Recent Progress of KAERI Atomic Database

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Presented by Hyun-Kyung Chung (IAEA)

2 November 2015, IAEA Headquarters, Vienna, Austria

Outline

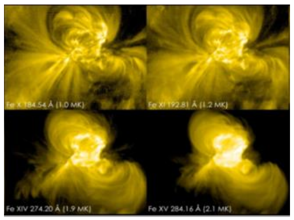
1. Research Activities of KAERI Atomic Data Center

2. KAERI Atomic Database Updates

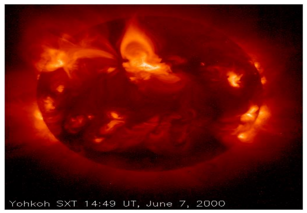
3. Summary and Outlook

Research Activities

1. **State-of-the-art calculations** for the **electron-impact ionization** and **recombination, and photoionization data** which are essential in modeling for laboratory and astrophysical plasmas

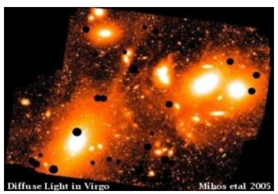


Sun

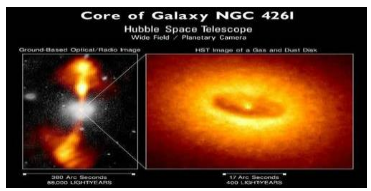


Star

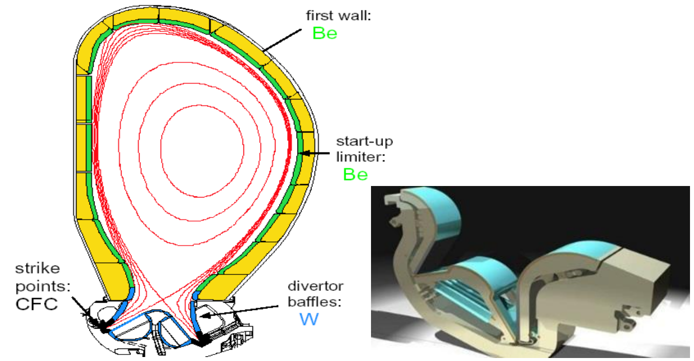
SNR



Galaxy

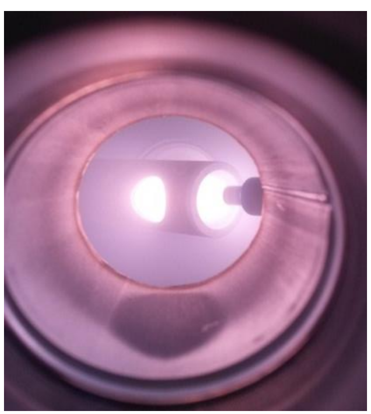


AGN

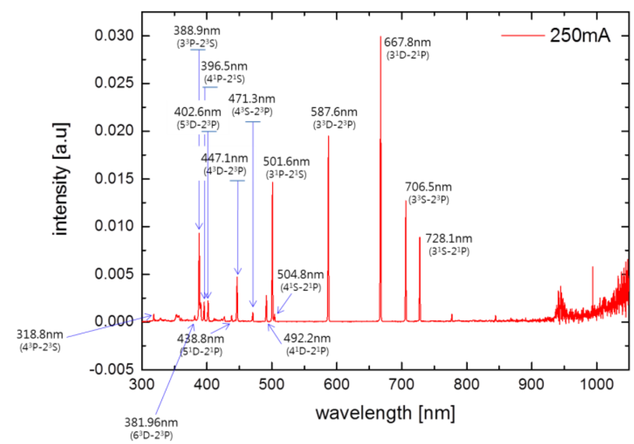


ITER wall design

2. **Spectroscopic measurement** in plasma devices and **collisional radiative modeling** for analysis on the measured spectra



Hollow Cathode Discharge (HCD)



