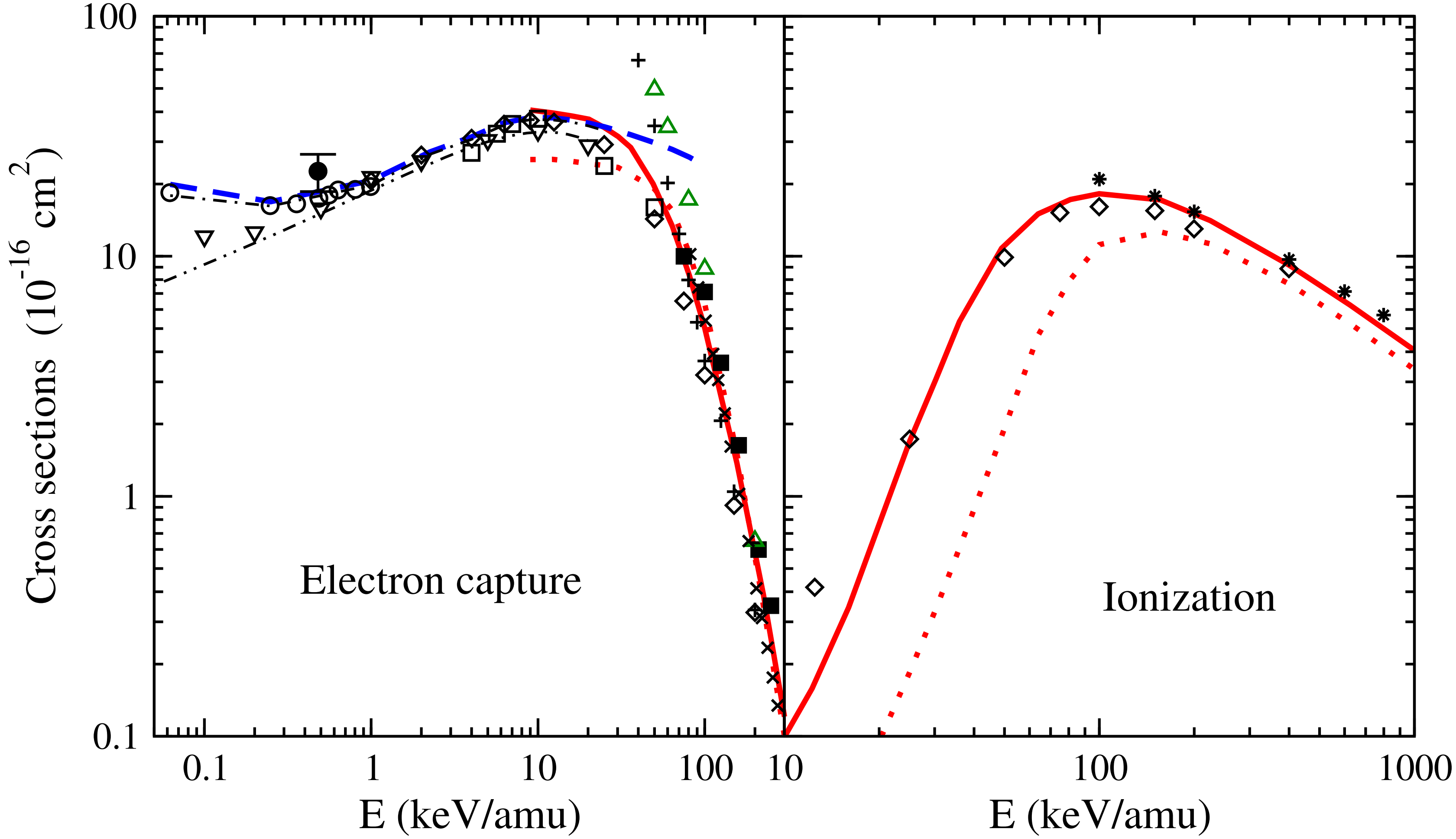
O’Mullane (2006)

B^{5+} + H(1s) collisions.

