The 1st IAEA Research Coordination Meeting on Data for Atomic Processes of Neutral Beams in Fusion Plasma , Vienna，June 19-21, 2017

State-resolved cross section calculations for excitation, ionization and charge transfer in collisions between hydrogen neutrals and the principal fully stripped impurity ions

Y. Wu[1], L. Liu[1], J. G. Wang[1] and S. B. Zhang[2]

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

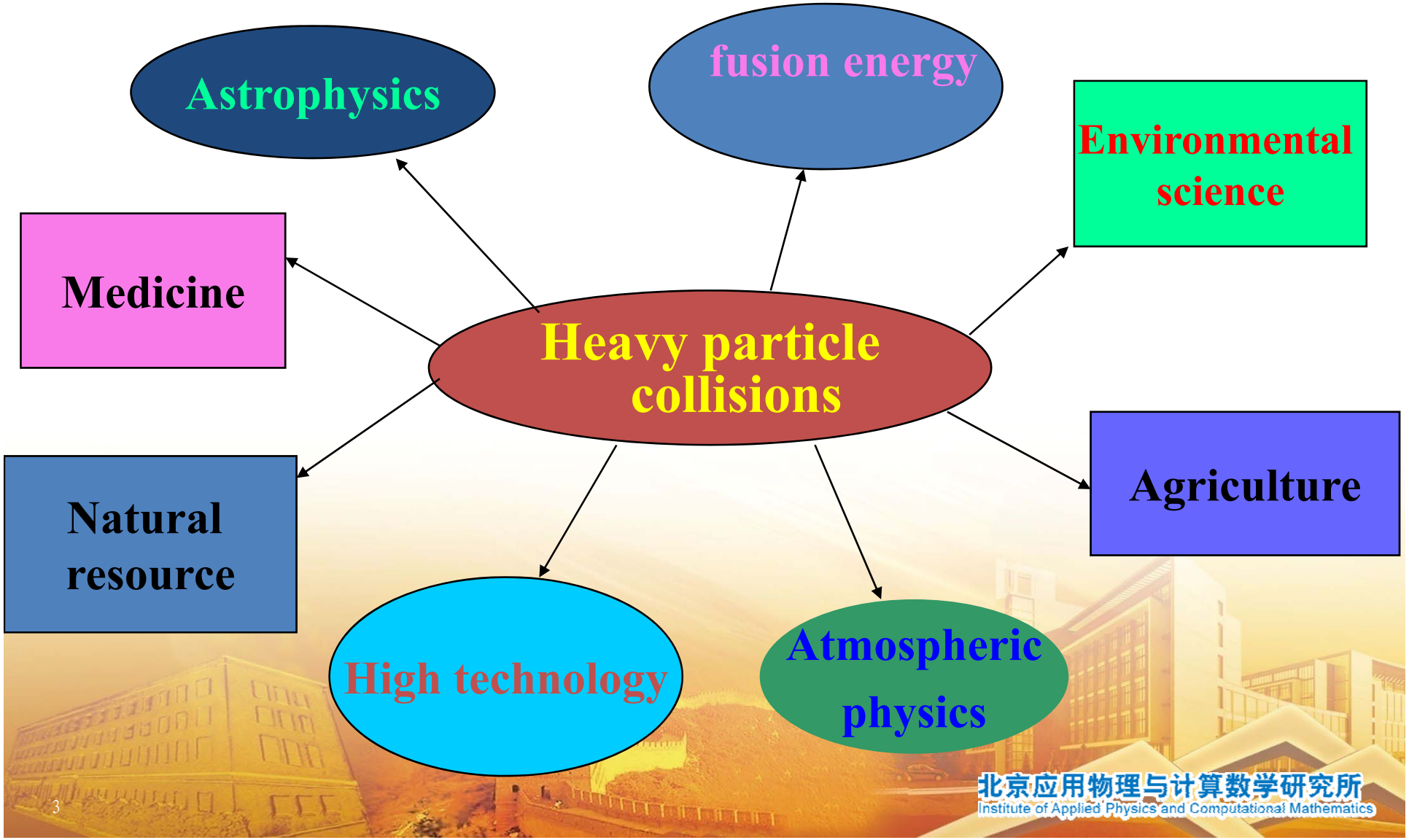
[2]*Shanxi Normal university, Xi'an, China*

北京应用物理与计算数学研究所
Institute of Applied Physics and Computational Mathematics

IAPCM

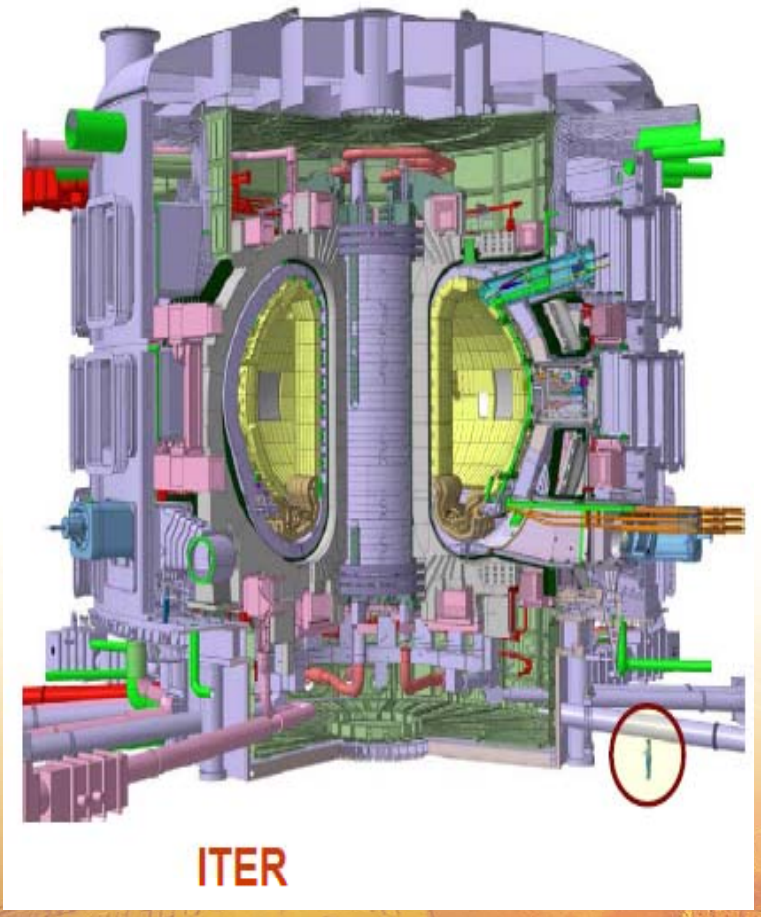
outline

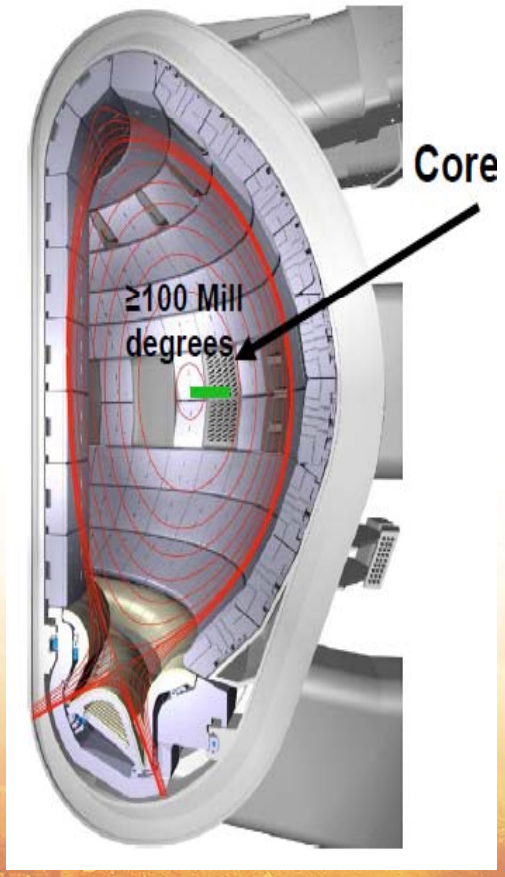
- Motivation
- Theoretical methods
- Scattering cross sections calculations
- X-ray spectra following highly charged ion-atom/molecule collisions
- Work plan


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

Divertor and core region in ITER

ITER – the biggest tokamak ever built





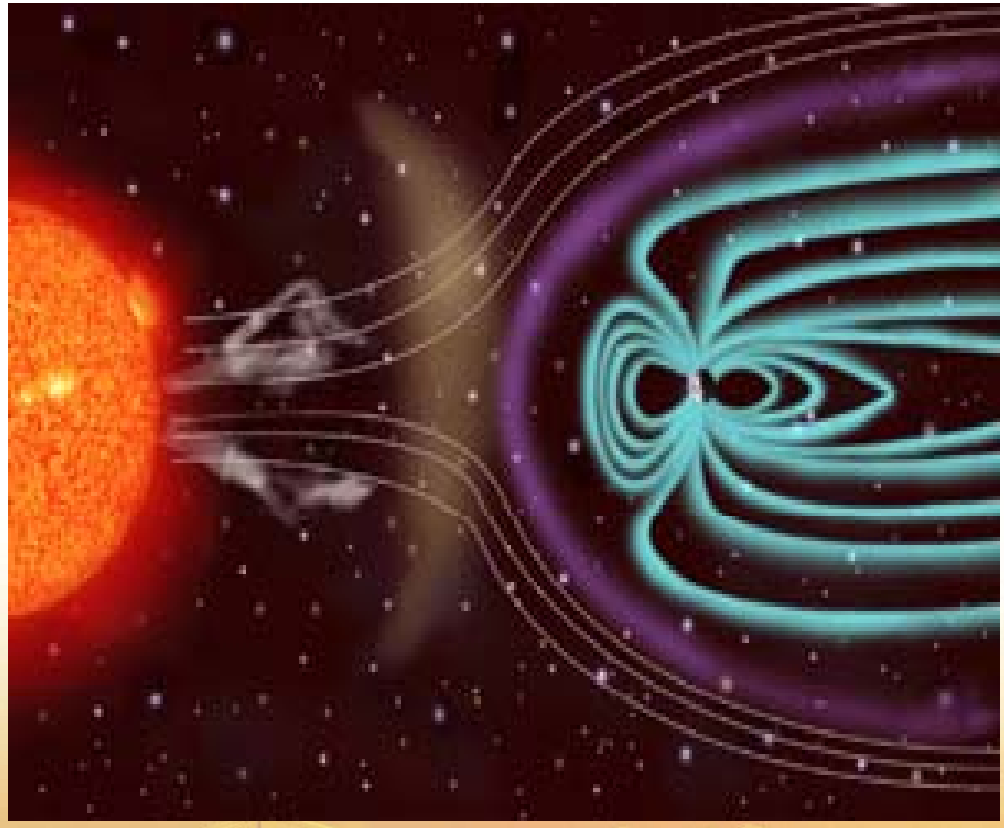
- All chemical bonds broken
- Impurity ions fully or highly stripped
- CX/ionization/recombination processes dominant

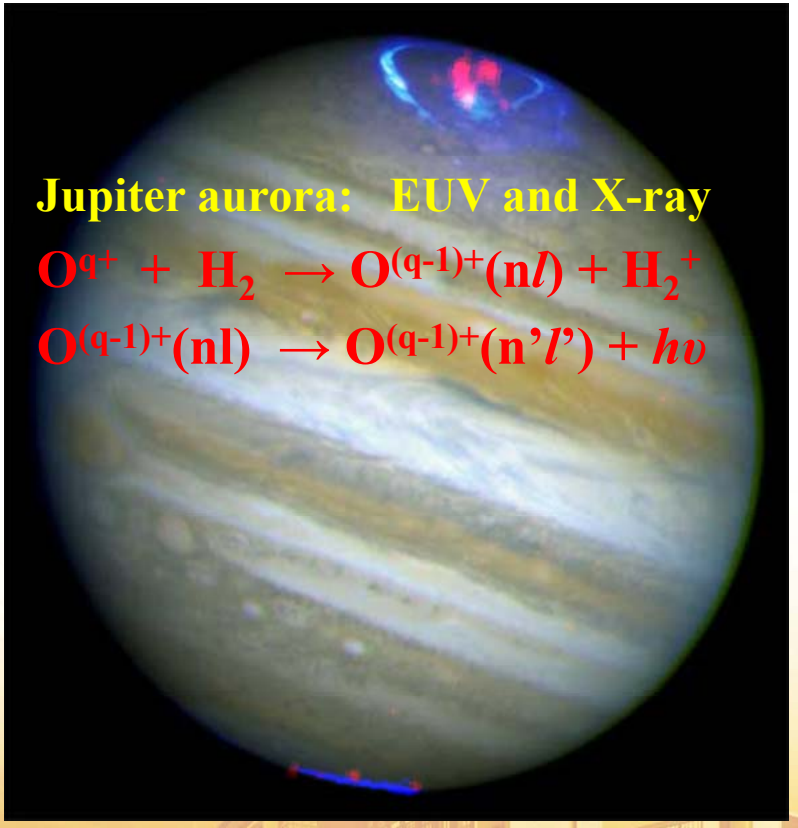
Atomic data models for hot plasma spectroscopy

- Interpretation
- Line shape modelling
- Diagnostics of the plasma condition

IAPCM

Jupiter aurora





北京应用物理与计算数学研究所
Institute of Applied Physics and Computational Mathematics

The study of charge transfer spectra

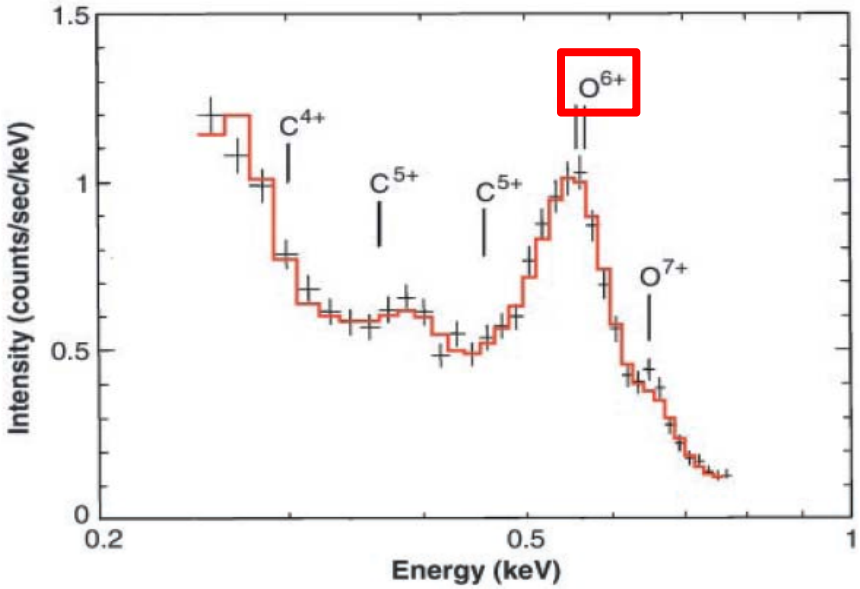


Fig. 2. Intensity versus photon energy. Soft x-ray spectrum of comet C/LINEAR 1999 S4 obtained on July 14, 2000, by the Chandra X-ray Observatory ACIS-S instrument. The solid red line is from a six-line best-fit "model" in which the line positions were fit parameters. The observational full-width half-maximum energy resolution was $\Delta E = .11$ keV. The positions of several transition lines from multiply charged ions known to be present in the solar wind are indicated but were not part of the data fit. Adapted from (*22*).