Research Activities

1. Electron-Impact Ionization (EII)
   - **P-like** isoelectronic sequences from **P** to **Zn**
   - **W** ions (**W^{17+}** and **W^{+}**)

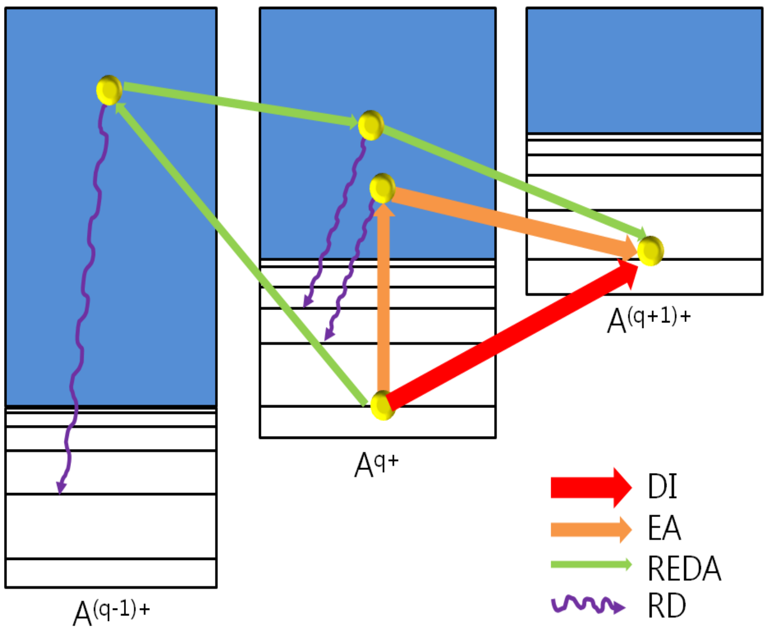
2. Dielectronic Recombination (DR)
   - **W^{45+}**

3. Photoionization
   - **Mg-like** isoelectronic sequences from Mg to Ar (except for P)

4. Spectroscopic measurement and Collisional Radiative (CR) modeling
   - **He I**

KAERI

EII pathways



Direct ionization (DI)

$$A^{q+} + e \rightarrow A^{(q+1)+} + e' + e''$$

Excitation-autoionization (EA)

$$A^{q+} + e \rightarrow A^{q+**} + e'$$
$$\rightarrow A^{(q+1)+} + e' + e''$$

Resonant excitation-double autoionization (REDA)

$$A^{q+} + e \rightarrow A^{(q-1)+**}$$
$$\rightarrow A^{q+*} + e'$$
$$\rightarrow A^{(q+1)+} + e'' + e'''$$

Resonant excitation-auto double ionization (READI)

$$A^{q+} + e \rightarrow A^{(q-1)+**} \rightarrow A^{(q+1)+} + e'' + e'''$$

Cross section

Total EII cross section in an *Independent Process-Isolated Resonance* (IP-IR) approximation is given by

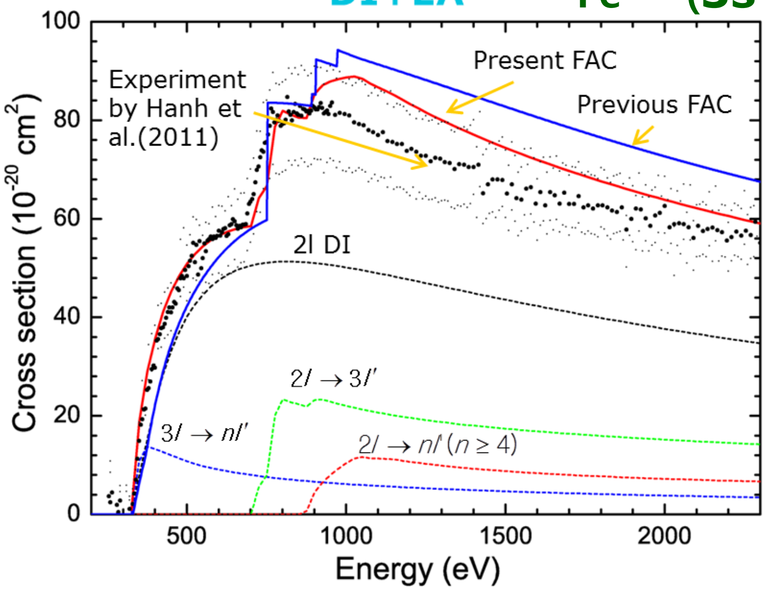
$$\sigma_{tot} = \sum_f \sigma_f^{DI} + \sum_j \sigma_j^{CE} B_j^{a} + \sum_k \bar{\sigma}_k^{DC} B_k^{da}$$

