Charge transfer cross section calculation and evaluation for Be^{q+} + H collisions

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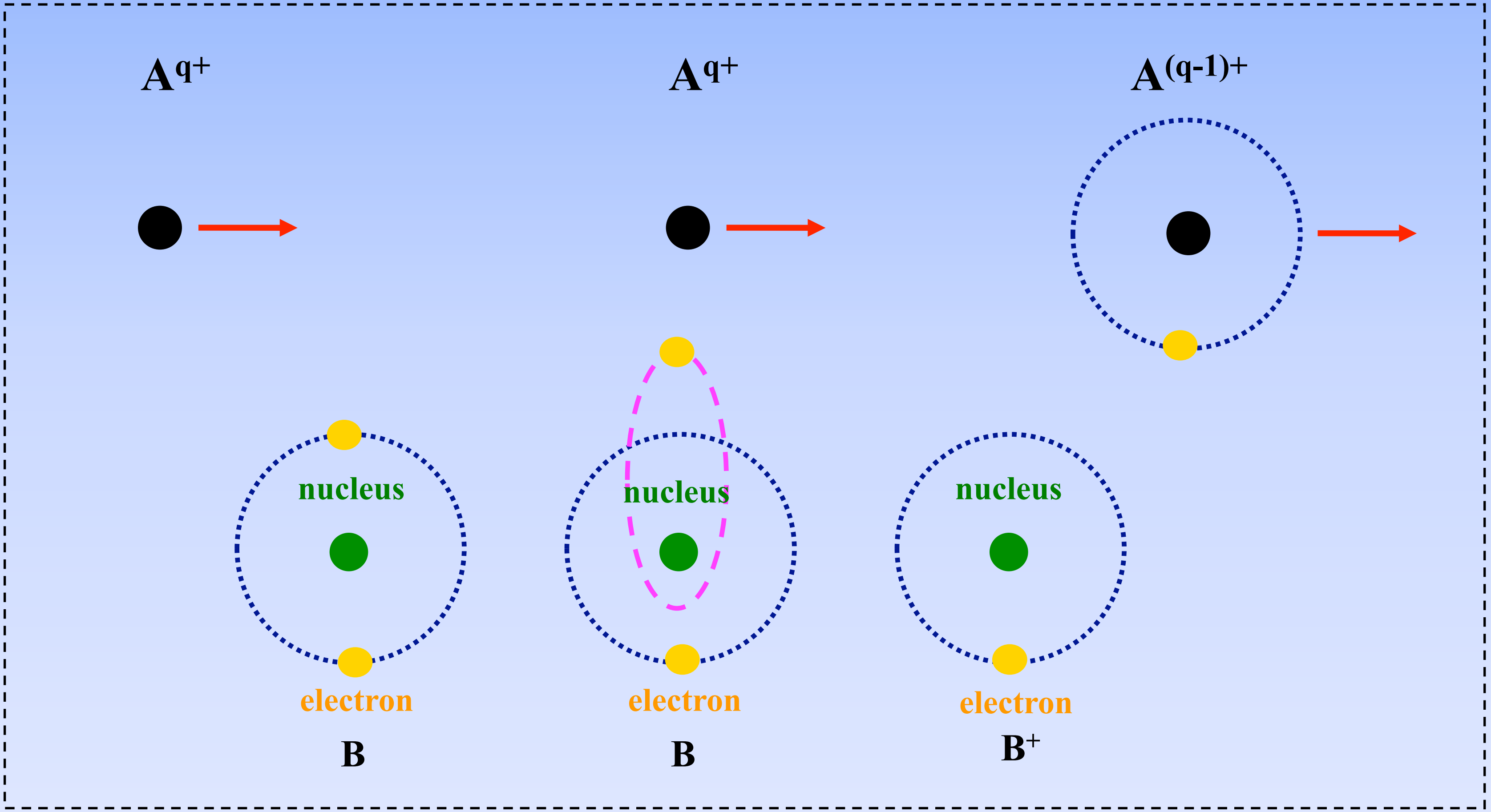
Charge Transfer Process



Outline

- **Motivation**
- **Theoretical methods**

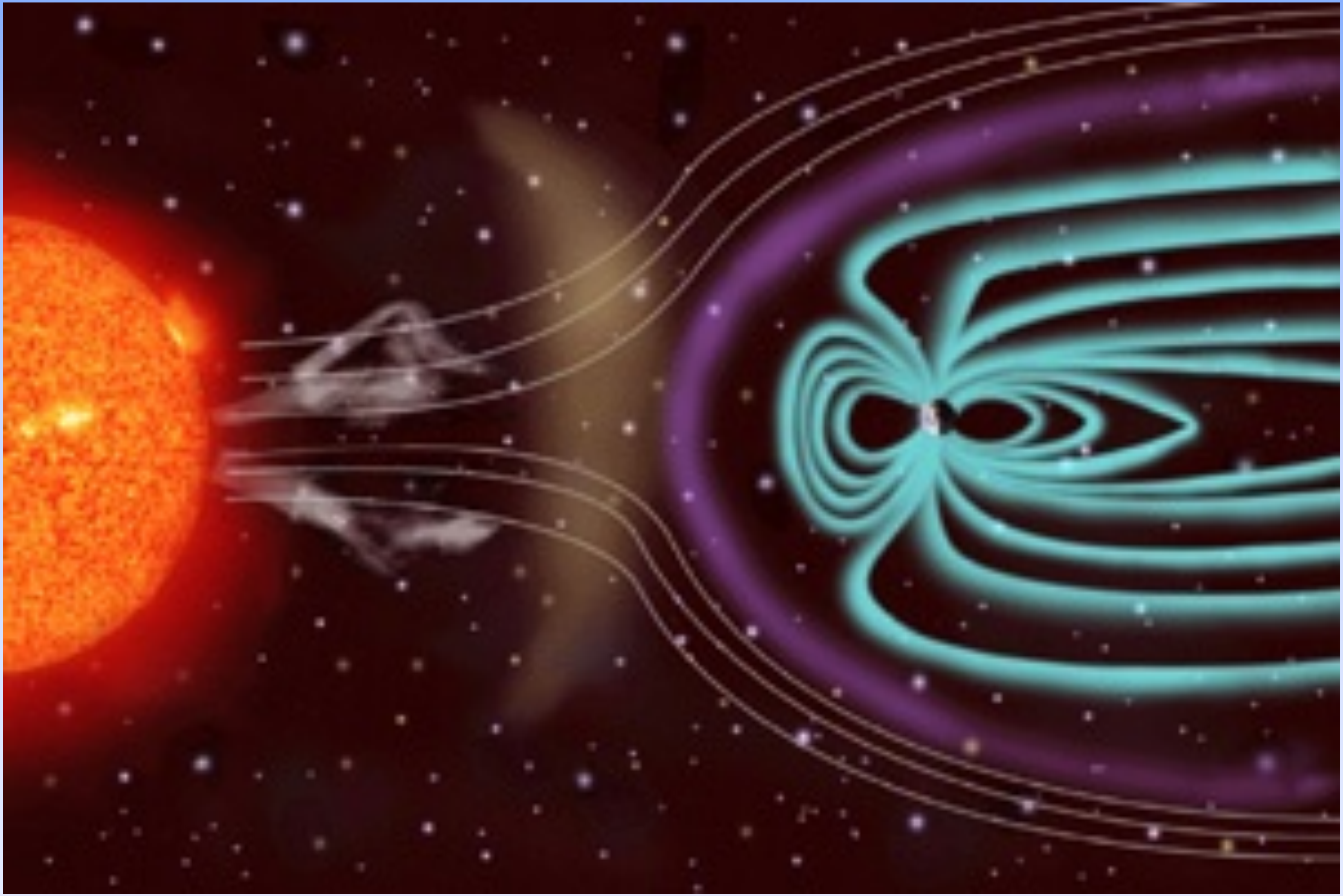
  QMOCC / AOCC

- **Results and discussions**

  Be^{q+} + H

- **Summary**

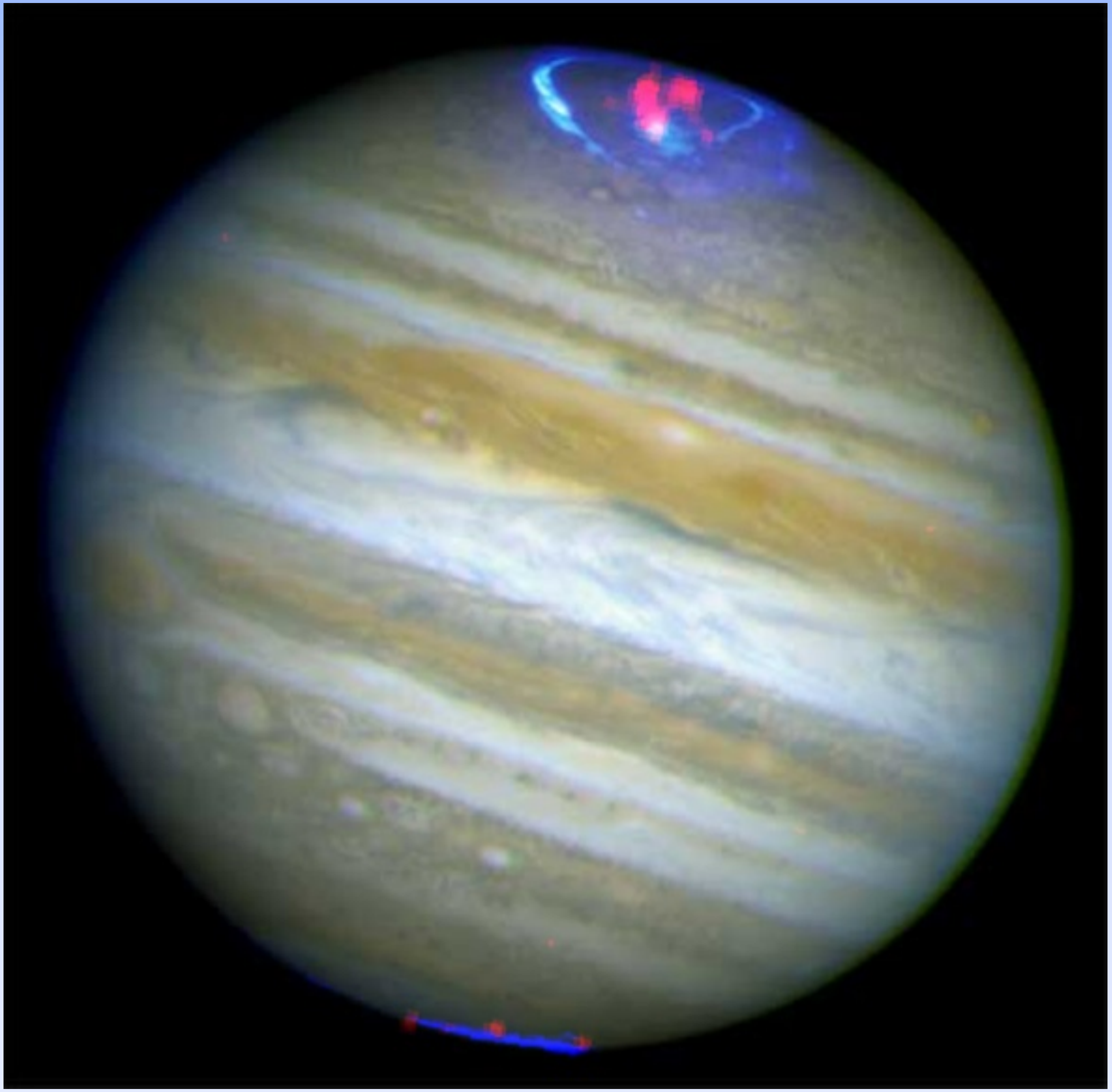
Solar Wind : O^{q+}, S^{q+}, Ne^{q+},…



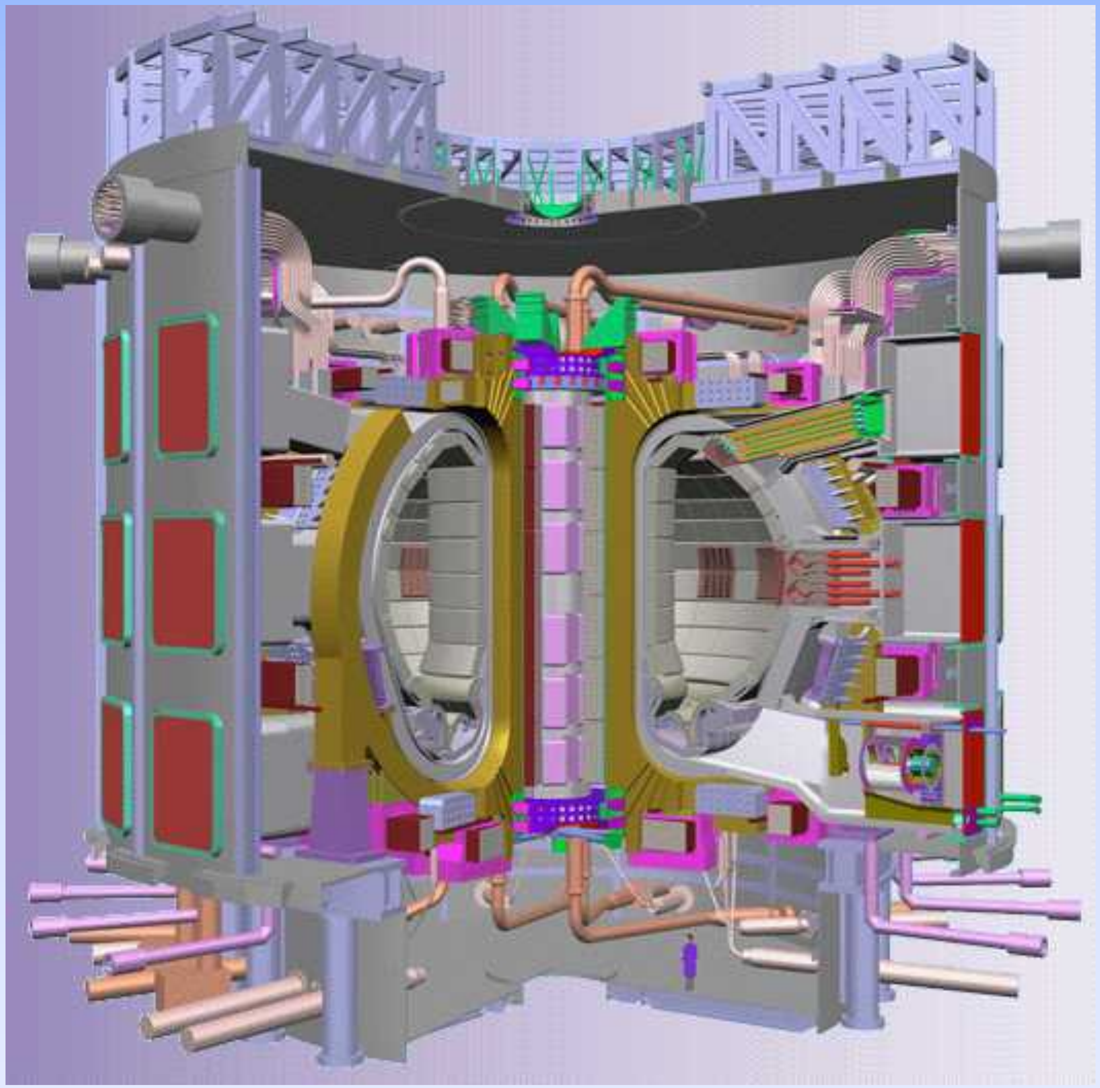
Jupiter : EUV and X-ray

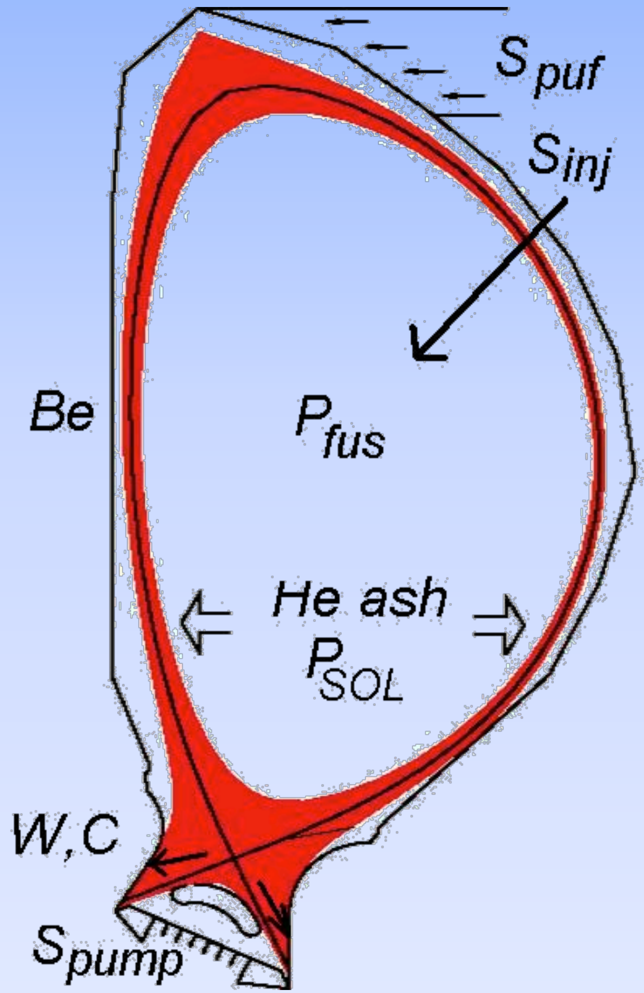
$$O^{q+} + H_2 \rightarrow O^{(q-1)+}(nl) + H_2^+$$