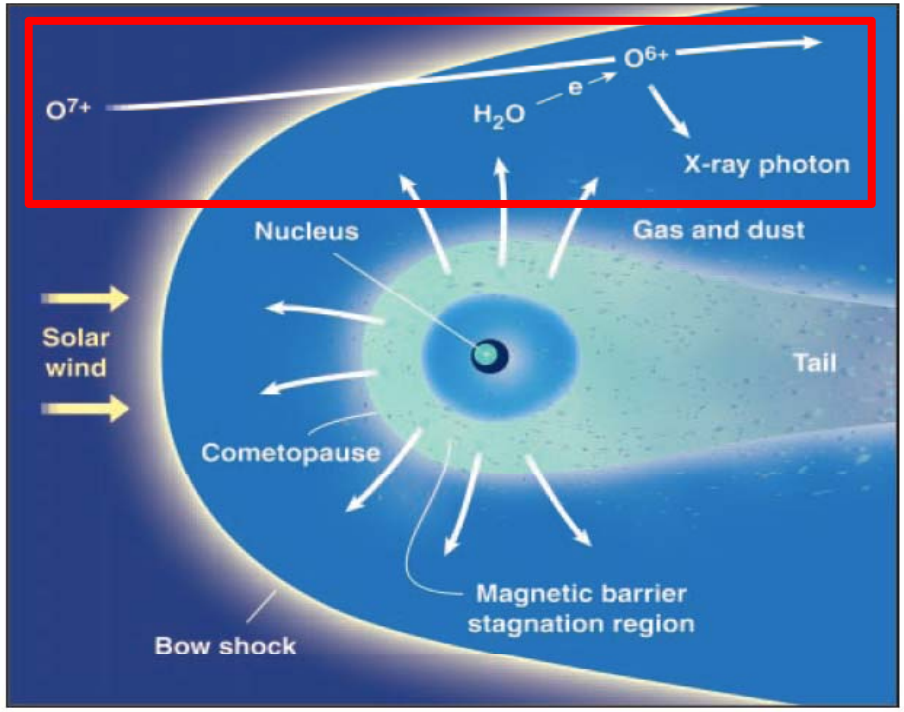


Fig. 3. Scheme of the solar wind/comet interaction. The location of the bow shock, magnetic barrier, and tail are shown. Also represented is a CT collision between a heavy solar wind ion and a cometary neutral water molecule, followed by the emission of an x-ray photon. The Sun is toward the left.

Science

AAAS

X-ray Emission from Comets
T. E. Cravens, *et al.*
Science **296**, 1042 (2002);
DOI: 10.1126/science.1070001

IAPCM

outline

- Motivation
- Theoretical methods
- Scattering cross sections calculations
- X-ray spectra following highly charged ion-atom/molecule collisions
- Work plan

IAPCM

Theoretical Methods

- **MOCC (Molecular orbital close-coupling)**
- **AOCC (Atomic orbital close-coupling)**
- TDDFT (Time-dependent DFT)
- TDSE (Time-dependent Schrödinger equation)
- MCTDH (Multi-reference time-dependent Hartree)
- CDW (Continuum distorted wave)
- CTMC (Classical orbital Monte-Carlo)
- MCLZ (Multi-channel Landau-Zener)

IAPCM

MOCC Method

- **Full quantum， appropriate for low energy collision $E \leq 10$ keV amu^{-1} ； electron correlation effect and multi-electron processes can be treated well.**
- **Structure calculations: potentials, couplings matrix element; MRDCI (the multi-reference single-and double-excitation configuration interaction method);**
- **Limitation on ionization treatment.**

Hamiltonian (diatomic molecules)

$$\mathbf{H}_{q_1 q_2}(\mathbf{R}) = [-\frac{1}{2\mu}\frac{\partial^2}{\partial R^2} + \frac{\mathbf{J}^2 - 2\mathbf{J}_z\mathbf{L}_z + \mathbf{L}_z^2}{2\mu R^2} + V_e^{q_2}(R)]\delta_{q_1,q_2}$$

$$-\frac{1}{\mu R^2}(\mathbf{J}_+ - \mathbf{J}_-) < \Psi_e^{q_1} \mid i\mathbf{L}_y \mid \Psi_e^{q_2} >$$

$$-\frac{1}{2\mu}(2 < \Psi_e^{q_1} \mid \frac{\partial}{\partial R} \mid \Psi_e^{q_2} > \frac{\partial}{\partial R} + < \Psi_e^{q_1} \mid \frac{\partial^2}{\partial R^2} \mid \Psi_e^{q_2} >)\delta_{\Lambda_{q_1}\Lambda_{q_2}}$$

$$\text{adiabatic} \rightarrow \text{diabatic} \qquad \mathbf{A}(R)\mathbf{C}(R) + \frac{\partial}{\partial R}\mathbf{C}(R) = 0$$

$$\overline{\mathbf{H}}_{q_1 q_2}(\mathbf{R}) = [-\frac{1}{2\mu}\frac{\partial^2}{\partial R^2} + \frac{\mathbf{J}^2 - 2\mathbf{J}_z\mathbf{L}_z + \mathbf{L}_z^2}{2\mu R^2}]\delta_{q_1,q_2} + \overline{V}_e(R) + \overline{V}_{q_1 q_2}^{C}(R)$$

$$\begin{cases} i\frac{\partial}{\partial t}\overline{\Psi}_N^{q,J}(\mathbf{R},t) = \overline{\mathbf{H}}_{q'q}(\mathbf{R})\overline{\Psi}_N^{q,J}(\mathbf{R},t) \\ \overline{\Psi}_N^{q,J}(\mathbf{R},t) = \phi_N^{q,J}(R,t)\overline{D}_{M,\Lambda_q}^{J}(\alpha,\beta,\gamma) \\ \overline{\Psi}_N^{q,J}(\mathbf{R},t=0) = \phi_N^{q_0,J_0}(R,t=0)\overline{D}_{M_0,\Lambda_{q_0}}^{J_0}(\alpha,\beta,\gamma) \end{cases}$$

IAPCM

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

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

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

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

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

AOCC method

- Two-center atomic orbital close-coupling (TC-AOCC) method
- The straight-line approximation for the relative nuclear motion $R(t) = \vec{b} + \vec{v}t$
- Atomic orbital basis
- Intermediate energy range

~100eV/amu < E < ~100 keV/amu

IAPCM

Schrödinger equation for the collision system:

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

$V_{A,B}(r_{A,B})$ are the interactions between the active electron and the targets (B) and the projectiles (A). We use the model potentials to describe the above interactions.

The total wave function for the collision system:

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

IAPCM

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

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

Slater type basis

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

Inserting $\Psi(\vec{r},t)$ into the Schrödinger equation, we can obtain the first-order coupled equations for the amplitude $a_i(t)$ and $b_j(t)$

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

S is the overlap matrix, H is direct coupling matrix and K is the electron exchange matrix.

$$S_{ji} = \int \phi_j^*(\vec{r}_B, t)\phi_i(\vec{r}_A, t)\exp(\mathrm{i}\vec{v}\cdot\vec{r})\,\mathrm{d}\vec{r},$$

$$H_{ii'} = \int \phi_i^*(\vec{r}_A, t)\phi_{i'}(\vec{r}_A, t)V_B(r_B)\,\mathrm{d}\vec{r}_A,$$

$$\bar{H}_{jj'} = \int \phi_j^*(\vec{r}_B, t)\phi_{j'}(\vec{r}_B, t)V_A(r_A)\,\mathrm{d}\vec{r}_B,$$

$$K_{ij} = \int \phi_j^*(\vec{r}_B, t)\phi_i(\vec{r}_A, t)\exp(\mathrm{i}\vec{v}\cdot\vec{r})V_B(r_B)\,\mathrm{d}\vec{r},$$

$$\bar{K}_{ij} = \int \phi_j(\vec{r}_B, t)\phi_i^*(\vec{r}_A, t)\exp(-\mathrm{i}\vec{v}\cdot\vec{r})V_A(r_A)\,\mathrm{d}\vec{r}.$$

IAPCM

The above equations can be solved under the initial conditions: $a_i(-\infty) = \delta_{1i}, b_j(-\infty) = 0$

The cross sections for the excitation, charge transfer and ionization processes are calculated as:

$$\sigma_{exc,i} = 2\pi \int_0^\infty |a_i(+\infty)|^2 \, bdb$$

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

$$\sigma_{ion} = \sigma_{ion}^{tc} + \sigma_{ion}^{pc}$$

$$\sigma_{ion}^{tc} = 2\pi \int_0^\infty |a_i^c(+\infty)|^2 \, bdb$$

$$\sigma_{ion}^{pc} = 2\pi \int_0^\infty |b_j^c(+\infty)|^2 \, bdb$$

X-ray spectra

$$A^{q+} + B \rightarrow A^{(q-1)+}(nl) + B^{+}$$
$$\downarrow \quad h\nu : emission$$
$$A^{(q-1)+}(n'l') + B^{+}$$

Line intensity:

$$I^{\nu}_{nl\rightarrow n'l'}(E_{\nu}) = [N^{\nu}_{nl\rightarrow n'l'} / (N^{P} N^{T})] \frac{1}{\sqrt{2\pi}\Gamma} \exp\left[-\frac{(E_{\nu} - E_{\nu_0})^2}{\Gamma^2} \right]$$

$$N^{\nu}_{nl,n'l'} = N^{P} N^{T} \nu B_{nl,n'l'} (\sigma_{nl} + \sum_{n''>n} C_{n''l'',nl} \sigma_{n''l''})$$

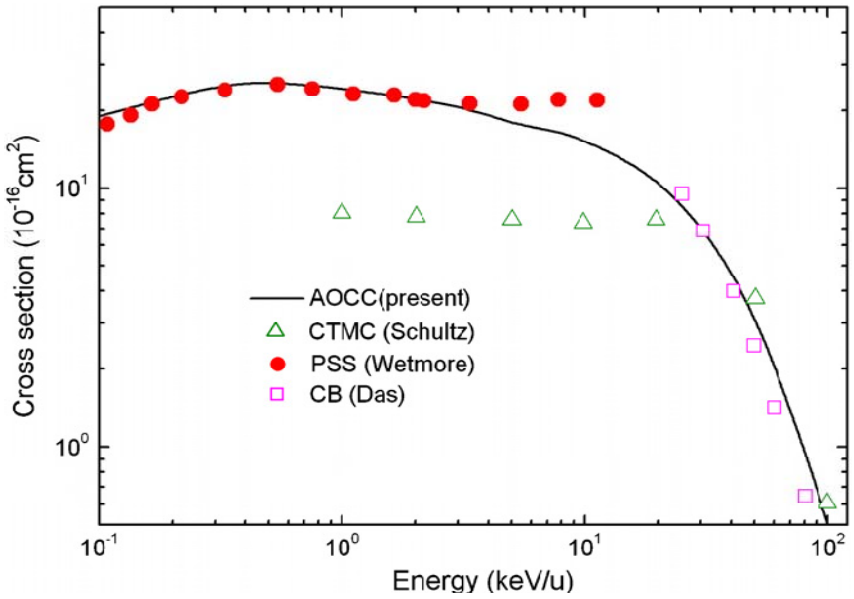
IAPCM

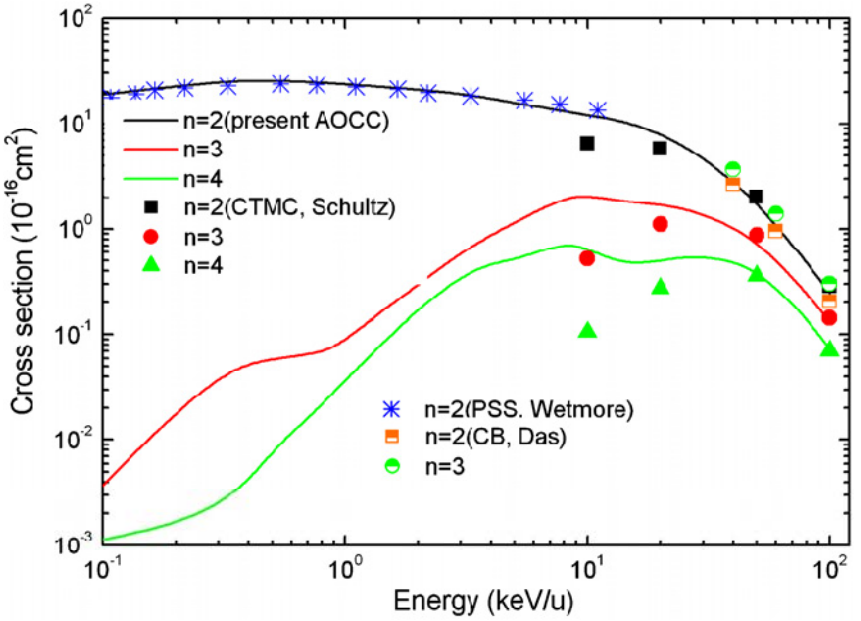
outline

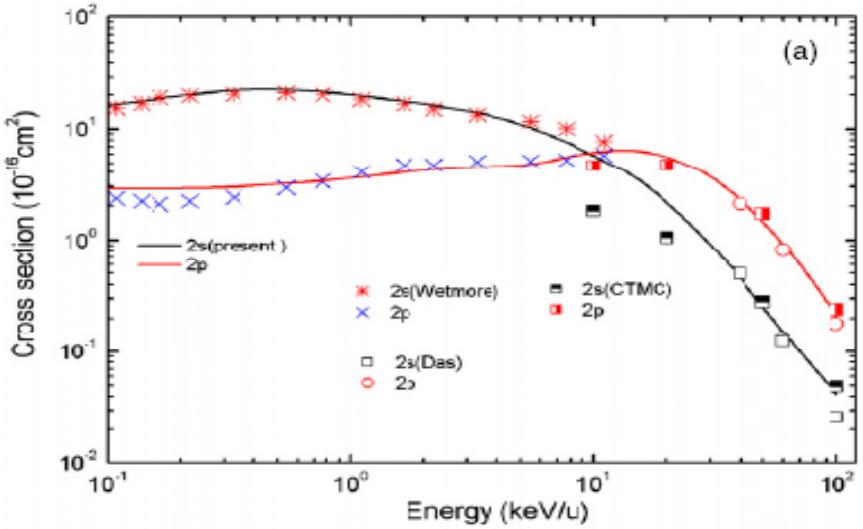
- Motivation
- Theoretical methods
- Scattering cross sections calculations ←
- X-ray spectra following highly charged ion-atom/molecule collisions
- Work plan