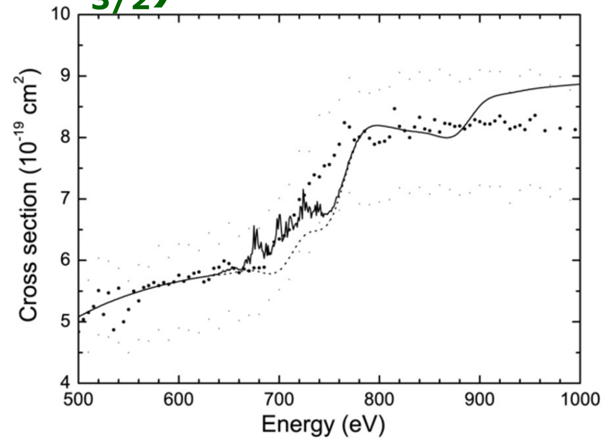
Autoionization (AI) branching ratio (BR) and double AI-BR : All of the branching ratios must be solved for recursively.

$$B_j^{a} = \frac{\sum_s A_{js}^{a} B_s^{r} + \sum_t A_{jt}^{r} B_t^{a}}{\sum_s A_{js}^{a} + \sum_t A_{jt}^{r}}, \quad B_k^{da} = \frac{\sum_{j'} A_{kj'}^{a} B_{j'}^{a}}{\sum_{j'} A_{kj'}^{a} + \sum_{t'} A_{jt}^{r}}$$