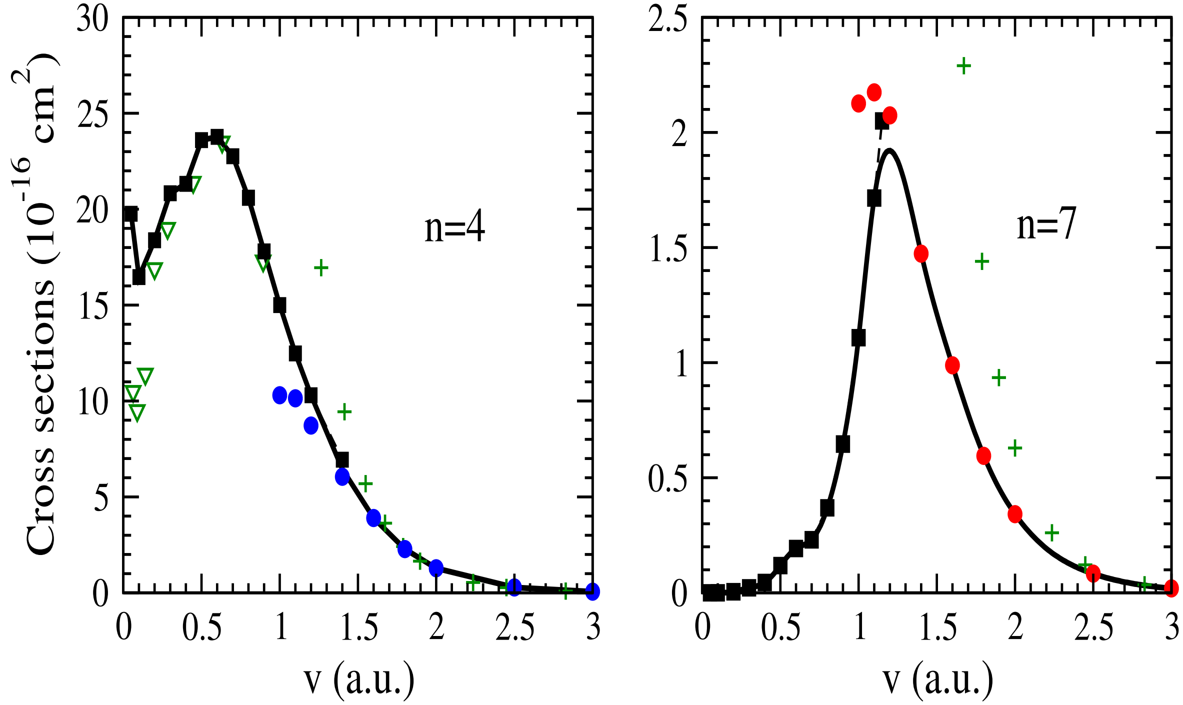


Present results for total capture cross sections.

B^{5+} + H(1s) collisions.



Partial cross sections



Line, recommended data.

■, semiclassical calculation

●, ●, CTMC calculations

+, Belkič $et\ al$,*At. Data Nucl. Data Tables* **51** 76 (1992)

▽,Fritsch and Lin, *Phys. Rev. A* **29** 3039 (1982)

Li^{+} + H(1s) and H^{+}+Li collisions.

- **Interest:**
  Diagnostics with Lithium beams:

  (4) $^{7}\mathrm{Li}(1\mathrm{s}^{2}2\mathrm{s}) + \mathrm{H}^{+} \rightarrow {}^{7}\,\mathrm{Li}^{+}(1\mathrm{s}^{2}) + \mathrm{H}(\mathrm{nl})$ CT

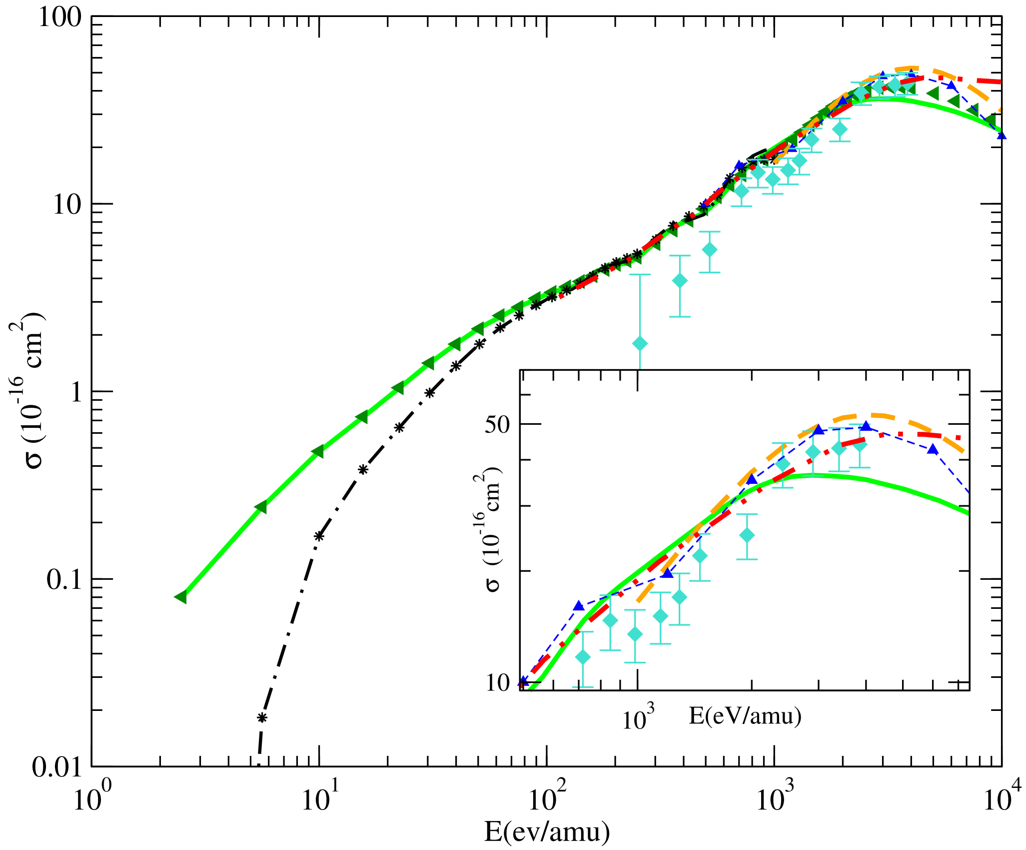
  Presence of Li impurities in the plasma edge:

  (5) $^{7}\mathrm{Li}^{+}(1\mathrm{s}^{2}) + \mathrm{H}(1\mathrm{s}) \rightarrow {}^{7}\,\mathrm{Li}(1\mathrm{s}^{2}\mathrm{nl}) + \mathrm{H}^{+}$ CT

  (6) $^{7}\mathrm{Li}^{+}(1\mathrm{s}^{2}) + \mathrm{H}(1\mathrm{s}) \rightarrow {}^{7}\,\mathrm{Li}^{+}(1\mathrm{s}^{2}) + \mathrm{H}(\mathrm{nl})$ EX

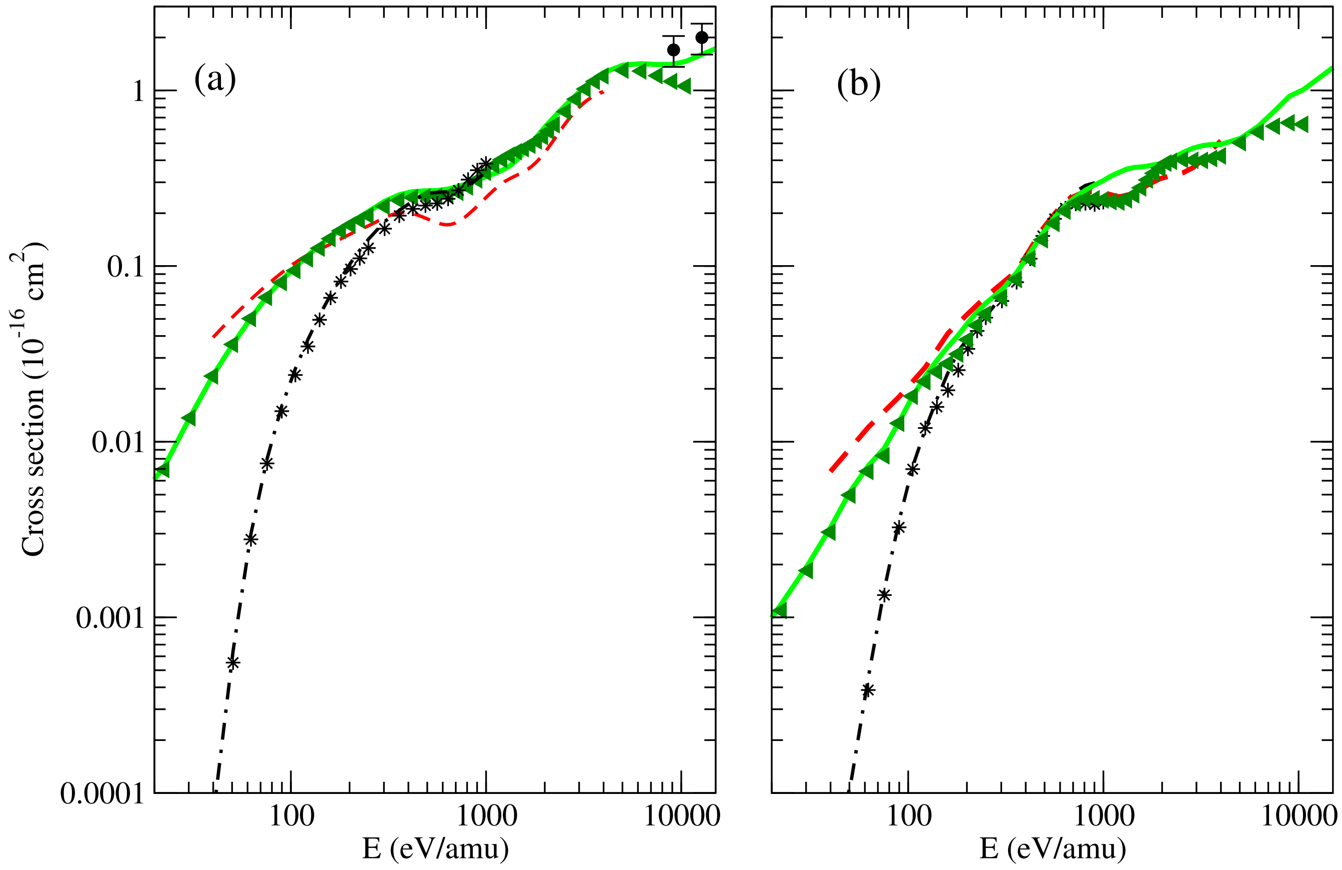
- **Calculations:**
  - Semiclassical approach with a molecular basis
  - Quantal molecular treatment (E $\leq$ 300 eV/amu)