Ion-atom/molecule (ground state) collisions

$Be^{2+}+H(1s)\rightarrow Be^{+}(1s^2nl)+H^{+}$: AOCC





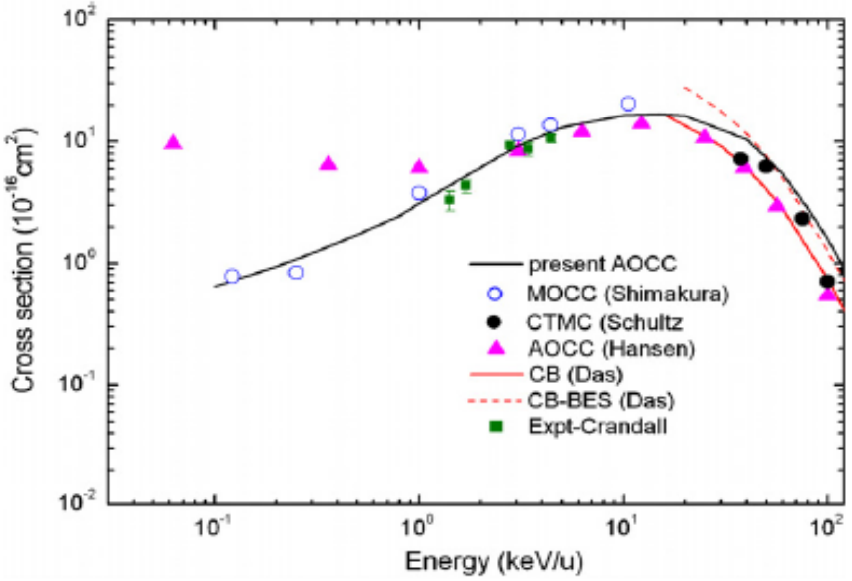


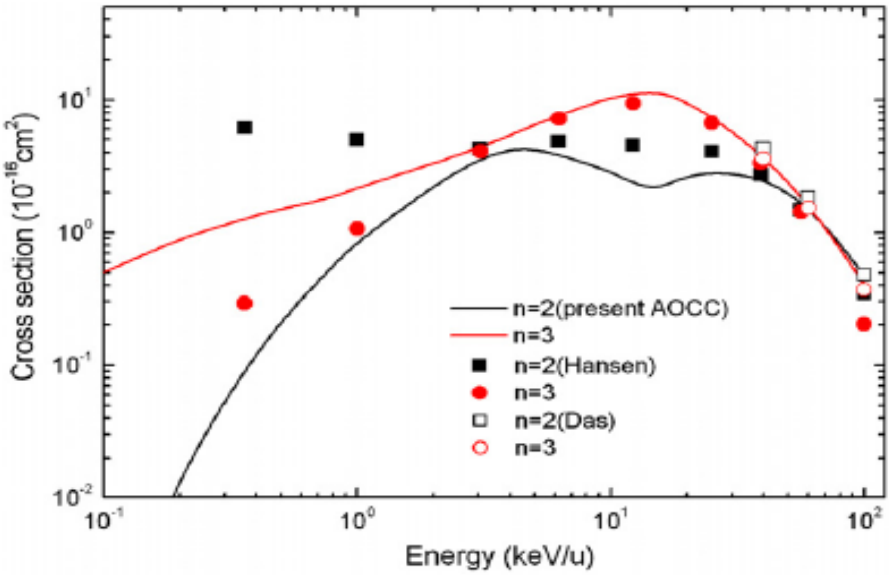
Model potential:

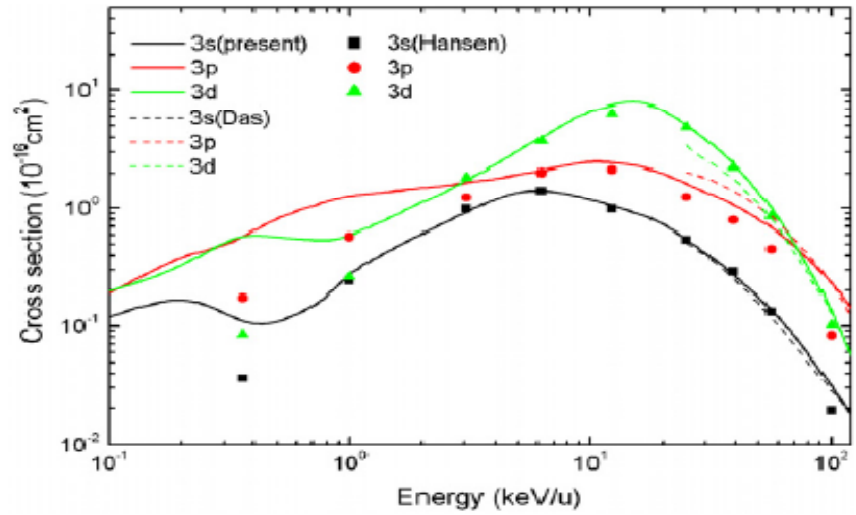
$$V_{Be^{2+}}(r) = -\frac{2}{r} - \frac{2}{r}(1+1.7308r)e^{-4.3792r}$$

L. Liu, *et al*, J. P. B 43, 144005 (2010)

$B^{3+}+H(1s)\rightarrow B^{2+}(1s^2nl)+H^{+}$: AOCC







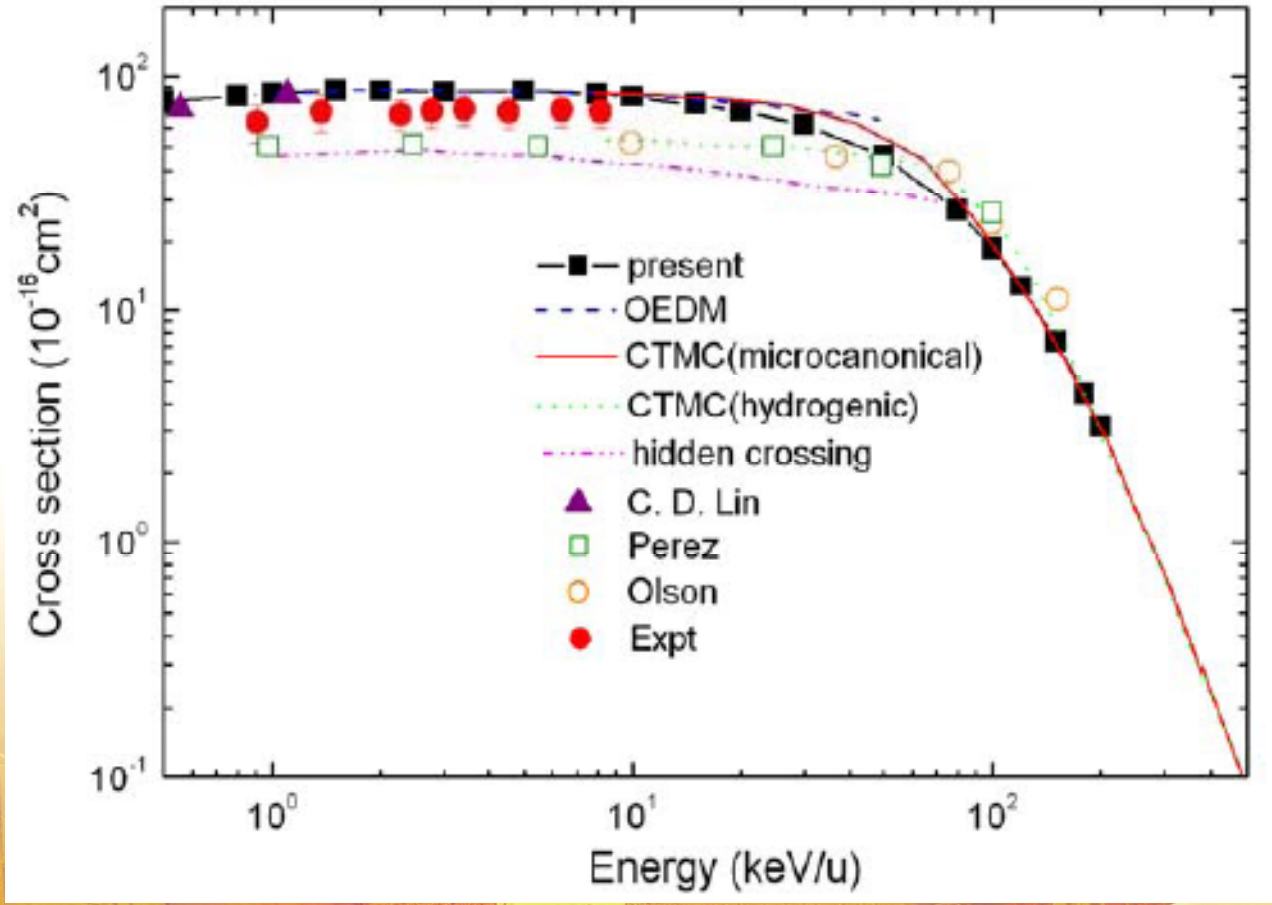
Model potential:

$$V_{B^{3+}}(r) = -\frac{3}{r} - \frac{2}{r}(1+3.04085r)e^{-6.0817r}$$

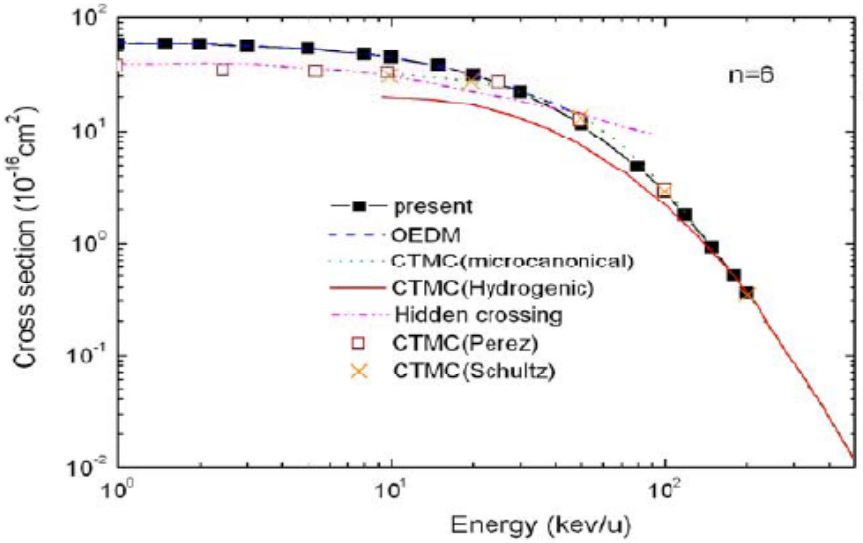
L. Liu, *et al*, J. P. B 43, 144005 (2010)

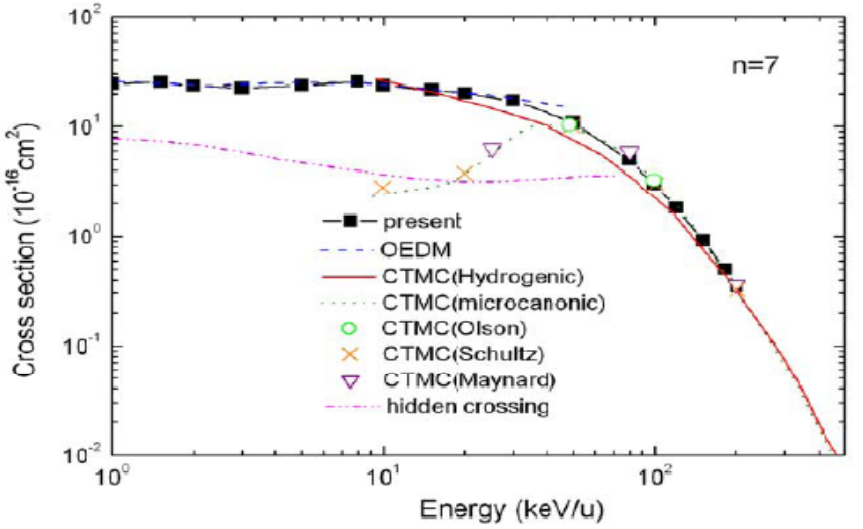
$$Ne^{10+} + H(1s) \rightarrow Ne^{9+}(nl) + H^{+}$$

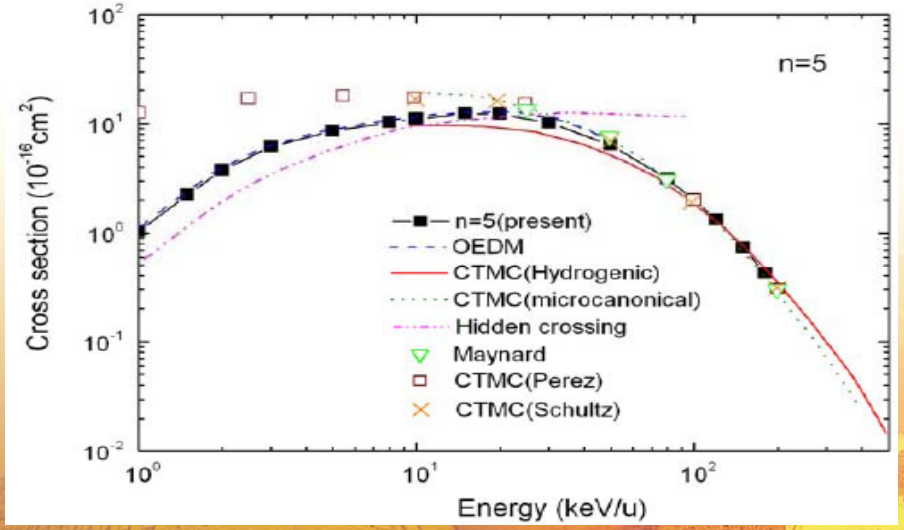
Total charge transfer cross section: AOCC