EII for P-like ions

DI+EA **Fe^{11+} ($3s^2\ 3p^3\ ^4S_{3/2}$)** **REDA**

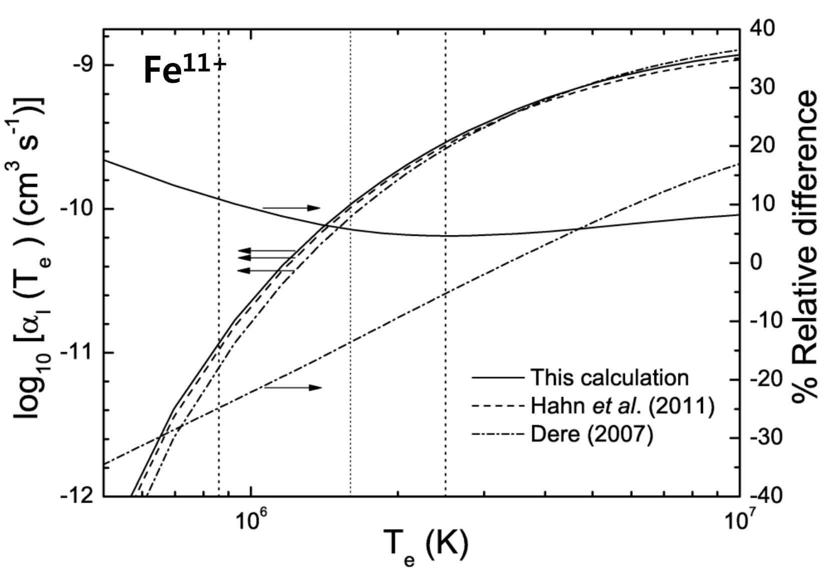


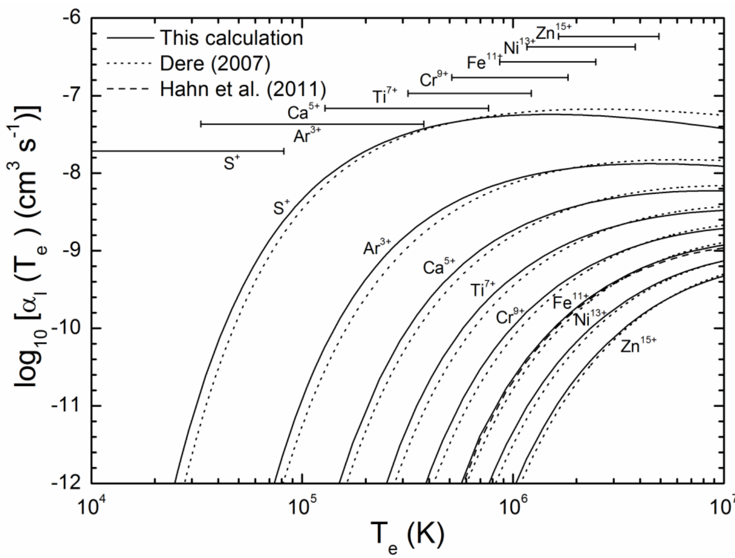


REDA contribution is within about 4% in rate coefficient