$$O^{(q-1)+}(nl) \rightarrow O^{(q-1)+}(n'l') + h\nu$$



ITER Tokomak (edge / divertor) neutral beam injection, diagnosis





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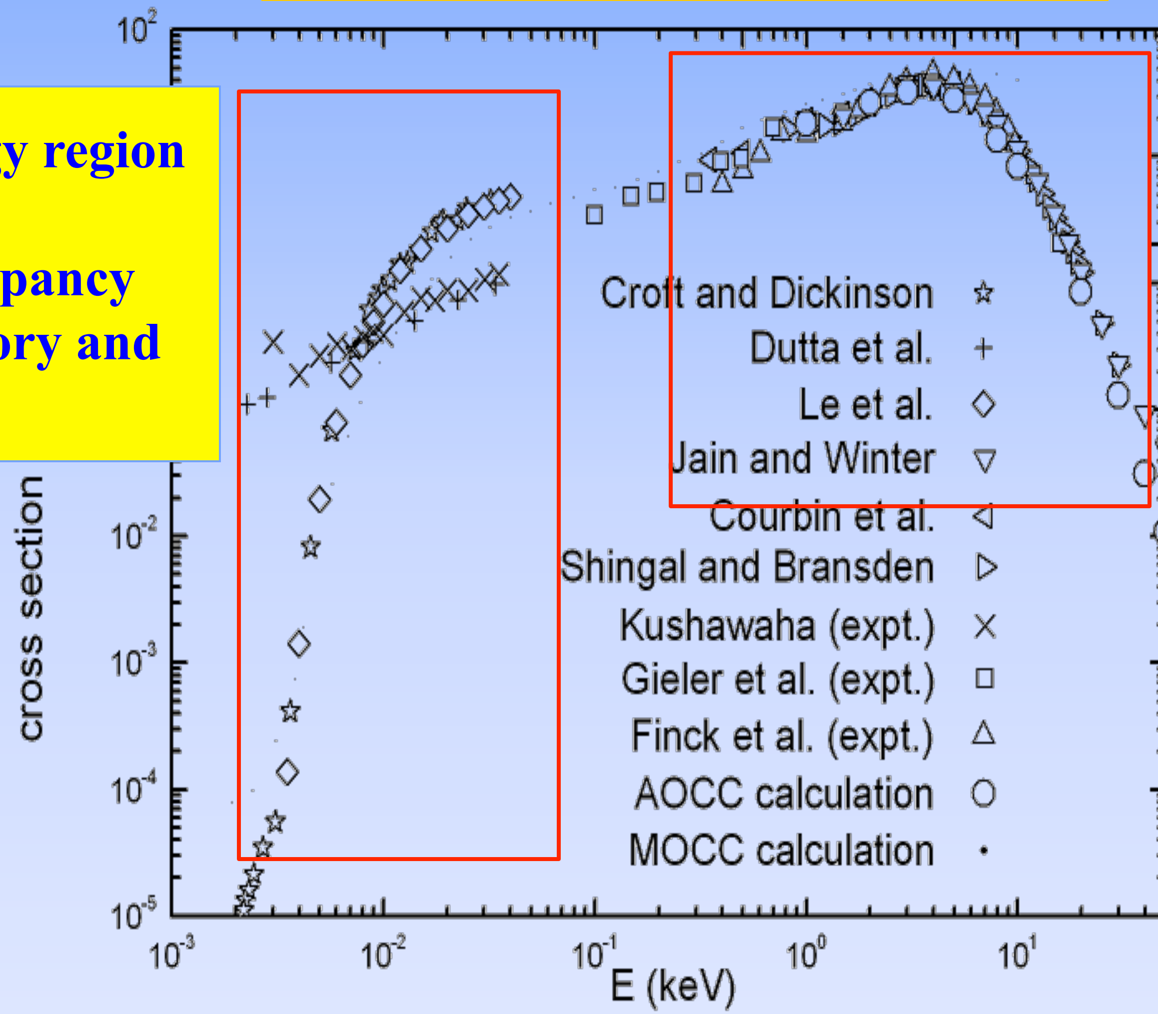
Total charge transfer cross sections

Na(3*s*) + H⁺ → Na⁺ + H(*n*=2)

Lower energy region

Large discrepancy between theory and experiment



Middle, and high energy region:

good agreement between theory and experiment

C. H. Liu, Y. Z. Qu et al., Phys. Rev. A 78, 024703 (2008).

Theoretical methods

CTMC （$E \geq 1$ keV/amu）

COBM （1-- 25 keV/amu）

AOCC （0.1-- n×100 keV/amu）

SMOCC （0.1--n×10 keV/amu）

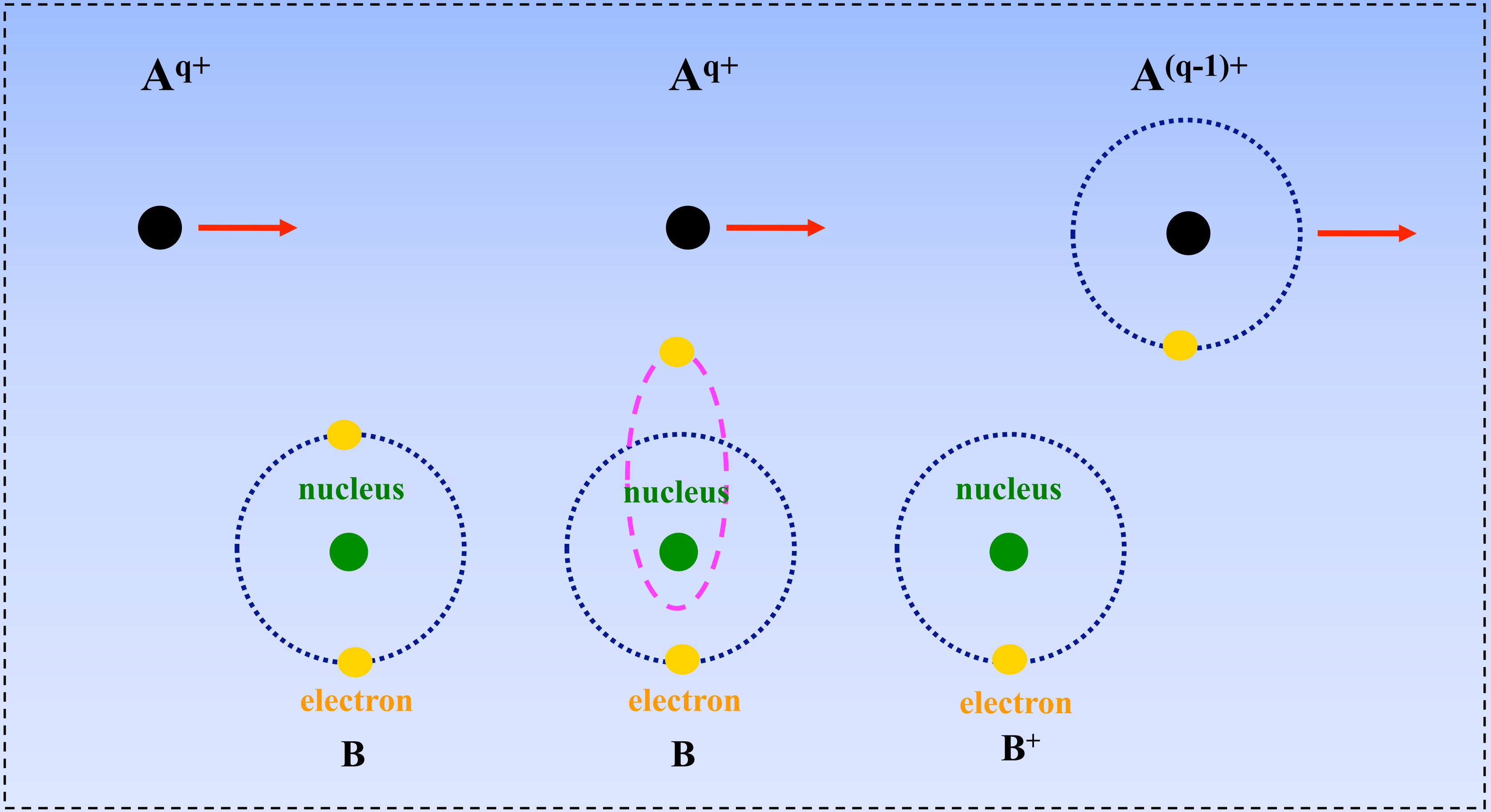
MCLZ （$E \geq$ keV/amu）

TDSE （$E \geq$ n×100 eV/amu）

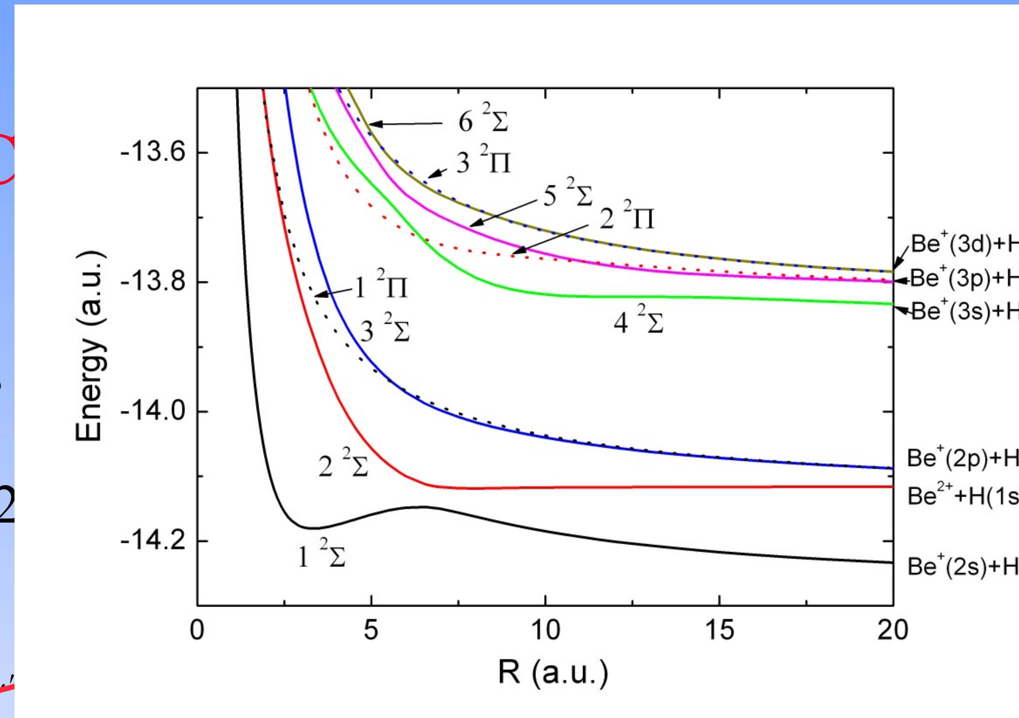
QMOCC （ < n keV/amu）

… …

QMOCC


A^{q+}
A^{q+}
A^{(q-1)+}
nucleus
nucleus
nucleus
electron
electron
electron
B
B
B^{+}

QMOC



The radial coupled equations

$$\left[\frac{d^2}{dR^2} - \frac{J(J+1) - \lambda^2}{R^2} + 2\mu E\right] g_\gamma^J - 2$$

where $U_{\gamma,\gamma'}(R) \equiv [C(u-P)C^{-1}]_{\gamma\gamma'}$

$$\frac{dC}{dR} + AC = 0, \quad \lim R \to \infty, \quad \mathrm{C}(R) \to \overset{\vee}{I}$$

rotational couplings

$$A_{ij}^{\theta} = \langle i | iL_y | j \rangle$$

$$P_{mn} = \pm \frac{1}{\mu R^2} \left[\left(J \,\mathrm{m} \lambda_m \right) \left(J \pm \lambda_m + 1 \right) \right]^{1/2} A_{mn}^{\theta} \delta\left(\lambda_m, \lambda_n \pm 1 \right)$$

The potentials, radial and rotational couplings are calculated by the multireference single- and double-excitation configuration interaction (MRD-CI) method **R J Buenker, Univ. of Wuppertal, Germany**

$$\lim_{R\to\infty} g_{\gamma}^{l}(R) \to \frac{1}{\sqrt{k_{\gamma'}}}\left[\delta_{\gamma,\gamma'} j_l\left(k_\gamma R\right) + K_{\gamma,\gamma'}^{l}\eta_l\left(k_{\gamma'}R\right)\right],$$

$$k_\gamma = \sqrt{2\mu\left[E - \varepsilon_\gamma(\infty)\right]}$$

$$\sigma_{i\to j} = \frac{\pi}{k_i^2}\sum_l \left(2l+1\right)\left|S^l - I\right|_{i,j}^2, \quad \text{where} \quad S^l = \frac{I + iK^l}{I - iK^l}$$

References:

1. T. G. Heil, *et al.*, Phys. Rev. A, 23, 1100 (1981).

2. B. Zygelman, *et al.*, Phys. Rev. A, 46, 3846 (1992).

AOCC method

- **Semi-classical method for middle and high collision region**

$$(H - i\frac{\partial}{\partial t})\Psi = 0 \qquad H = -\frac{1}{2}\nabla_r^2 + V_A(r_A) + V_B(r_B)$$

$V_{A,B}(r_{A,B})$ **are the electron interactions with the target and projectile**

The atomic orbital states $\phi_{nlm}(\vec{r})$ can be obtained as

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

$$\chi_{klm}(\vec{r}) = N_l(\xi_k) r^l e^{-\xi_k r} Y_{lm}(\hat{r}) \qquad \xi_k = \alpha\beta^k, k = 1, 2, \ldots, N$$

The total wave function of the collision system (TCAO)

$$\Psi(\vec{r}, t) = \sum_i a_i(t)\phi_i^A(\vec{r}, t) + \sum_j b_j(t)\phi_j^B(\vec{r}, t)$$

The resulting first-order coupled equations for the amplitude $a_i(t)$ and $b_j(t)$ are

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

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

The above equations can be solved under the initial conditions:

$$a_i(-\infty) = \delta_{1i}, b_j(-\infty) = 0$$

The cross sections for excitation and charge transfer are:

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

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Theoretical methods

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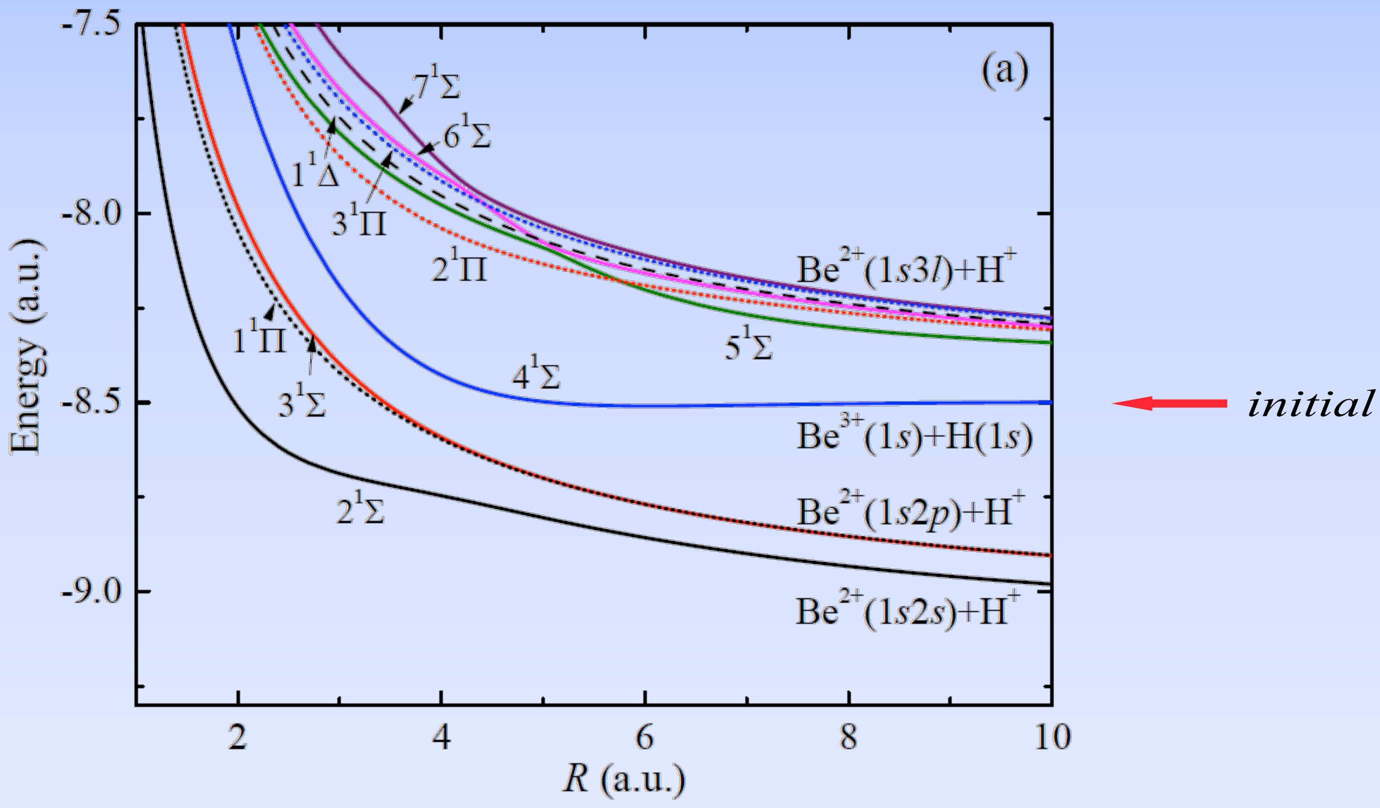
Be^{q+} + H ⬅