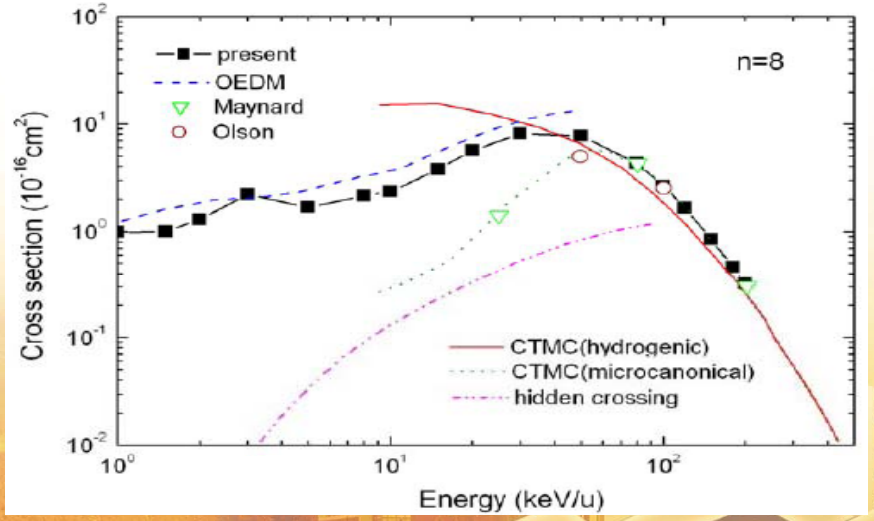


n-state-selective cross section: AOCC





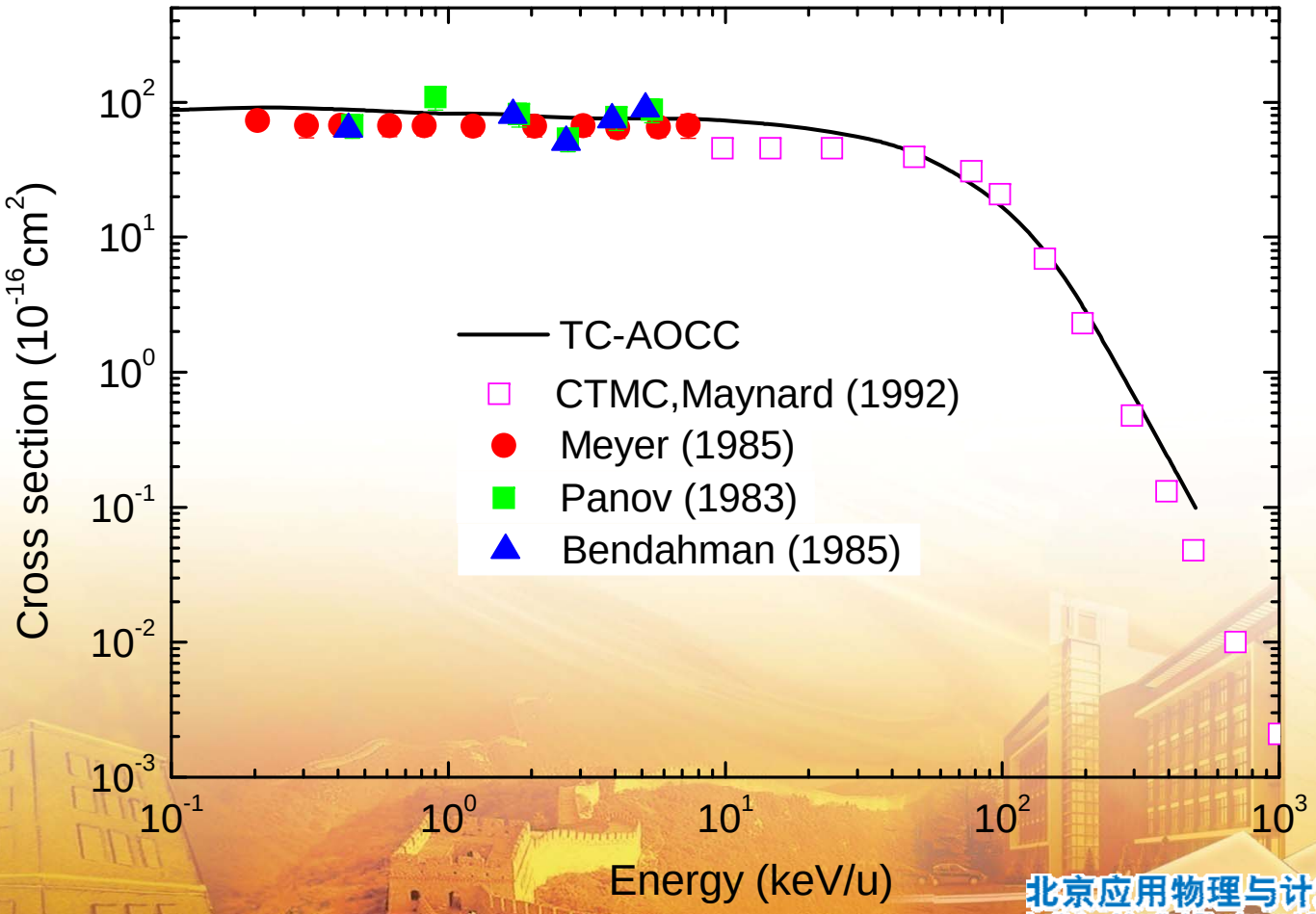




IAPCM

$$Ne^{9+}(1s)+H(1s)\rightarrow Ne^{8+}(1snl)+H^{+}$$

Total charge transfer cross section: AOCC

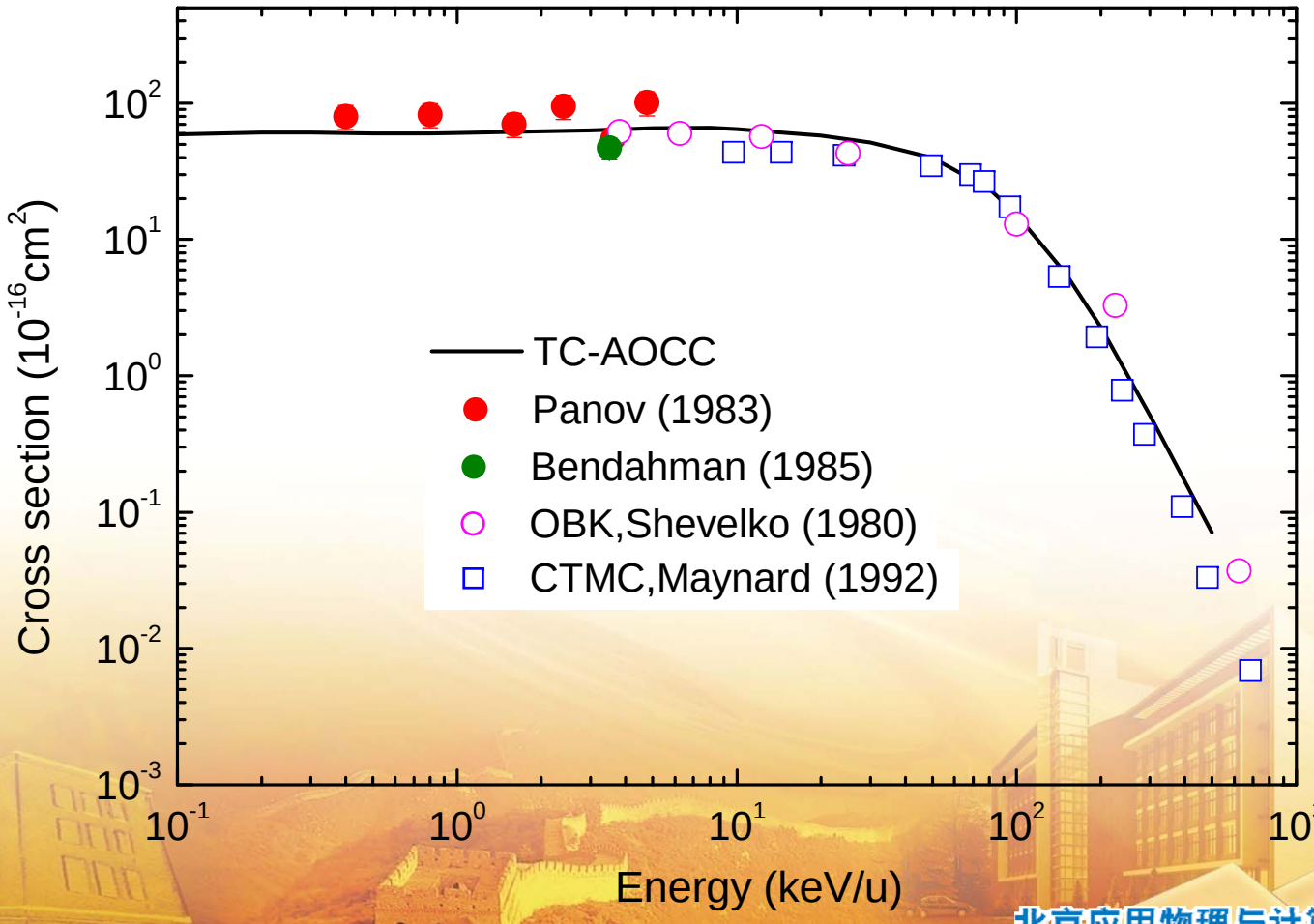


北京应用物理与计算数学研究所
Institute of Applied Physics and Computational Mathematics

IAPCM

$$Ne^{8+}(1s^2)+H(1s)\rightarrow Ne^{7+}(1s^2nl)+H^+$$

Total charge transfer cross section: AOCC



北京应用物理与计算数学研究所
Institute of Applied Physics and Computational Mathematics

Ion-atom collisions: AOCC&MOCC

$$C^{5+}(1s)+H(1s)\rightarrow C^{4+}(1snl)+H^{+}$$

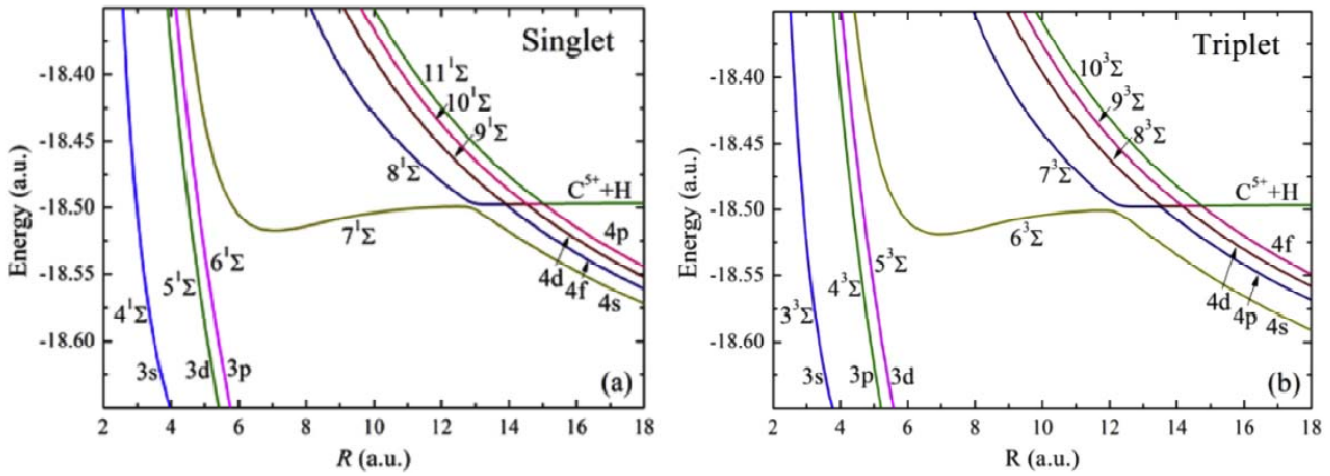
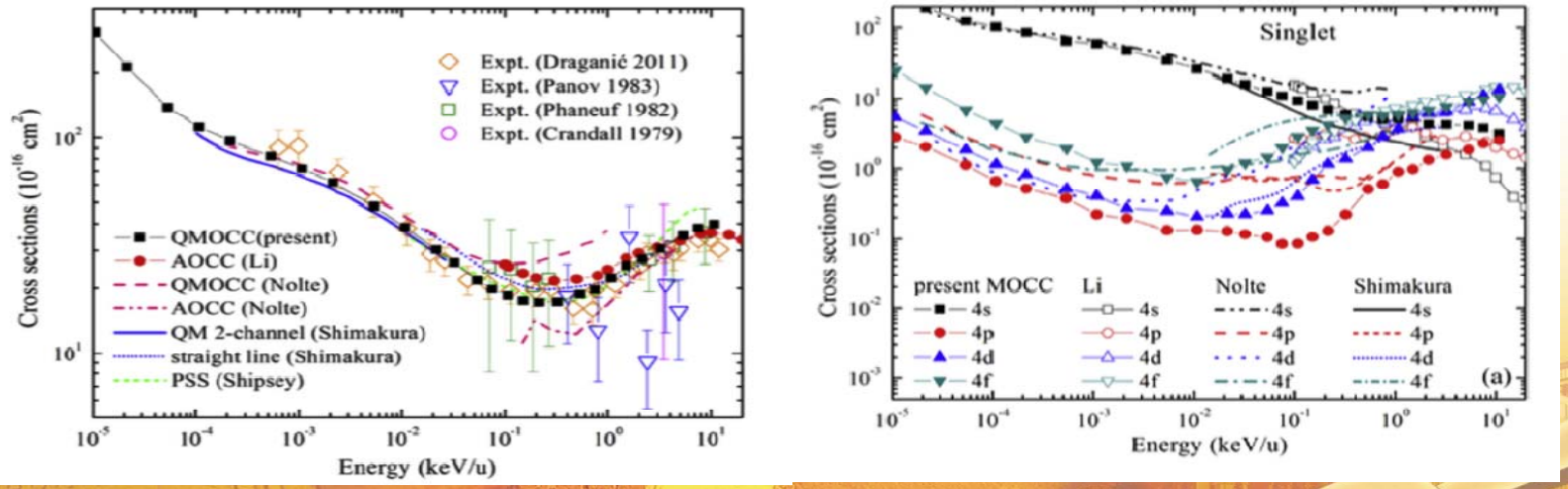
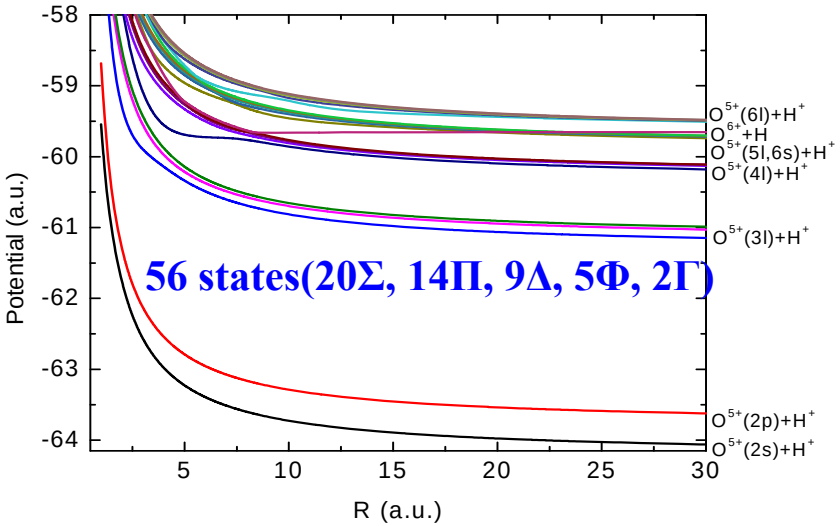


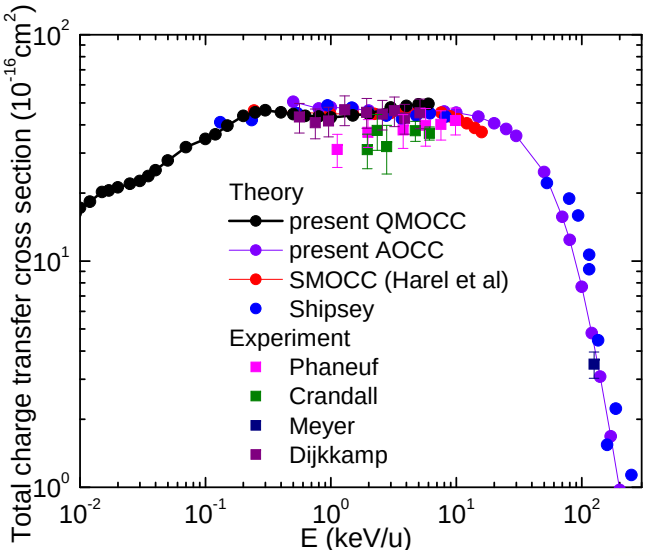
Figure 2. Enlarged view of adiabatic energies for Σ states. (a) Singlet states; (b) triplet states.

