Beryllium ion collisions and free-free transition in H plasma

L. Liu[1], S. B. Zhang[2], C.H.Liu[3], Y. Wu[1], J.G.Wang[1] and R.K.Janve[4]

[1] Institute of Applied Physics and Computational Mathematics, Beijing, China

[2] Shaanxi Normal University, Xi'an, China

[3] Southeast University, Nanjing, China

[4] Macedonian Academy of Sciences and Arts, Skopje, Macedonia

The IAEA 1th RCM on Vapour Shielding, Vienna, 2019.03.13

Part 1
Beryllium ion collisions

Outline

- **Motivation** ←
- **Theoretical method**
- **Results and discussions**

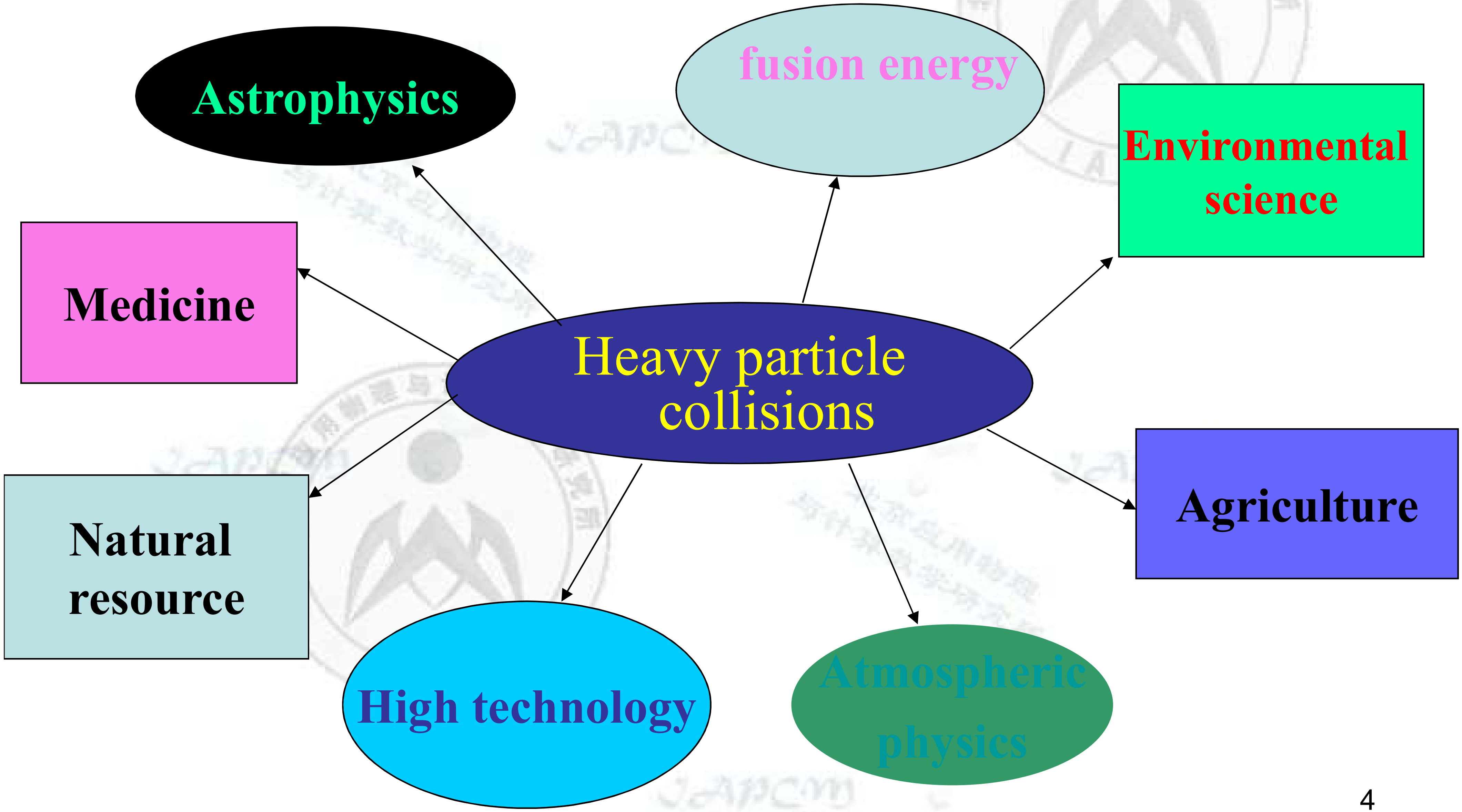
H^+-$Be^+ \rightarrow H(nl)+Be^{2+}$

$\rightarrow H^+ + Be^+(1s^2nl)$, n>2

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

Be^{3+}-$Li \rightarrow Be^{2+}+Li^+$

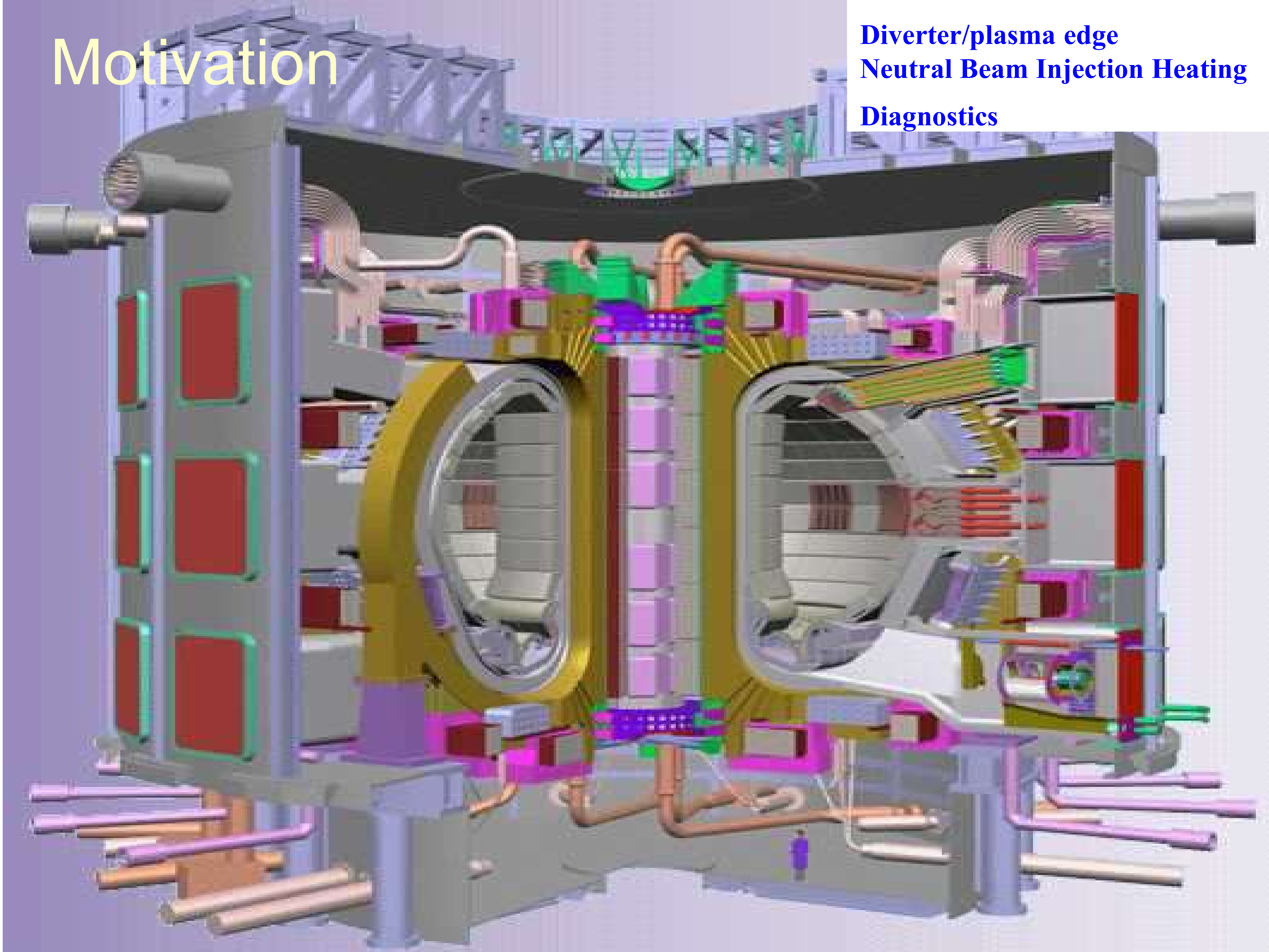
- **Summary**


Astrophysics
fusion energy
Environmental science
Medicine
Heavy particle collisions
Agriculture
Natural resource
High technology
Atmospheric physics

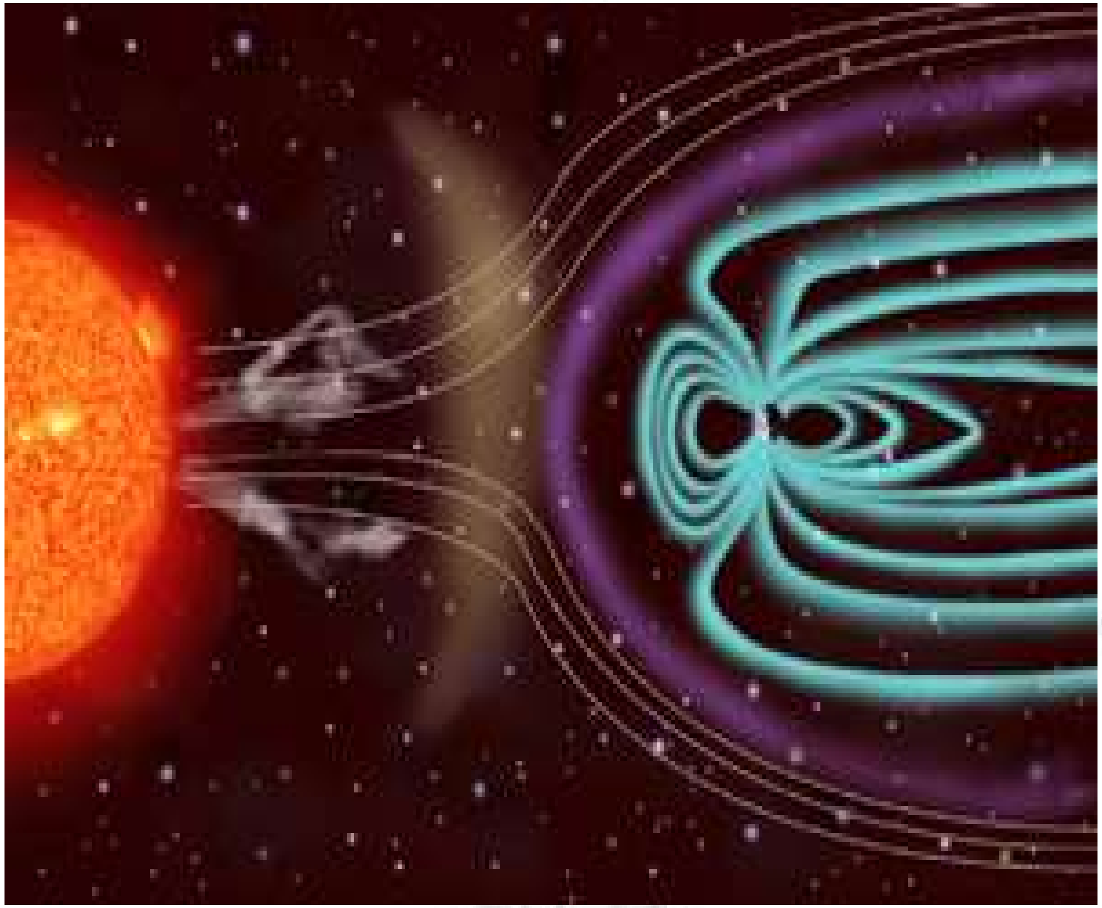
Motivation

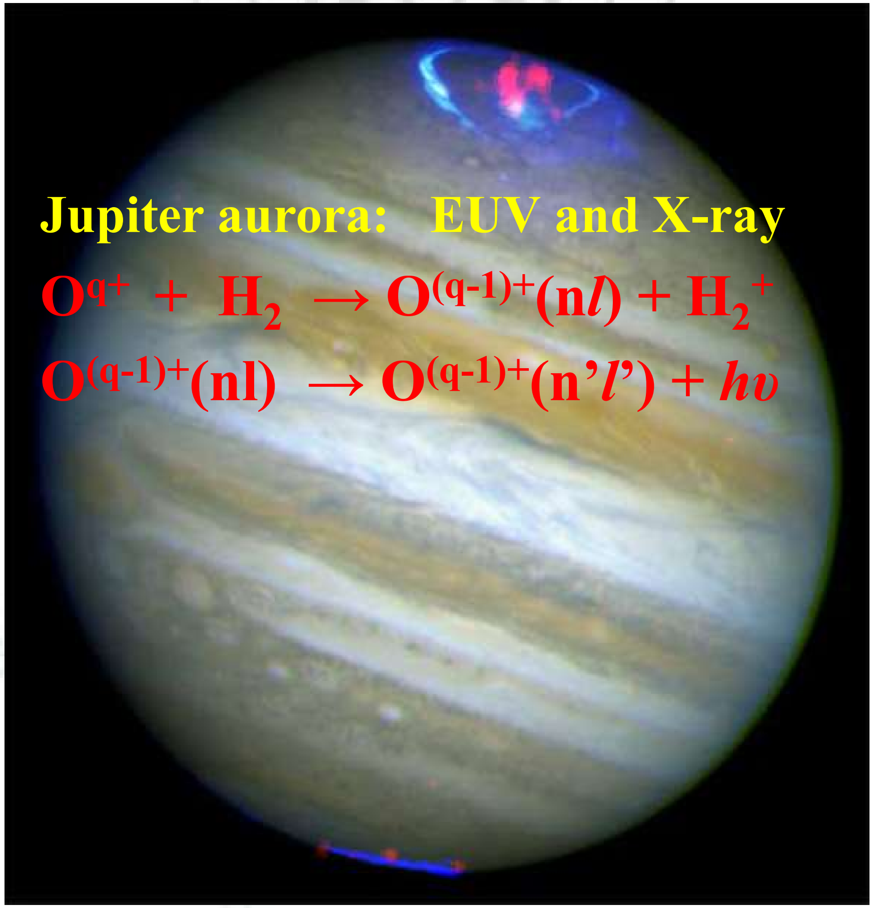
Diverter/plasma edge
Neutral Beam Injection Heating

Diagnostics



Jupiter aurora





Outline

- **Motivation**
- **Theoretical method** ←
- **Results and discussions**

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

$\rightarrow H^+ + Be^+(1s^2nl)$, n>2

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

$Be^{3+}\text{-}Li \rightarrow Be^{2+} + Li^+$

- **Summary**

Theoretical method

- **Fully quantum mechanical molecular orbital close-coupling (MOCC) method**
- **Two-center atomic orbital close-coupling (TC-AOCC) method**

MOCC method

- **Molecular structure calculations**

  Multi-reference single- and double-excitation configration interaction (MRDCI) approach

  (Collaborated with Prof. R. Buenker)

- **Scattering calculations**

  Close-coupling approach

  (Collaborated with Prof. P. C. Stancil)

MOCC method

Approximations:

- Born-Oppenheim approximation (BO)
- Perturbed stationary-state approximation (PSS)

$$\psi(R,\rho_i) = \sum_{\gamma} F_\gamma(R)\phi_\gamma(\rho_i \mid R)$$

System Hamilton:

$$H(R,\rho_i) = -\frac{1}{2\mu_R}\nabla_R^2 + H_{ad}(\rho_i \mid R)$$

$$H_{ad}(\rho_i \mid R)\phi_\gamma(\rho_i \mid R) = \varepsilon_\gamma(R,)\phi_\gamma(\rho_i \mid R)$$

Total wave function can be written as

$$\psi(R,\rho_i) = \sum_{\gamma} F_{\gamma}(R)\phi_{\gamma}(\rho_i \mid R)$$

By the variation theory, the adiabatic close-coupling scattering equation is obtained:

$$\left(-\frac{1}{2\mu}\nabla_R^2 \overleftrightarrow{\mathrm{I}} - \overleftrightarrow{\epsilon}(R) + E\overleftrightarrow{\mathrm{I}} + \frac{1}{2\mu}\left[2\vec{\mathrm{A}}(\vec{\mathrm{R}})\cdot\nabla_R + \vec{\mathrm{B}}(\vec{\mathrm{R}})\right]\right) F^{a}(\vec{\mathrm{R}}) = 0$$