Summary

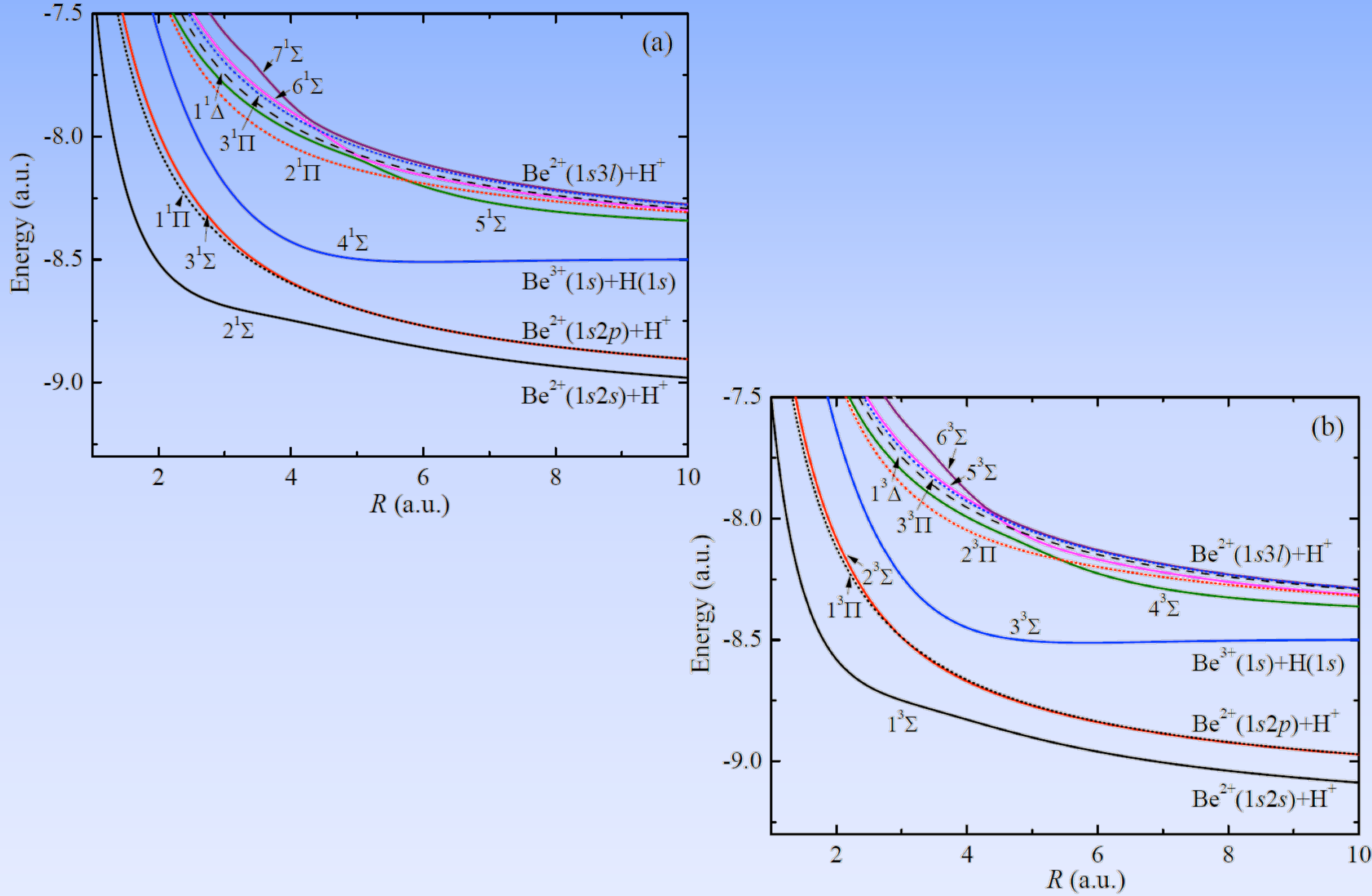
- **Charge transfer of** $Be^{3+}(1s) + H$

$$Be^{3+}(1s) + H \rightarrow Be^{2+}(1snl) + H^{+} \quad \text{non-radiative CT}$$

$$\rightarrow Be^{2+} + H^{+} + h\nu \quad \text{radiative CT}$$



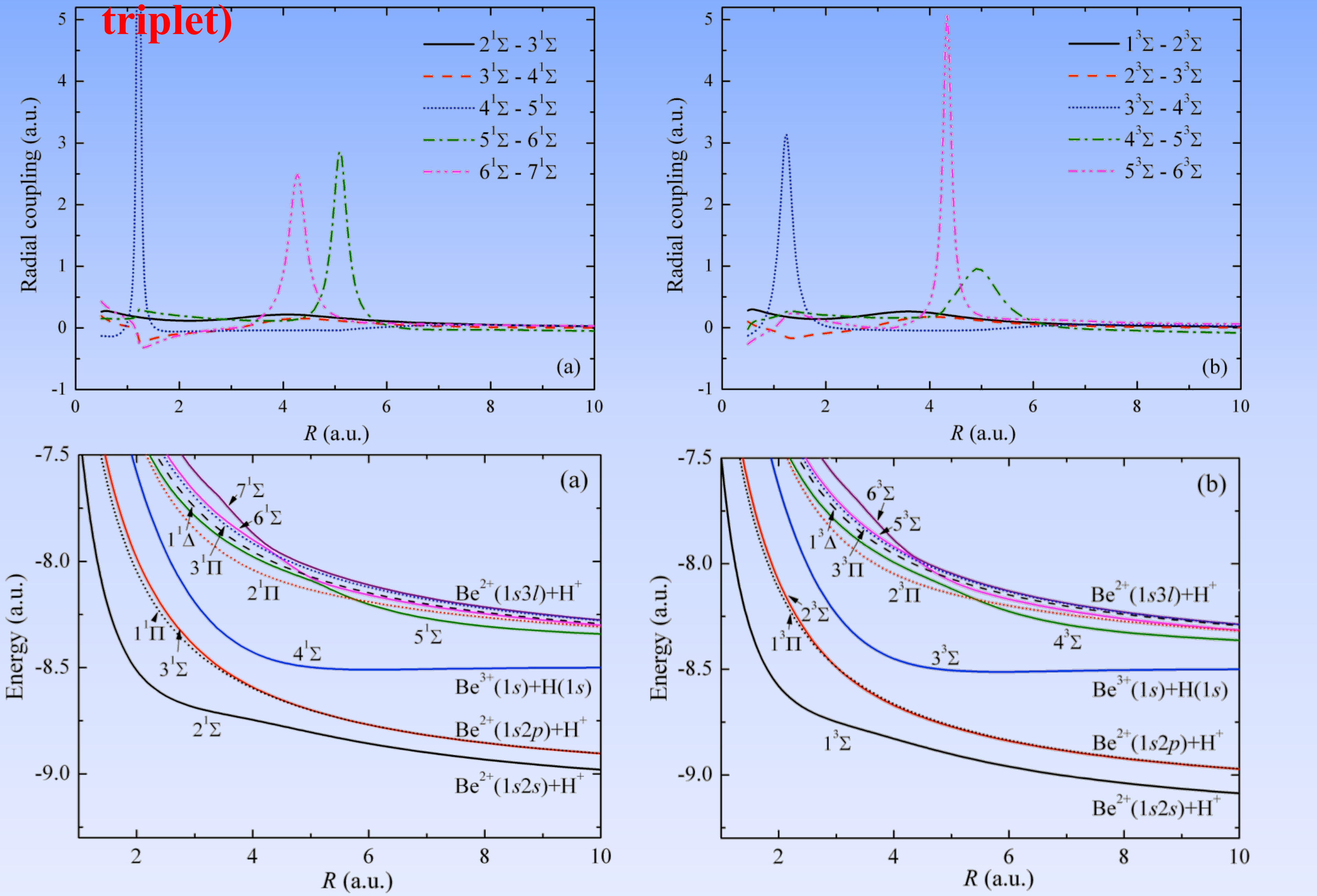
Potential curves for BeH^{3+} (singlet / triplet)



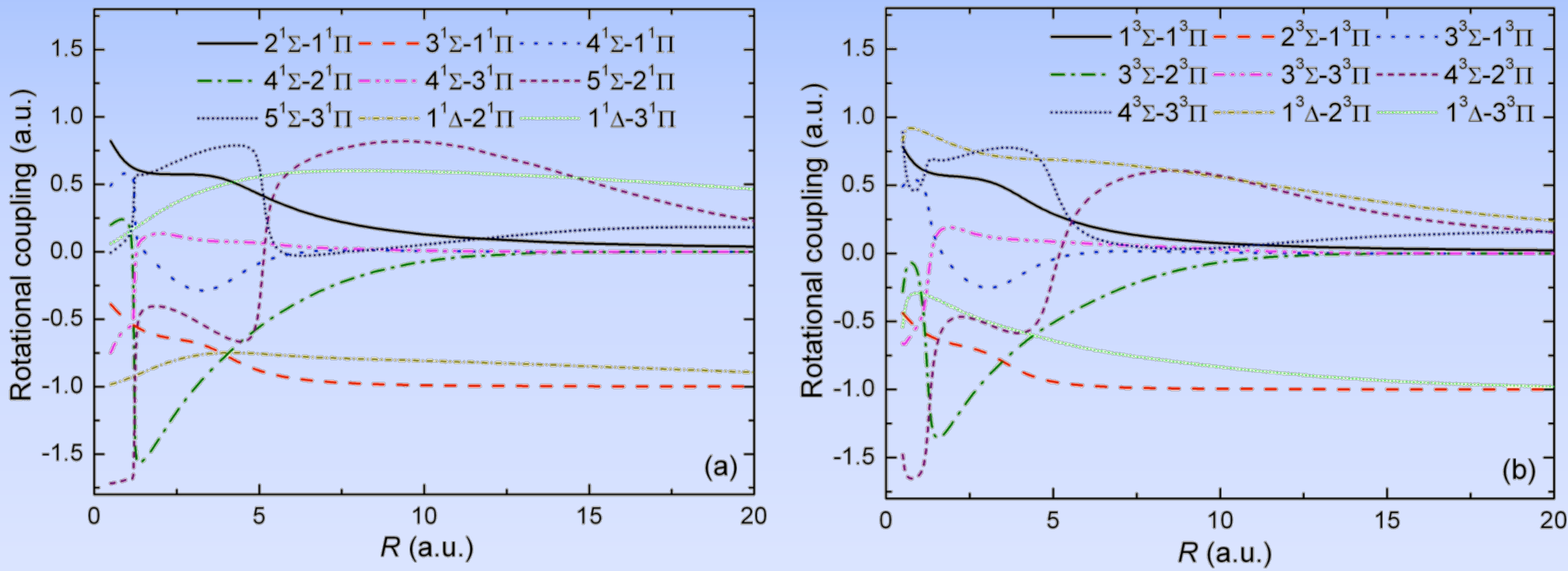
Asymptotic separated-atom energies of BeH^{3+}

Molecular state	Asymptotic atomic states	Energy (eV)		
		present	NIST	errors
$1\,^3\Sigma$	$Be^{2+}(1s2s)[^3S]+H^+$	-21.48	-21.70	0.22
$2\,^1\Sigma$	$Be^{2+}(1s2s)[^1S]+H^+$	-18.55	-18.64	0.09
$2\,^3\Sigma$, $1\,^3\Pi$	$Be^{2+}(1s2p)[^3P]+H^+$	-18.34	-18.37	0.03
$3\,^1\Sigma$, $1\,^1\Pi$	$Be^{2+}(1s2p)[^1P]+H^+$	-16.52	-16.63	0.11
$4\,^1\Sigma$, $3\,^3\Sigma$	$Be^{3+}(1s)+H(1s)$	0	0	0
$4\,^3\Sigma$	$Be^{2+}(1s3s)[^3S]+H^+$	-1.219	-1.285	0.066
$5\,^1\Sigma$	$Be^{2+}(1s3s)[^1S]+H^+$	-0.450	-0.484	0.034
$5\,^3\Sigma$, $2\,^3\Pi$	$Be^{2+}(1s3p)[^3P]+H^+$	-0.379	-0.403	0.024
$6\,^3\Sigma$, $3\,^3\Pi$, $1\,^3\Delta$	$Be^{2+}(1s3d)[^3D]+H^+$	0.028	-0.020	0.048
$6\,^1\Sigma$, $2\,^1\Pi$, $1\,^1\Delta$	$Be^{2+}(1s3d)[^1D]+H^+$	0.036	-0.018	0.054
$7\,^1\Sigma$, $3\,^1\Pi$	$Be^{2+}(1s3p)[^1P]+H^+$	0.161	0.097	0.064

Radial coupling matrix elements (singlet / triplet)

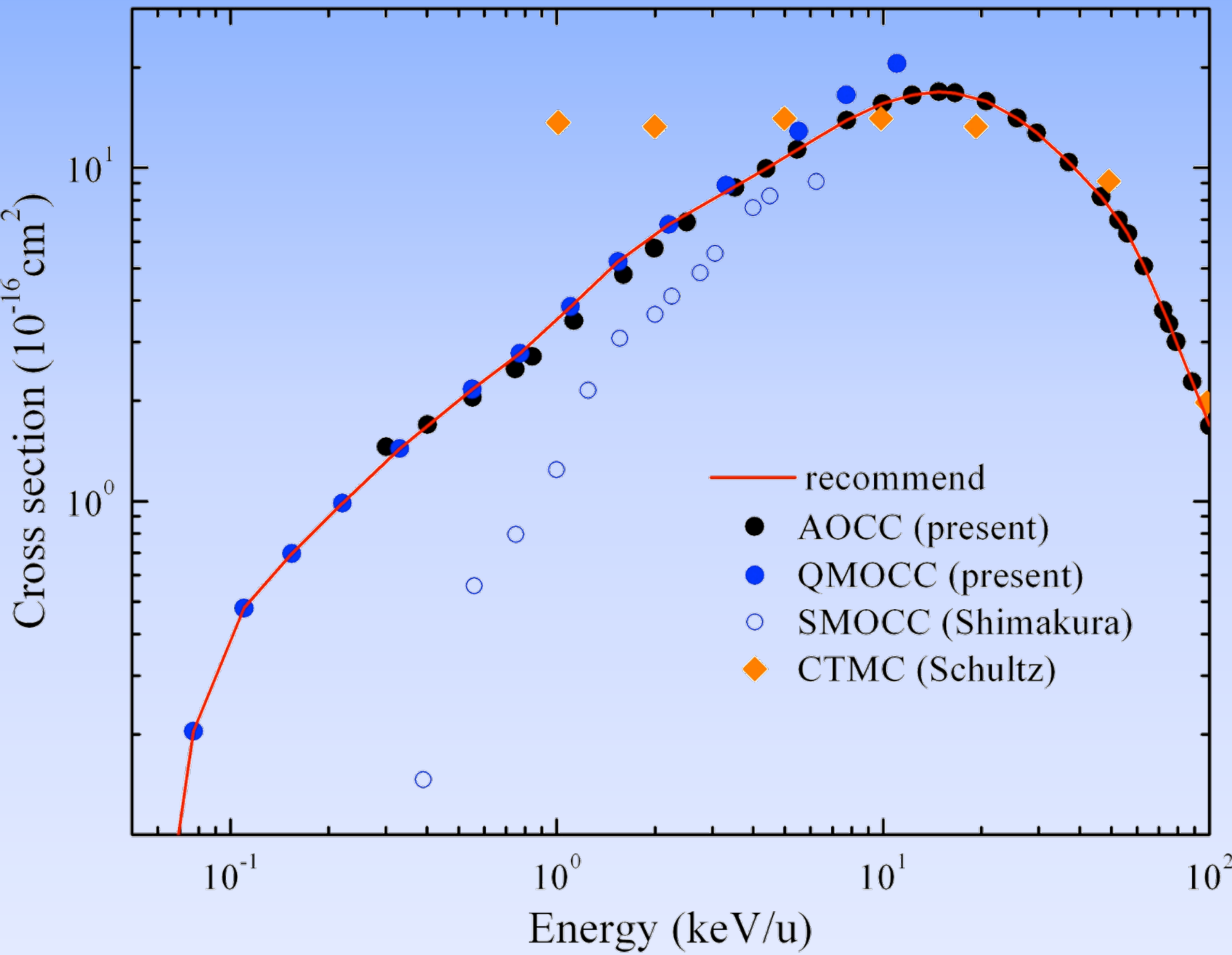


Rotational coupling matrix elements (singlet / triplet)