$$e^- + 2s^2 2p^6 3s^2 3p^{3\,4}S_{3/2}$$

$$\rightarrow 2[s,p]^7 3s^2 3p^3 n_1\ell_1 n_2\ell_2$$



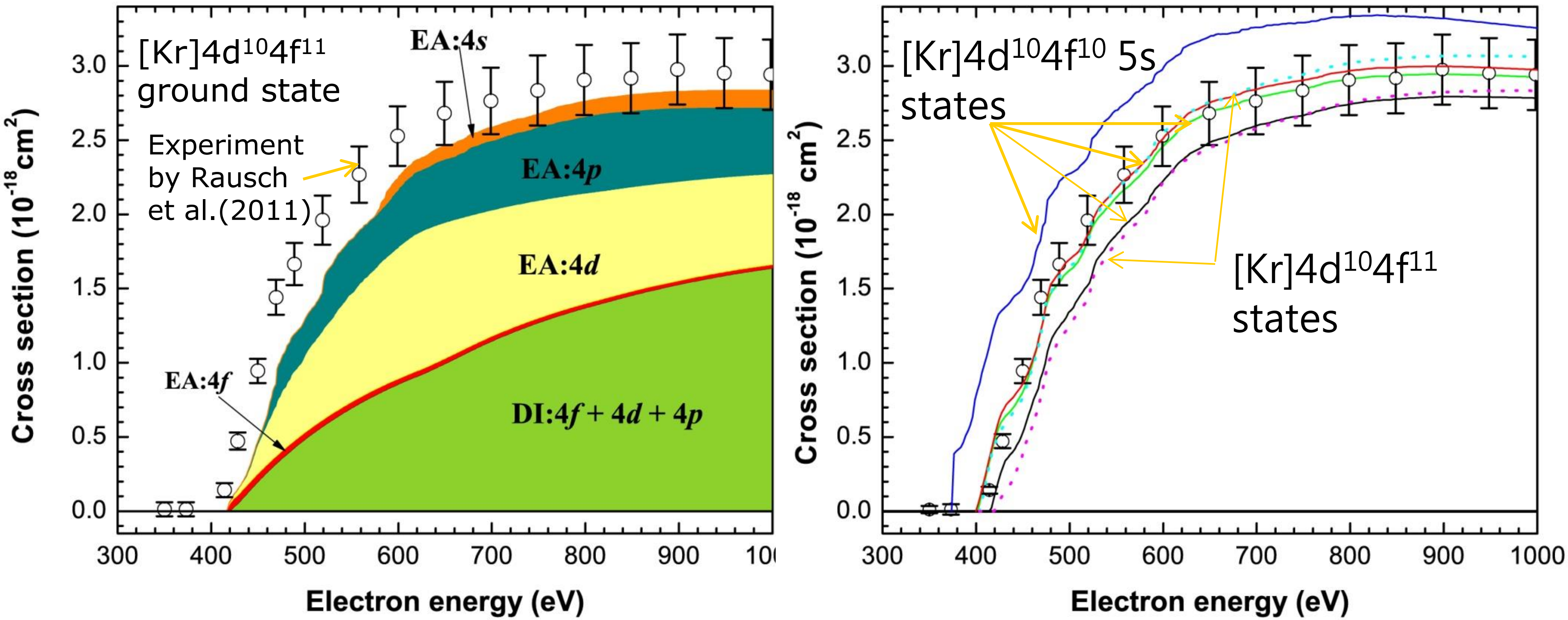


7~50% relative differences from previous FAC results

D.-H. Kwon and D. W. Savin, Astrophys. J **784**, 13 (2014)