The coupled equations are transformed to a diabatic representation:

$$\left\{\nabla_R^2 + 2\mu_R\left[E - \varepsilon_{\gamma}^{d}(R,\theta)\right]\right\} F_{\gamma}(R,\theta) = 2\mu_R \sum_{\gamma'\neq\gamma} V_{\gamma,\gamma'}^{d} F_{\gamma'}(R,\theta)$$

Using a partial wave decomposition method, the radial wavefunction and the S-matrix are obtained:

$$\lim_{R\to\infty} f_{\gamma}^{lm}(R) \to \frac{1}{\sqrt{k_{\gamma'}}}\{\delta_{\gamma,\gamma'} j_l(k_\gamma R) + K_{\gamma,\gamma'}^{l} \eta_l(k_{\gamma'} R)\}$$

$$S^{l} = \frac{I + iK^{l}}{I - iK^{l}}$$

The differential and integrate total cross sections are respectively:

$$\frac{d\sigma(\theta)}{d\Omega} = \frac{1}{4k^2}[\sum_{l} (2l+1) S_{i,j}^{l} P_l(\cos\theta)]^2$$

$$\sigma_{tot}(k) = \frac{\pi}{k_i^2}\sum_{l} (2l+1)(\left|\delta_{ij} - S^{l}\right|_{i,j}^{2})$$

AOCC method

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

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

even-tempered basis

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

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

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

The total wave function of the collision system

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

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 calculated as:

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

Outline

- **Motivation**
- **Theoretical method**
- **Results and discussions** ←

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

$\rightarrow H^+ + Be^+(1s^2nl)$, n>2

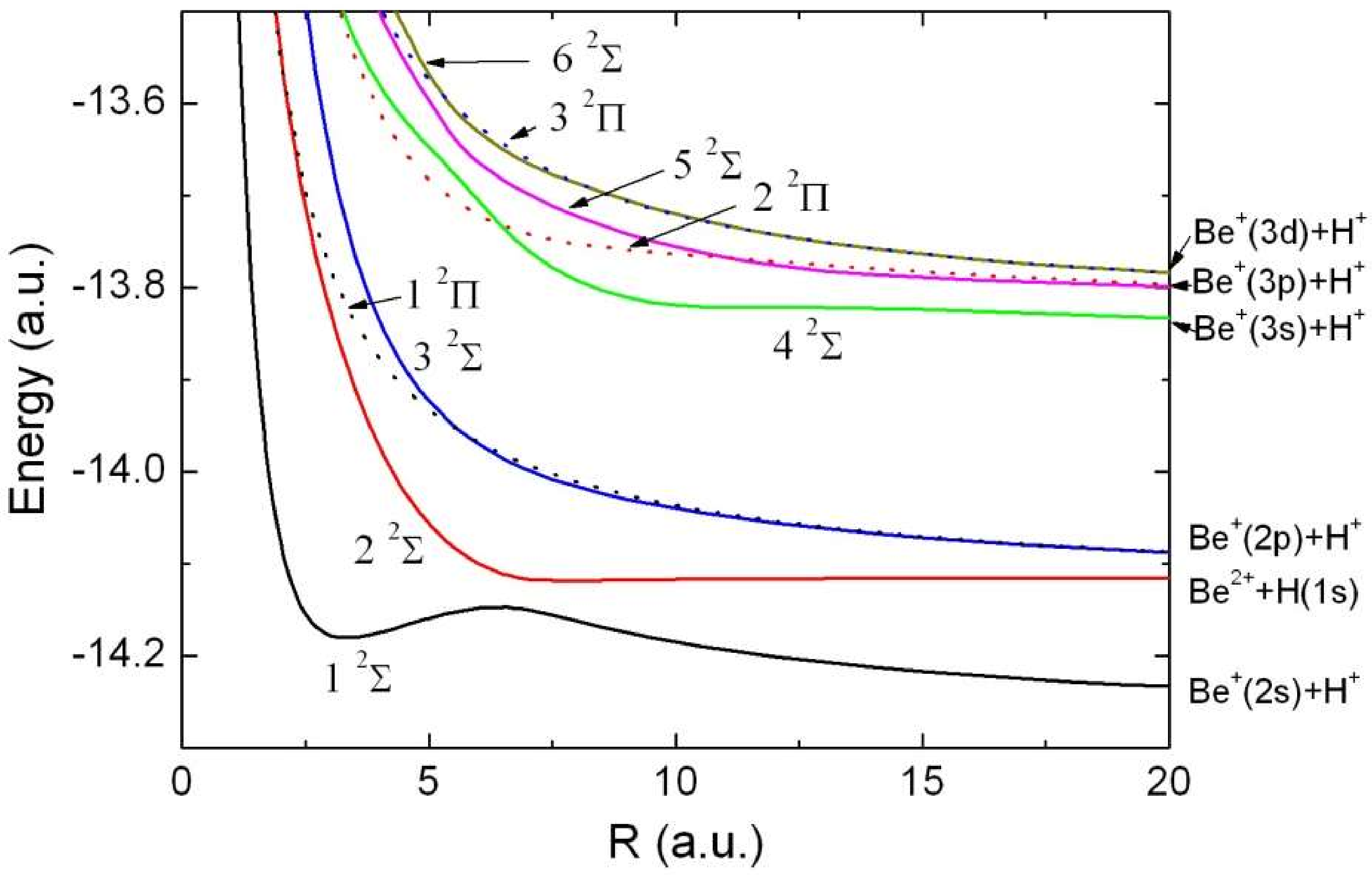
$\rightarrow H^+ + Be^{2+}(1s^2)+e$

Be^{3+}-$Li \rightarrow Be^{2+}+Li^+$

- **Summary**

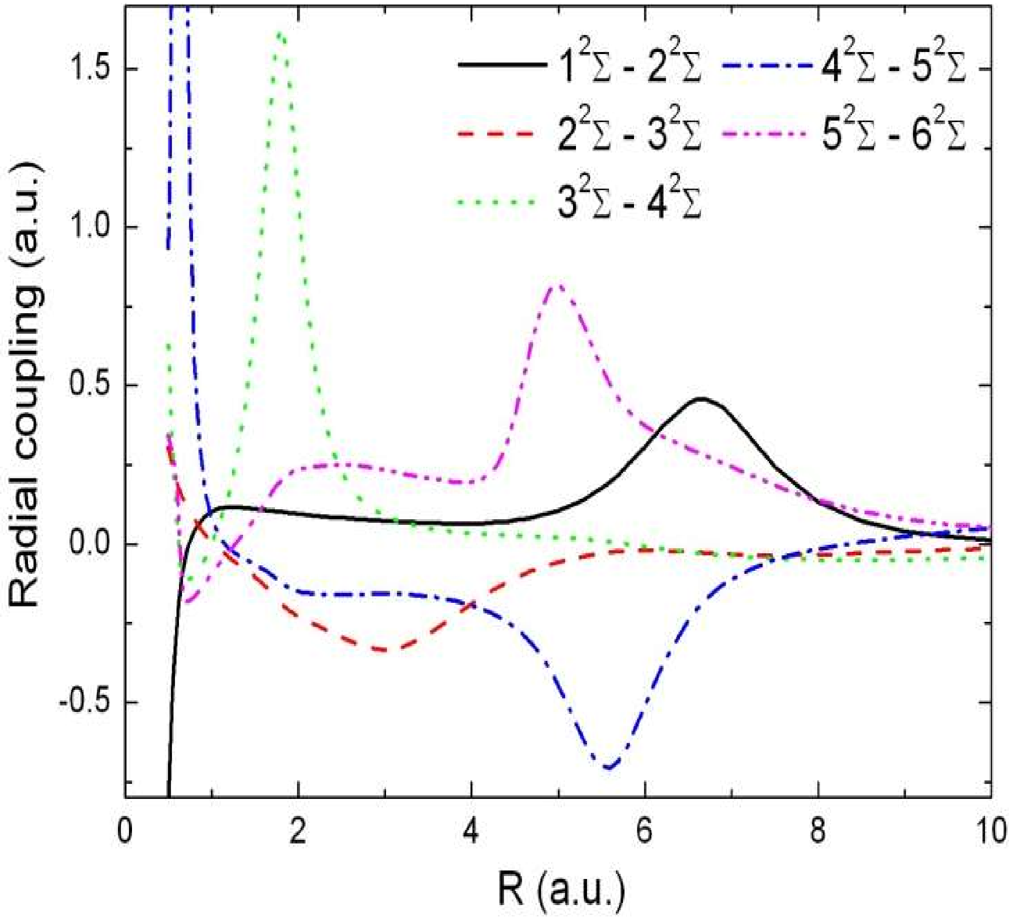
$H^+ + Be^+(1s^2 2l) \rightarrow H(nl) + Be^{2+}$ / $H^+ + Be^+(1s^2 nl)$, n>2

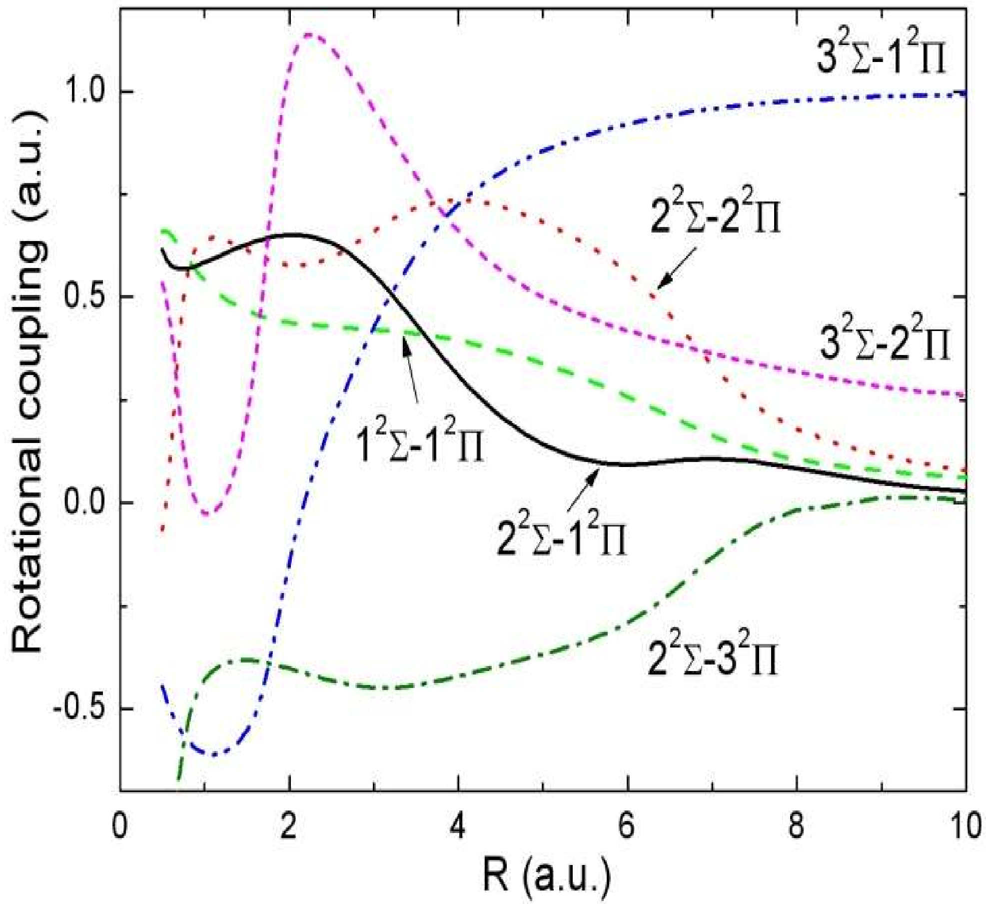
Adiabatic potential curves for $(BeH)^{2+}$ system



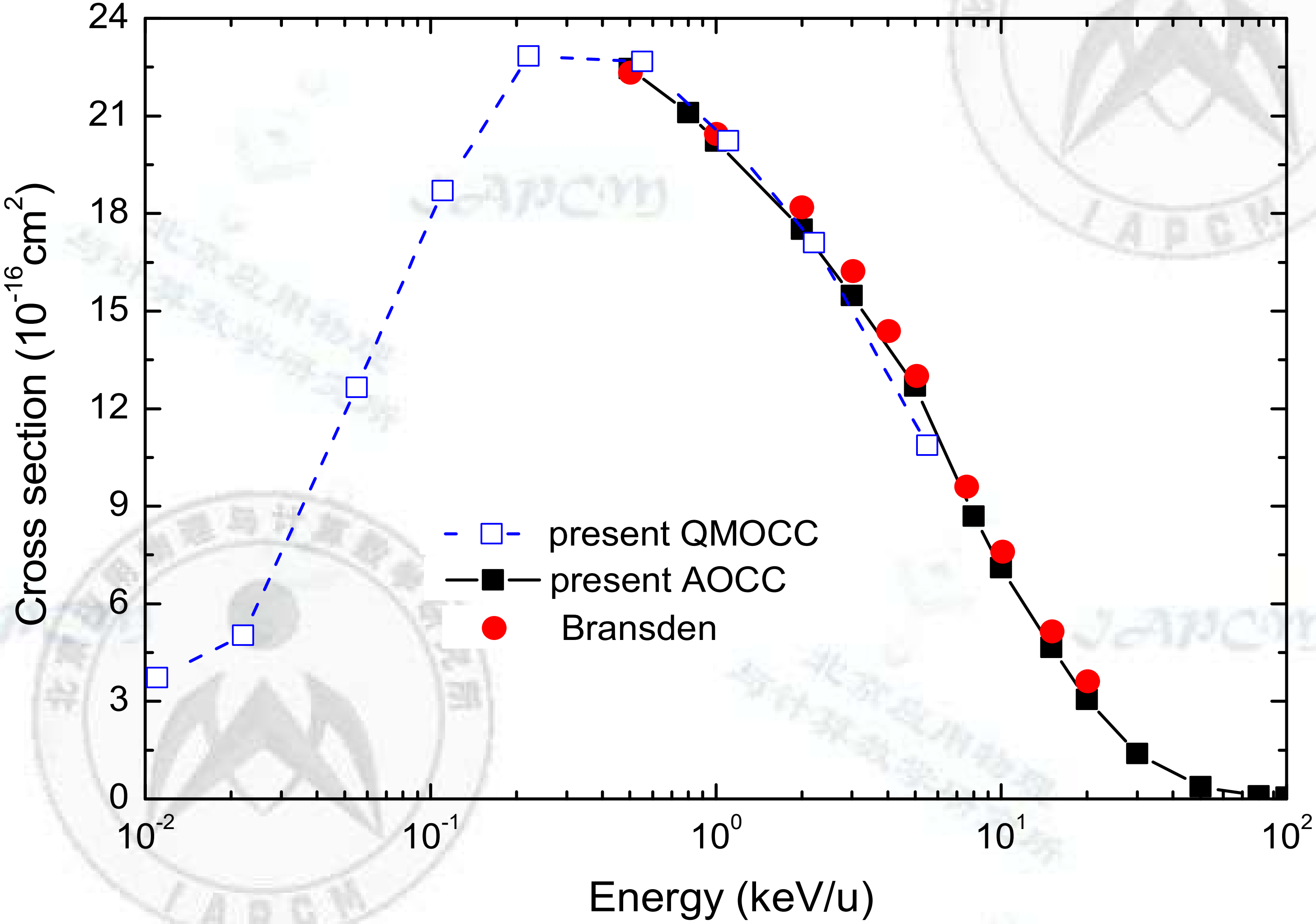
The solid and dotted lines represent the $^2\Sigma$ and $^2\Pi$ states, respectively.