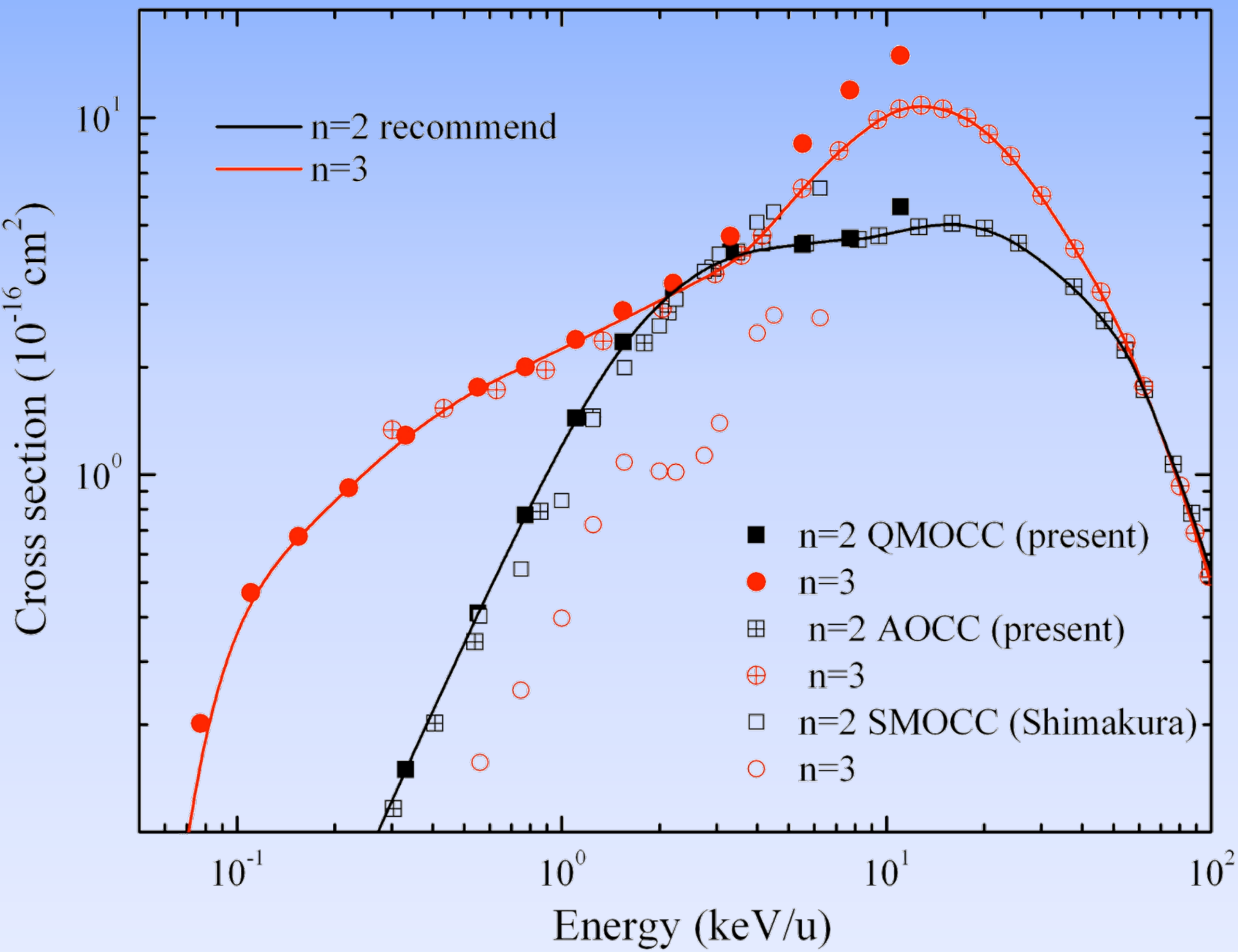
Total CT cross section

$Be^{3+} + H \rightarrow Be^{2+} + H^{+}$



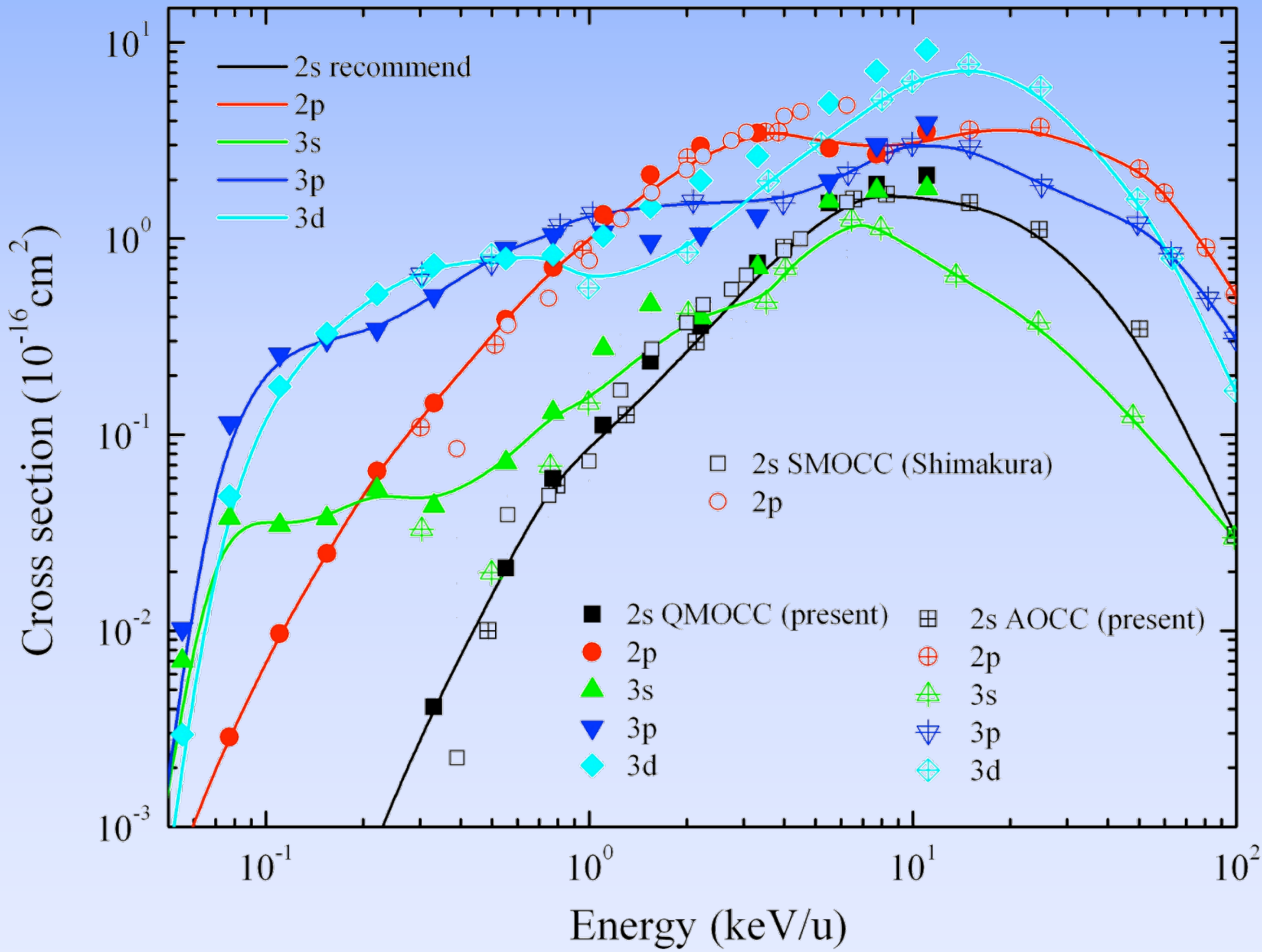
n state-selective cross sections

$Be^{3+} + H \rightarrow Be^{2+}(nl) + H^{+}$



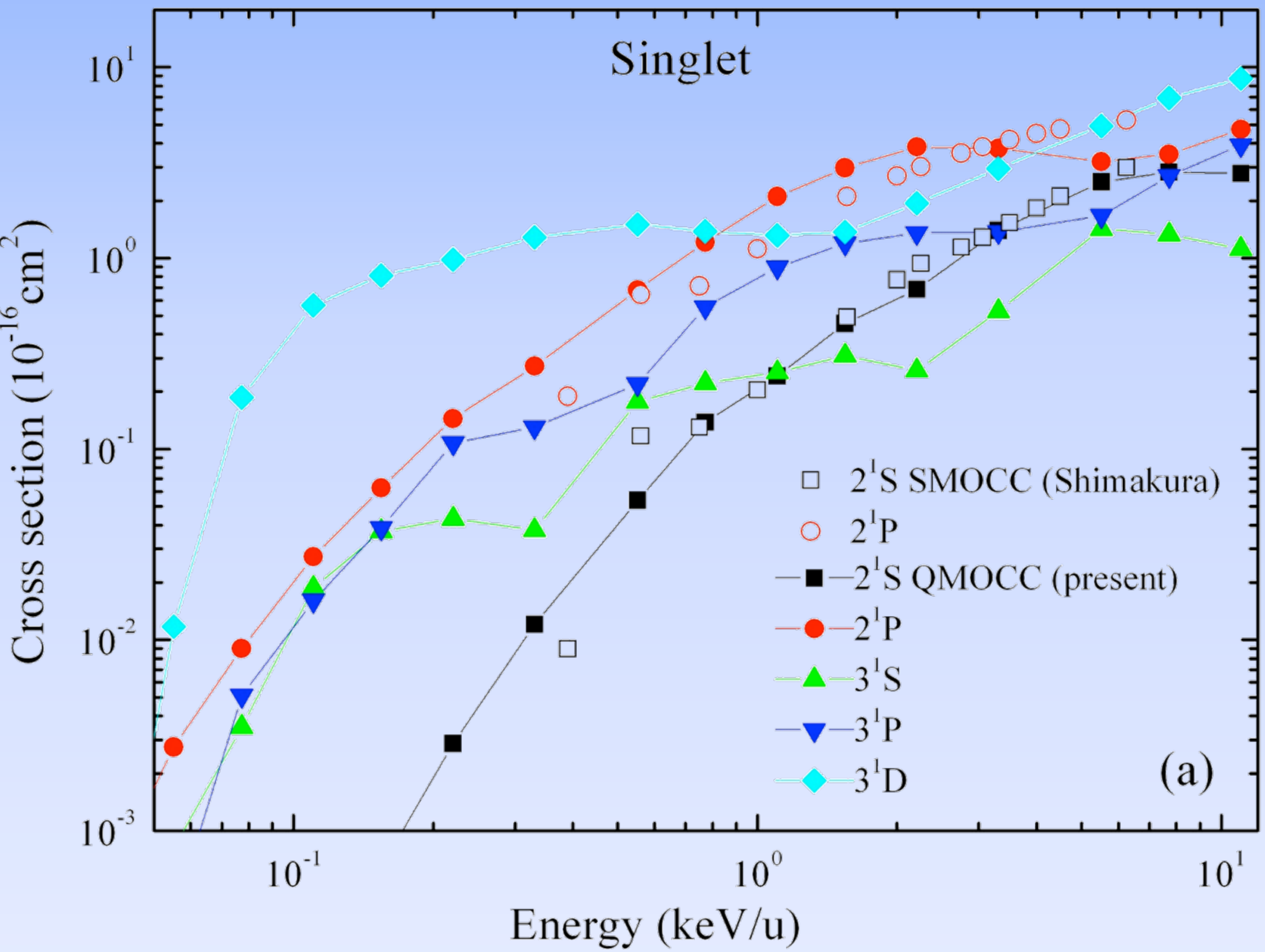
nl state-selective cross sections

$Be^{3+} + H \rightarrow Be^{2+}(1snl) + H^{+}$



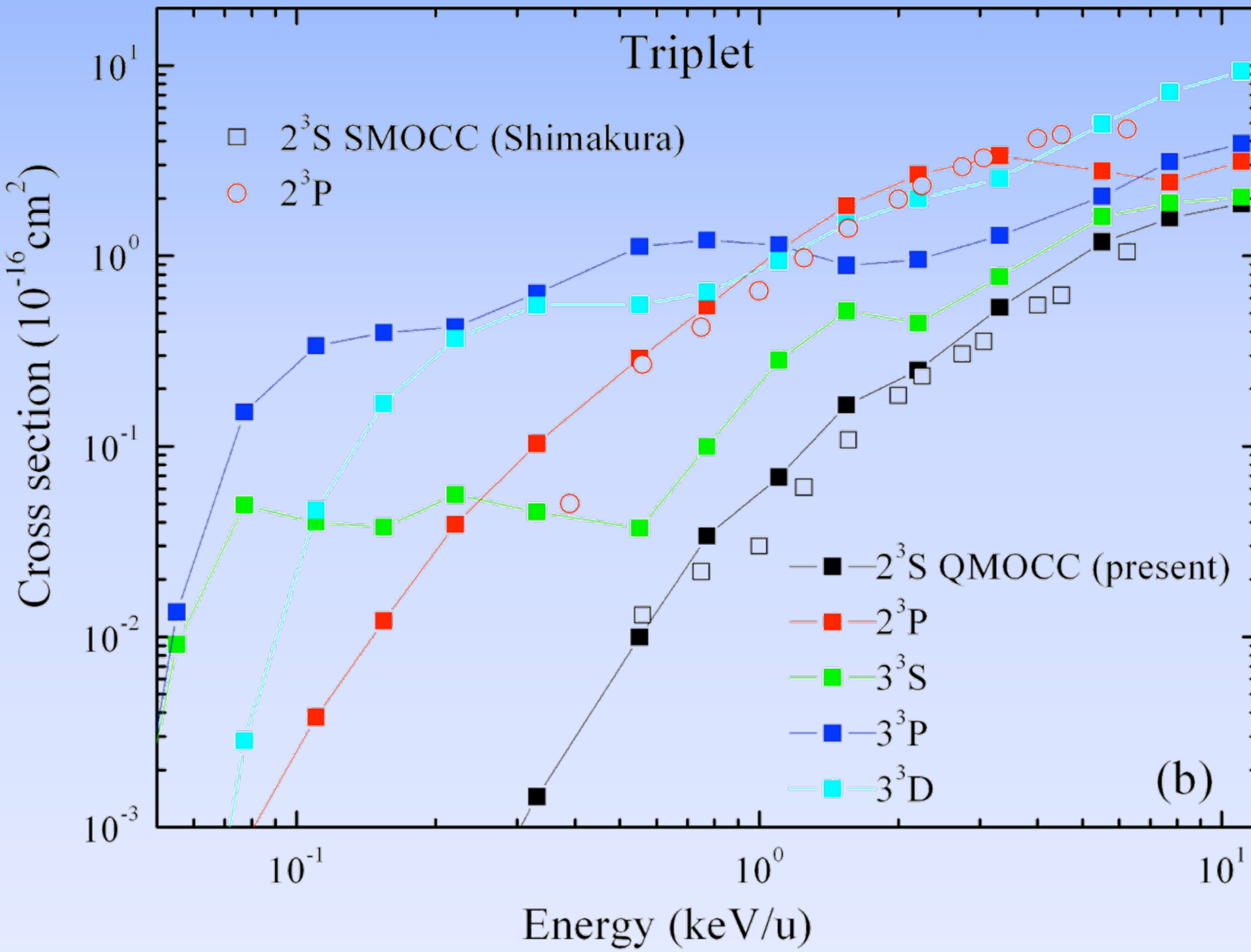
nl state-selective cross sections (singlet)

$$Be^{3+} + H \rightarrow Be^{2+}(1snl) + H^{+}$$



nl state-selective cross sections (triplet)