H^+ + Li collisions.



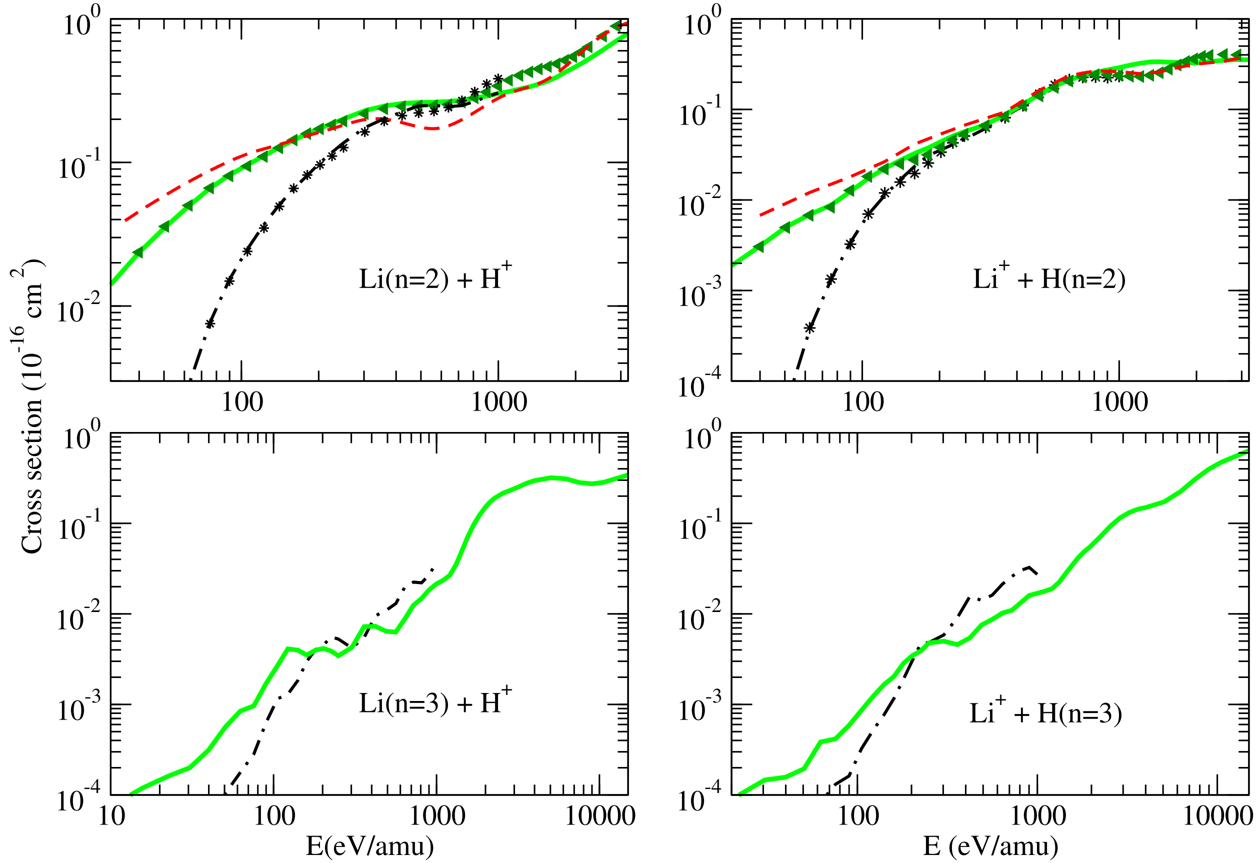
- Present CT results: 17MO *ab initio* basis set: —, semiclassical calculation; — · —·, quantal calculation. Calculations with the 7MO basis set: ◀, eikonal and ∗, quantal results.
- Experimental results: ◆ (Varghese et al. 1984).
- Previous calculations for total CT: —▲—, results of Fritsch and Lin (1984); - ·· -, results of Salas (2000); - - - , results of Schweinzer et al. (1999) for target electron loss.

Li$^+$ + H(1s) collisions.