Radial and rotational coupling matrix elements for BeH^{2+}



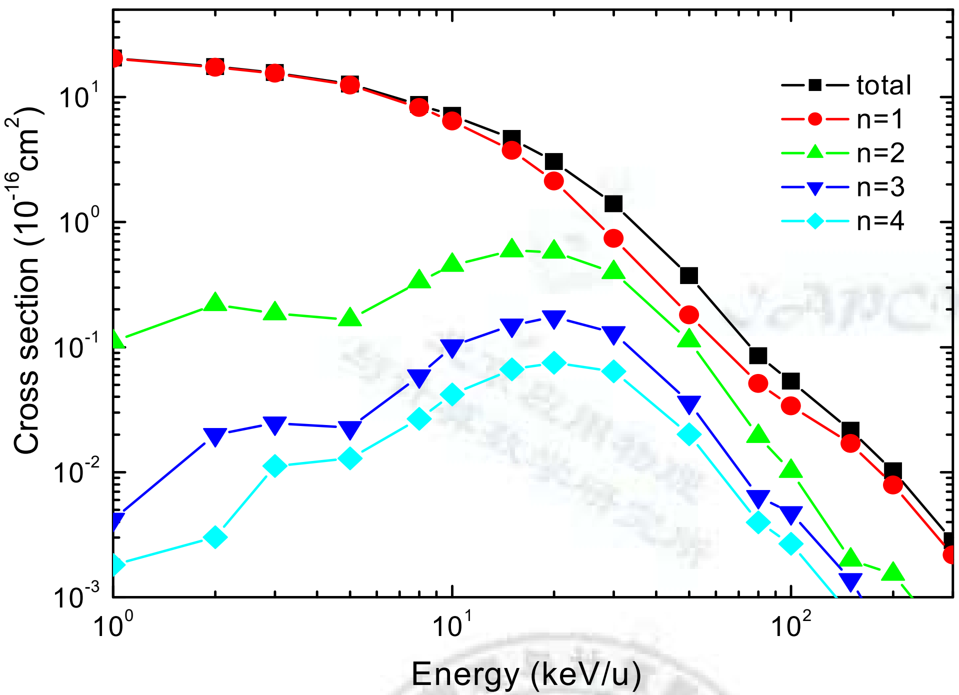


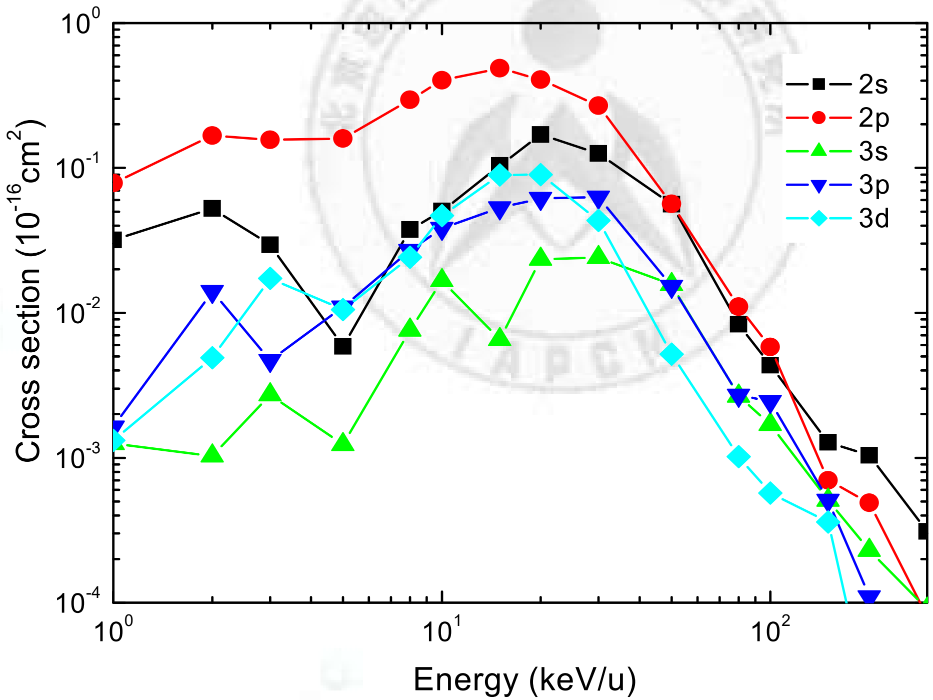
Cross section results: $Be^+(1s^2 2s)$ initial state

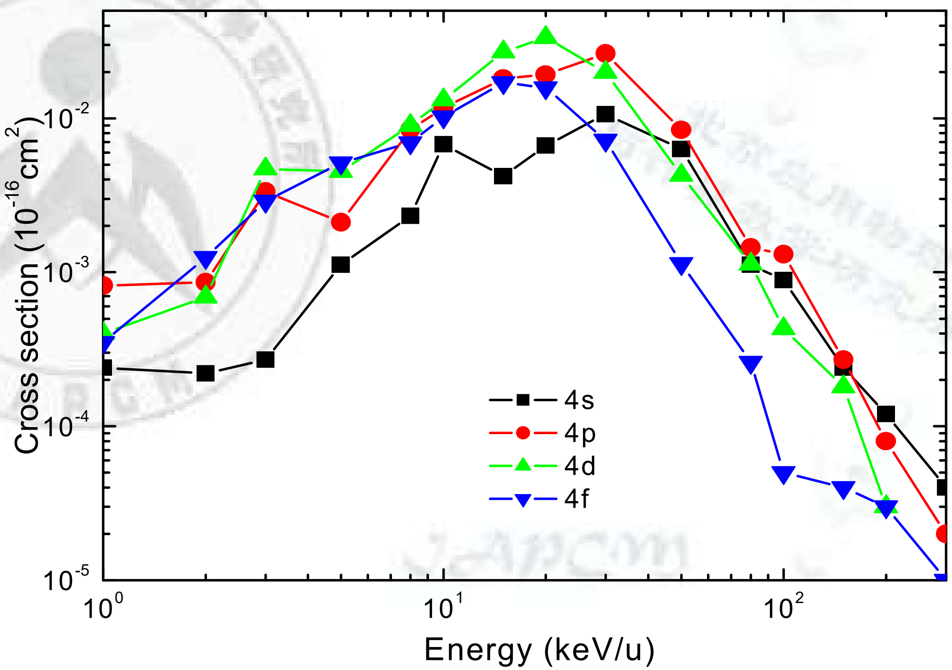


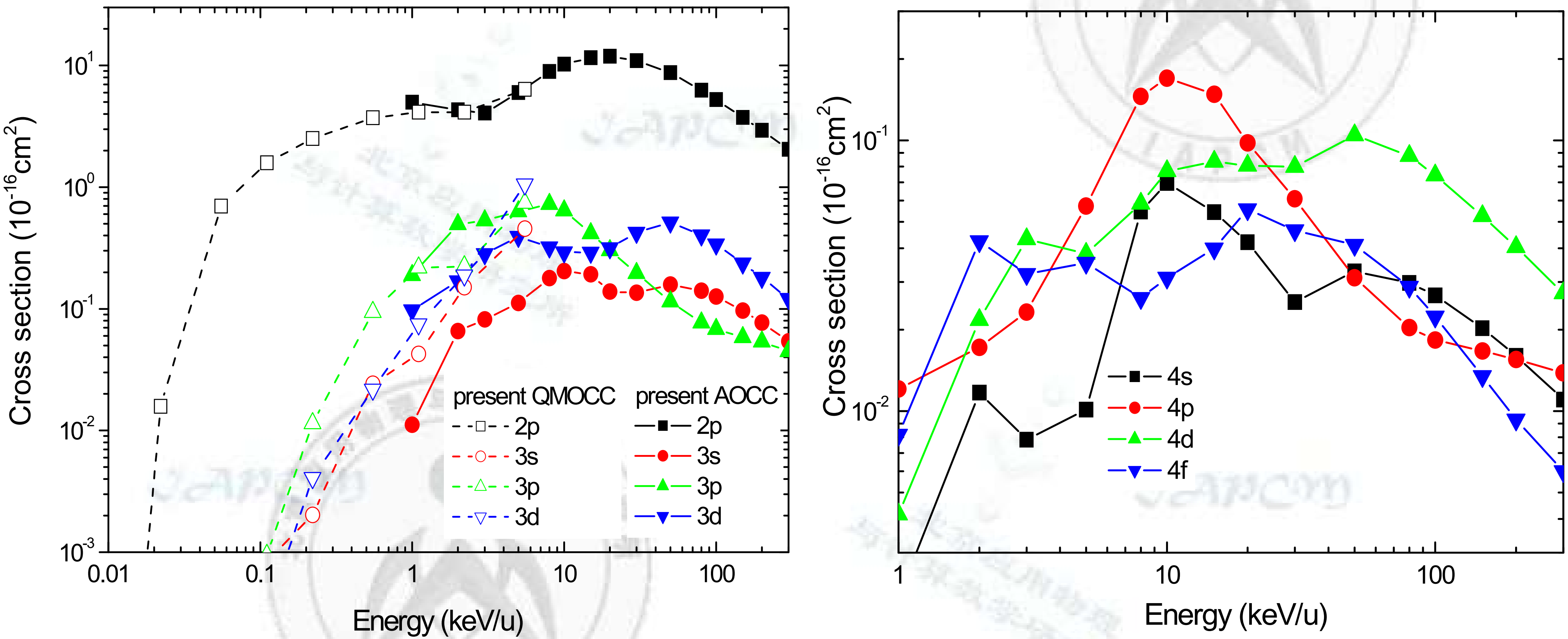
Total electron capture cross section for H^+-$Be^+(2s)$ collisions.

n- and *nl*-partial electron capture cross section for H^+-$Be^+(2s)$ collisions

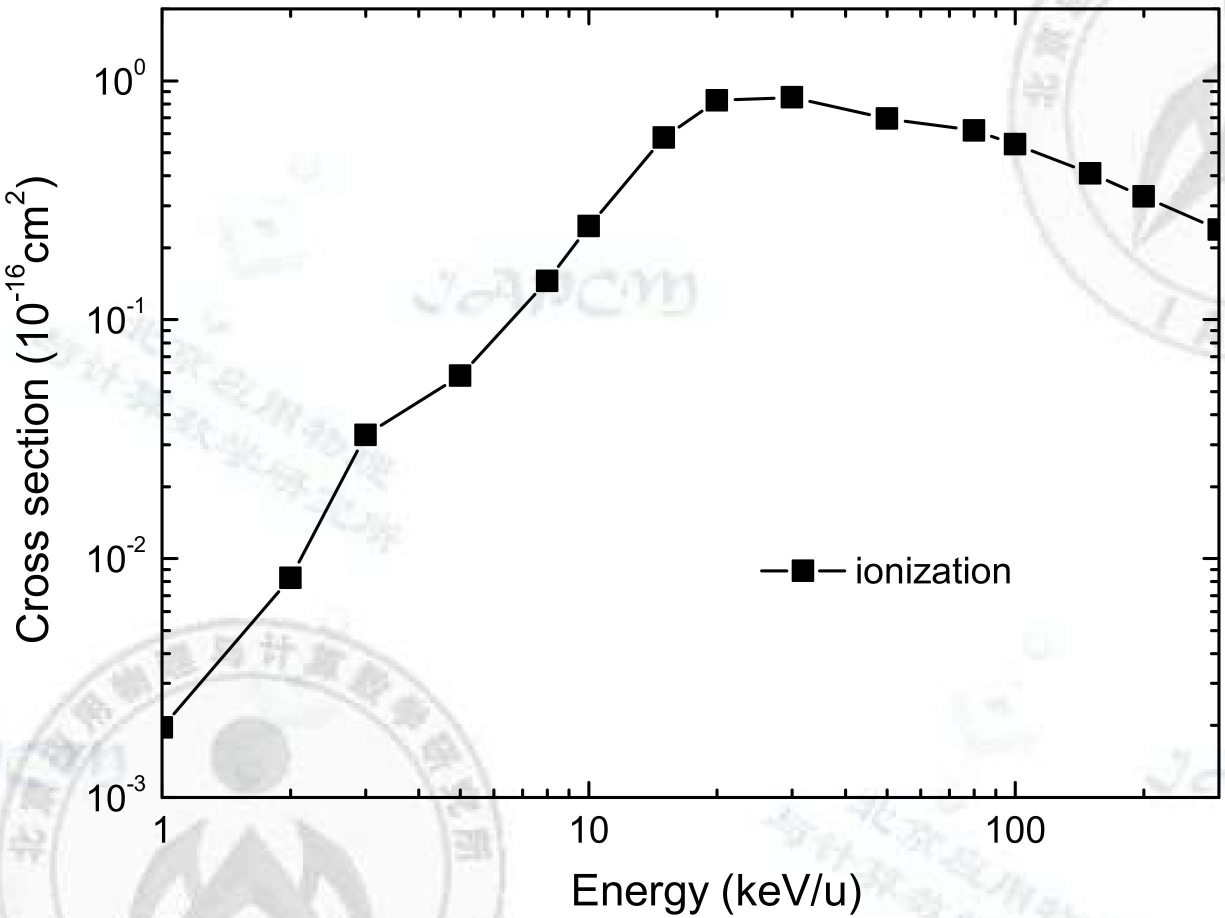






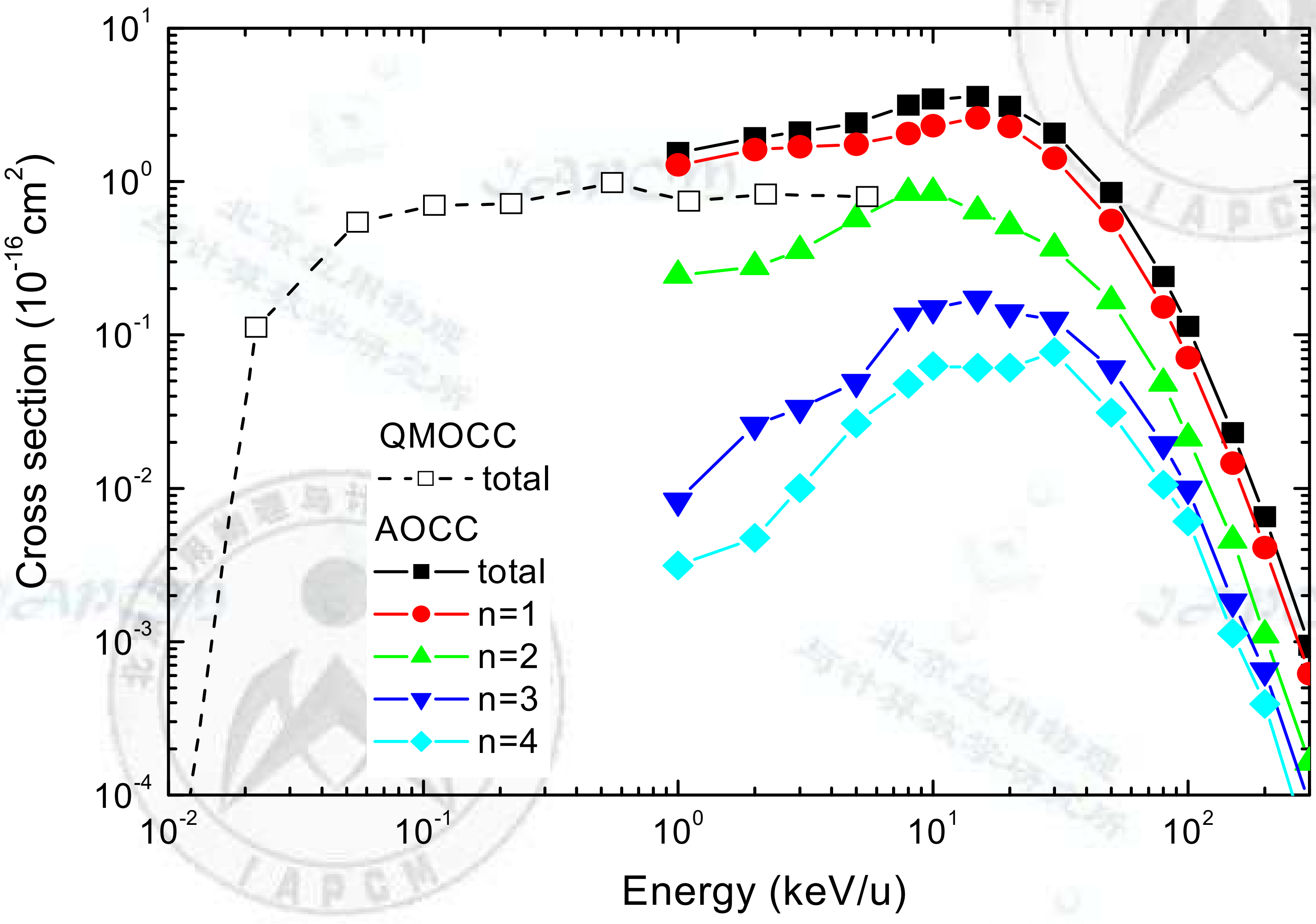


Cross sections for excitation to *2p*, *3l* and *4l* states of Be^+ in H^+-$Be^+(1s^22s)$ collisions.