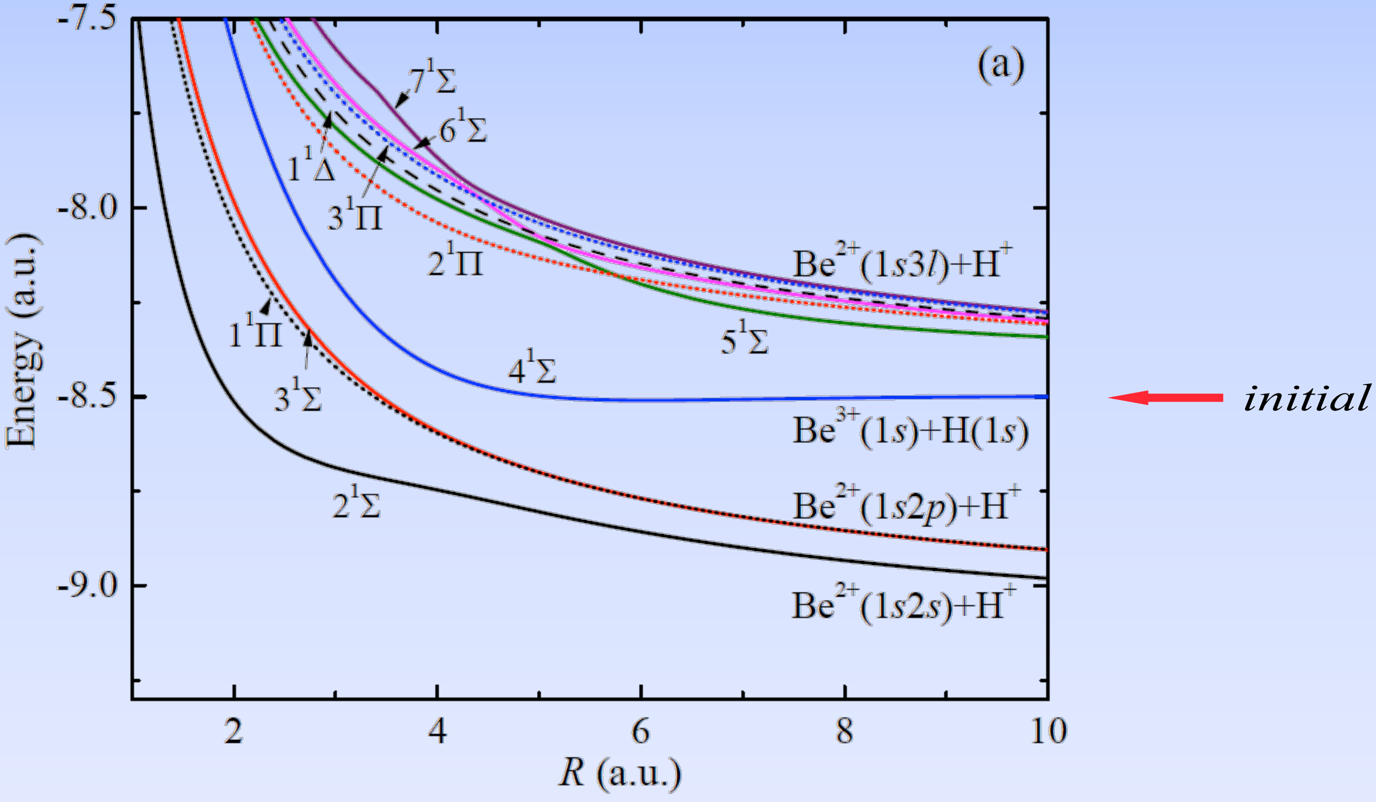
$$Be^{3+} + H \rightarrow Be^{2+}(1snl) + H^{+}$$



- **Charge transfer of** $Be^{3+}(1s) + H$

$$Be^{3+}(1s) + H \rightarrow Be^{2+}(1snl) + H^{+} \qquad \text{non-radiative CT}$$

$$\rightarrow Be^{2+} + H^{+} + h\nu \qquad \text{radiative CT}$$



Quantumal approach for radiative CT

Total cross section $$\sigma = \int_{\omega_{\min}}^{\omega_{\max}} \frac{d\sigma}{d\omega} d\omega$$

where $$\frac{d\sigma}{d\omega} = \frac{8}{3}\left(\frac{\pi}{k_A}\right)^2 \frac{\omega^3}{c^3} \sum_J \left[J M_{J,J-1}^2(k_A, k_X) + (J+1)\ M_{J,J+1}^2(k_A, k_X) \right]$$

$$M_{J,J'}(k_A, k_X) = \int_0^\infty dR f_J^A(k_A R) D(R) f_{J'}^X(k_X R)$$

$$\left\{ \frac{d^2}{dR^2} - \frac{J(J+1)}{R^2} - 2\mu\left[V_i(R) - V_i(\infty)\right] + k_i^2 \right\} f_J^i(k_i R) = 0$$

$$k_A = \sqrt{2\mu\left[E - V_A(\infty)\right]}$$

$$k_X = \sqrt{2\mu\left[E - V_X(\infty) - \hbar\omega\right]}$$

B. Zygelman, and A. Dalgarno, Phys. Rev. A 38, 1877 (1988)

Theoretical methods for radiative decay

Semiclassical method (relatively high energy region)

$$\sigma(E) = 2\pi\sqrt{\frac{2\mu}{E}}\int p\,dp\int_{R_A^{\mathrm{ctp}}}^{\infty} dR\,\frac{A(R)}{\sqrt{1 - V_A(R)/E - p^2/R^2}}$$

Optical potential method

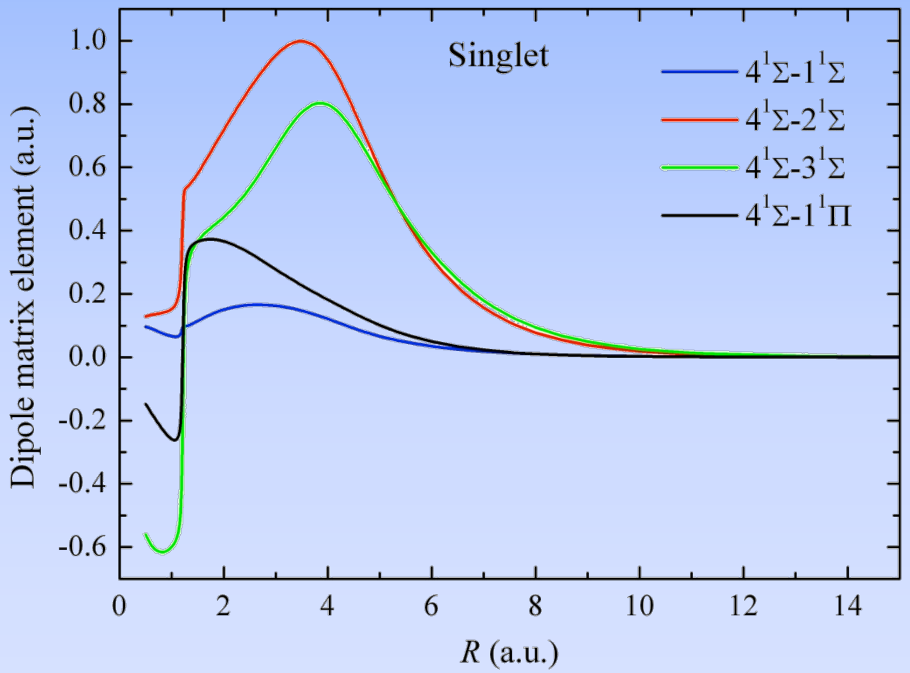
$$\left[-\frac{1}{2\mu}\nabla_{\vec{R}}^2 + V_A(R) - E\right]F_A(\vec{R}) = \frac{i}{2}A(R)F_A(\vec{R})$$

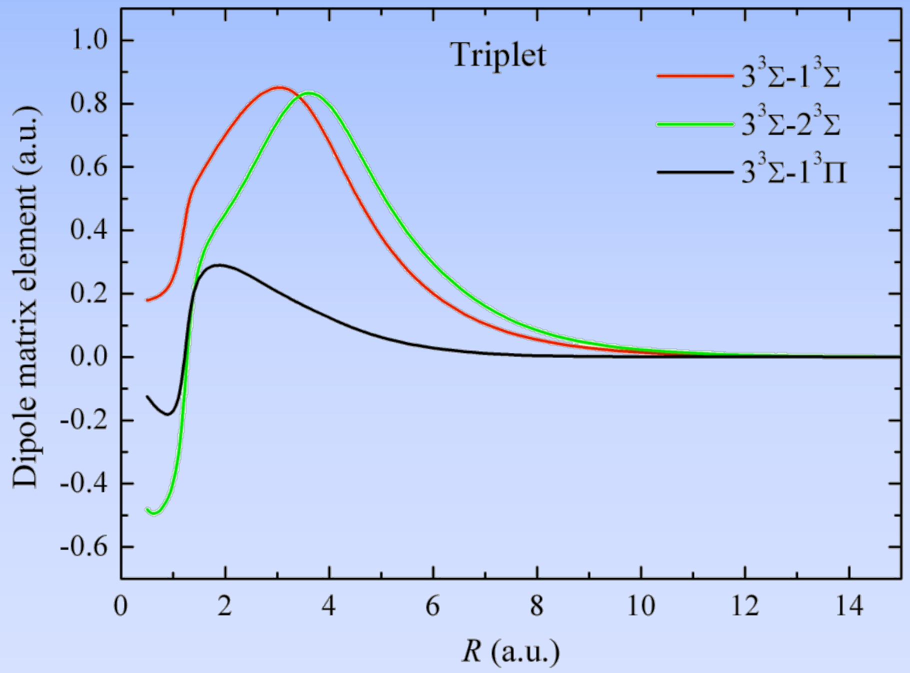
where Einstein coefficients $A(R) = \frac{4}{3}D^2(R)\frac{|V_A(R) - V_X(R)|^3}{c^3}$

$$\sigma(E) = \frac{\pi}{k_A^2}\sum_J^{\infty}(2J+1)[1 - \exp(-4\eta_J)]$$

B. Zygelman, and A. Dalgarno, Phys. Rev. A 38, 1877 (1988)

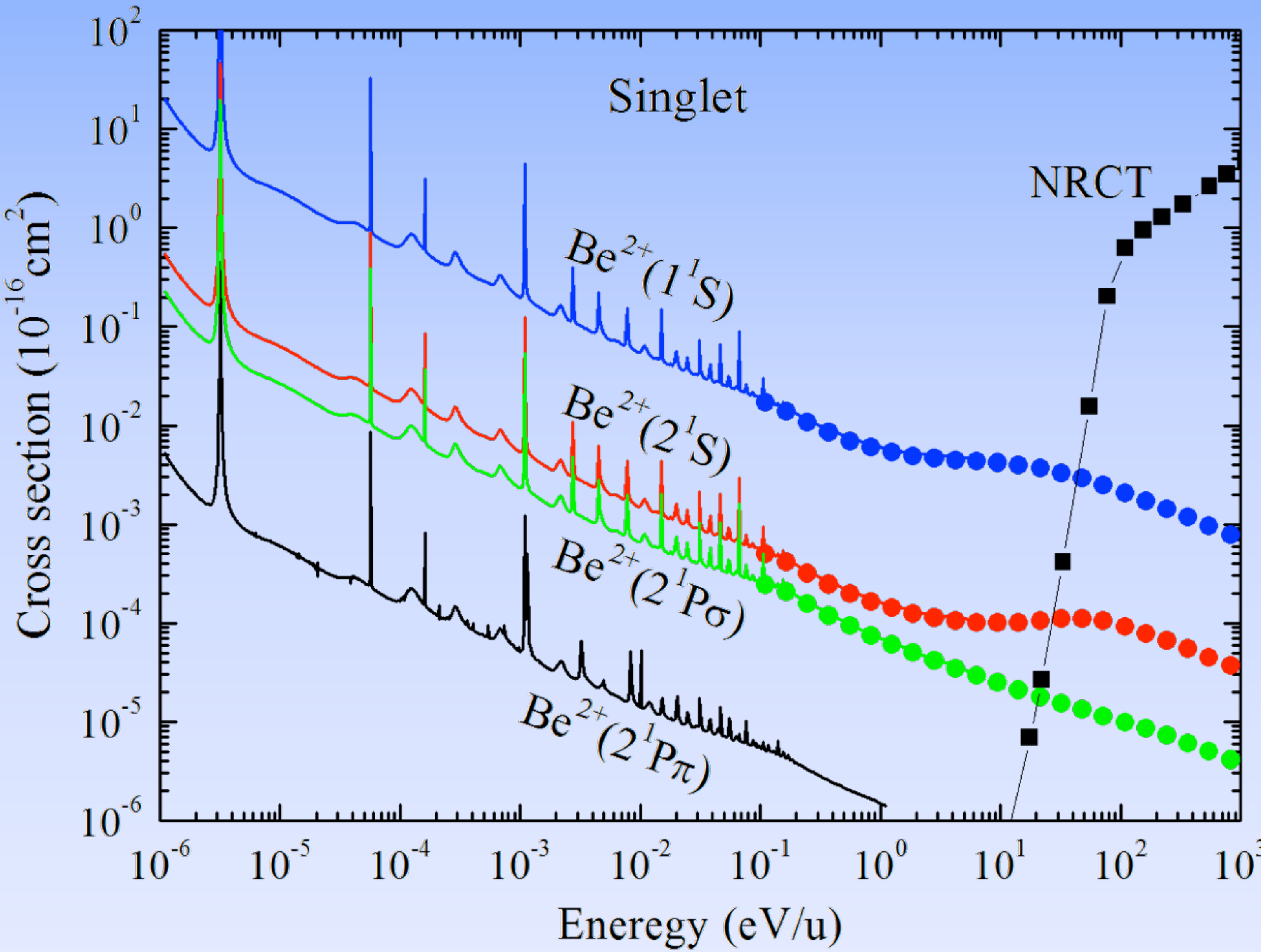
Dipole transition matrix elements





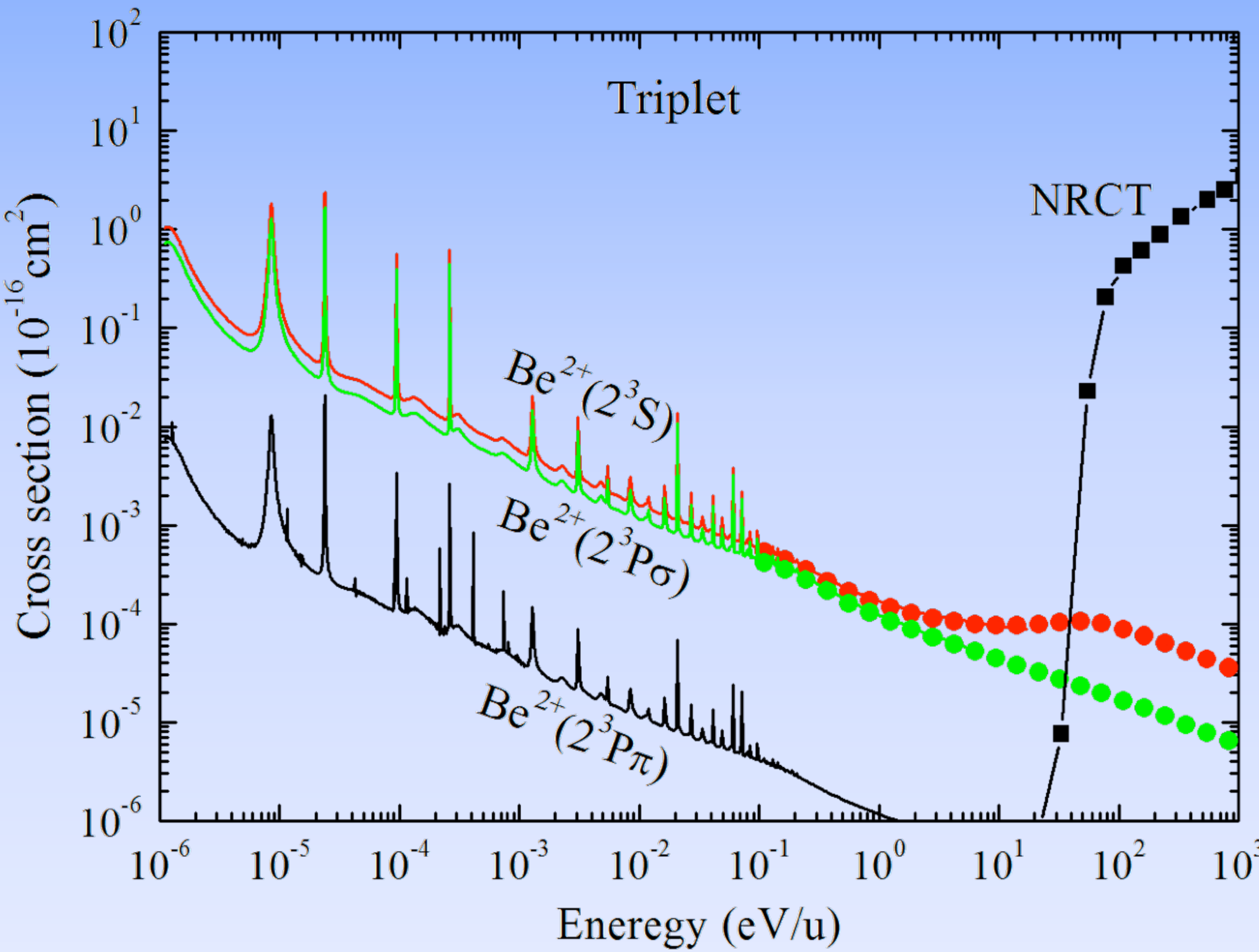
Radiative charge transfer – Singlet states