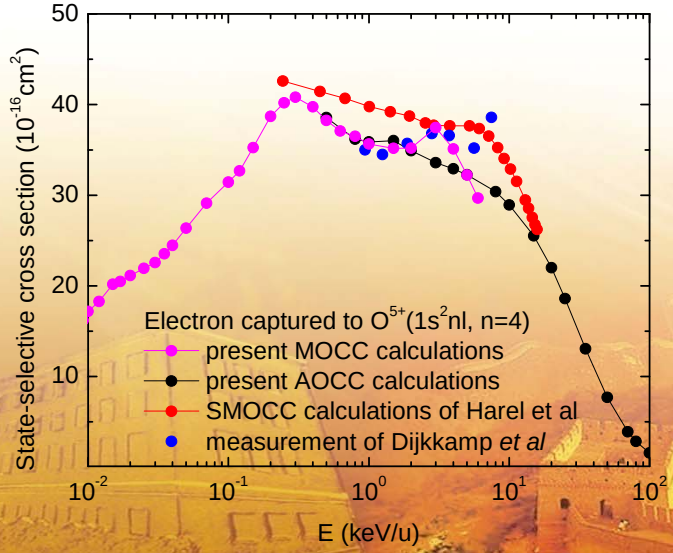


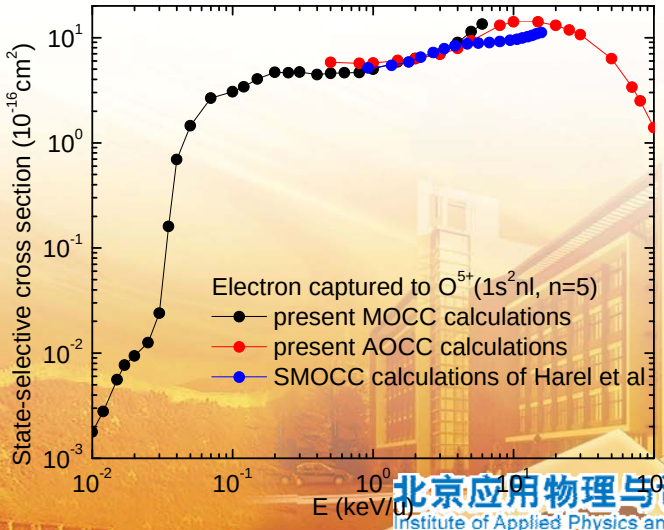
C.H. Liu et al, JPB (2016)

$O^{6+}(1s^2)+H(1s) \rightarrow O^{5+}(1s^2nl)+H^+$: AOCC&MOCC



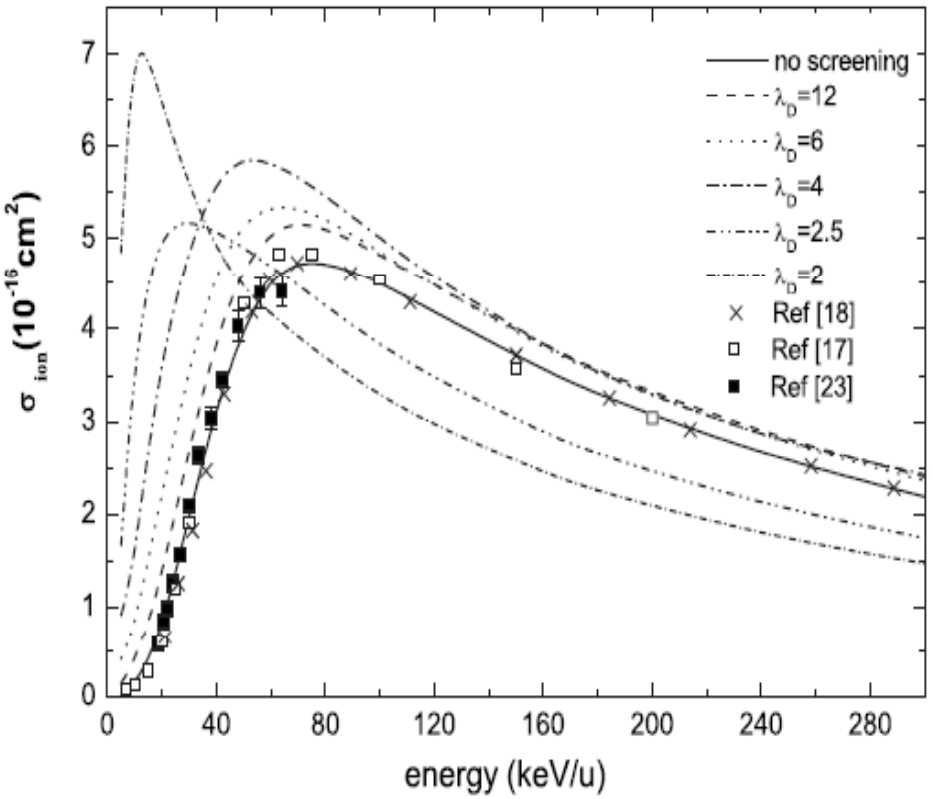






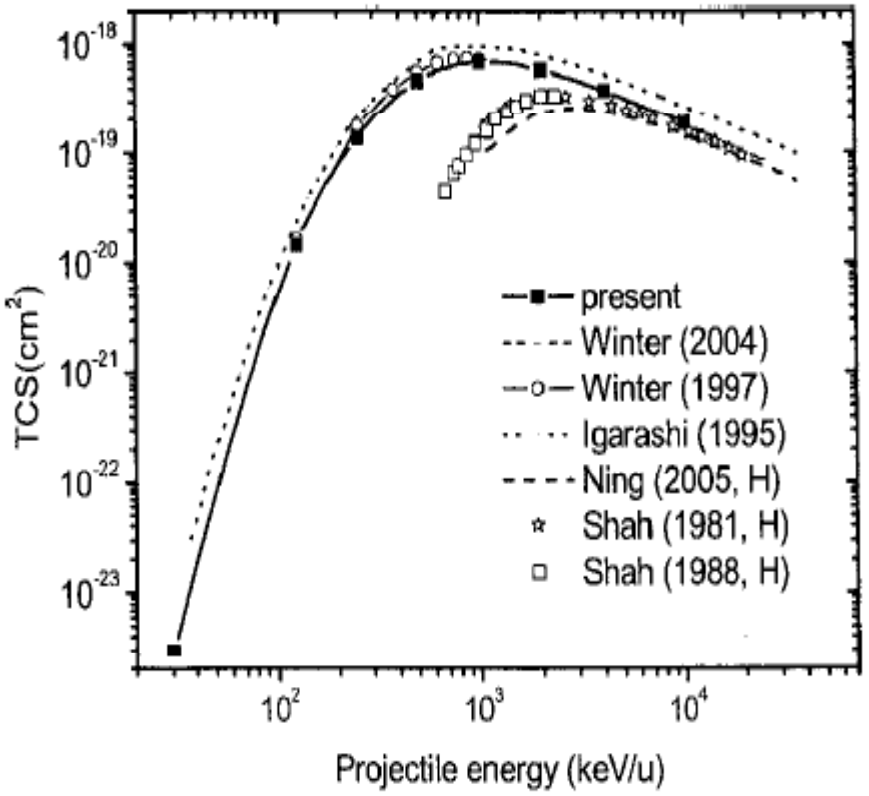
Ion-atom ionization: AOCC&CDW

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



PHYSICAL REVIEW A 77, 042712 (2008)

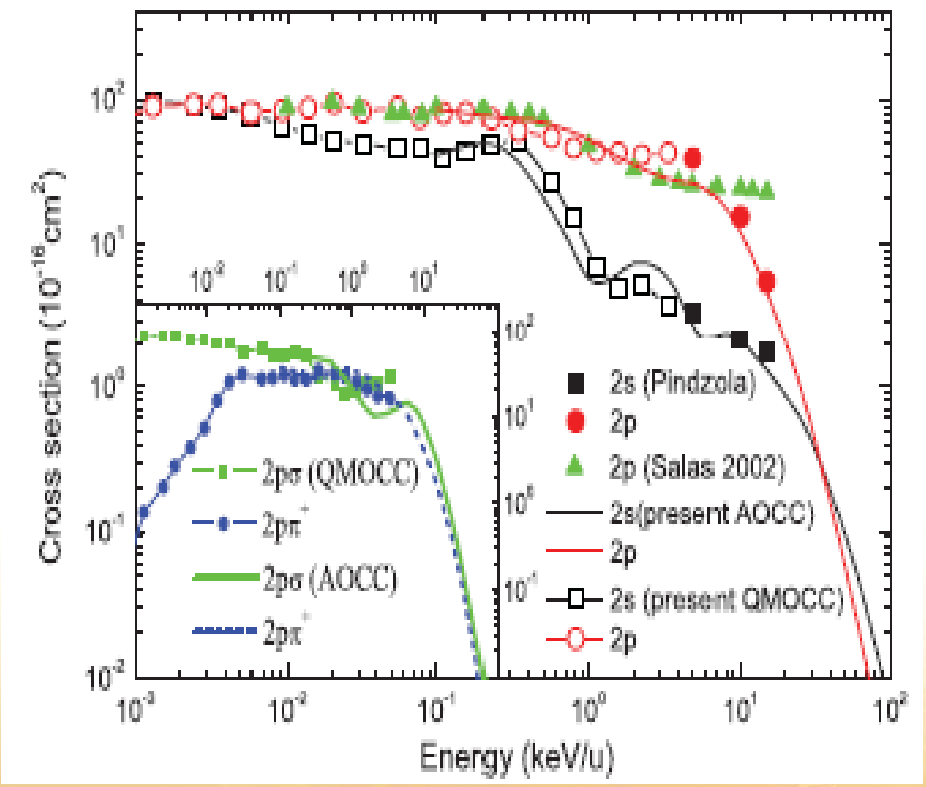
$$He^{2+} + C^{5+}(1s) \rightarrow He^{2+} + C^{6+} + e$$



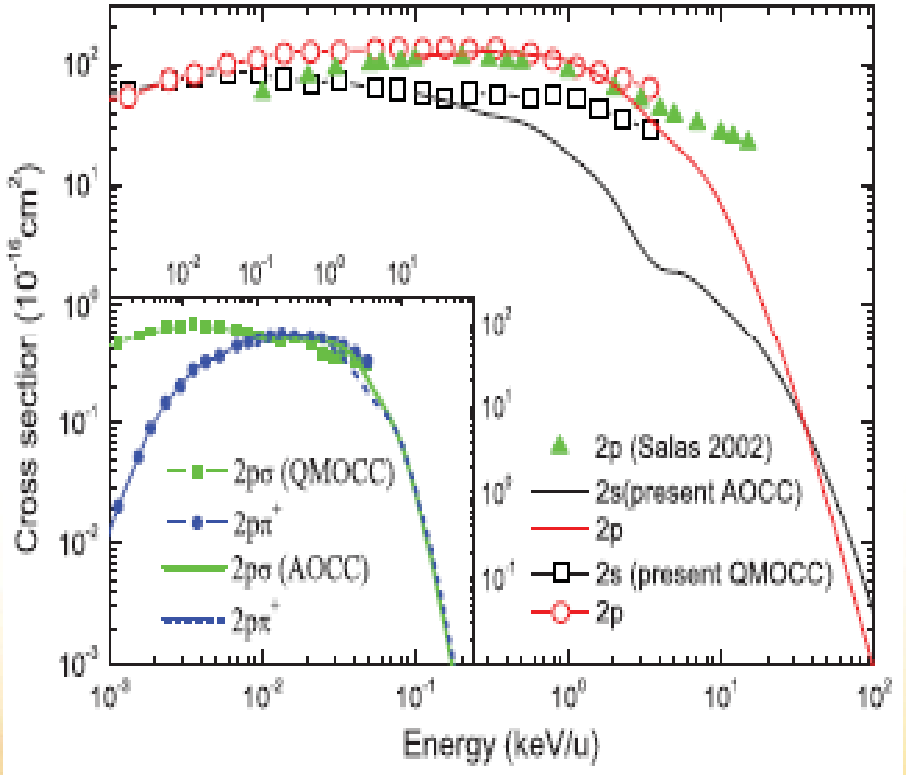
PHYSICAL REVIEW A 72, 022702 (2005)

Ion-atom (excited state) collisions: AOCC&MOCC

$$H^+ + Li(2p\sigma, \pi^{\pm}) \rightarrow H(2l) + Li^+$$



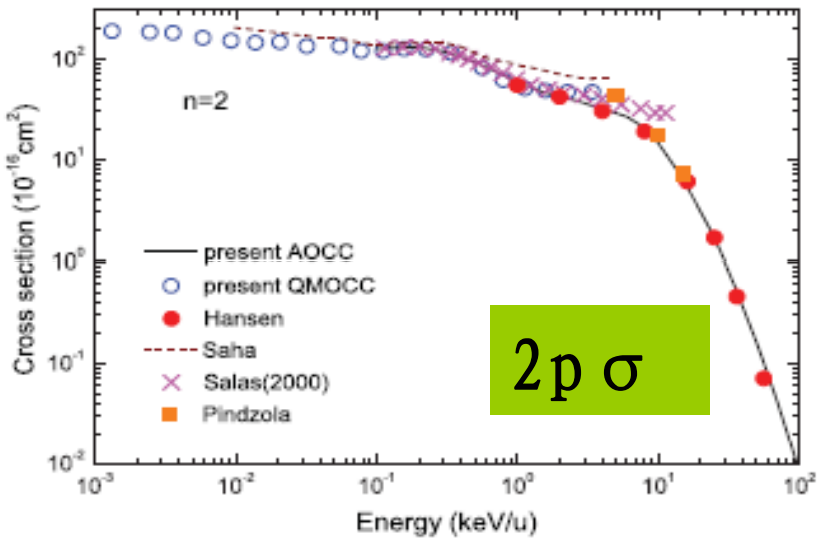
H$^+$-Li(2pσ)

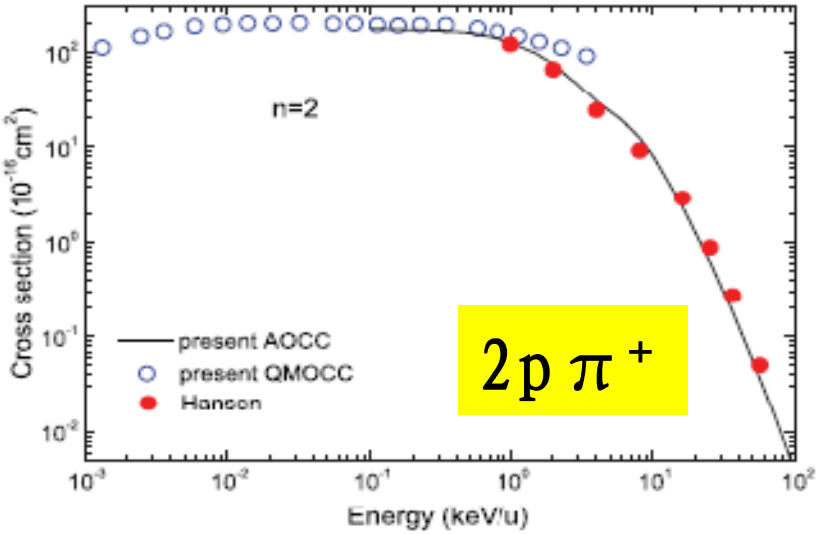


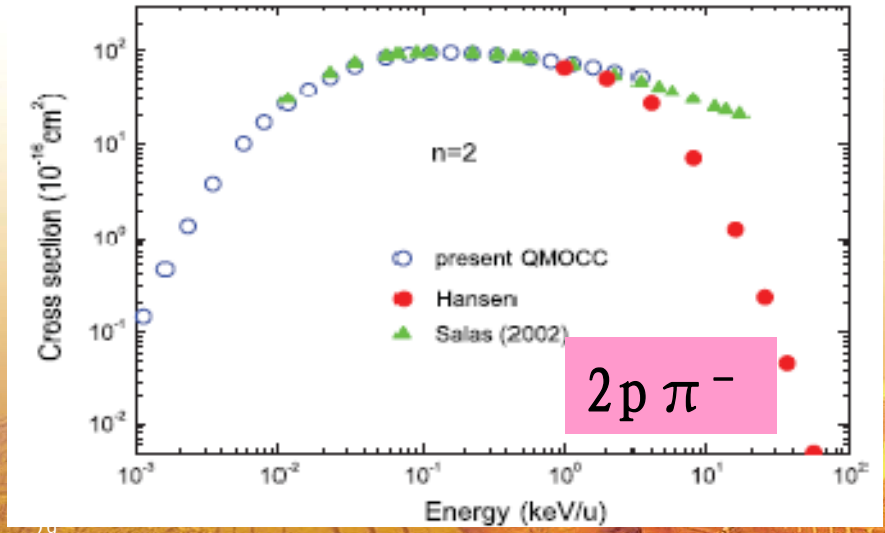
H$^+$-Li(2pπ$^+$)