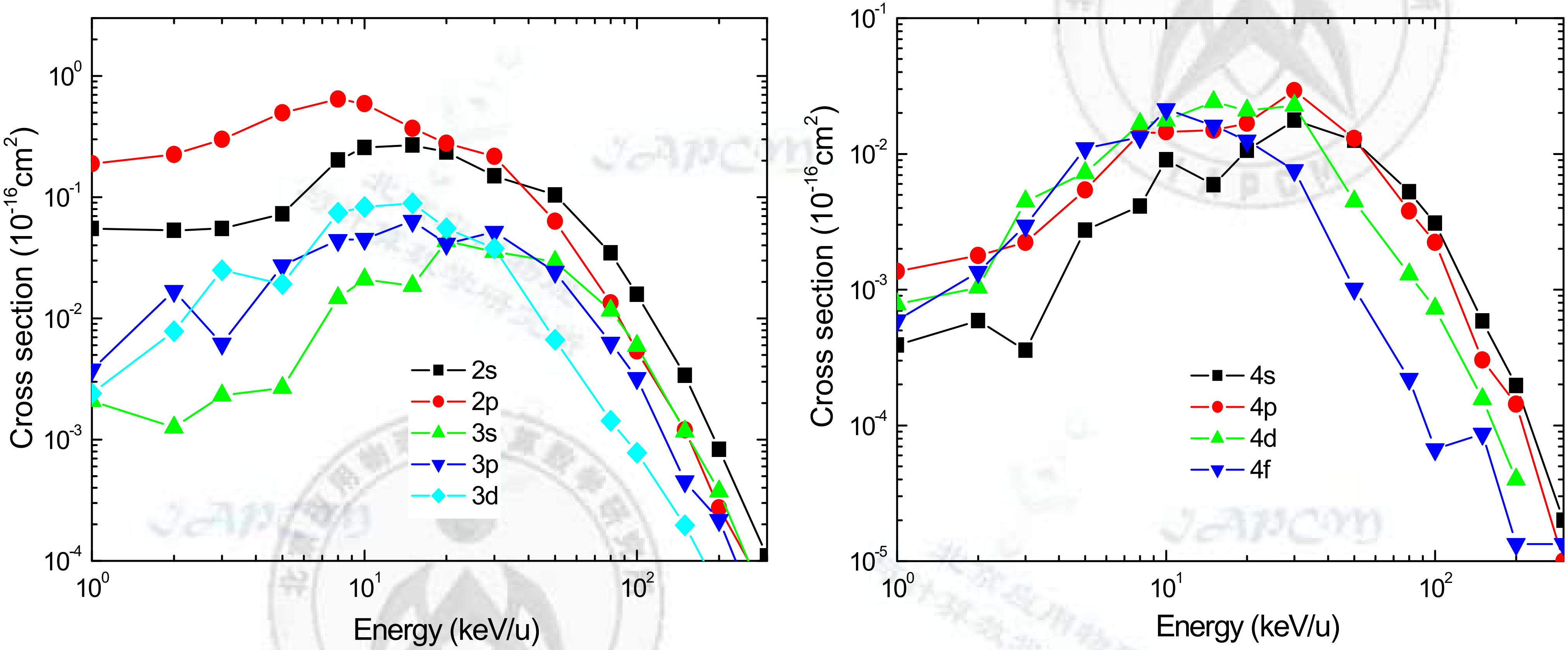


AOCC ionization cross sections in H^+-$Be^+(1s^22s)$ collisions.

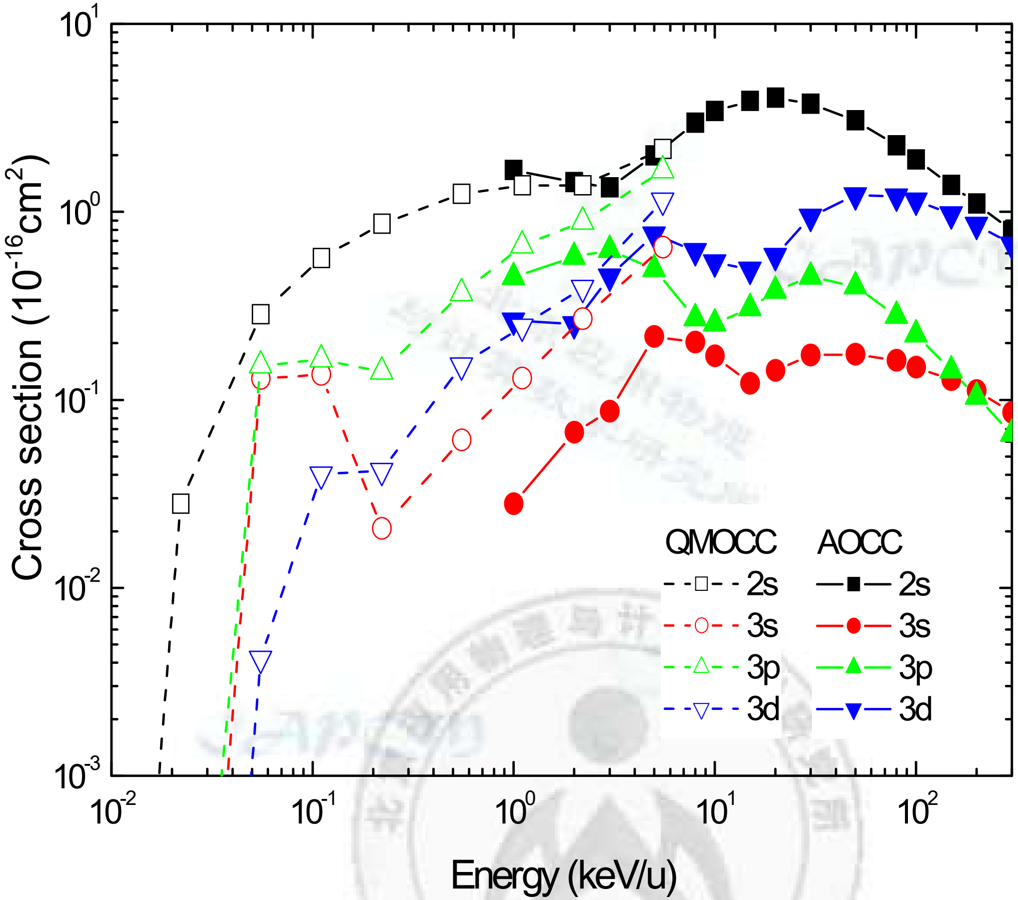
Cross section results: $Be^{+}(1s^22p)$ initial state



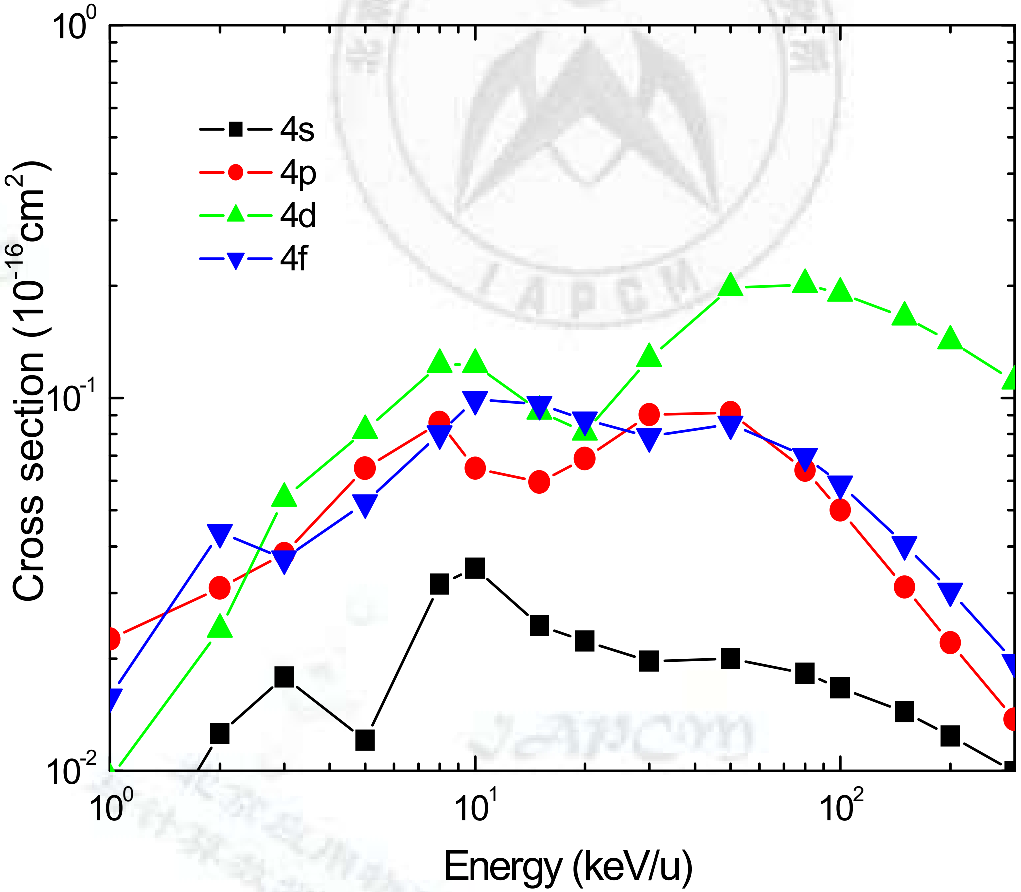
Total and n-shell AOCC and *1s* QMOCC electron capture cross sections in H^{+}-$Be^{+}(1s^22p)$ collisions.



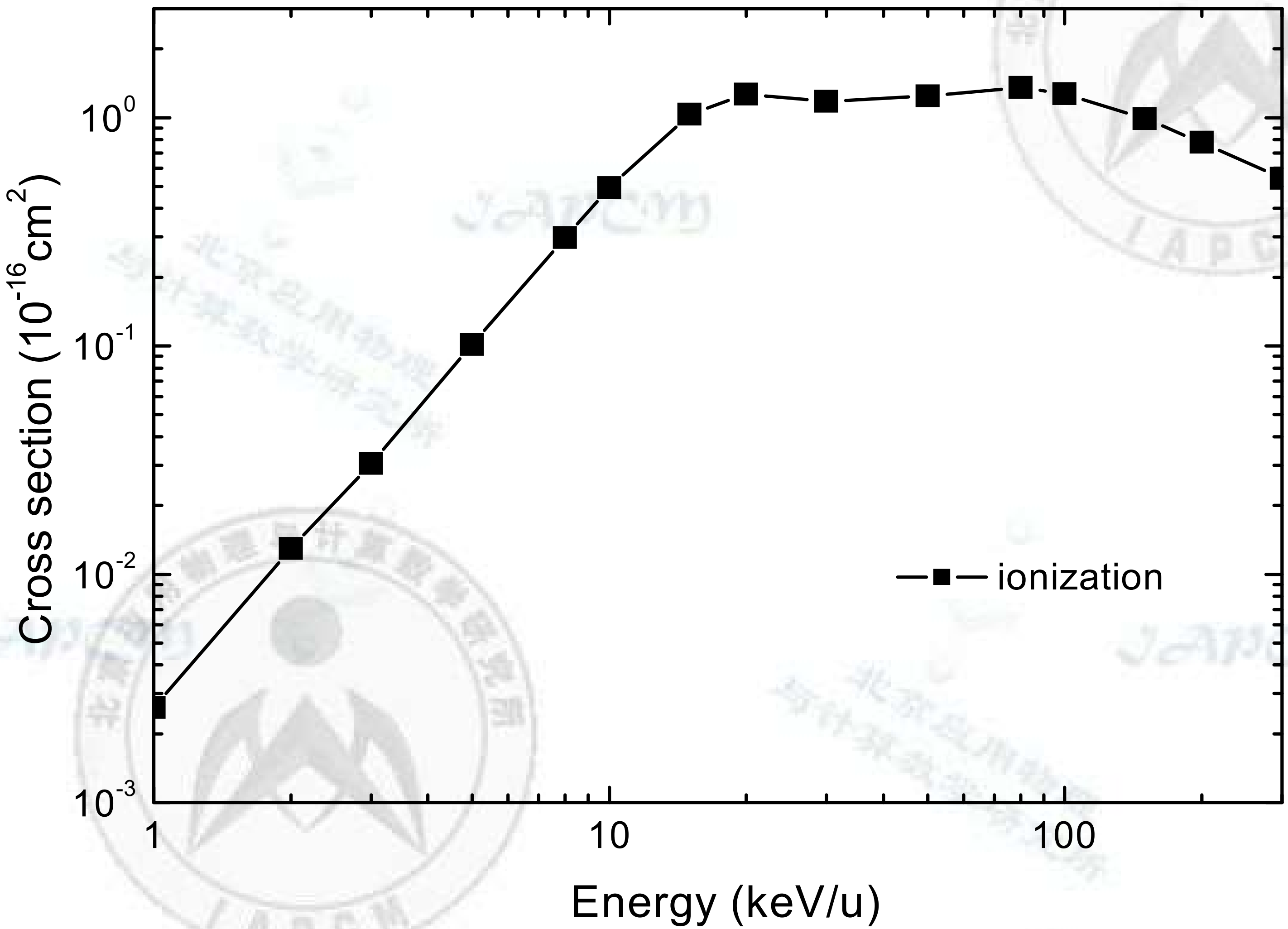
AOCC cross sections for electron capture to 4*l* states of H in H^+-$Be^+(1s^22p)$ collisions.



Cross sections for **excitation** to the 2*s* and 3*l* states of Be^+ in H^+-$Be^+(1s^22p)$ collisions.



AOCC cross sections for **excitation** to 4*l* states of Be^+ in H^+-$Be^+(1s^22p)$ collisio

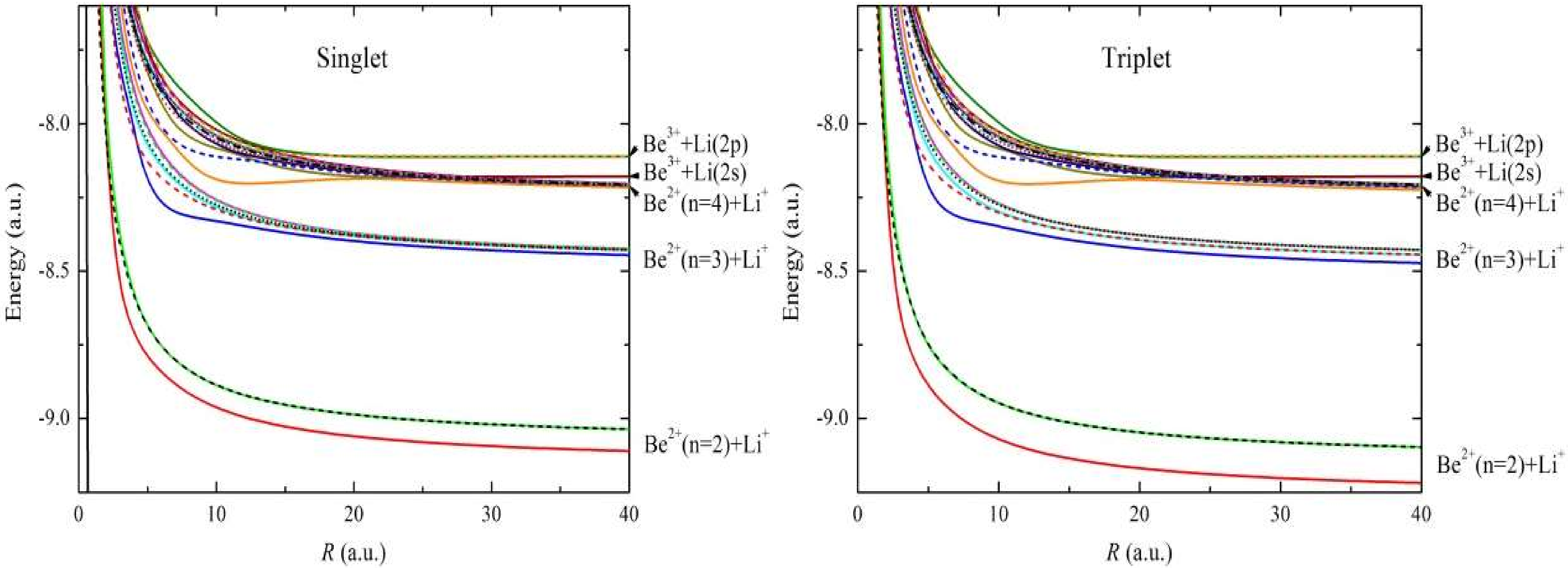


AOCC ionization cross section H^+-Be^+(*1s²2p*) collisions.