$Be^{3+} + H \rightarrow Be^{2+} + H^{+} + h\nu$

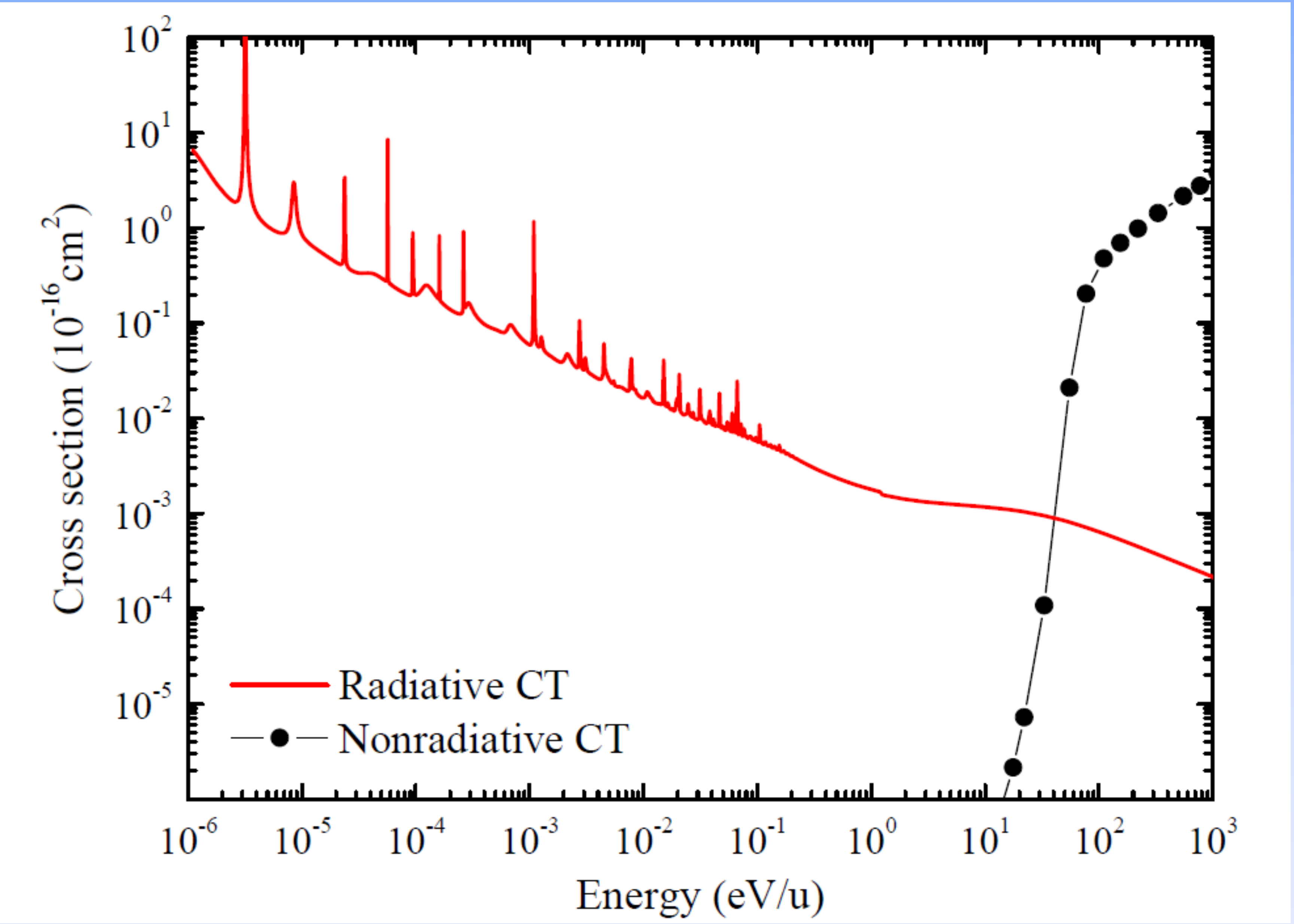


Radiative charge transfer – Triplet states

$Be^{3+} + H \rightarrow Be^{2+} + H^{+} + h\nu$



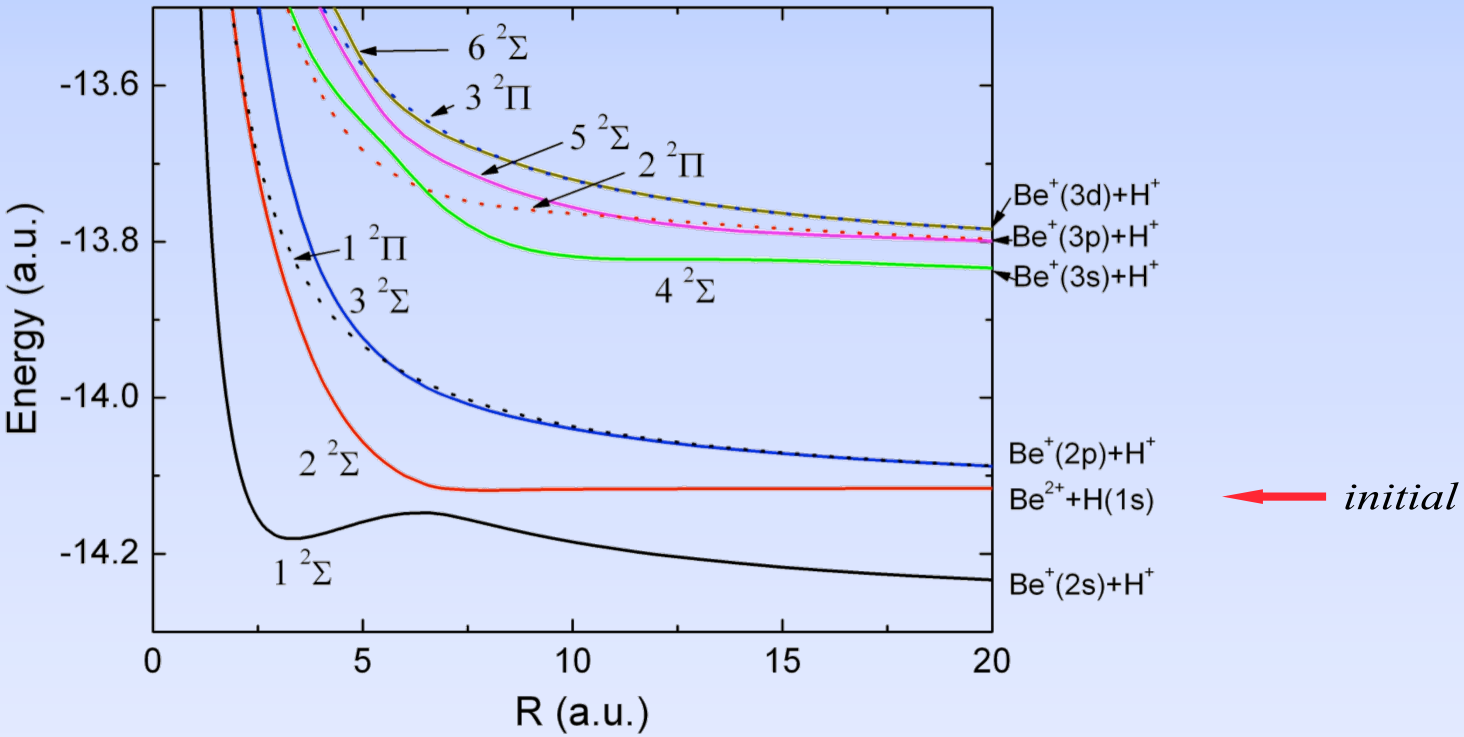
Total radiative charge transfer cross sections



$Be^{2+}(1s^2) + H$

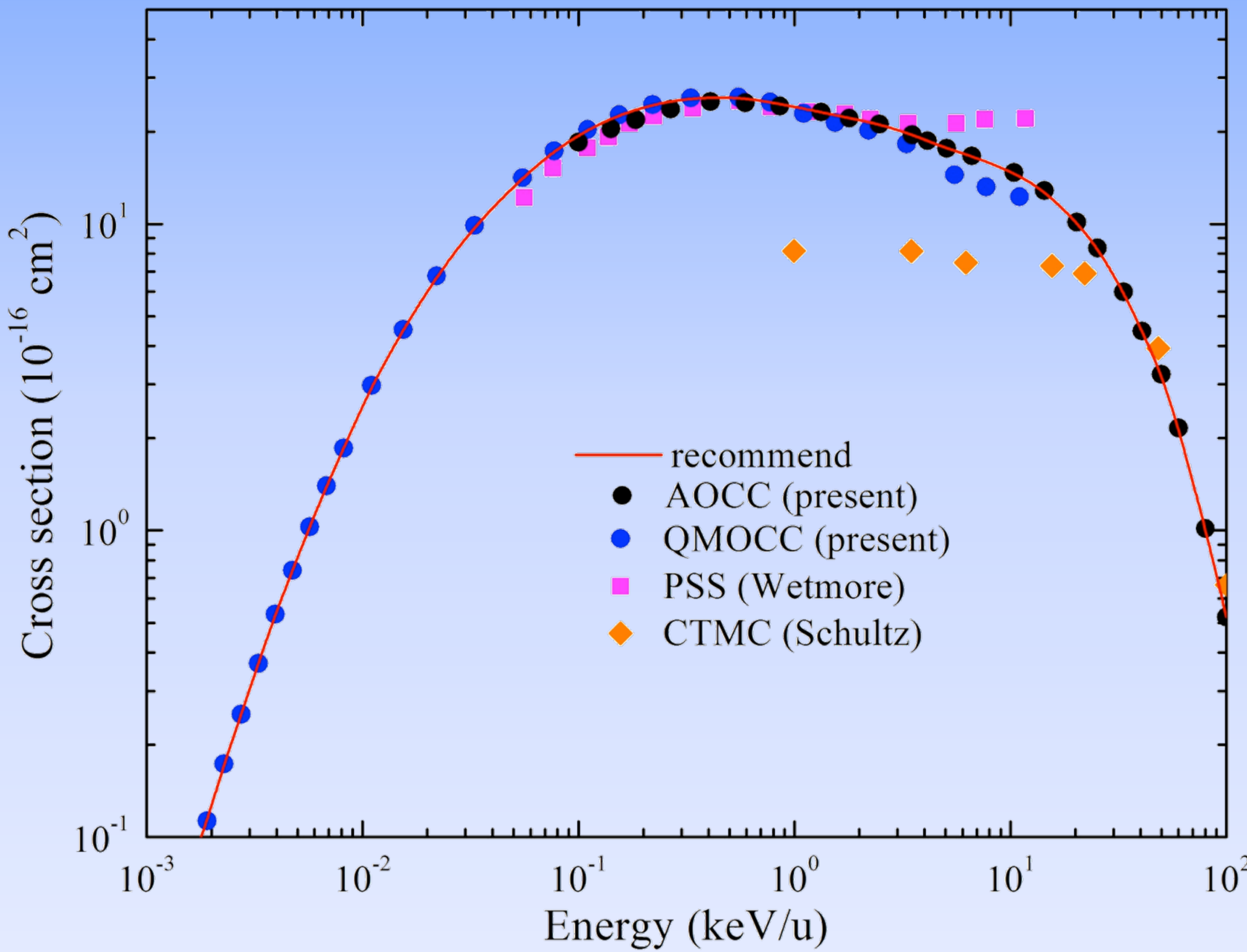
$Be^{2+} + H \rightarrow Be^{+}(1s^2 nl) + H^{+}$ non-radiative CT

$\rightarrow Be^{+}(1s^2 2s) + H^{+} + h\nu$ radiative CT

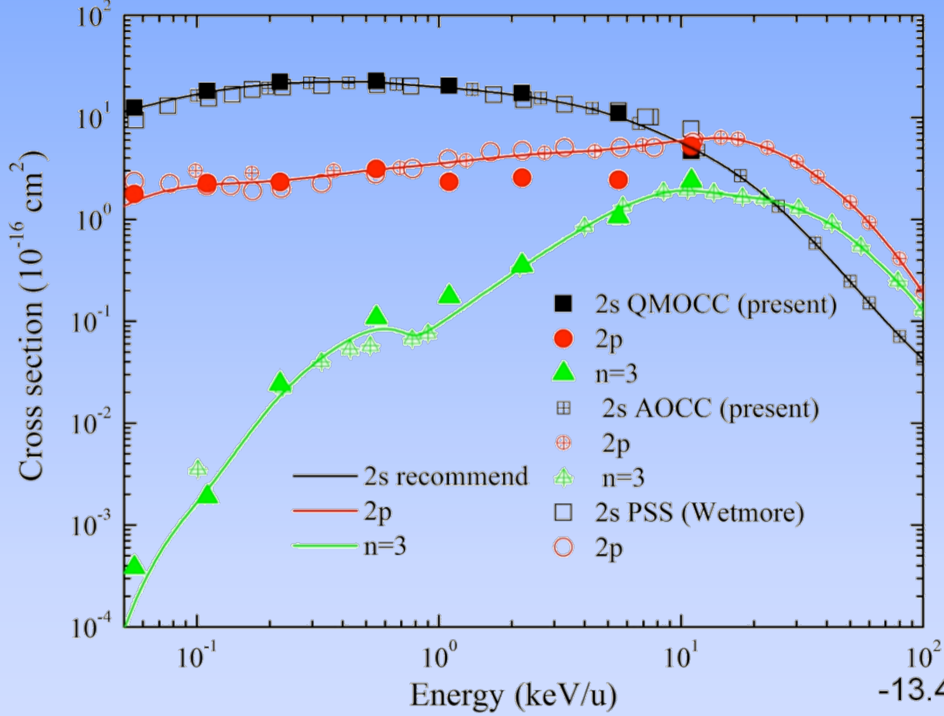


Total CT cross section

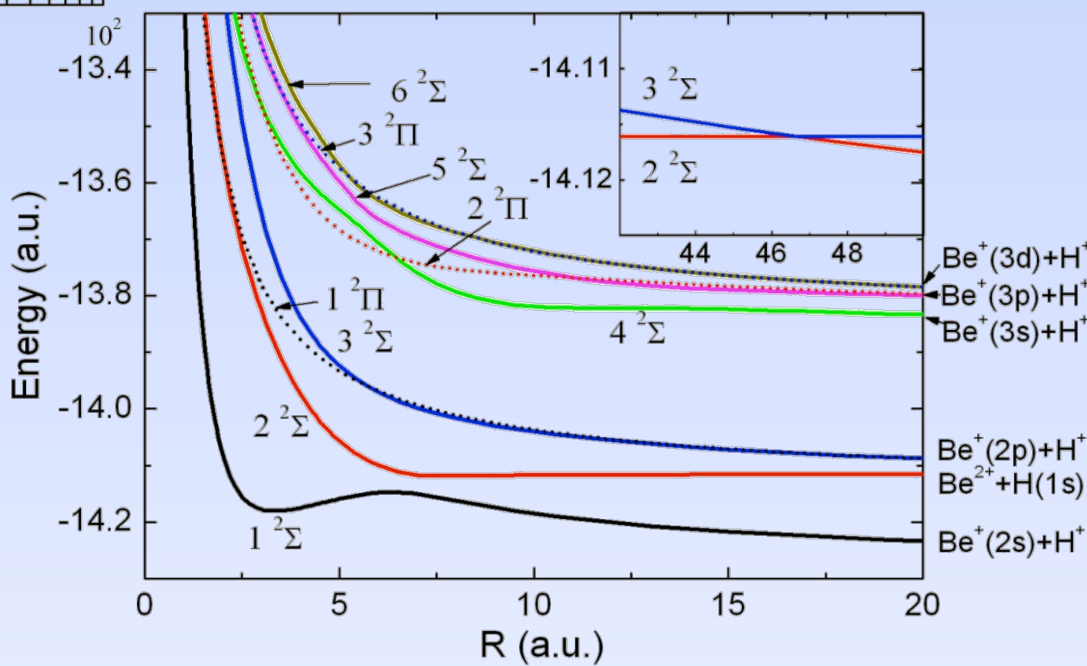
$Be^{2+} + H \rightarrow Be^{+} + H^{+}$