L. Liu et al, Phys. Rev. A 84, 032710 (2011)

$$H^+ + Li(2p\sigma, \pi^{\pm}) \rightarrow H(n=2) + Li^+$$







- **A strong alignment dependence on the initial state is found for electron capture cross sections at low energies.**

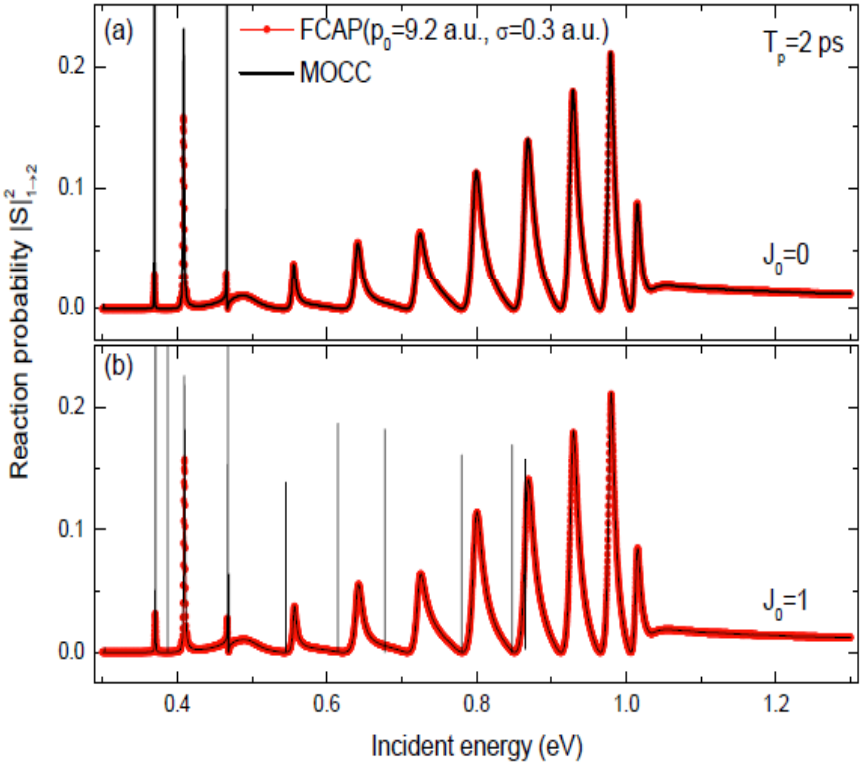
L. Liu et al, Phys. Rev. A 84, 032710 (2011)

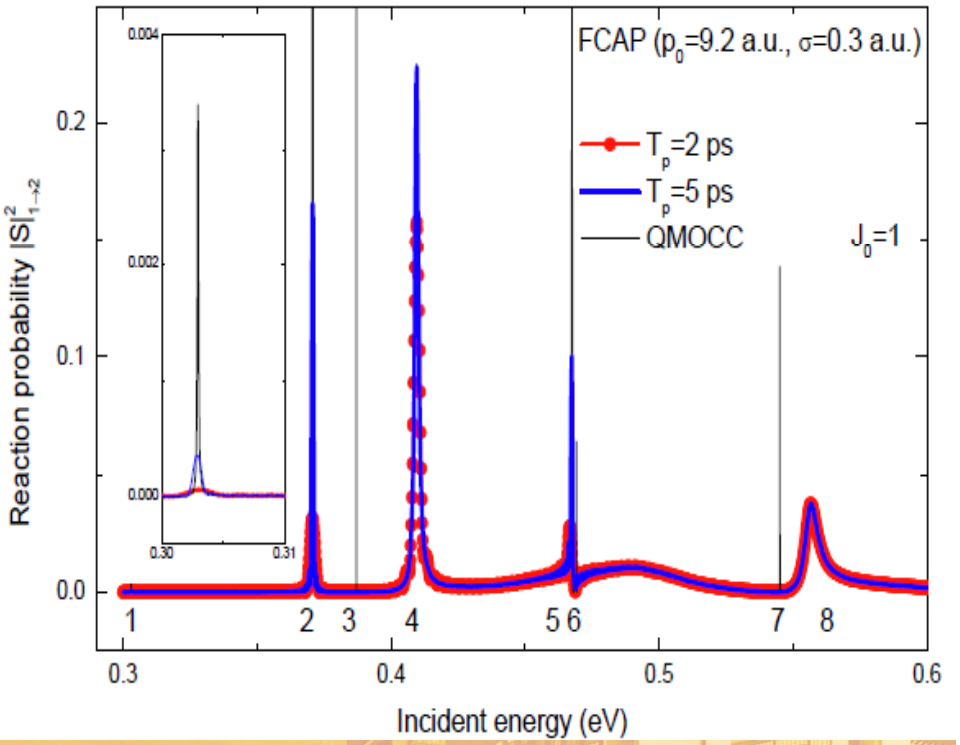
IAPCM

$H^-(1s^2)+Li(1s^22s) \rightarrow H(1s)+Li^-(1s^22s^2)$

$\rightarrow H(1s)+Li^-(1s^22s2p)$

MCTDH calculations





J Chem. Phys. 145, 224306 (2016)

北京应用物理与计算数学研究所
Institute of Applied Physics and Computational Mathematics

IAPCM

$H^+ + H_2O \rightarrow H_2O^+ + \ldots$

$H^+ + H_2O \rightarrow H + \ldots$

TDDFT calculations

PHYSICAL REVIEW A **93**, 062706 (2016)

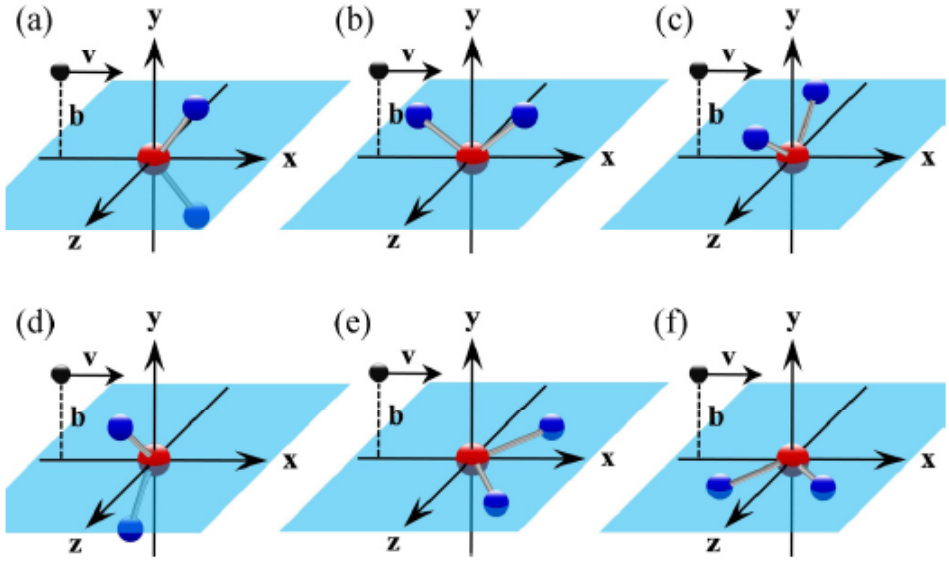
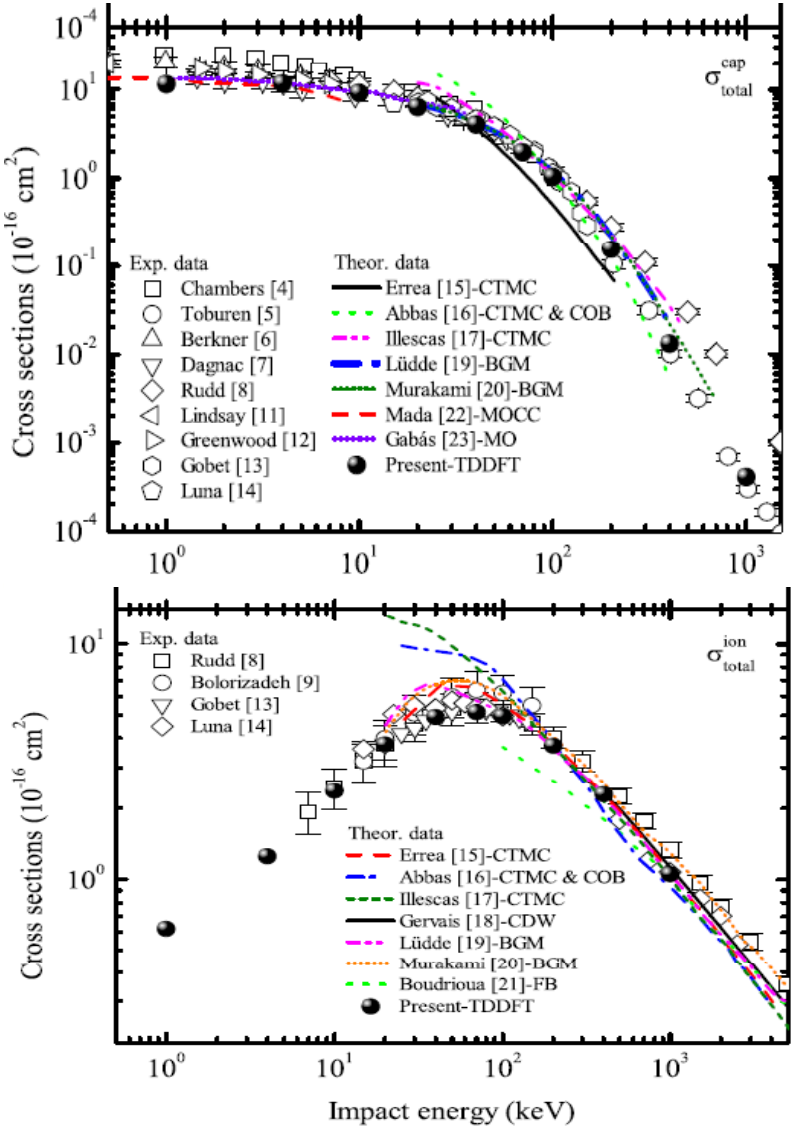


FIG. 1. Geometrical diagrams of collisions between protons and water molecules. The proton, hydrogen atom, and oxygen atom are represented by different-sized circles. Water molecules are located (a), (b) in the xy half-plane with $x > 0$ and $y > 0$, (c), (d) in the yz half-plane with $y > 0$ and $z > 0$, and (e), (f) in the xz half-plane with $x > 0$ and $z > 0$. The velocity vector $\mathbf{v}$ of the incident proton is oriented along the x direction. The impact parameter b is oriented along the y direction.



He^{2+} - H collision in magnetic field **(TDSE)**

1. The effect to the initial target (H) state

H Hamilton in magnetic field

(The magnetic field direction: z-axis)

$$H = H_0 + \frac{1}{2}\gamma L_z + \frac{1}{8}\gamma^2 r^2 \sin^2(\theta)$$

$$H_0 = -\frac{1}{2}\nabla^2 - \frac{1}{r}; \frac{1}{2}\gamma L_z : \text{The paramagnetic term;}$$

$$\frac{1}{8}\gamma^2 r^2 \sin^2(\theta) : \text{The diamagnetic term}$$

The effect of Magnetic field

H Hamilton in the magnetic field

$$H^{(0)}_{n'l'm',nlm} = \left\langle n'l'm' \middle| H_0 \middle| nlm \right\rangle = E_{nl}\delta_{n'n}\delta_{l'l}\delta_{m'm}$$

$$H^{(1)}_{n'l'm',nlm} = \left\langle n'l'm' \middle| \frac{1}{2}\gamma L_z \middle| nlm \right\rangle = \frac{1}{2}\gamma m\delta_{n'n}\delta_{l'l}\delta_{m'm}$$

$$H^{(2)}_{\alpha'\beta'\gamma',\alpha\beta\gamma} = \left\langle \alpha'\beta'\gamma' \middle| \frac{1}{8}\gamma^2 r^2 \sin^2(\theta) \middle| \alpha\beta\gamma \right\rangle = \frac{1}{8}\gamma^2 r_\alpha^2 \sin^2(\theta_\beta)\delta_{\alpha'\alpha}\delta_{\beta'\beta}\delta_{\gamma'\gamma}$$

$$H^{SR} = H^{(0)} + H^{(1)} + L^{+}H^{(2)}L$$

Magnetic field effect

1. H(1s) energy in magnetic field：

Magnetic intensity	0	0.05	0.1	0.15	0.2
H(1s) energy	-0.5	-0.4994	-0.4975	-0.4945	-0.494

Magnetic intensity in unit of γ:

$$\gamma = \frac{B}{B_0}$$

B_0=2.35*10^{5}T， the magnetic intensity of H(1s)

Magnetic field effect

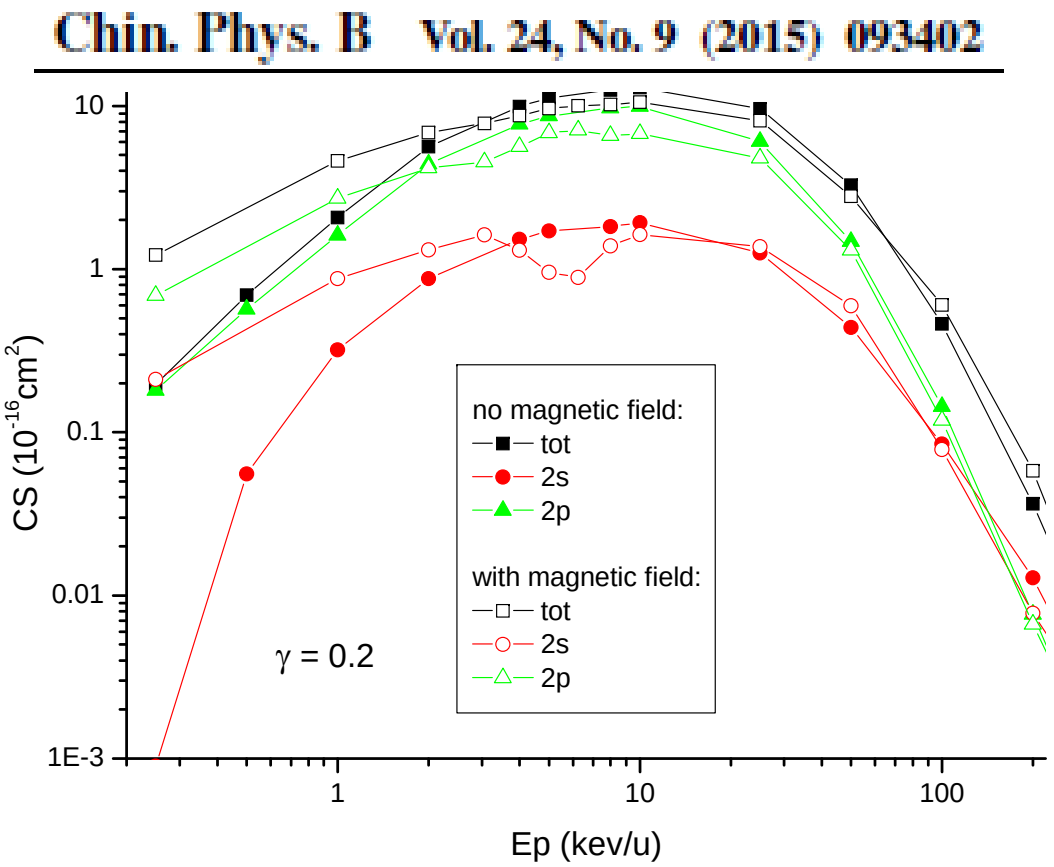
2. **The electron evolve under the actions of magnetic field and incident ion：**

$$H = -\frac{\nabla^2}{2} - \frac{1}{r} + \frac{1}{\left|\vec{R} - \vec{r}\right|} + \frac{1}{2}\gamma\hat{L}_z + \frac{1}{8}r^2\sin^2(\theta)\gamma^2$$

$$\psi(t+\Delta t) = e^{-iH_0\Delta t/2}e^{-i\tilde{V}(t)\Delta t}e^{-iH_0\Delta t/2}\psi(t)$$

The incident ion is along the Z direction。

The charge transfer cross section comparison in He^{2+} +H collisions



1,Cross sections vary significantly under the action of the magnetic field.