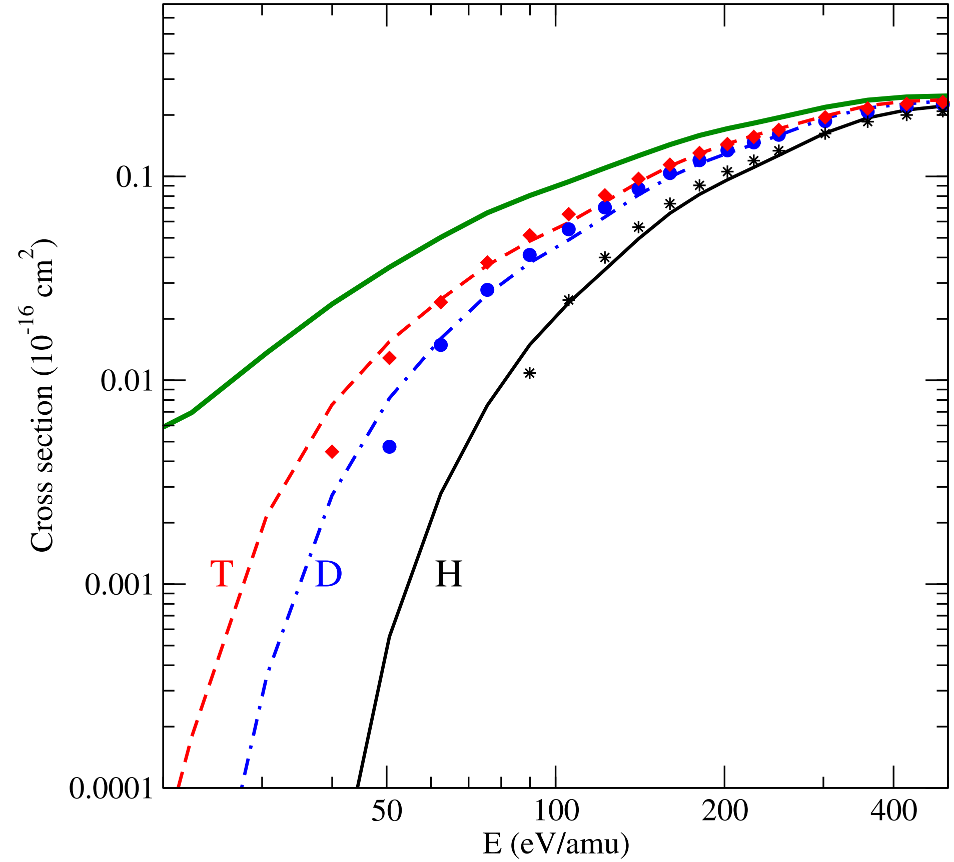
CT (a) and EX (b) in Li$^+$+ H(1s) collisions. Calculations with the 17MO *ab initio* basis set: —, eikonal and – · –·, quantal. 7MO *ab initio* basis set: ◀, eikonal and ∗, quantal. - - - , eikonal calculation with a model potential 7MO basis set. •, experimental results of Shah et al. (1978).

Li^+ + H(1s) collisions.



n-resolved cross sections CT into Li(n=2,3) + H^+ and H excitation to H(n=2,3) in Li^+ + H(1s) collisions. The minimal 7MO basis is sufficient to obtain converged $n = 2$ CT and EX cross sections.

Li^+ + H (D, T)(1s) collisions.



Cross sections for charge transfer in Li^+ + H (D, T) (1s) collisions. Thick line, eikonal calculation. Thin lines, quantal results for the different H isotopes. Points, Coulomb trajectory model:

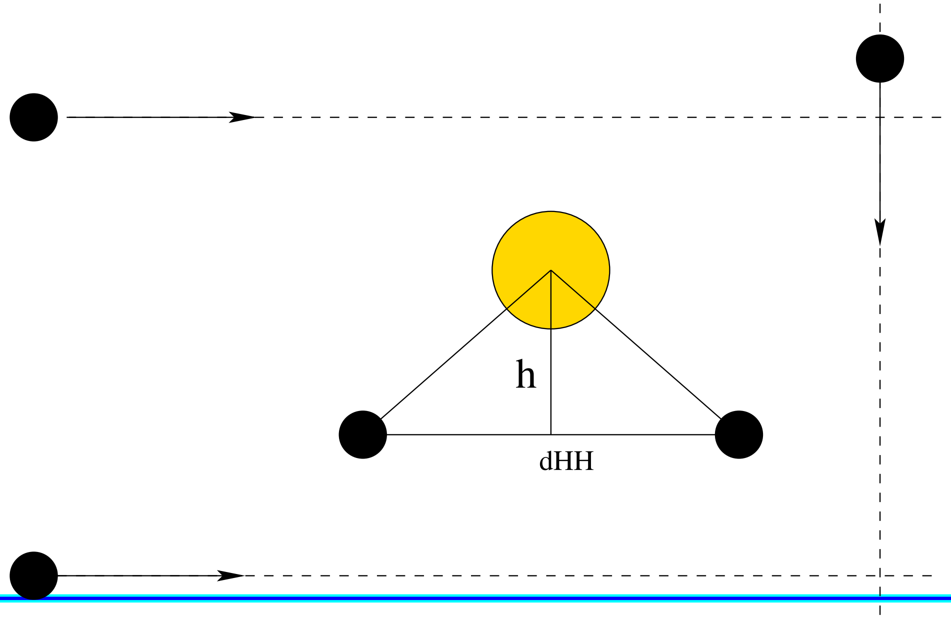
$$\sigma(v) \approx \sigma^{\mathrm{eik}}(v)\left[1 - \frac{2q}{\mu v^2 R_0}\right]$$