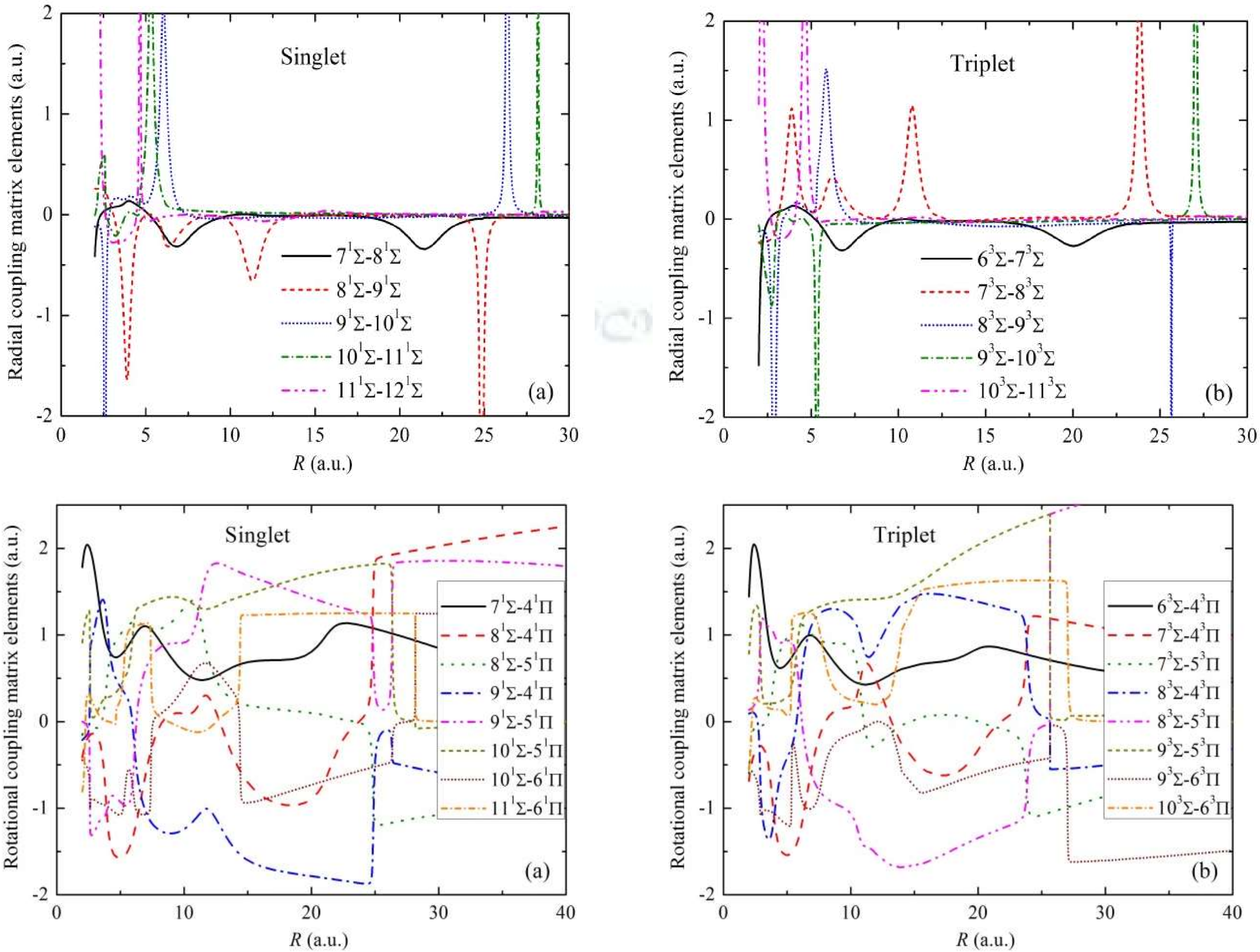
Table 1. Asymptotic separated-atom energies of $BeLi^{3+}$ molecule.

Molecular state	Asymptotic atomic state	Energy (eV)		
		Expt. [13]	Theor.	error
$1^3\Sigma$	$Be^{2+}(1s2s)[^3S]+Li^+$	-29.913	-29.676	0.237
$2^1\Sigma$	$Be^{2+}(1s2s)[^1S]+Li^+$	-26.854	-26.724	0.13
$2^3\Sigma$, $1^3\Pi$	$Be^{2+}(1s2p)[^3P]+Li^+$	-26.583	-26.363	0.22
$3^1\Sigma$, $1^1\Pi$	$Be^{2+}(1s2p)[^1P]+Li^+$	-24.836	-24.715	0.121
$3^3\Sigma$	$Be^{2+}(1s3s)[^3S]+Li^+$	-9.495	-9.363	0.132
$4^1\Sigma$	$Be^{2+}(1s3s)[^1S]+Li^+$	-8.687	-8.634	0.053
$4^3\Sigma$, $2^3\Pi$	$Be^{2+}(1s3p)[^3P]+Li^+$	-8.613	-8.591	0.022
$5^3\Sigma$, $3^3\Pi$, $1^3\Delta$	$Be^{2+}(1s3d)[^3D]+Li^+$	-8.231	-8.155	0.076
$5^1\Sigma$, $2^1\Pi$, $1^1\Delta$	$Be^{2+}(1s3d)[^1D]+Li^+$	-8.221	-8.150	0.071
$6^1\Sigma$, $3^1\Pi$	$Be^{2+}(1s3p)[^1P]+Li^+$	-8.106	-8.052	0.054
$6^3\Sigma$	$Be^{2+}(1s4s)[^3S]+Li^+$	-2.786	-2.579	0.207
$7^1\Sigma$	$Be^{2+}(1s4s)[^1S]+Li^+$	-2.450	-2.347	0.103
$7^3\Sigma$, $4^3\Pi$	$Be^{2+}(1s4p)[^3P]+Li^+$	-2.429	-2.327	0.102
$8^3\Sigma$, $5^3\Pi$, $2^3\Delta$	$Be^{2+}(1s4d)[^3D]+Li^+$	-2.271	-2.151	0.12
$8^1\Sigma$, $4^1\Pi$, $2^1\Delta$	$Be^{2+}(1s4d)[^1D]+Li^+$	-2.266	-2.148	0.108
$9^1\Sigma$, $5^1\Pi$, $3^1\Delta$	$Be^{2+}(1s4f)[^1F]+Li^+$	-2.263	-2.138	0.125
$9^3\Sigma$, $6^3\Pi$, $3^3\Delta$	$Be^{2+}(1s4f)[^3F]+Li^+$	-2.263	-2.138	0.125
$10^1\Sigma$, $6^1\Pi$	$Be^{2+}(1s4p)[^1P]+Li^+$	-2.224	-2.084	0.140
$11^1\Sigma$, $10^3\Sigma$	$Be^{3+}(1s)+Li(2s)$	0	0	0
$12^1\Sigma$, $11^3\Sigma$, $7^{1,3}\Pi$	$Be^{3+}(1s)+Li(2p)$	1.848	1.848	0

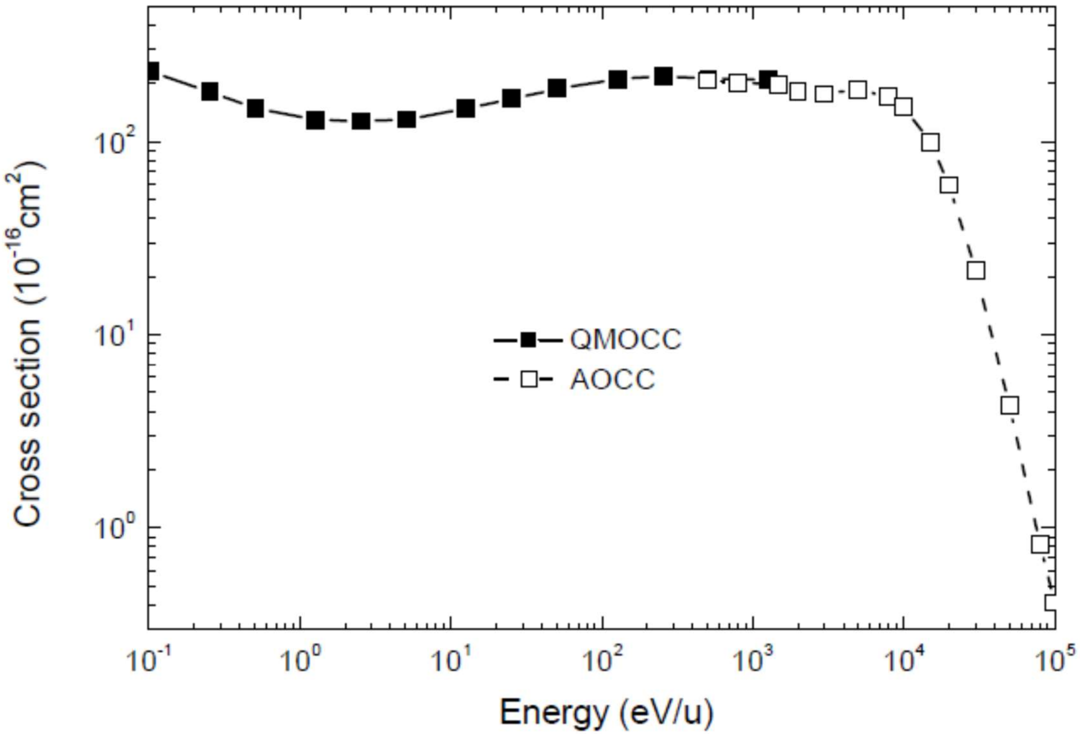
Be^{3+}-Li

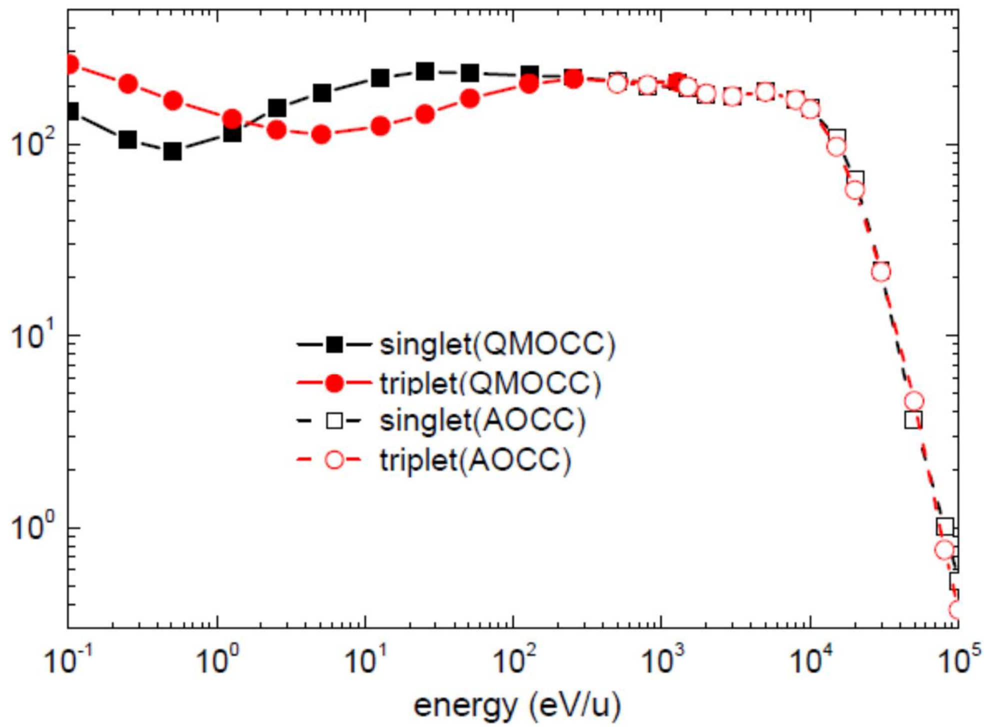


Adiabatic energies of $BeLi^{3+}$ molecular ion. The solid, dashed, dotted and dash-dotted lines represent the Σ, Π, Δ and Φ states, respectively. (a) singlet states; (b) triplet states.



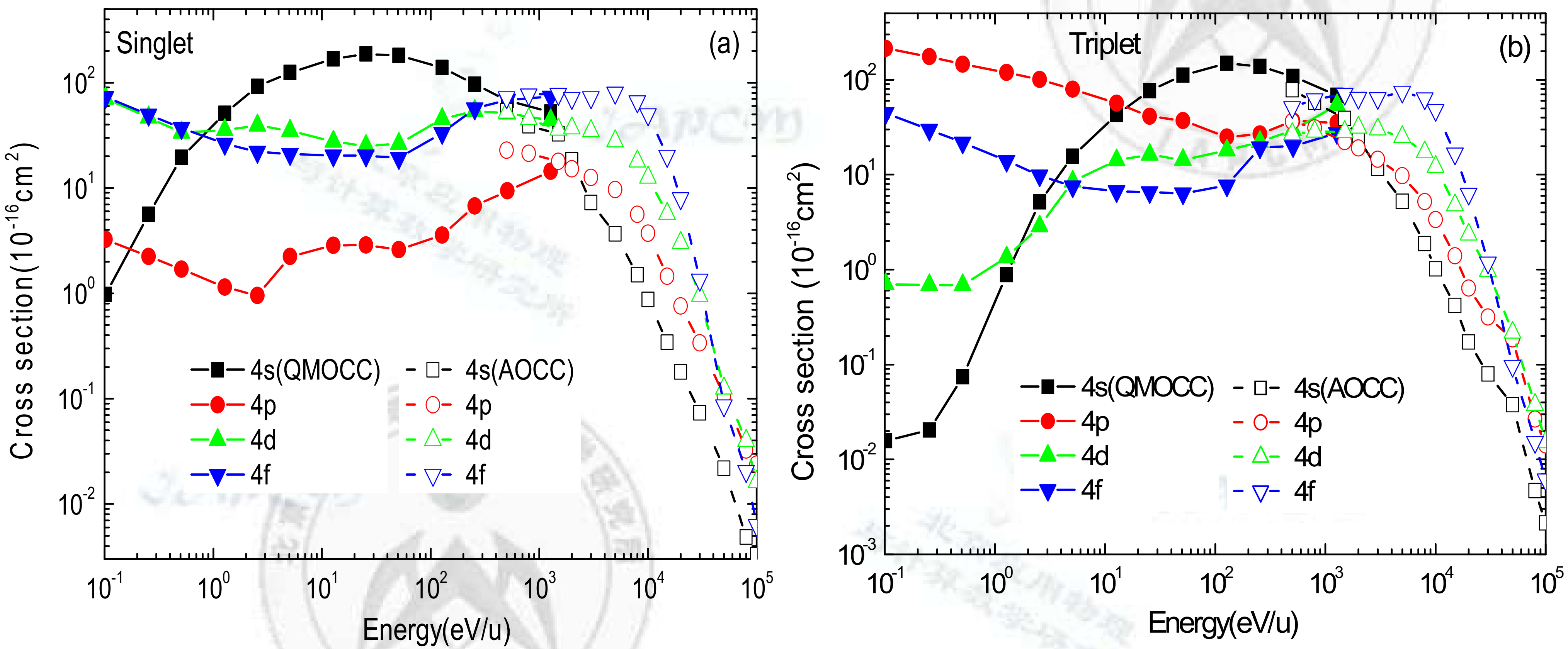
Radial and rotational coupling matrix elements for the singlet and triplet states.