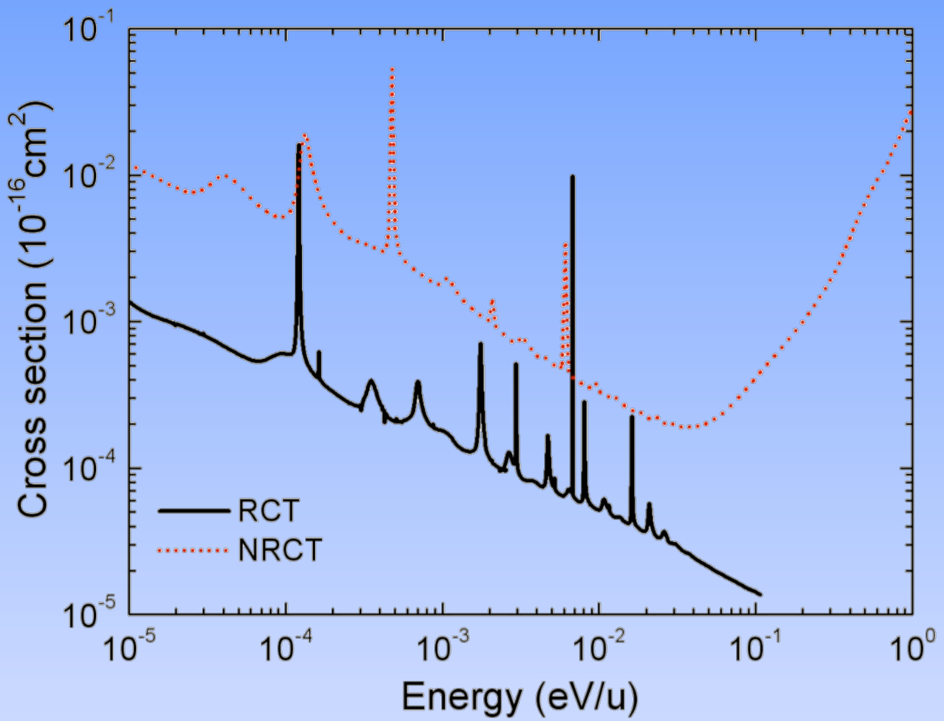


State-selective cross sections

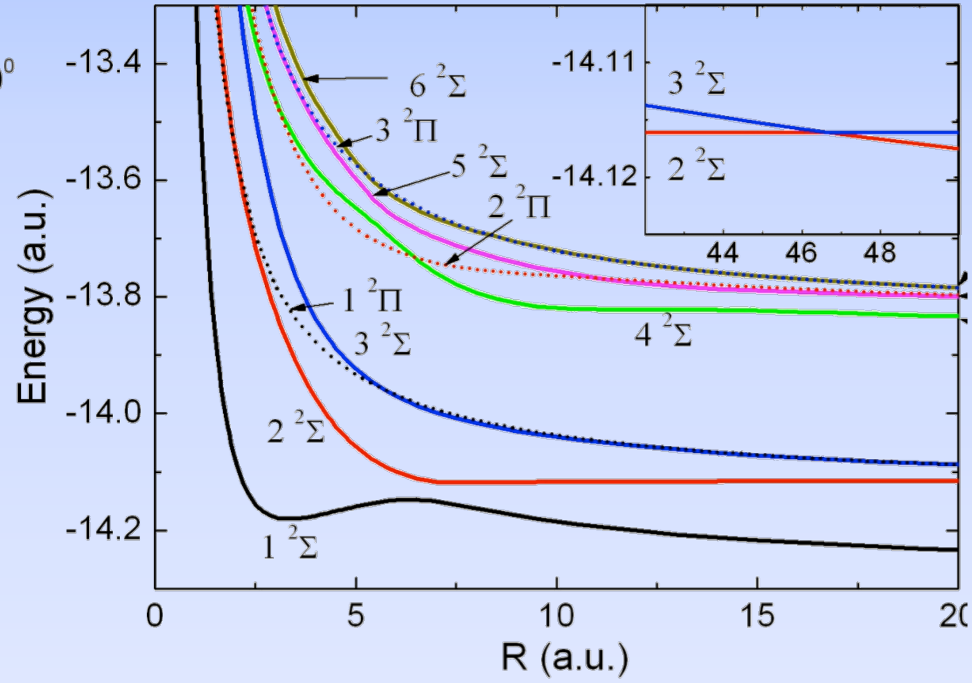


$$Be^{2+} + H \rightarrow Be^{+}(2s) + H^{+}$$
$$\rightarrow Be^{+}(2p) + H^{+}$$
$$\rightarrow Be^{+}(n=3) + H^{+}$$



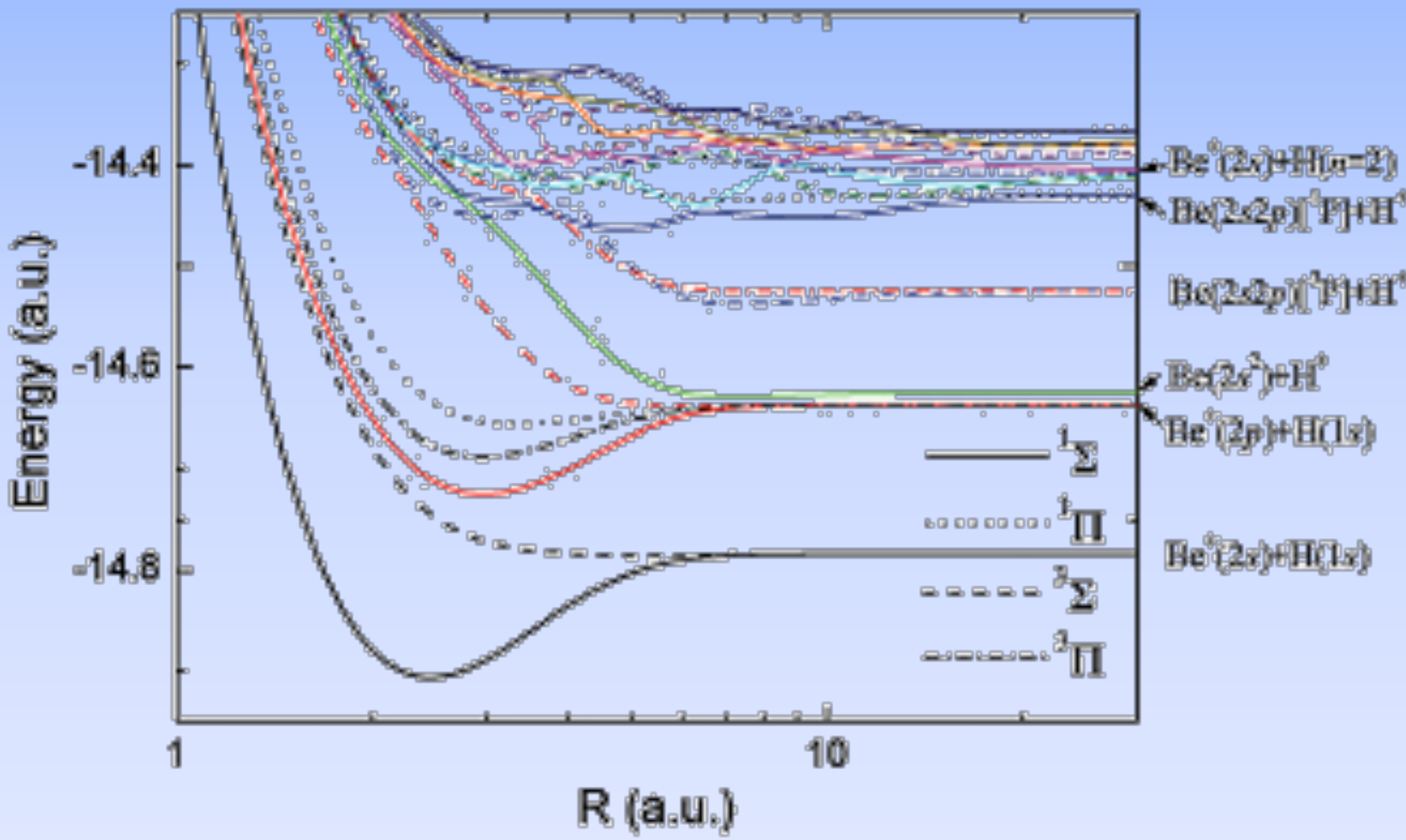


$Be^{2+} + H \rightarrow Be^{+} + H^{+} + h\nu$



C H Liu, LLiu, Y. Z. Qu et al., Phys. Rev. A 82, 022710 (2010).

$Be^{+}(2s) + H \rightarrow Be + H^{+}$

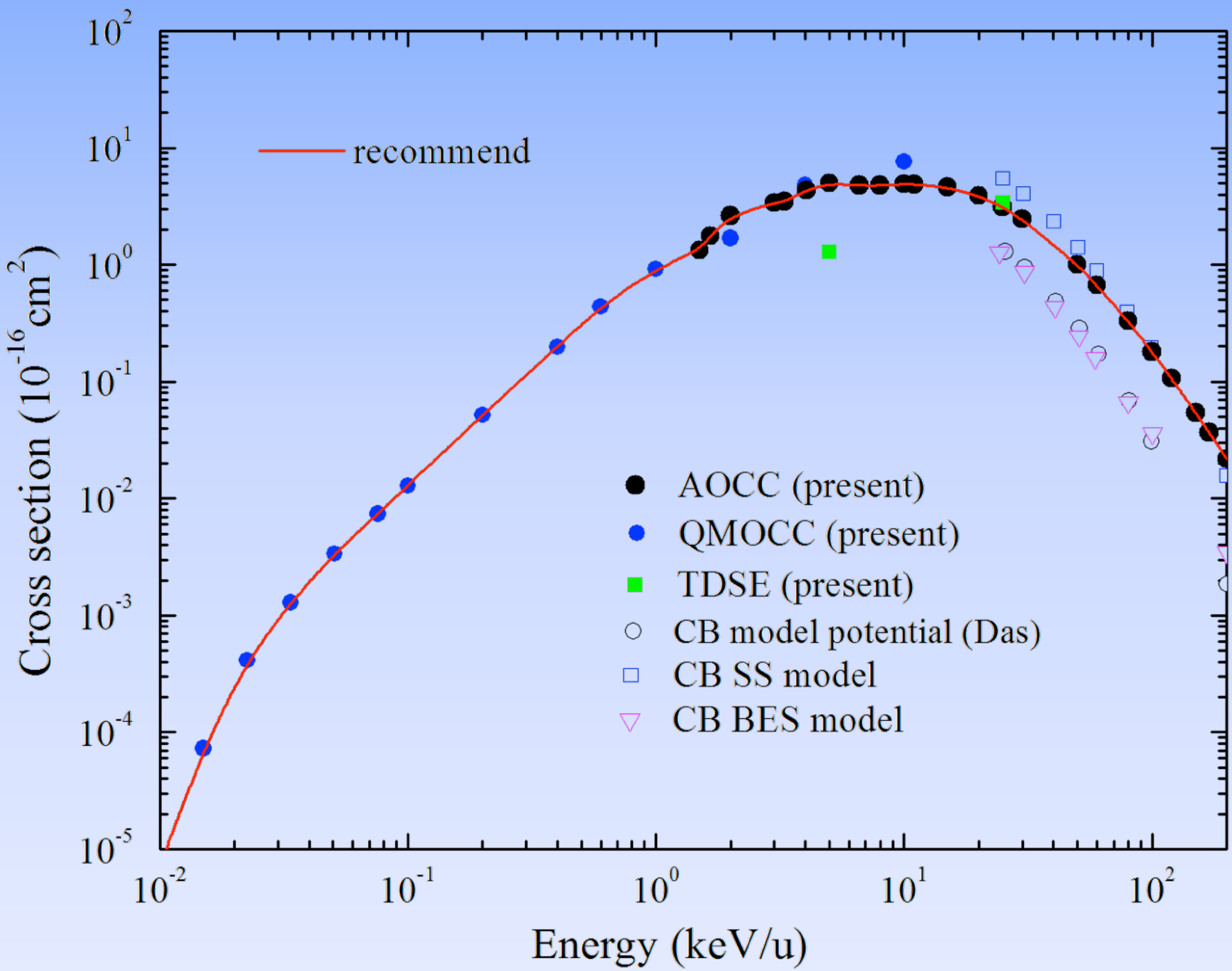


initial

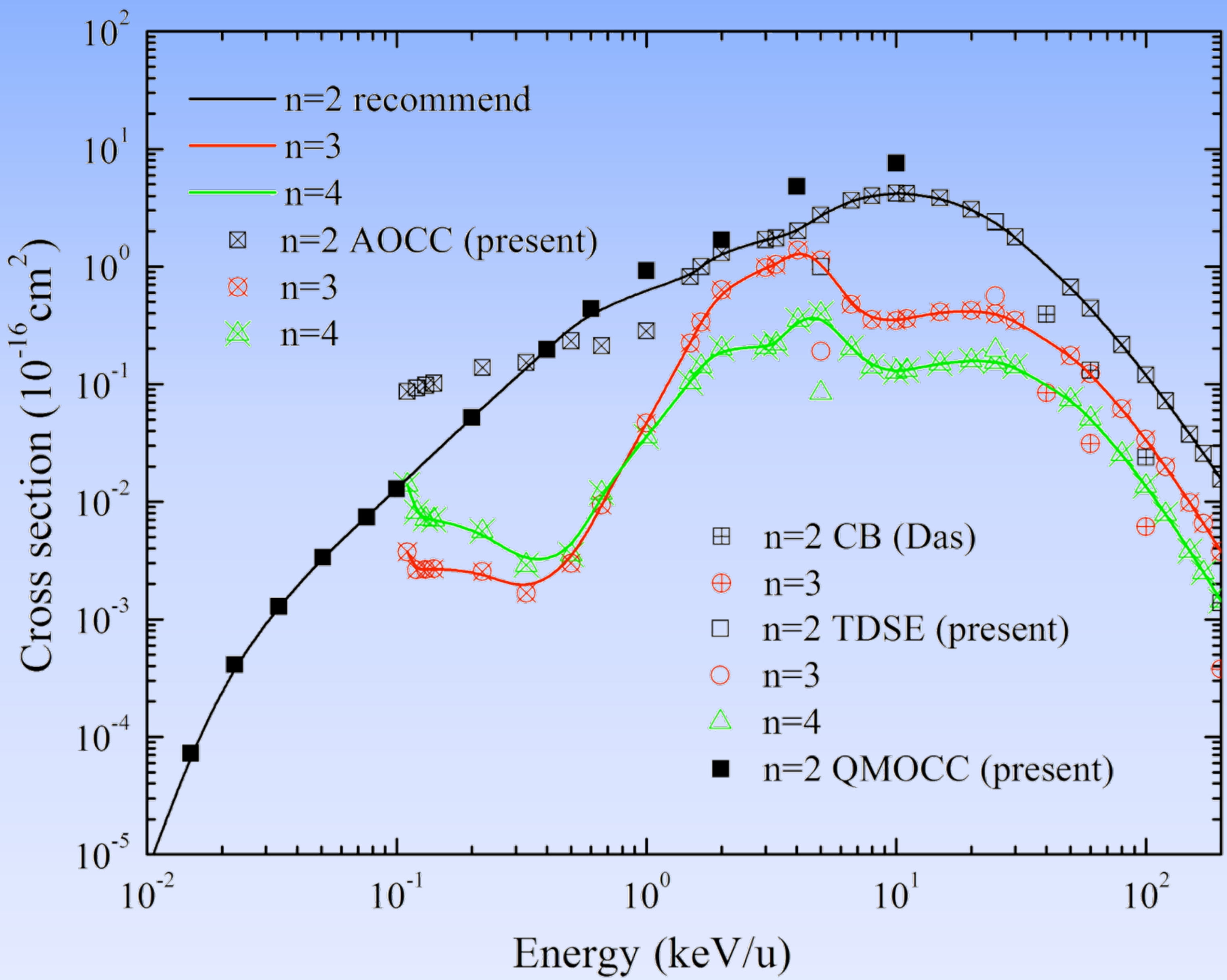
C H Liu, J G Wang et al., J Phys. B 43, 144006 (2010).