which has a threshold at $v_t = \sqrt{\frac{2q}{\mu R_0}}$ for each μ.

Application to ion-molecule collisions.

- Effective Coulomb potential: $V_{\rm ef} = -Z_{\rm ef}/r$
- The IPM approach.
- Orientation average.

$$\sigma^{\rm X}(E) = 2\pi \int_0^\infty \left[b + \frac{1}{6}(d_{HH}/2 + h) \right] P^X(b, E){\rm d}b$$



IPM for H^+ + H_2O collisions.

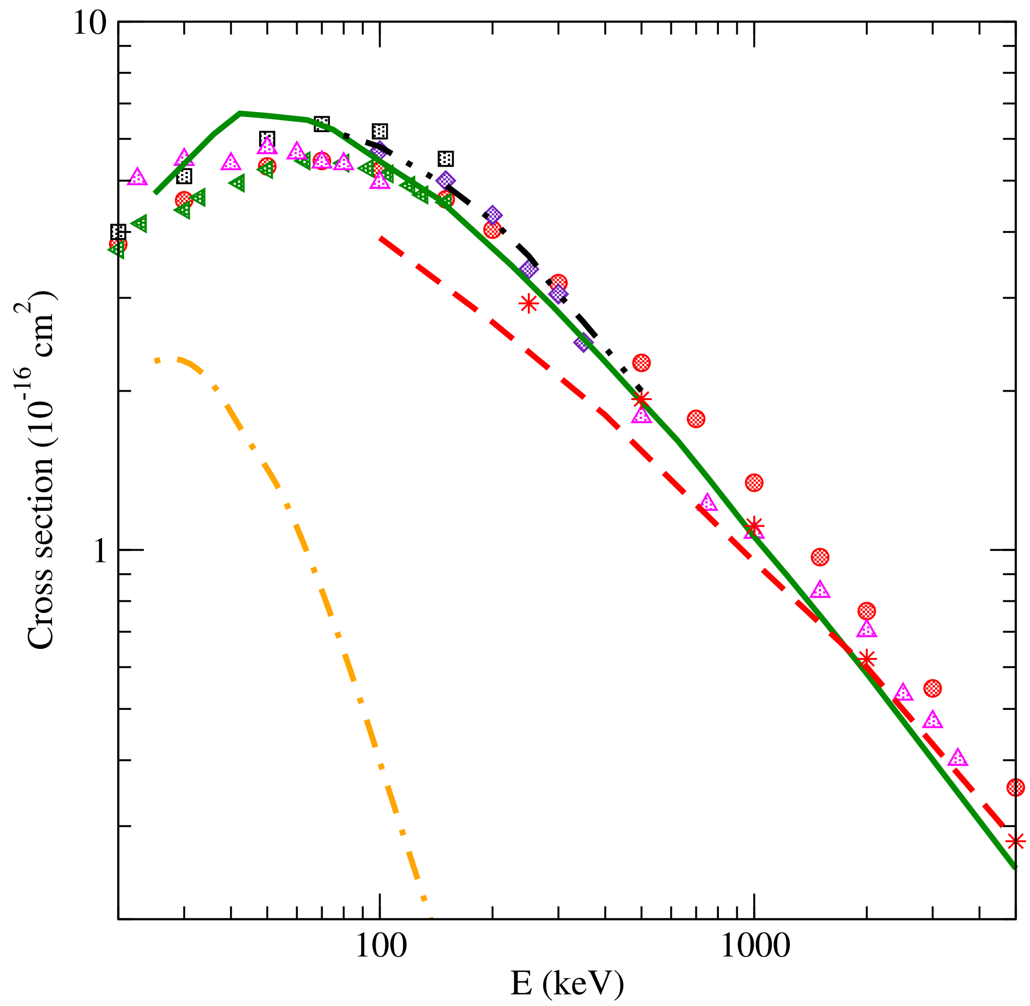
- Electron emission from 1b$_1$, $E_{\text{ion}} = 12.61$ eV ⇒ One-electron probabilities: p_1^{ion}, p_1^{cap}
- Electron emission from 3a$_1$, $E_{\text{ion}} = 15.57$ eV ⇒ p_2^{ion}, p_2^{cap}
- Electron emission from 1b$_2$, $E_{\text{ion}} = 19.83$ eV ⇒ p_3^{ion}, p_3^{cap}
- Electron emission from 3a$_1$, $E_{\text{ion}} = 36.88$ eV ⇒ p_4^{ion}, p_4^{cap}