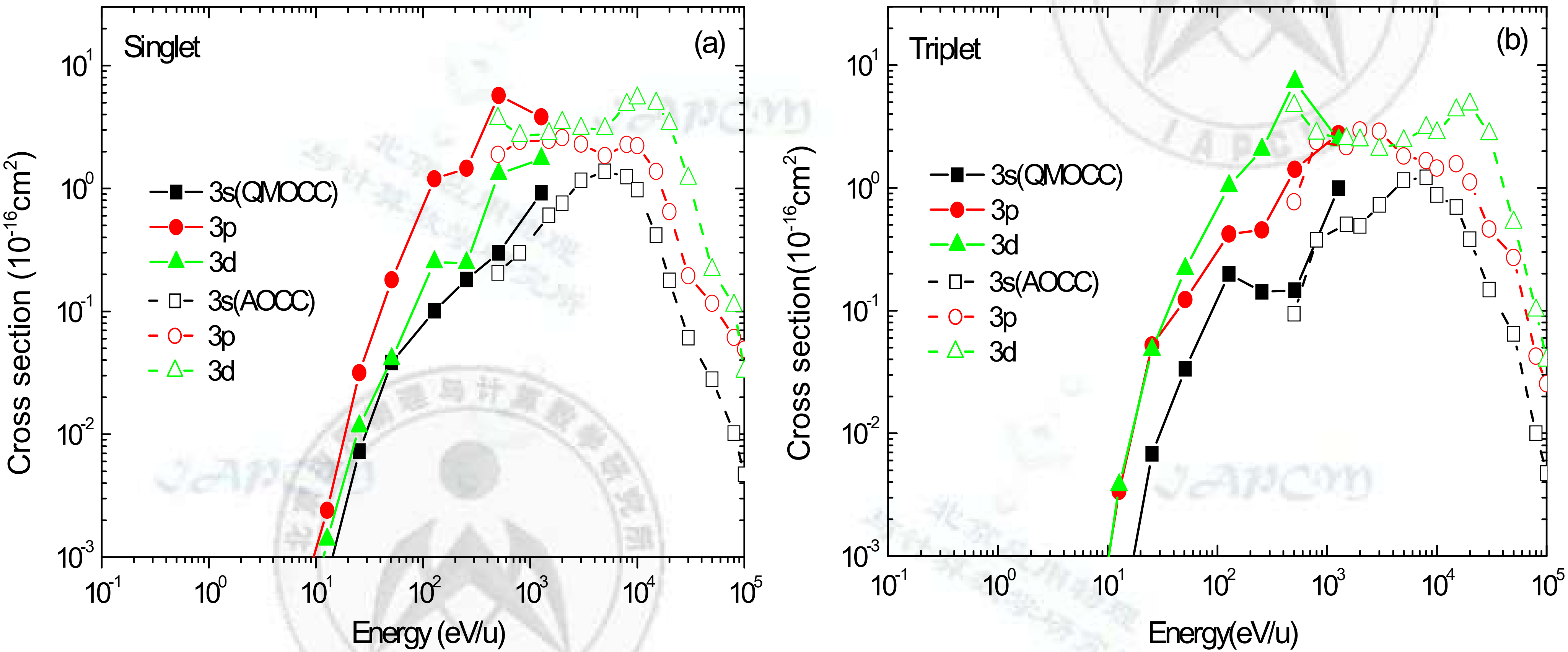


Total electron capture cross section in Be^{3+}-Li(2s) collisions.

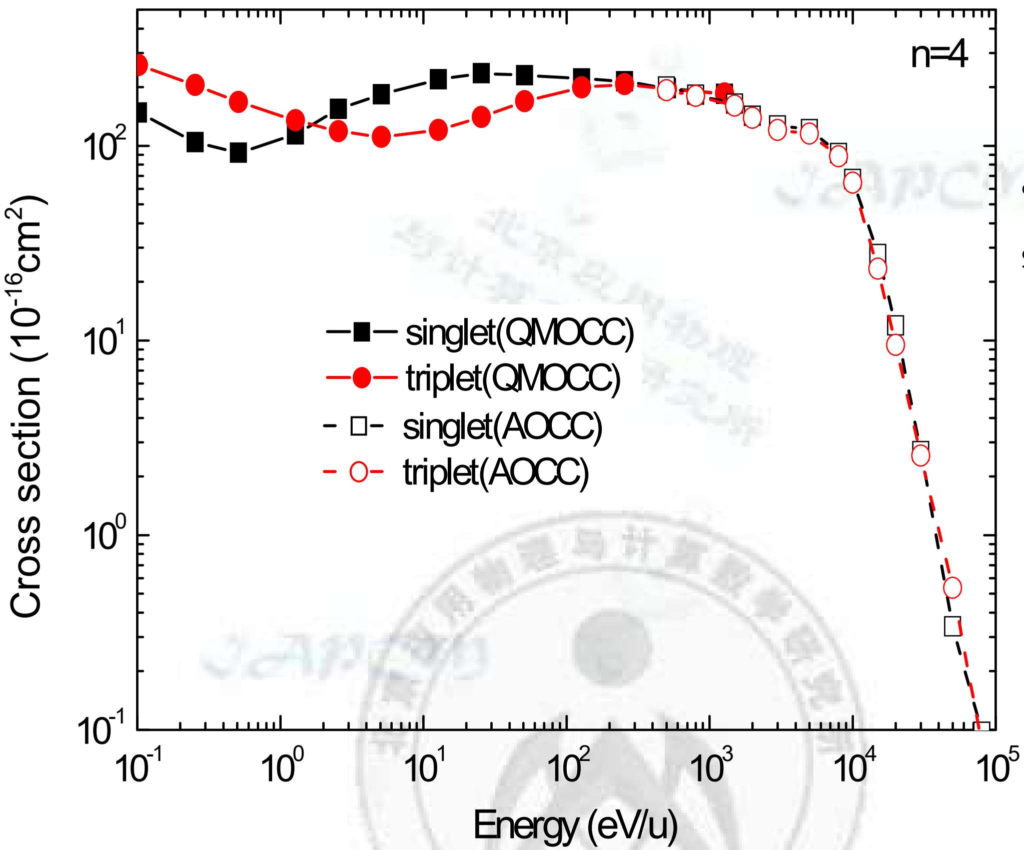
Spin-resolved cross sections

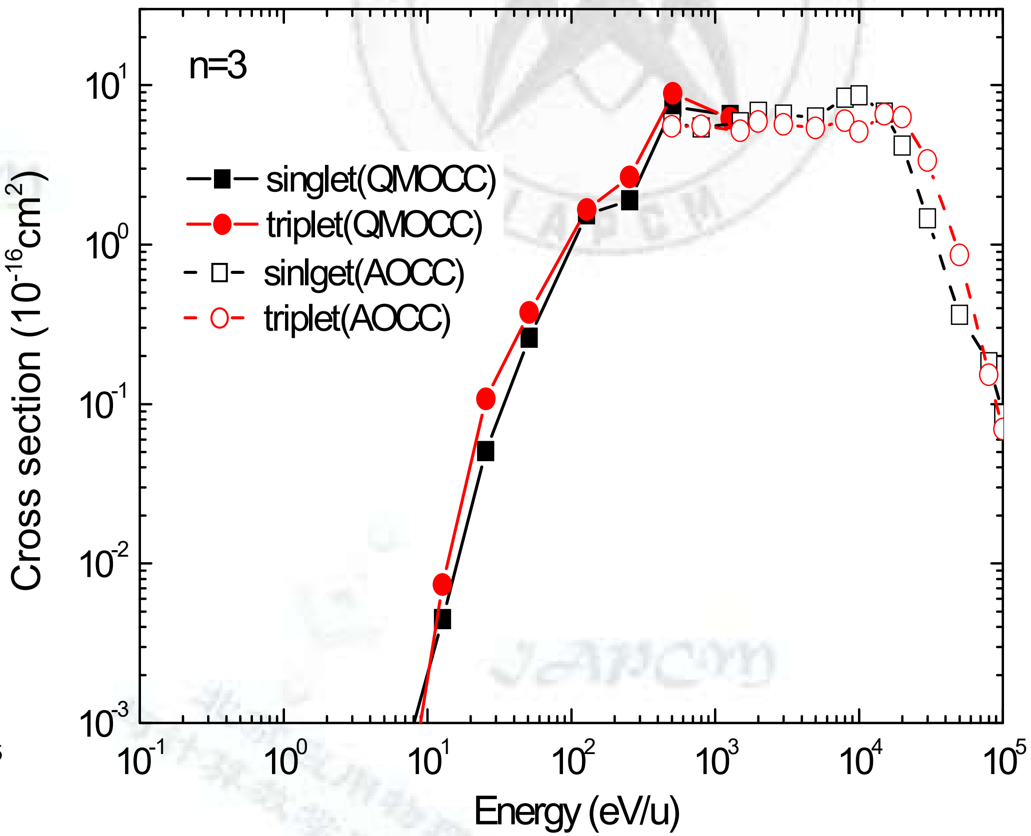


Cross sections for electron capture to 4*l* singlet and triplet states of Be^{2+} ion.



Cross sections for electron capture to 3*l* singlet and triplet states of Be^{2+} ion.





Cross sections for electron capture to the *n*=4 and n=3 shells of singlet and triplet states of Be^{2+} ion.

Outline

- **Motivation**
- **Theoretical method**
- **Results and discussions**

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

$\rightarrow H^+ + Be^+(1s^2nl)$, n>2

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

Be^{3+}-$Li \rightarrow Be^{2+} + Li^+$

- **Summary** ←

- **Using the MOCC and AOCC methods, the reliable CT and EXC data can be obtained in a large energy range.**
- **Multi–electron system and very high charge ion problems are still challenges.**

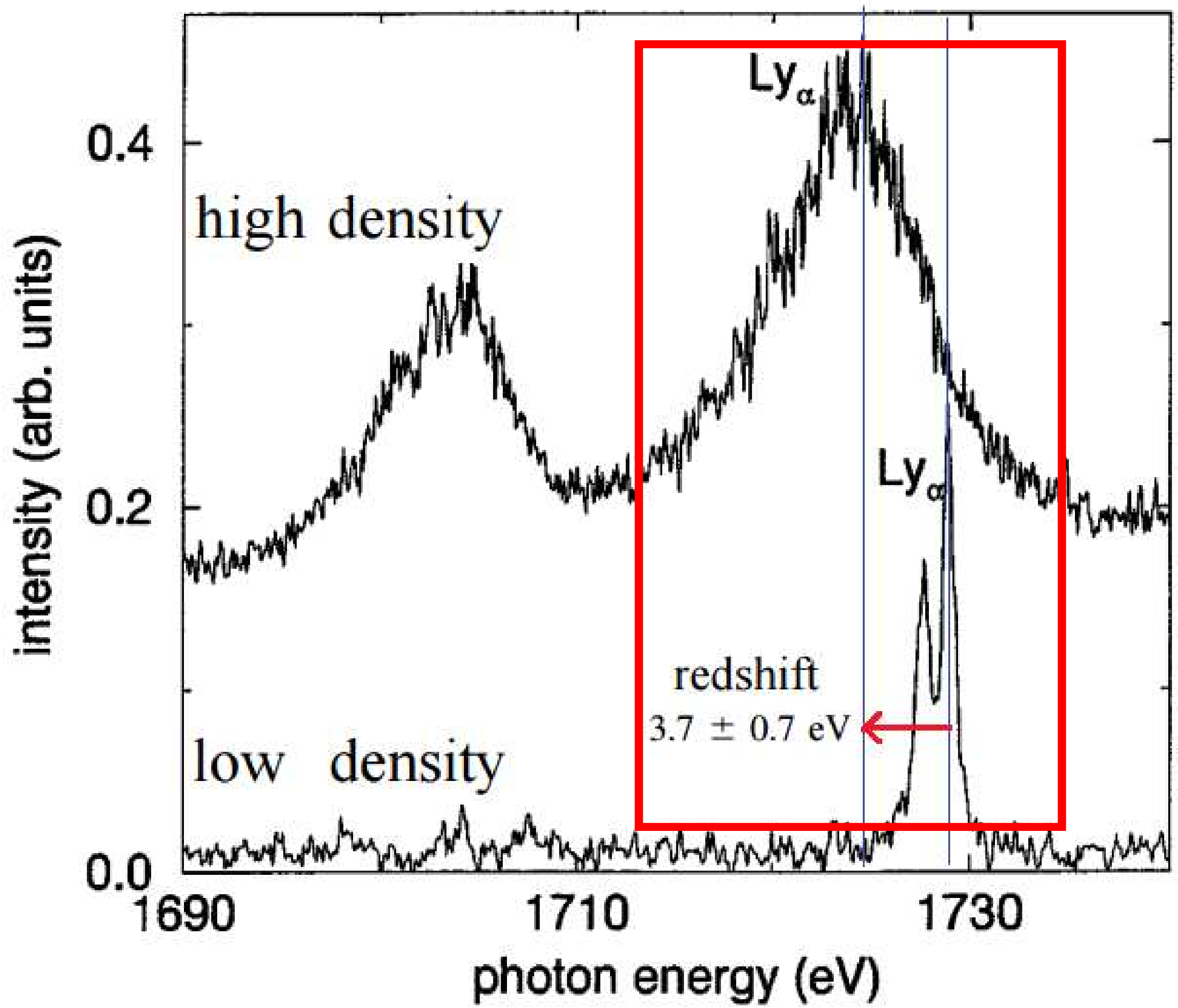
Future works

- **H^+-$Be^{(0,2,3)+}$, H^+-Ne^{q+}(q=0-9), H^+-Ar^{q+}(q=0-17)**

Part 2
Free-free transition in H plasma

K-shell emission spectra of solid Aluminum laser produced plasma

T=~300eV
n=(5-10)×10^{23}/cm^3



Saemann et al. Phys. Rev. Lett. **82**, 4843 (1999)

plasma screening

The Coulomb interaction screening is a general phenomenon in plasma;
it is a collective effect of correlated many-particle Interactions;
it strongly depends on the plasma environments;
it strongly affects the electronic structure (spectral) properties of atoms/molecules and properties of their collision processes with respect to those for isolated systems.

Coupling parameter

$$\Gamma = \langle Ze \rangle^2 / (\frac{3}{4\pi n_e})^{1/3} k_B T_e$$

Degeneracy parameter

$$\Theta = k_B T_e / E_F$$

$$\begin{cases} \Gamma = 1 & \text{nearly ideal} \\ \Gamma \le 1 & \text{weakly nonideal} \\ \Gamma > 1 & \text{strongly coupled} \end{cases}$$

$$\begin{cases} \Theta > 1 & \text{nondegenerate} \\ \Theta < 1 & \text{degenerate} \end{cases}$$

Debye plasma

weakly coupled classical hot-dense plasma ($\Gamma<<1,\Theta>1$)

e.g., laser induced plasmas, ICF plasma, stellar interiors …

pair-wise correlation approximation

$$\frac{Z}{r} \rightarrow \frac{Z}{r} e^{-\frac{r}{D}} \text{ (Debye-Hückel potential)}$$

Hamiltonian

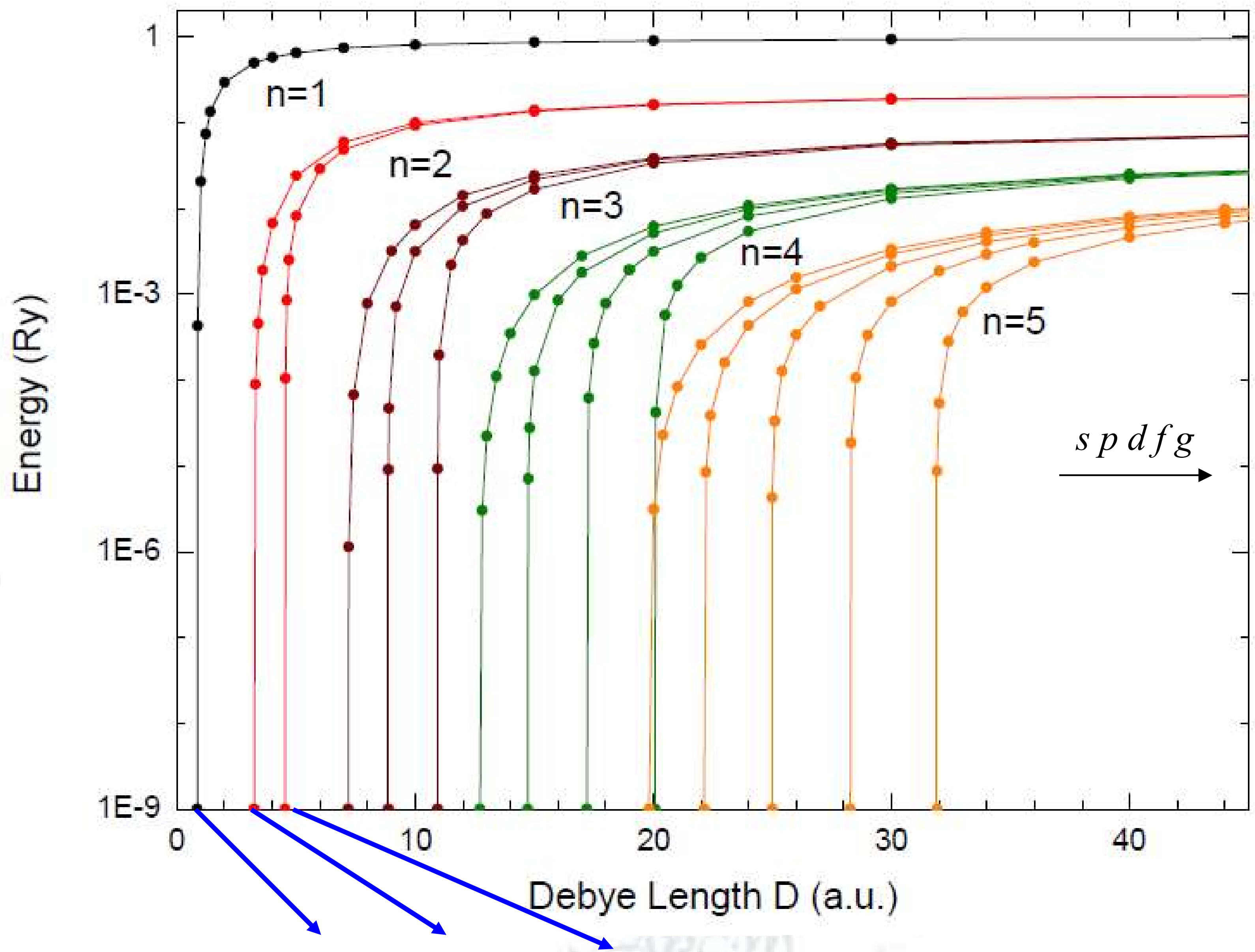
$$H = \sum_{n=1} [-\frac{1}{2}\nabla_n^2 - \frac{Z}{r_n} \times e^{-r_n/D} + \sum_{m>n} \frac{1}{r_{mn}} \times e^{-r_{mn}/D}]$$