Total CT cross section

$Be^{+} + H \rightarrow Be + H^{+}$

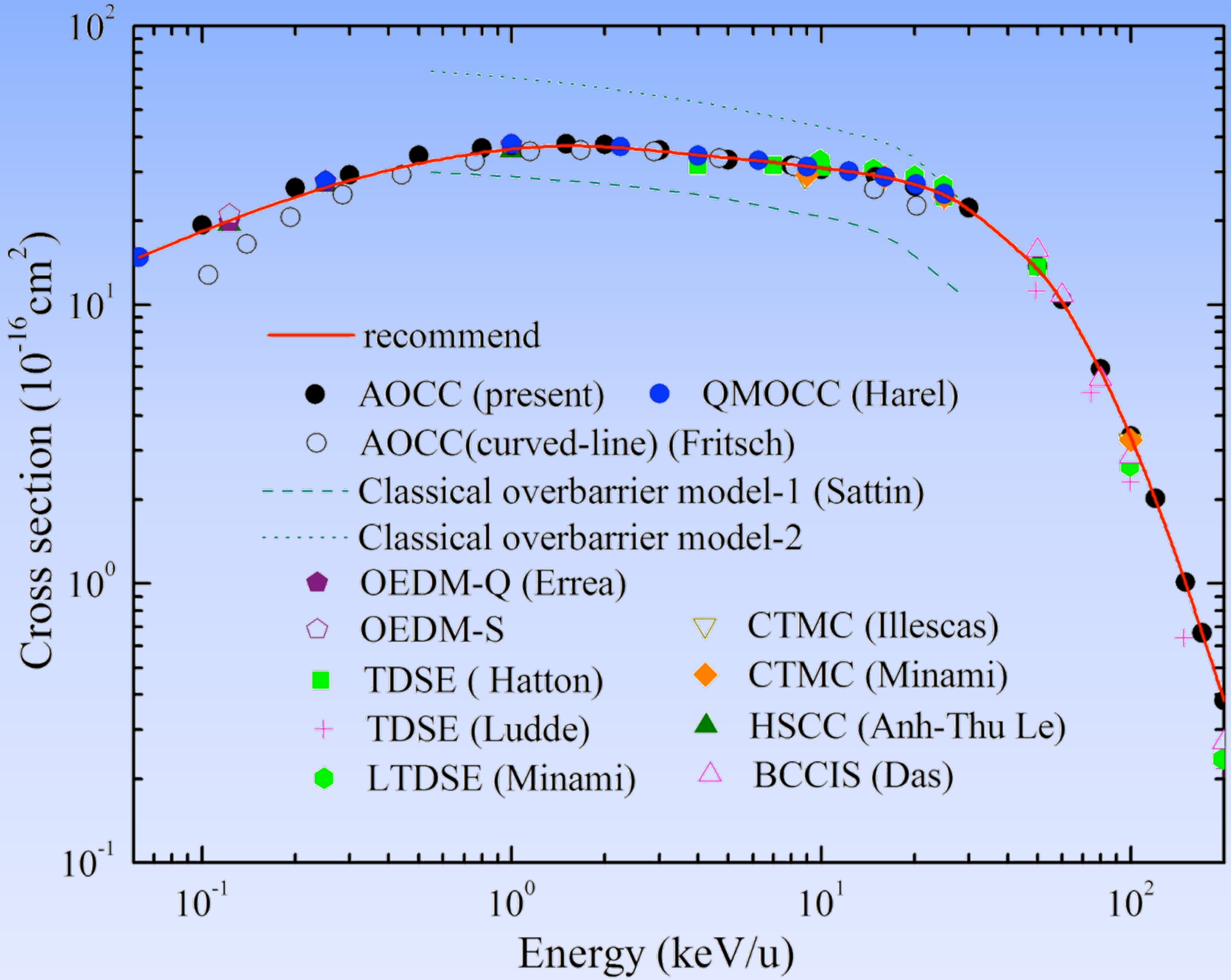


n state-selective cross sections

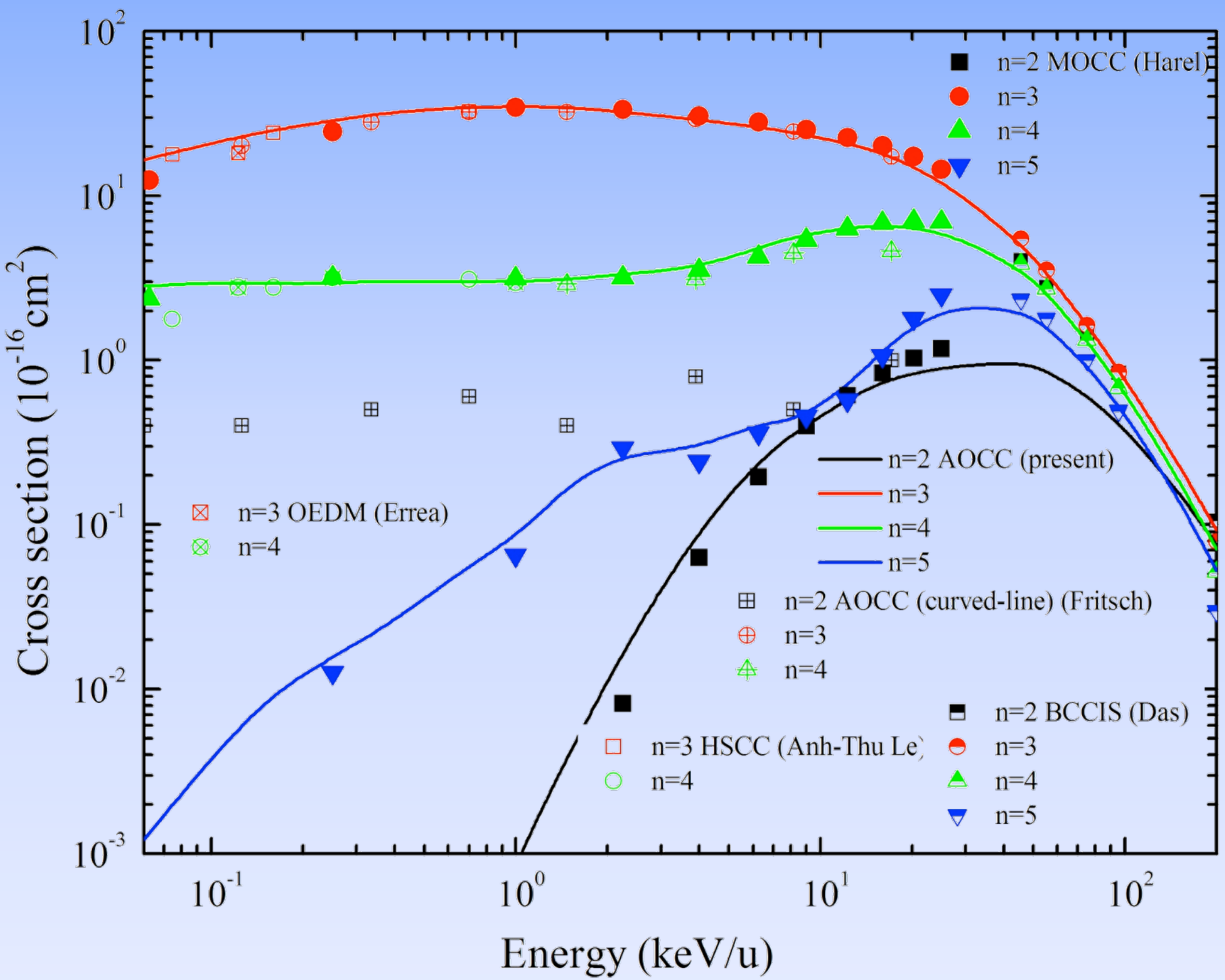


Total CT cross section

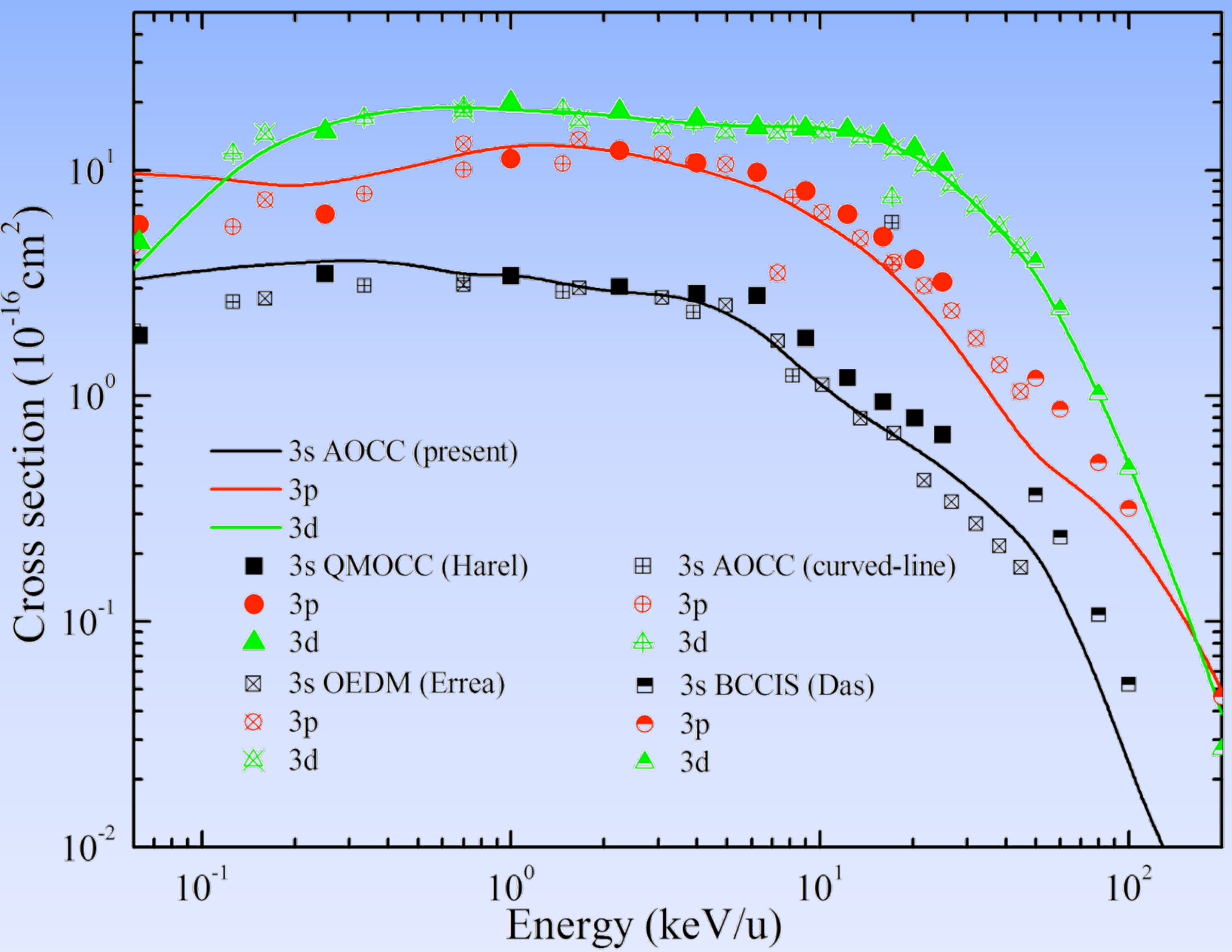
$Be^{4+} + H \rightarrow Be^{3+} + H^{+}$



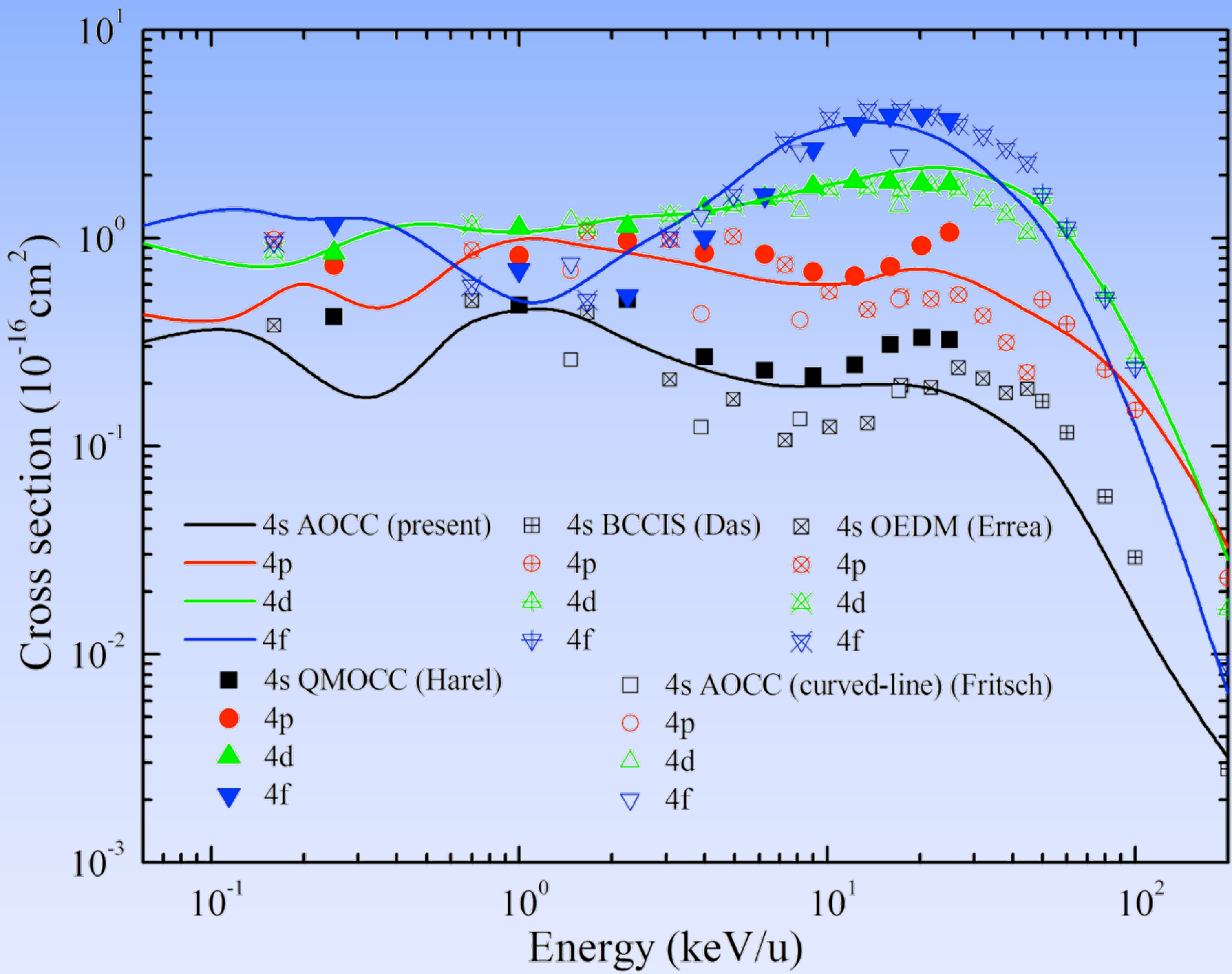
n state-selective cross sections



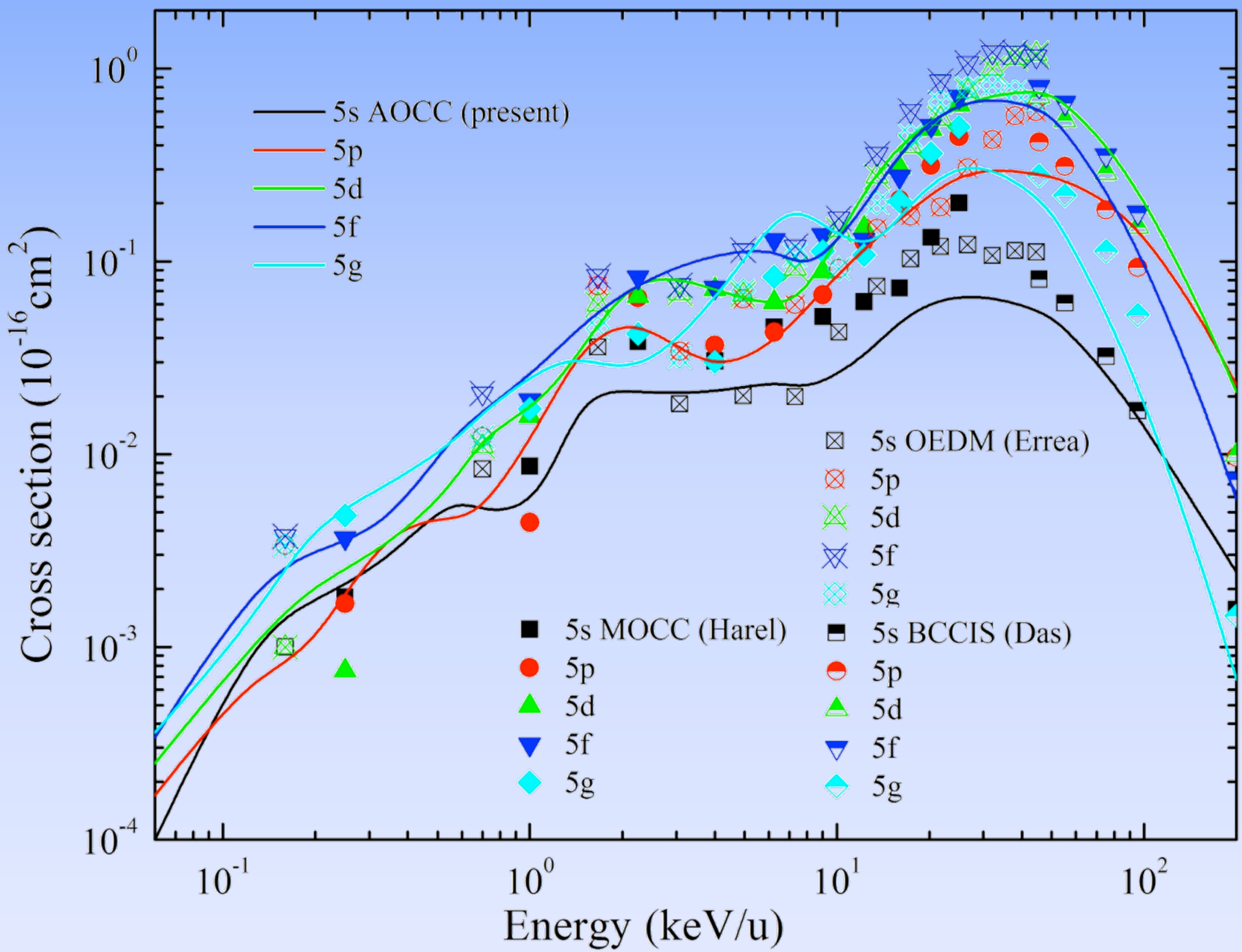
nl state-selective cross sections



nl state-selective cross sections



nl state-selective cross sections



Summary

- **Theoretical methods**

  QMOCC / AOCC /

  TDSE / CTMC/ TDDFT …

- **Be^{q+} + H (q = 1, …, 4)**
- **wide energy range, NRCT, RCT**
- **total, n, nl, spin-resolved recommended cross section**
- **experimental cooperation**

Thanks to the NSFC, CAS

Thank you!