EII for W ions

W^{17+}

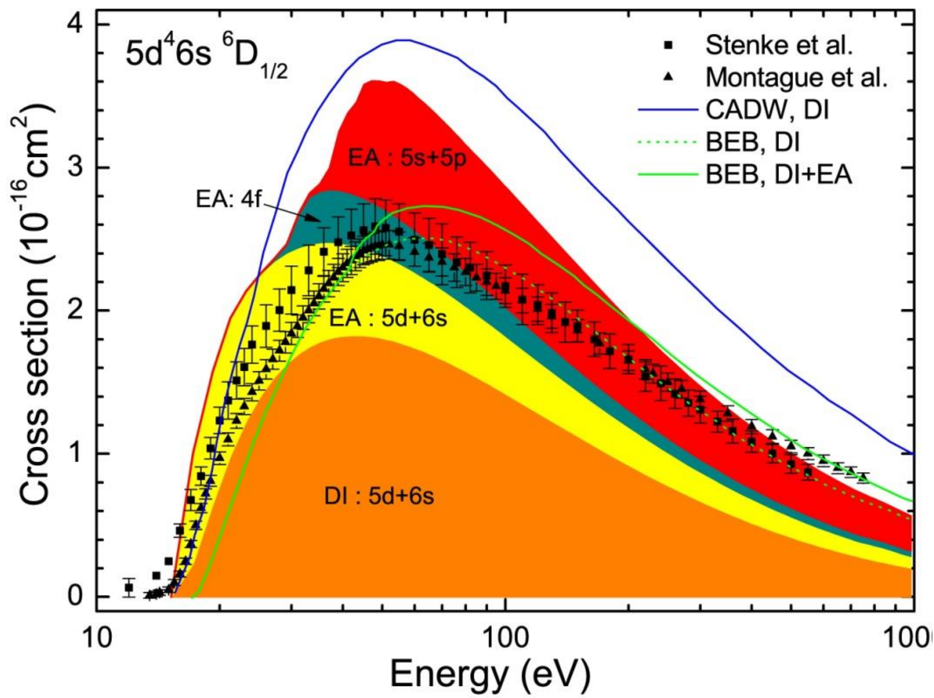


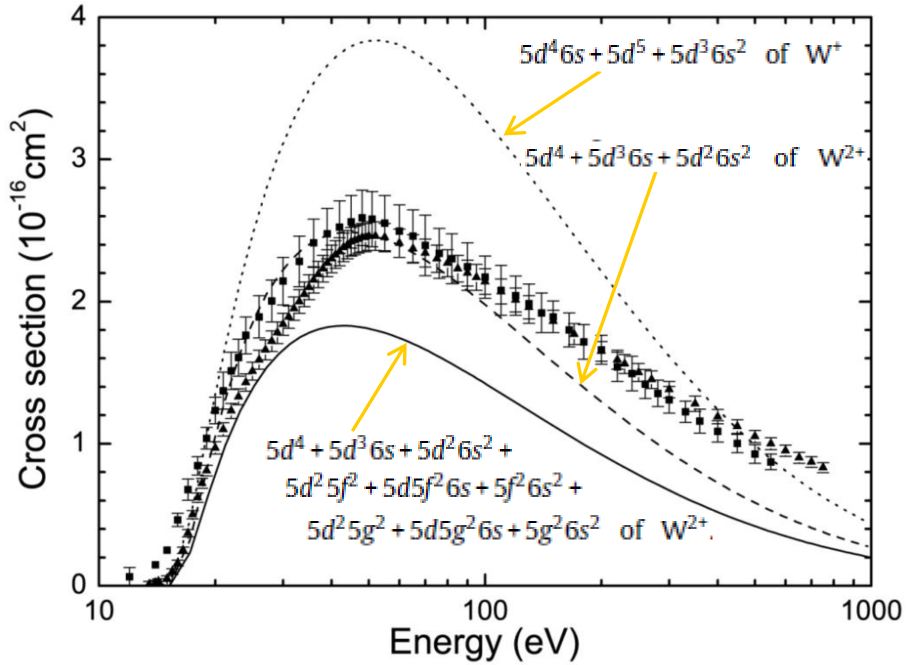
There are many long lived excited states and parent ion beams are mixed in ground and excited states. Good agreement is shown between theoretical calculation and experiment

D.-H. Zhang and D.-H. Kwon, J Phys. B **47**, 075202 (2014)