What we have done in Debye plasmas

* Electronic structure
* Emission spectra
* Photoionization (non-relativistic & relativistic)
* Fast electron impact ionization
* Low energy electron impact excitation
* Low energy electron-impact ionization
* Heavy particle collisions (excitation、charge transfer、ionization)
* free-free trantion

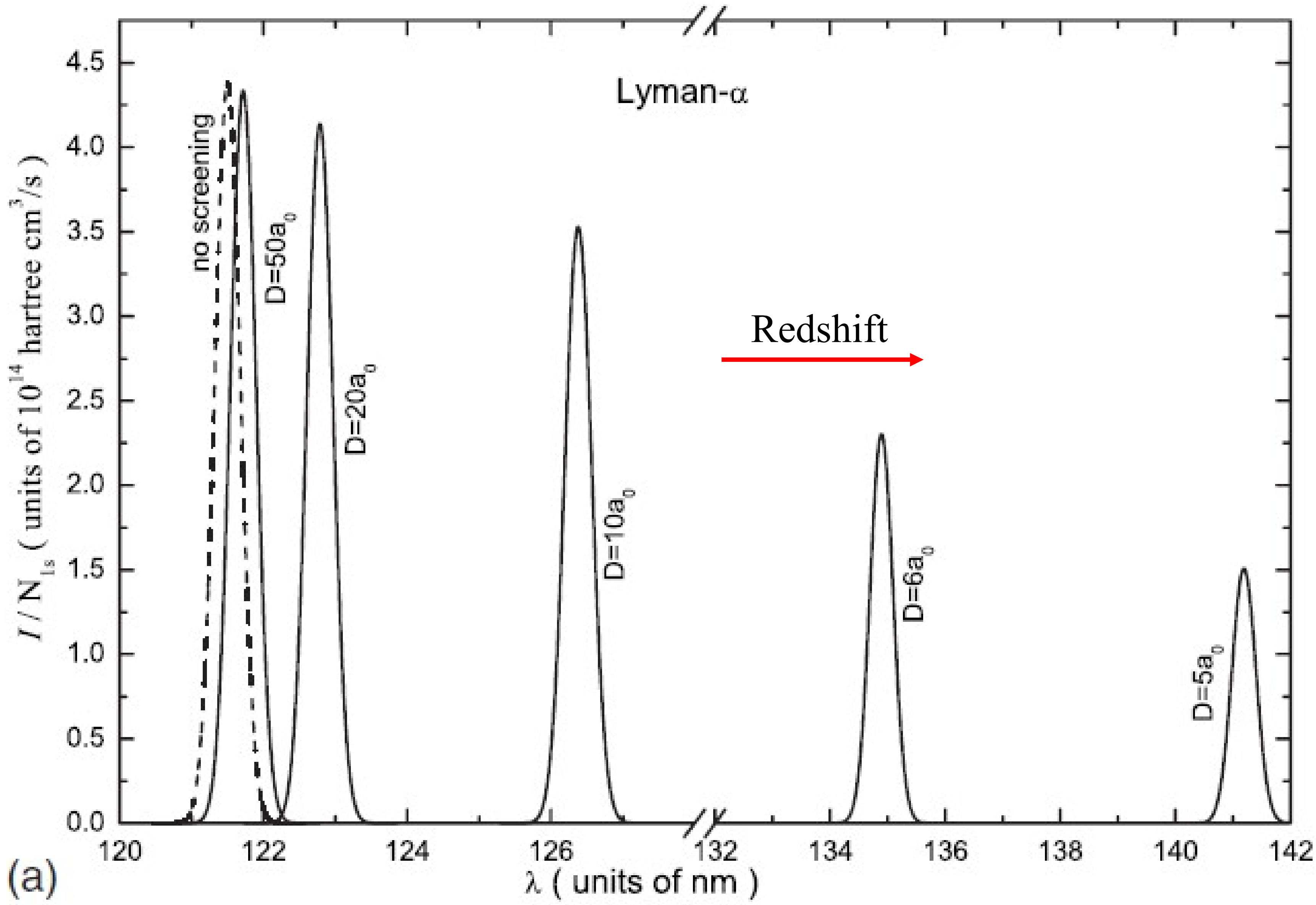
R.K. Janev, S.B. Zhang, and J.G. Wang, Matter and Radiation at Extremes **1**, 237 (2016).

Energy levels (Ryd) of H in Debye plasma



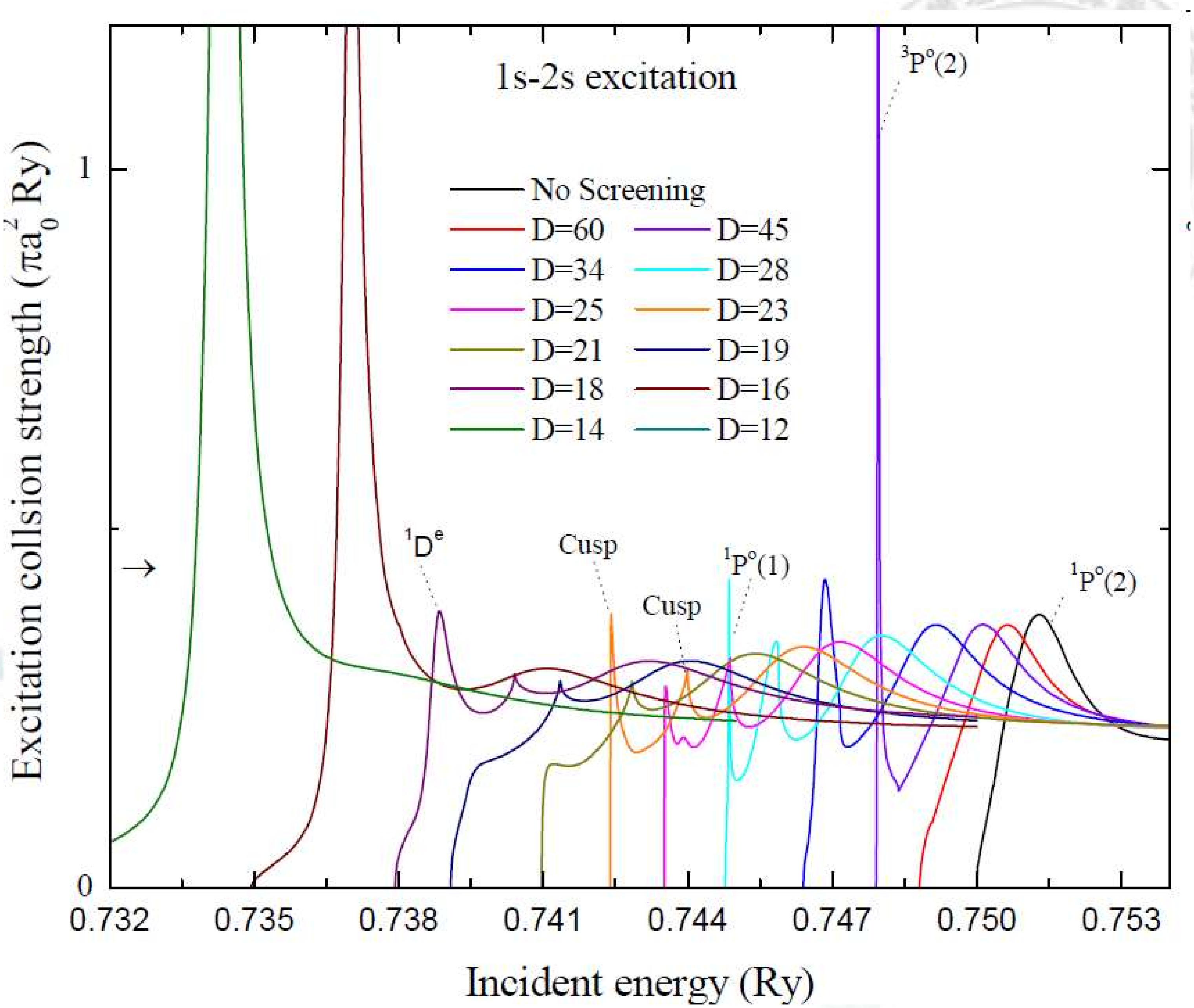
Critical Debye length: 0.8403, 3.2267, 4.54104 a.u.

Lyman-α emission spectra of hydrogen



Qi et al. Phys. Rev. A **78**, 062511 (2008)

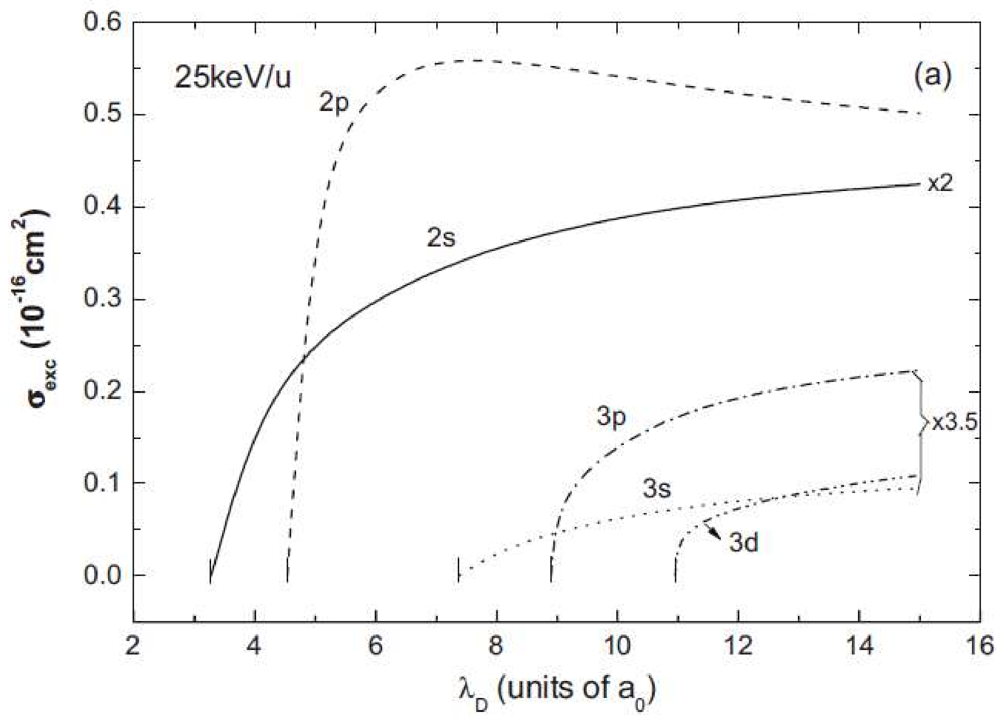
Low energy electron impact excitation of hydrogen



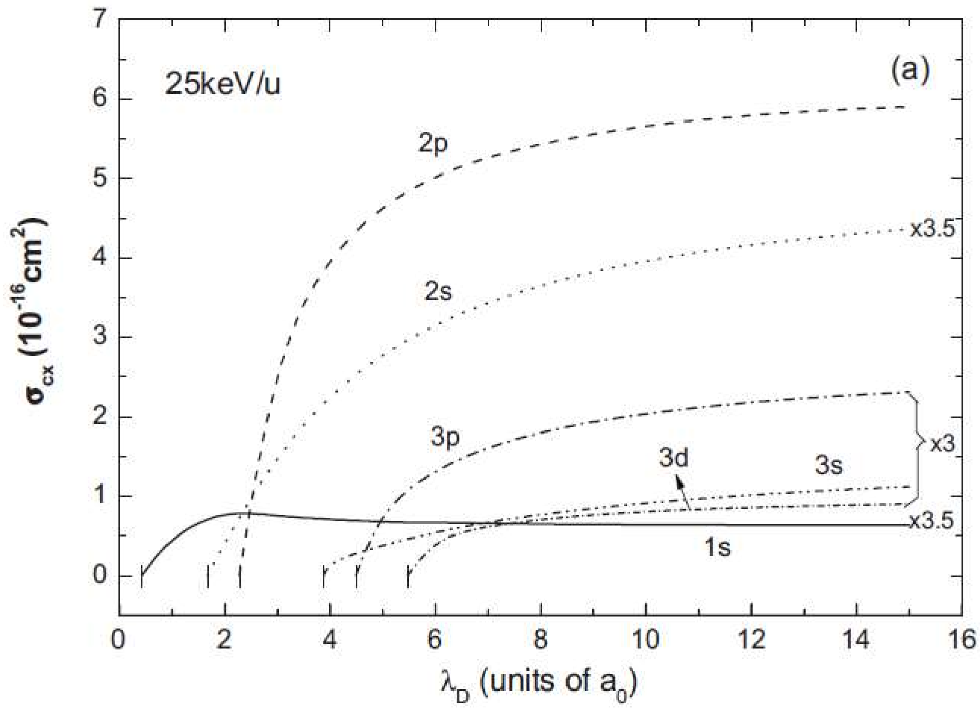
S.B. Zhang, J.G. Wang and R.K. Janev, Phys. Rev. Lett. **104**, 023203 (2010)

Heavy particle collisions: excitation & charge transfer

$$He^{2+} + H(1s) \rightarrow \begin{cases} He^{2+} + \ H(nl) & \text{excitation} \\ He^{+}(nl) + H^{+} & \text{charge transfer} \end{cases}$$



excitation



charge transfer

Liu et al. Phys. Rev. A **77**, 032709 (2008)

free-free absorption cross sections

$$\mathrm{d}\sigma_e^{ab} = a_0^2 Z^2 \frac{64}{3}\left(\frac{e^2}{\hbar c}\right)\left[\left(\frac{Ry}{\hbar\omega}\right)^3 \frac{d(\hbar\omega)}{Ry}\right] k_i k_f \sum_{l=0}^{\infty}\left[(l+1)\tau_{l+1\leftarrow l}^2 + l\tau_{l-1\leftarrow l}^2\right],$$