Low E: enhanced 5 times

Intermediate E:

Decreased 18 % ;

High E: enhanced 48 %

2,Minimum for 2s cross section at 6keV/u

The total, 2s and 2p cross sections vary with the incident energy with and without magnetic field.

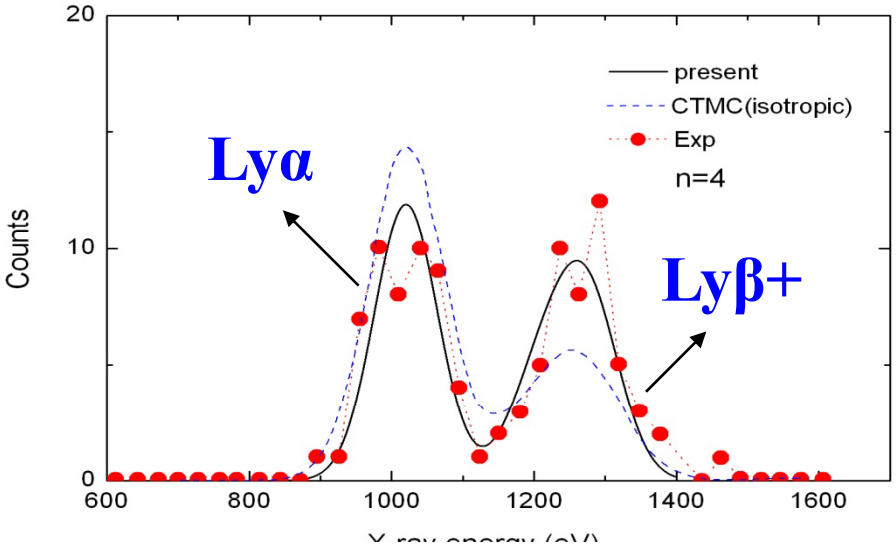
Magnetic intensity: γ = 0.2

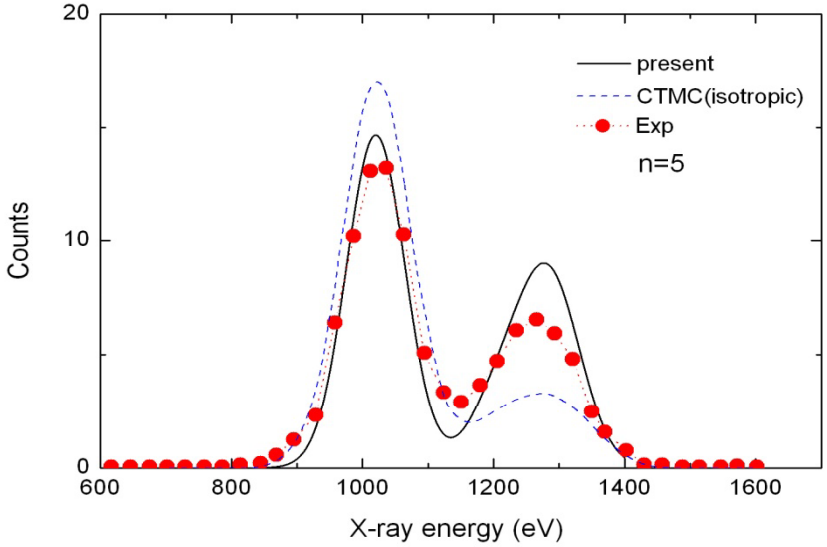
outline

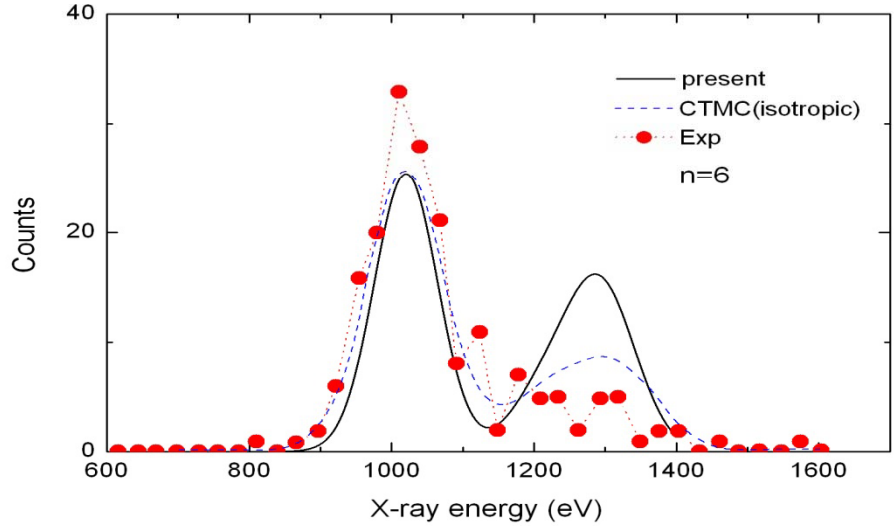
- Motivation
- Theoretical methods
- Scattering cross sections calculations
- X-ray spectra following highly charged ion-atom/molecule collisions
- Work plan

$$Ne^{10+} + He \rightarrow Ne^{9+}(nl) + He^{+}$$

$$Ne^{9+}(nl) \rightarrow Ne^{9+}(n'l') + hv$$







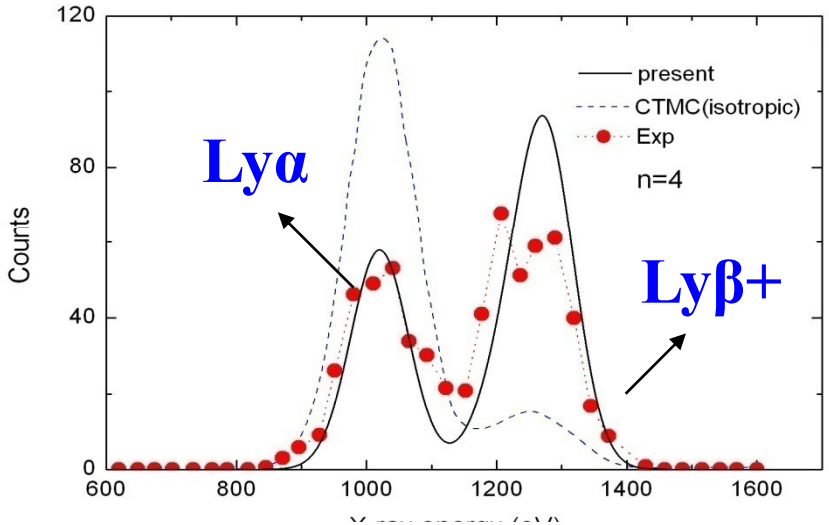
E=4.54keV/u

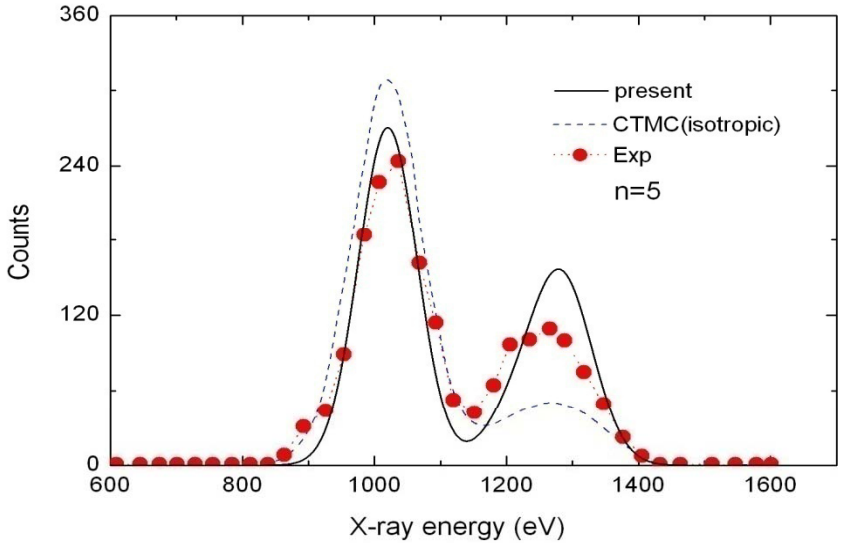
Lyβ+: n≥3→n=1

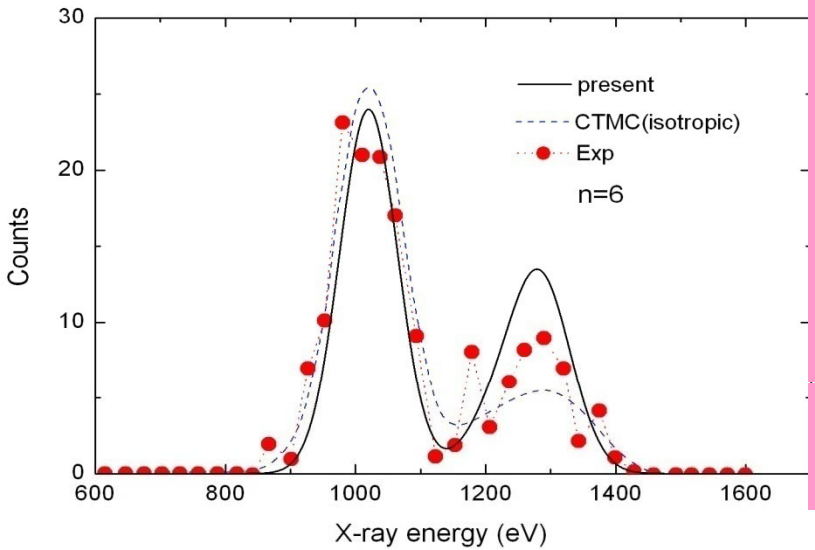
Exp: R. Ali et al., Astrophysical Journal Letters, 716, L95 (2010)

$$Ne^{10+} + Ne \rightarrow Ne^{9+}(nl) + Ne^{+}$$

$$Ne^{9+}(nl) \rightarrow Ne^{9+}(n'l') + h\nu$$



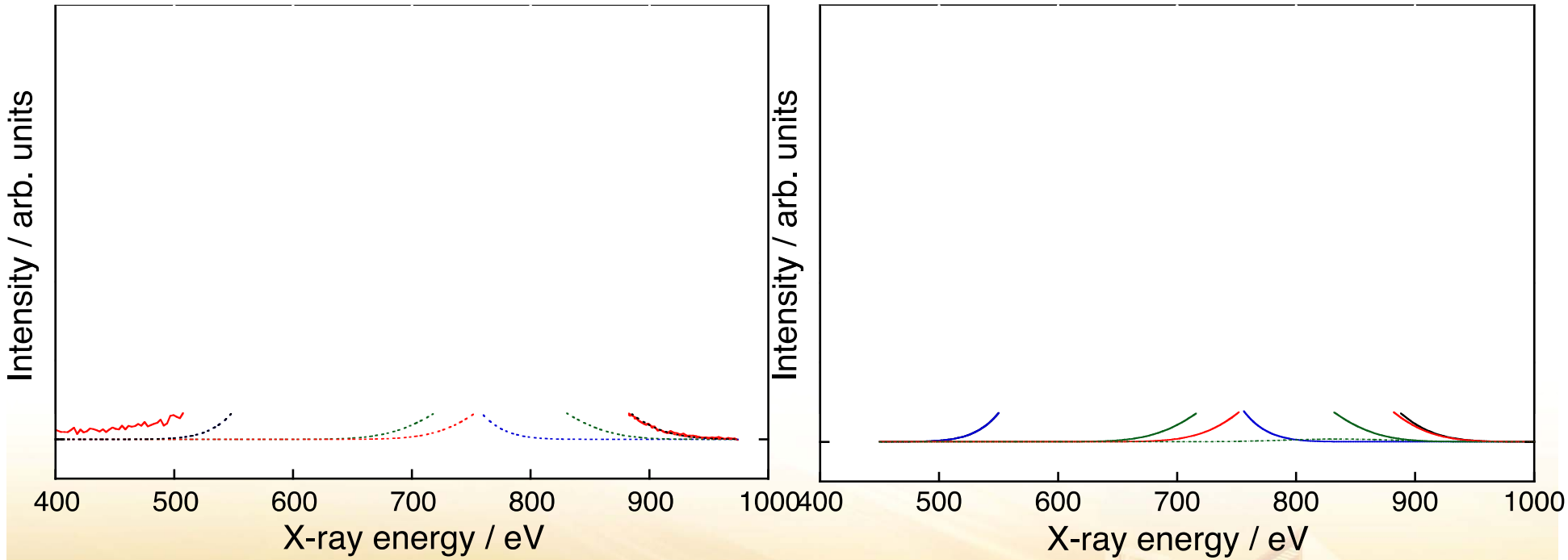




- **Our X-ray spectra results are in better agreement with the experimental data compared with CTMC results.**
- **Disagreement is from the use of model potentials and the competition of two-electron transition processes with the single electron capture process.**

$$O^{8+} + He \rightarrow O^{7+}(nl) + He^{+}$$

$$O^{7+}(nl) \rightarrow O^{7+}(n'l') + h\nu$$



The 1s-2p transition is dominant.