EII for W ions

W^+



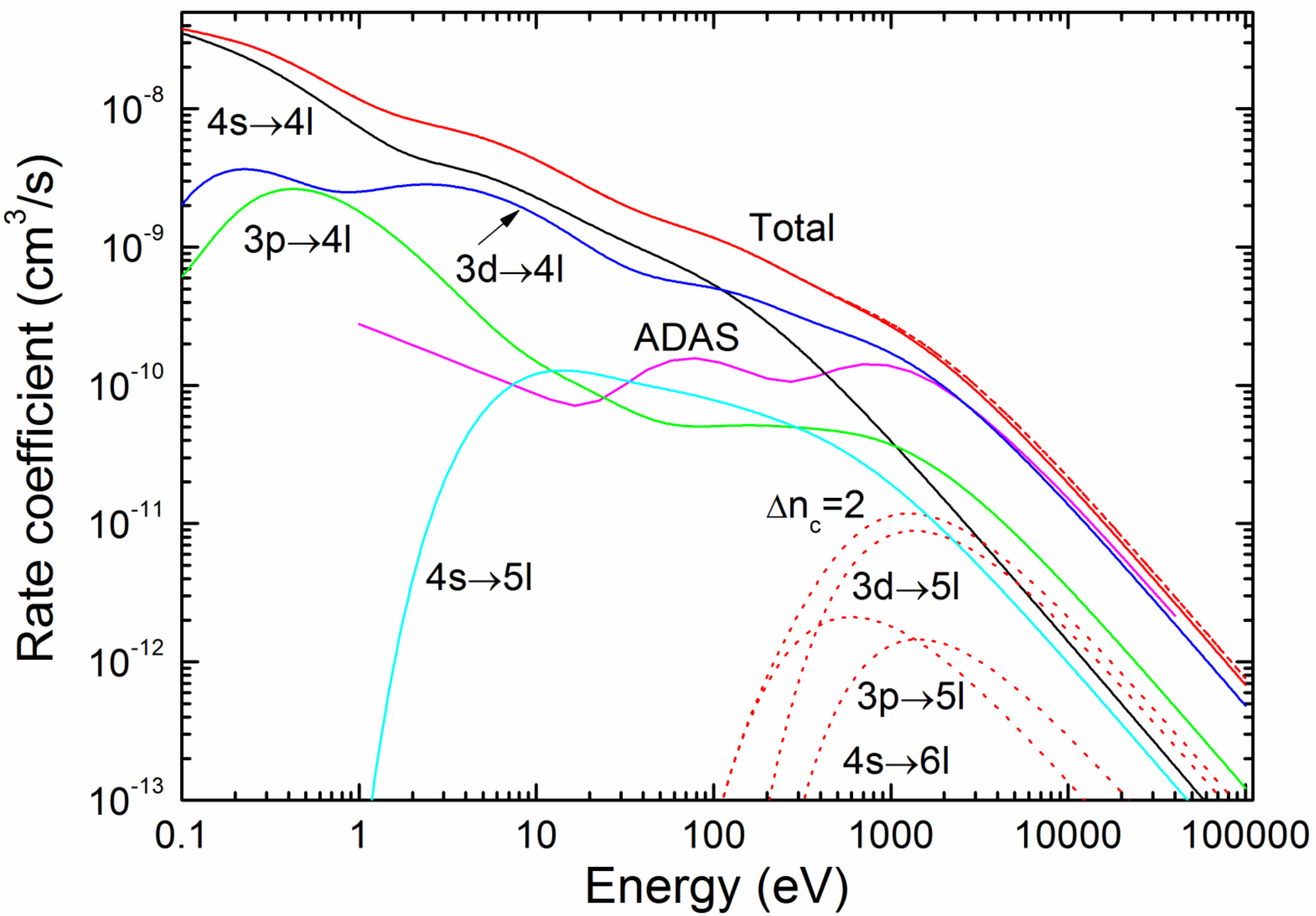


Large sensitivity of DI cross section to potential choices.

D.-H. Kwon, Y. S. Cho, and Y. O. Lee, Int. J. Mass Spect. **356**, 7 (2013)

Dielectronic Recombination (DR)