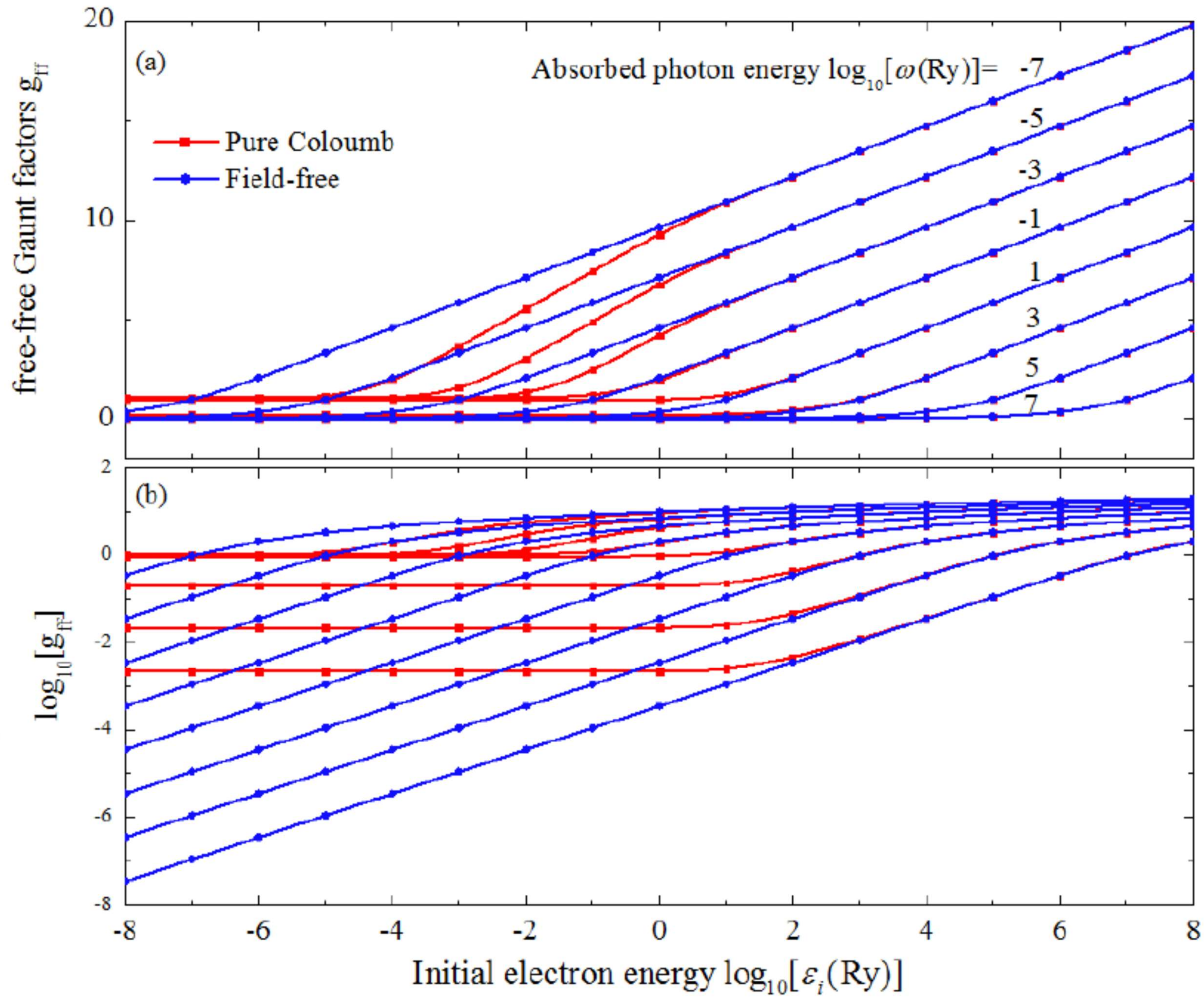
$$\varepsilon_f = \varepsilon_i + \hbar\omega \qquad \tau_{l'\leftarrow l} = \int_0^{\infty} r^2 \psi_{l'}^f(k_f r)\frac{1}{r^2}\psi_l^i(k_i r)dr$$

classical Kramers' cross sections

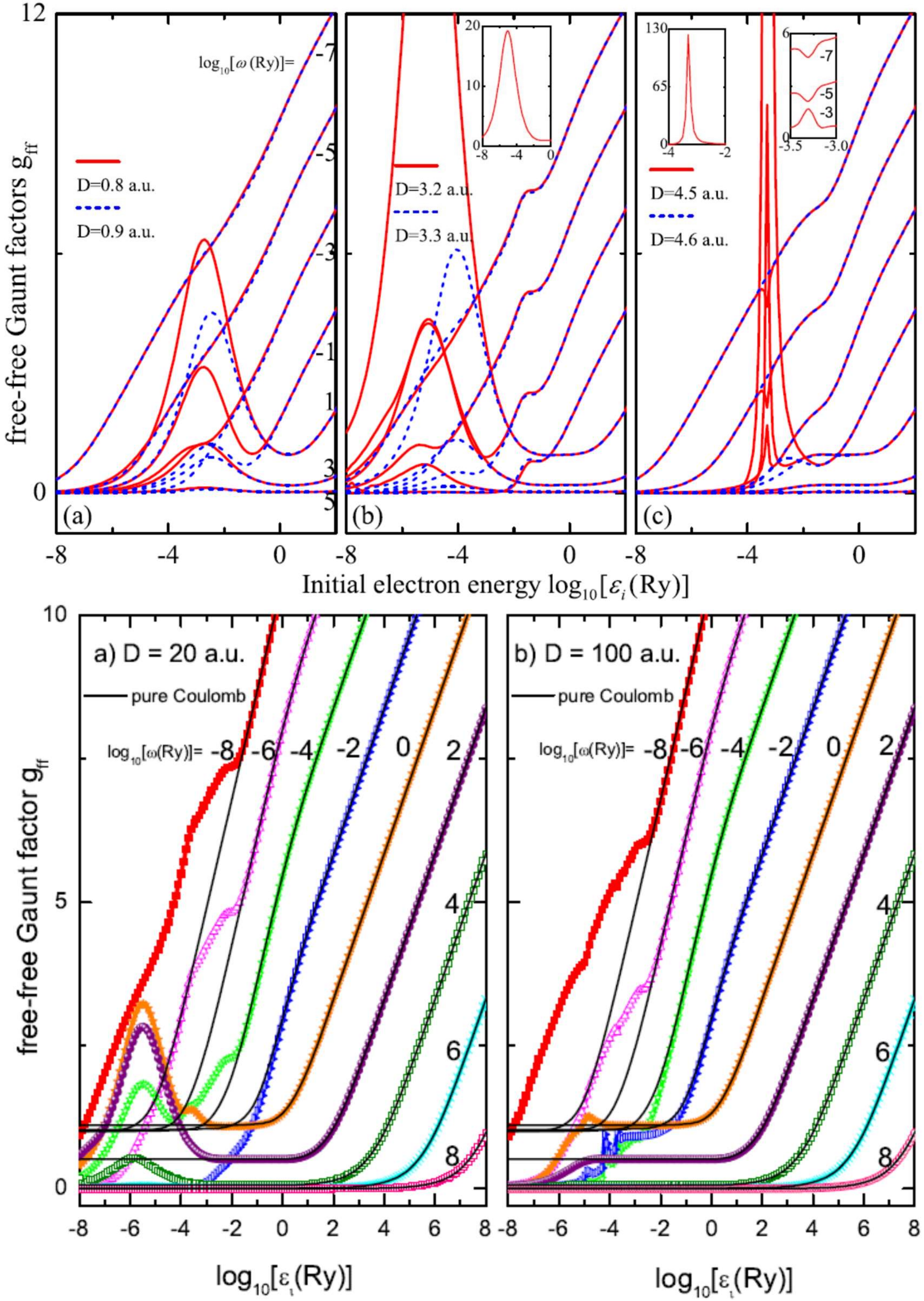
$$d\sigma_K = a_0^2 Z^2 \frac{32\pi}{3\sqrt{3}}\left(\frac{e^2}{\hbar c}\right)\left[\left(\frac{Ry}{\hbar\omega}\right)^3 \frac{d(\hbar\omega)}{Ry}\right].$$

free-free Gaunt factor

$$g_{ff}(\varepsilon_i,\omega) = \frac{\sigma_e^{ab}}{\sigma_K} = \frac{2\sqrt{3}}{\pi} k_i k_f \sum_{l=0}^{\infty}\left[(l+1)\tau_{l+1\leftarrow l}^2 + l\tau_{l-1\leftarrow l}^2\right].$$



Non-relativistic free-free absorption Gaunt factors for the pure Coulomb potential and field-free cases

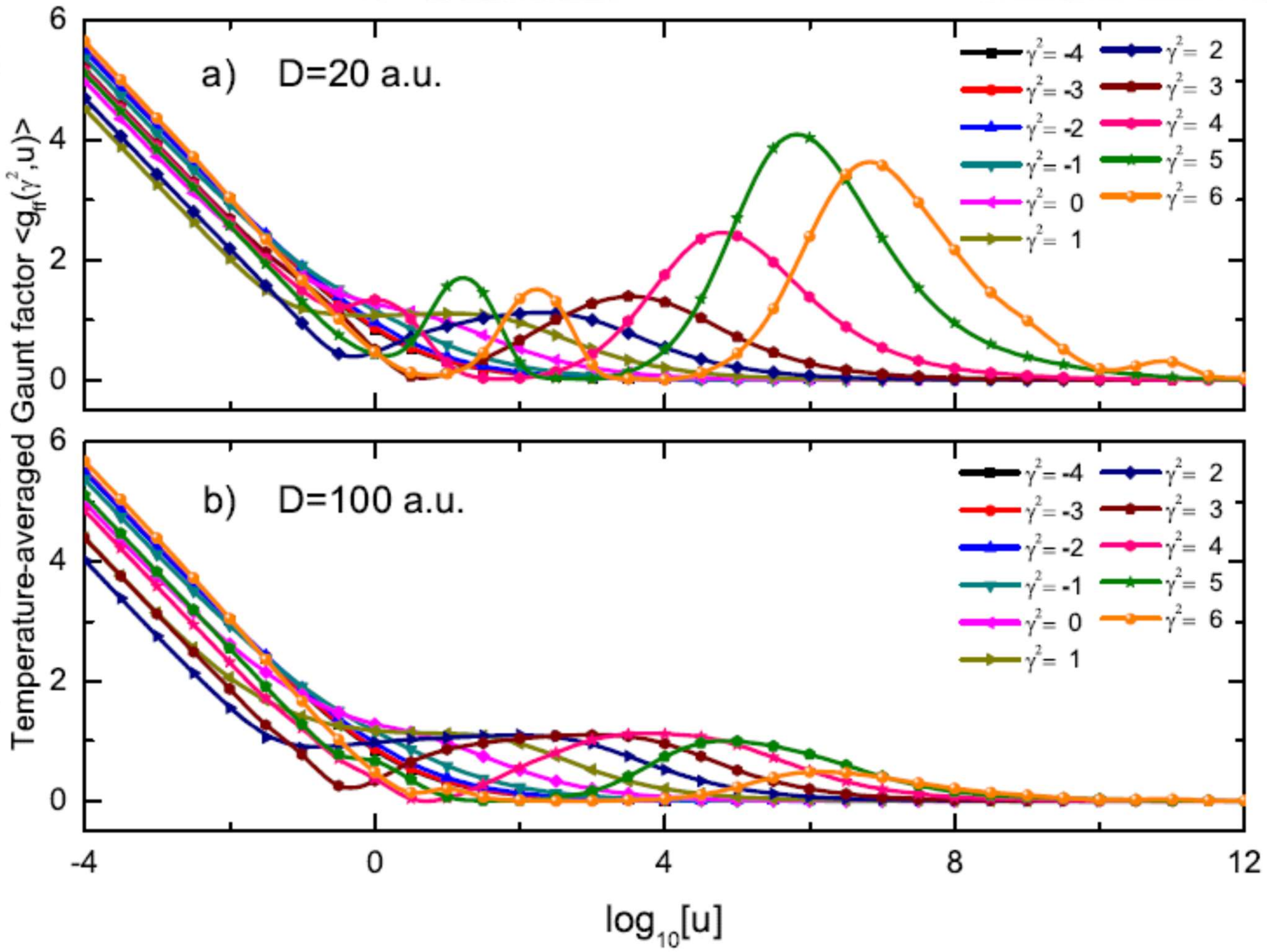


free-free absorption Gaunt factors for different screening lengths

Phys. Rev. A **99**, 012705 (2019)

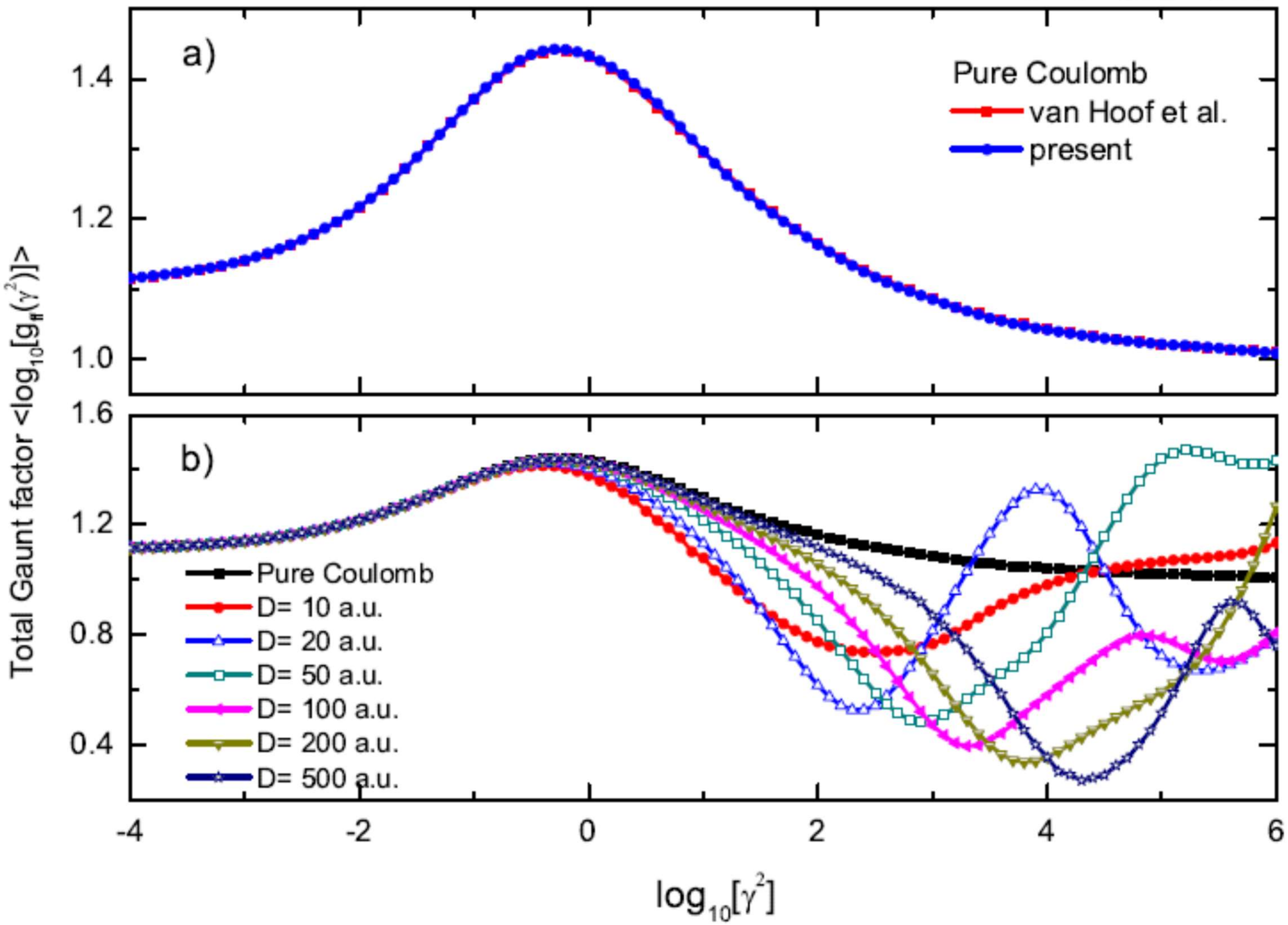
thermally averaged Gaunt factors

$$\left\langle g_{ff}\left(\gamma^2,u\right)\right\rangle = \int_0^\infty e^{-x} g_{ff}\left(\varepsilon_i = \frac{x}{\gamma^2}, \omega = \frac{u}{\gamma^2}\right) dx \qquad \gamma^2 = \frac{Z^2 Ry}{kT_e} \text{ and } u = \frac{h\nu}{kT_e}$$



Total thermally averaged Gaunt factors

$$\left\langle g_{ff}\left(\gamma^2\right)\right\rangle = \int_0^\infty e^{-u}\left\langle g_{ff}\left(\gamma^2,u\right)\right\rangle du$$



MNRAS (submitted)

Summary

Free-free Gaunt factors, (total) thermally averaged one in H Debye plasma have been numerically studied in the non-relativistic level.

Future works

different plasmas, relativistic level, different objects

Thanks for your attention!