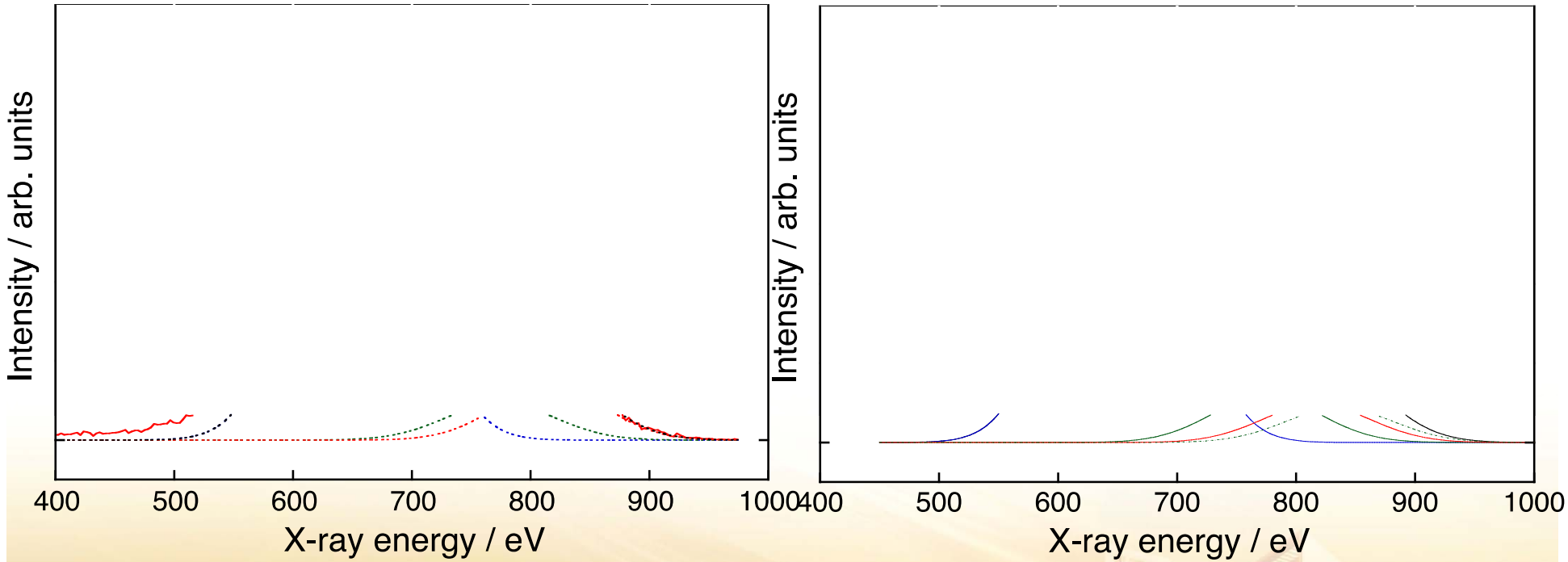
2p > 4p > 3p

2p > 4p > 3p

The experimental data is from H. Tanuma's group in Japan.

$$O^{8+} + H_2 \rightarrow O^{7+}(nl) + H_2^{+}$$

$$O^{7+}(nl) \rightarrow O^{7+}(n'l') + h\nu$$



The 1s-2p transition is dominant.

2p > 4p > 3p

2p > 3p ~ 4p ~ 5p

outline

- Motivation
- Theoretical methods
- Scattering cross sections calculations
- X-ray spectra following highly charged ion-atom/molecule collisions
- Work plan

Work plan

The AOCC, MOCC and CDW methods will be employed to calculate the excitation, charge transfer and ionization cross section in collisions between hydrogen (H, D, T) and the fully stripped ions of He, Be, C, N, O, Ne, Ar at hydrogen energy from about 1 keV to 1 MeV.

- 2017: He^{2+}, Be^{4+}, C^{6+}, N^{7+}-H collisions
- 2018: O^{8+}, Ne^{10+} -H collisions
- 2019: Ar^{18+} -H collisions

IAPCM

collaborators：

R. K. Janev: ***Macedonian Academy of Sciences and Arts, Macedonia***

R. J. Buenker: ***Bergische Universitat Wuppertal , Germany***

P. Krstic: ***Stony Brook University, USA***

P. C. Stancil: ***University of Georgia, USA***

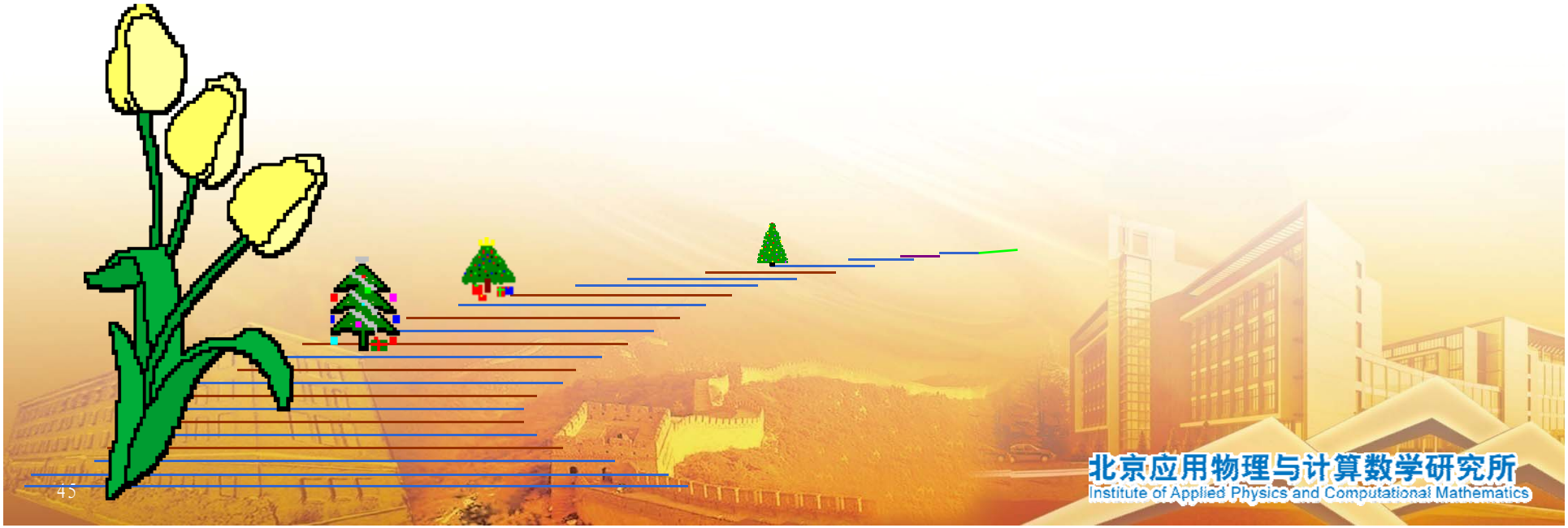
L. Mendez, I. Rabadan: ***Universidad Autonoma de Madrid , Spain***

A. Dubois: ***UPMC University Paris, France***

X. Ma: ***Institute of Modern Physics, China***

IAPCM

Thank you for your attention!



北京应用物理与计算数学研究所
Institute of Applied Physics and Computational Mathematics

TDDFT Method

The Kohn-Sham equation is:

$$i\frac{\partial\varphi_{k\mu}(r,t)}{\partial t}=\hat{H}_{KS}(t)\varphi_{k\mu}(r,t)=\left[-\frac{1}{2}\nabla^2+V_{KS}(r,t)\right]\varphi_{k\mu}(r,t)$$

Here $\varphi_{k\mu}(r,t)$ is the Kohn-sham orbital (KSO) and the electron density can be written as:

$$\rho(r,t)=\sum_{\mu=\uparrow\downarrow}\rho_{\mu}(r,t)=\sum_{\mu=\uparrow\downarrow}\sum_{k=1}^{4}n_{k\mu}\left|\varphi_{k\mu}(r,t)\right|^2$$

The Slater determinant can be obtained from the KSOs.

Nuclear motion: Velocity Verlet algorithm;

Electron propagation:

$$U(t+\Delta t,t)=\exp\left\{-i\frac{\Delta t}{2}H(t+\Delta t)\right\}\exp\left\{-i\frac{\Delta t}{2}H(t)\right\}$$

TDDFT Method

Electron capture probability is calculates as:

$$p_{i,j}(b) = \binom{N}{n=i-j} \int_T d\vec{r}_1, \cdots, d\vec{r}_n \int_{\bar{T}} d\vec{r}_{n+1}, \cdots, d\vec{r}_N \left| \Phi(\vec{r}_1, \cdots, \vec{r}_N, t_f; b) \right|^2$$

Electron loss probability is calculates as:

$$p_q(b) = \binom{N}{m=N-q} \int_T d\vec{r}_1, \cdots, d\vec{r}_m \int_{\bar{T}} d\vec{r}_{m+1}, \cdots, d\vec{r}_N \left| \Phi(\vec{r}_1, \cdots, \vec{r}_N, t_f; b) \right|^2$$

Here i and j are the ionic states of the projectile before and after collision. N is the total number of electron on the target before collision, n=i-j is the number of electrons transferred to the projectile, and q is the degree of ionization. $\Phi(\vec{r}_1,...,\vec{r}_N;t_f;b)$ is the Slater determinant, T represents the spatial area around the projectile and $\bar{T}$ is the spatial area outside it.

A coordinate space translation technique is employed to focus our investigation on some certain space of interest such as the regions around the projectile or target.

A absorbing complex potential added to Kohn-Sham potential to treat the ionization processes

The electron capture or electron loss cross section is determined by:

$$\sigma = 2\pi \int p(b) b \, db$$

TDSE method

$$i\frac{\partial\psi(x,t)}{\partial t}=H(x,t)\,\psi(x,t)$$

Pseudospectral method: a discrete variable representation for the radial coordinate, a two-dimensional Associated-Legendre-Function representation for the angles coordinate

$$\psi(\vec{r},t)=\sum_{nlm}\psi_{nlm}^{SR}(t)\frac{u_{nl}(r)}{r}P_{lm}(\theta)\frac{e^{im\phi}}{\sqrt{2\pi}}$$

The second-order split-operator method used for the wave function: propagation

$$\psi(r,t+\Delta t)=e^{-iH_0\Delta t/2}e^{-iV_{\text{int}}(t+\Delta t/2)\Delta t}e^{-iH_0\Delta t/2}\psi(r,t)$$

$$V_{\text{int}}(t)=\frac{1}{|\mathrm{R}(t,b)-r|}$$

The electron capture or electron loss cross section is determined by:

$$\sigma=2\pi\int b*\,p(b)db \qquad p(b)=\left|\Psi(t,T_f)\right|^2$$

Wavepacket → S-matrix → Cross section (JCP 105, 6778 (1996))

MCTDH

$$\frac{d}{dt}\langle\Psi|\Theta_\gamma|\Psi\rangle = i\langle\Psi|[H,\Theta_\gamma]|\Psi\rangle \qquad \Theta_\gamma = h(R_\gamma - R_{\gamma c})$$

flux operator $\hat{F}_\gamma \equiv i[H,\Theta_\gamma]$

Flux operator

$$\langle\Psi^+_{E\alpha\nu}|\hat{F}_\gamma|\Psi^+_{E\alpha\nu}\rangle = \frac{1}{2\pi}\sum_{\nu'}|S_{\gamma\nu',\alpha\nu}(E)|^2$$

$$|\Psi^+_{E\alpha\nu}\rangle = \frac{1}{2\pi\Delta(E)}\int_{-\infty}^{\infty} e^{-i(H-E)t}|\Phi_0\rangle dt$$

energy distribution $\Delta(E) = \langle\Psi^+_{E\alpha\nu}|\Phi_0\rangle$

Complex absorbing potential $\tilde{H} \equiv H - iW \qquad W = W_\alpha + W_\beta + \cdots$

$$\langle\Psi^+_{E\alpha\nu}|\hat{F}_\gamma|\Psi^+_{E\alpha\nu}\rangle = \frac{(2\pi)^{-2}}{|\Delta(E)|^2}\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt'\,\langle\Phi_0|e^{i(\tilde{H}^\dagger - E)t}\hat{F}_\gamma e^{-i(\tilde{H}-E)t'}|\Phi_0\rangle$$

$$\Phi(t) = e^{-iHt}\Phi_0$$

$$\sum_{\nu'}|S_{\gamma\nu',\alpha\nu}(E)|^2 = \frac{1}{\pi|\Delta(E)|^2}\int_0^{\infty}dt\int_0^{\infty}dt'\,\langle\Phi(t)|W_\gamma|\Phi(t')\rangle e^{-iE(t-t')}$$

$$\sum_{\nu'}|S_{\gamma\nu',\alpha\nu}(E)|^2 = \frac{2}{\pi|\Delta(E)|^2}\,\mathrm{Re}\int_0^{\infty}g(\tau)e^{-iE\tau}d\tau \qquad g(\tau) \equiv \int_0^{\infty}dt\langle\Phi(t+\tau)|W_\gamma|\Phi(t)\rangle$$

Excitation or transfer cross section $\sigma_{i\to j} = \frac{\pi}{k_i^2}\sum_J(2J+1)\left|S_{ij}^J\right|^2$

MCTDH

Hamiltonian (diatomic molecules)

$$\mathbf{H}_{q_1 q_2}(\mathbf{R}) = [-\frac{1}{2\mu}\frac{\partial^2}{\partial R^2} + \frac{\mathbf{J}^2 - 2\mathbf{J}_z\mathbf{L}_z + \mathbf{L}_z^2}{2\mu R^2} + V_e^{q_2}(R)]\delta_{q_1,q_2}$$

$$-\frac{1}{\mu R^2}(\mathbf{J}_+ - \mathbf{J}_-) < \Psi_e^{q_1} \mid i\mathbf{L}_y \mid \Psi_e^{q_2} >$$

$$-\frac{1}{2\mu}(2 < \Psi_e^{q_1} \mid \frac{\partial}{\partial R} \mid \Psi_e^{q_2} > \frac{\partial}{\partial R} + < \Psi_e^{q_1} \mid \frac{\partial^2}{\partial R^2} \mid \Psi_e^{q_2} >)\delta_{\Lambda_{q_1}\Lambda_{q_2}}$$

adiabatic $\rightarrow$ diabatic $\quad \mathbf{A}(R)\mathbf{C}(R) + \frac{\partial}{\partial R}\mathbf{C}(R) = 0$

$$\overline{\mathbf{H}}_{q_1 q_2}(\mathbf{R}) = [-\frac{1}{2\mu}\frac{\partial^2}{\partial R^2} + \frac{\mathbf{J}^2 - 2\mathbf{J}_z\mathbf{L}_z + \mathbf{L}_z^2}{2\mu R^2}]\delta_{q_1,q_2} + \overline{V}_e(R) + \overline{V}_{q_1 q_2}^{C}(R)$$

$$\begin{cases} i\frac{\partial}{\partial t}\overline{\Psi}_N^{q,J}(\mathbf{R},t) = \overline{\mathbf{H}}_{q'q}(\mathbf{R})\overline{\Psi}_N^{q,J}(\mathbf{R},t) \\ \overline{\Psi}_N^{q,J}(\mathbf{R},t) = \phi_N^{q,J}(R,t)\overline{D}_{M,\Lambda_q}^{J}(\alpha,\beta,\gamma) \\ \overline{\Psi}_N^{q,J}(\mathbf{R},t=0) = \phi_N^{q_0,J_0}(R,t=0)\overline{D}_{M_0,\Lambda_{q_0}}^{J_0}(\alpha,\beta,\gamma) \end{cases}$$