$$P^{\text{SI}} = \sum_{k=1}^4 P_k^{\text{SI}} = 2\sum_{k=1}^4 p_k^{\text{ion}} p_k^{\text{el}} \prod_{j\neq k} (p_j^{\text{el}})^2 \qquad \text{single ionization}$$

$$P^{\text{SEC}} = \sum_{k=1}^4 P_k^{\text{SEC}} = 2\sum_{k=1}^4 p_k^{\text{cap}} p_k^{\text{el}} \prod_{j\neq k} (p_j^{\text{el}})^2 \qquad \text{single electron capture}$$

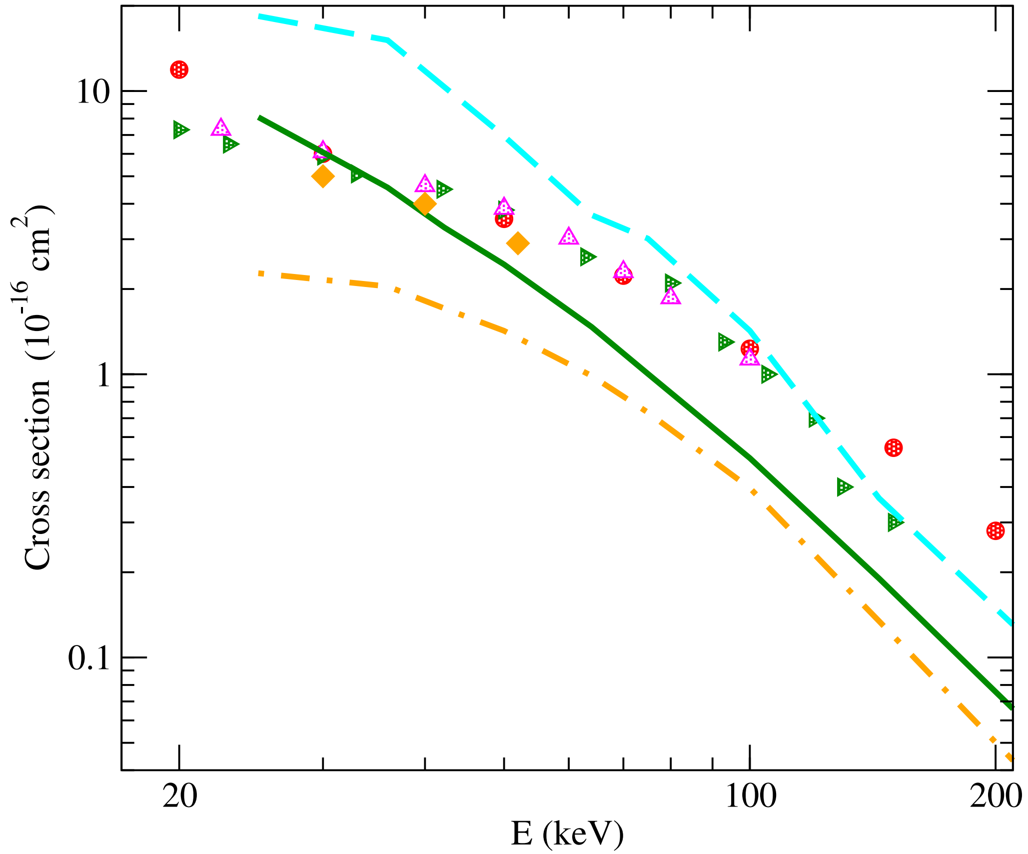
$$\begin{aligned} P^{\text{TI}} &= 4\sum_{k\neq l} p_k^{\text{cap}} p_l^{\text{ion}} p_k^{\text{el}} p_l^{\text{el}} \prod_{j\neq k,l} (p_j^{\text{el}})^2 + \\ &\quad +2\sum_k p_k^{\text{cap}} p_k^{\text{ion}} \prod_{j\neq k} (p_j^{\text{el}})^2 \qquad \text{transfer ionization} \end{aligned}$$

H^+ + H_2O collisions.



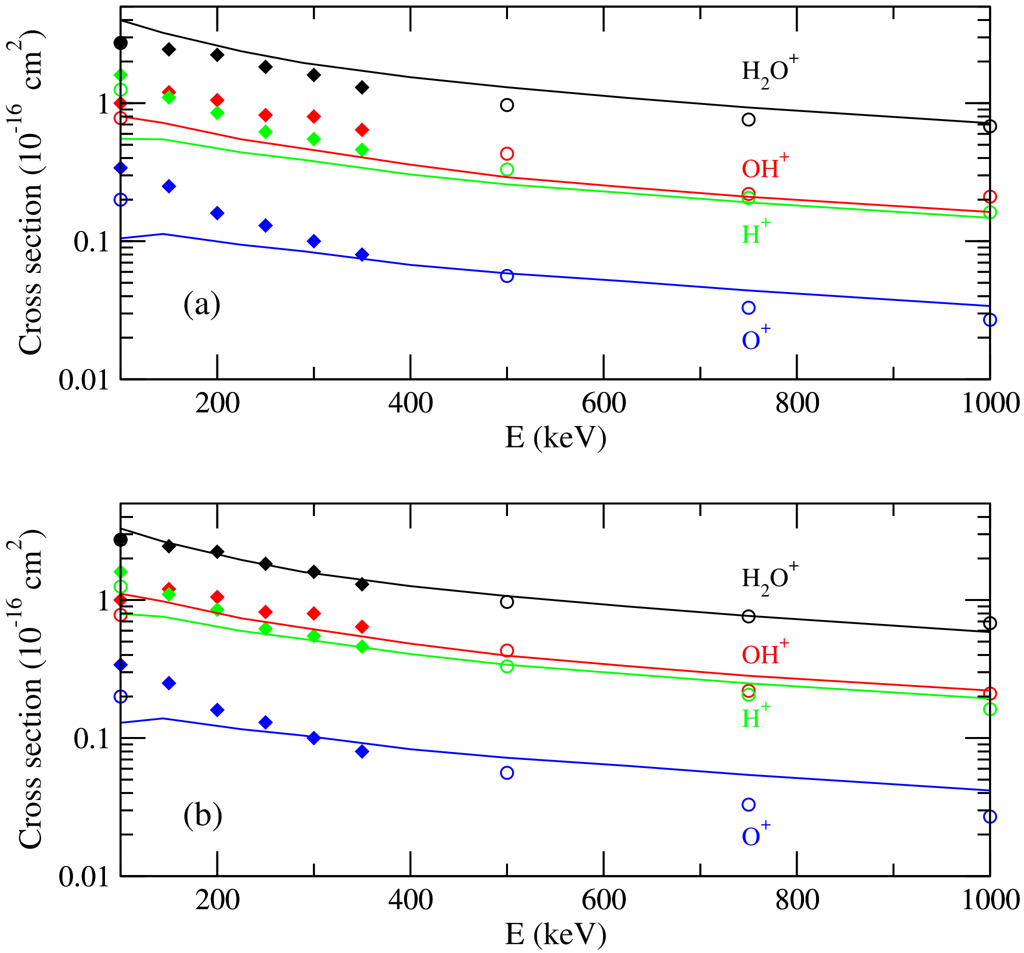
- Present results: —-, SI; - · - · TI.
- Previous calculations: - - -, Boudriuoua et al., 2007 (Born); - ·· -, Olivera et al. 1996; ⋆, Gervais et al., 2006 (CDW)
- Experimental data for SI: ●, Rudd et al. 1985; ■, Bolorizadeh and Rudd, 1986 ◆, Werner et al., 1995 ◀ Gobet et al., 2004
- Experimental data for SI + TI of Luna et al., 2007: ▲ .

$H^+ + H_2O$ collisions.



- Present results: —-, SEC. - · -, TI. - - -, Present results for SEC using the modified IPM treatment of Kircher et al 2000.
- Experimental data for SEC: ●,Rudd et al. 1985 ; ▶, Gobet et al., 2004.
- Experimental data for SEC + TI: ◆, Dagnac et al., 1970; ▲, Luna et al., 2007.

Fragmentation in SI.



Total cross sections for formation of H_2O^+, OH^+, H^+ and O^+ in the SI reaction, calculated using the branching ratios of Tan *et al.* (1978) (a) and Olivera *et al.* (1998) (b). Experimental data: ♦, Werner *et al.* (1995), ◯, Luna *et al.* (2007)

Summary.

- Use of complementary methods to cover a large energy range.
- Study of the overlap region:
  - Convergence of the molecular expansion.
  - Influence of the initial distribution in CTMC calculations.
- New recommended data for CX in B^{5+} + H(1s).
- New data for CX in Li^{+} + H(1s) at low-E.
- Results for total cross sections in H^{+}+H_2O collisions at intermediate-E, as an illustration of the application to small molecules of interest in fusion; e.g. small hydrocarbons.