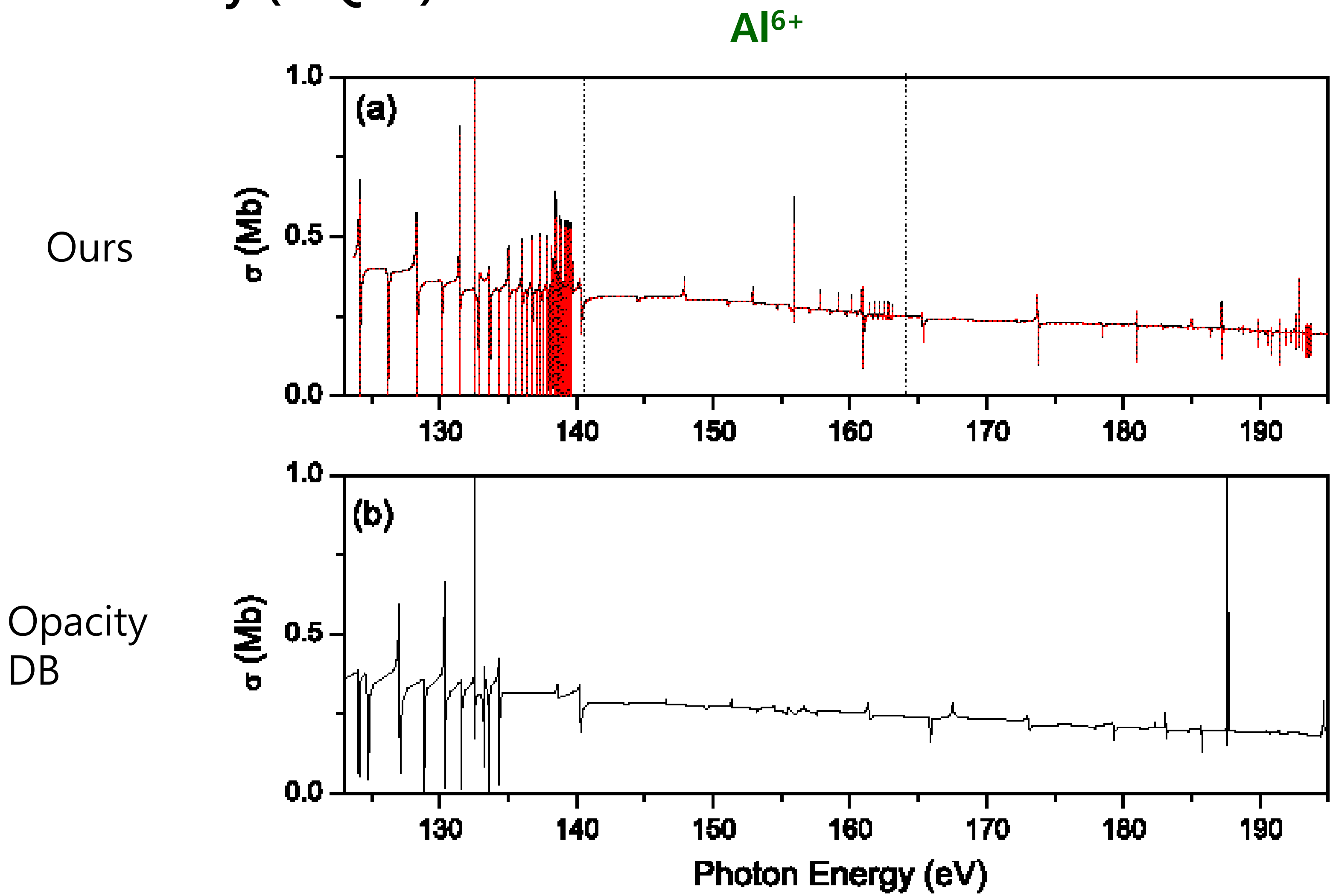
W^{45+}



D.-H. Kwon and W. Lee, J. Quant. Spectrosc. Radiat. Transfer, submitted.

Photoionization

Eigenchannel R-matrix approach connected with **multichannel quantum-defect theory (MQDT)**

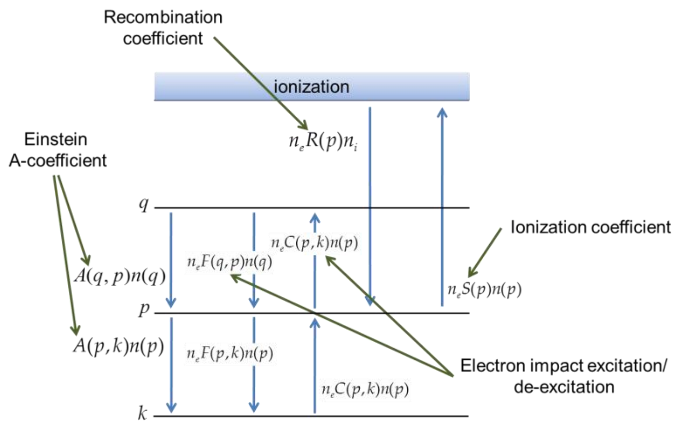


D.-S. Kim and D.-H. Kwon, J Phys. B **48**, 105004 (2015)

Collisional-Radiative Model

Collision-Radiative model is one of population model of any element (atom, ion, molecule, etc).

$$\frac{d}{dt}n(p)=\sum_{q<p}C(q,p)n_e n(q) - \left[\sum_{q<p}F(p,q)+\sum_{q>p}C(p,q)+S(p)+\frac{1}{n_e}\sum_{q<p}A(p,q)\right]n_e n(p) + \sum_{q>p}\left[F(q,p)n_e + A(q,p)\right]n(q) + \left[\alpha(p)n_e+\beta(p)+\beta_d(p)\right]n_e n^+$$



$$\frac{d}{dt}n(p)=0$$: quasi steady state (QSS)

formulation I for Helium

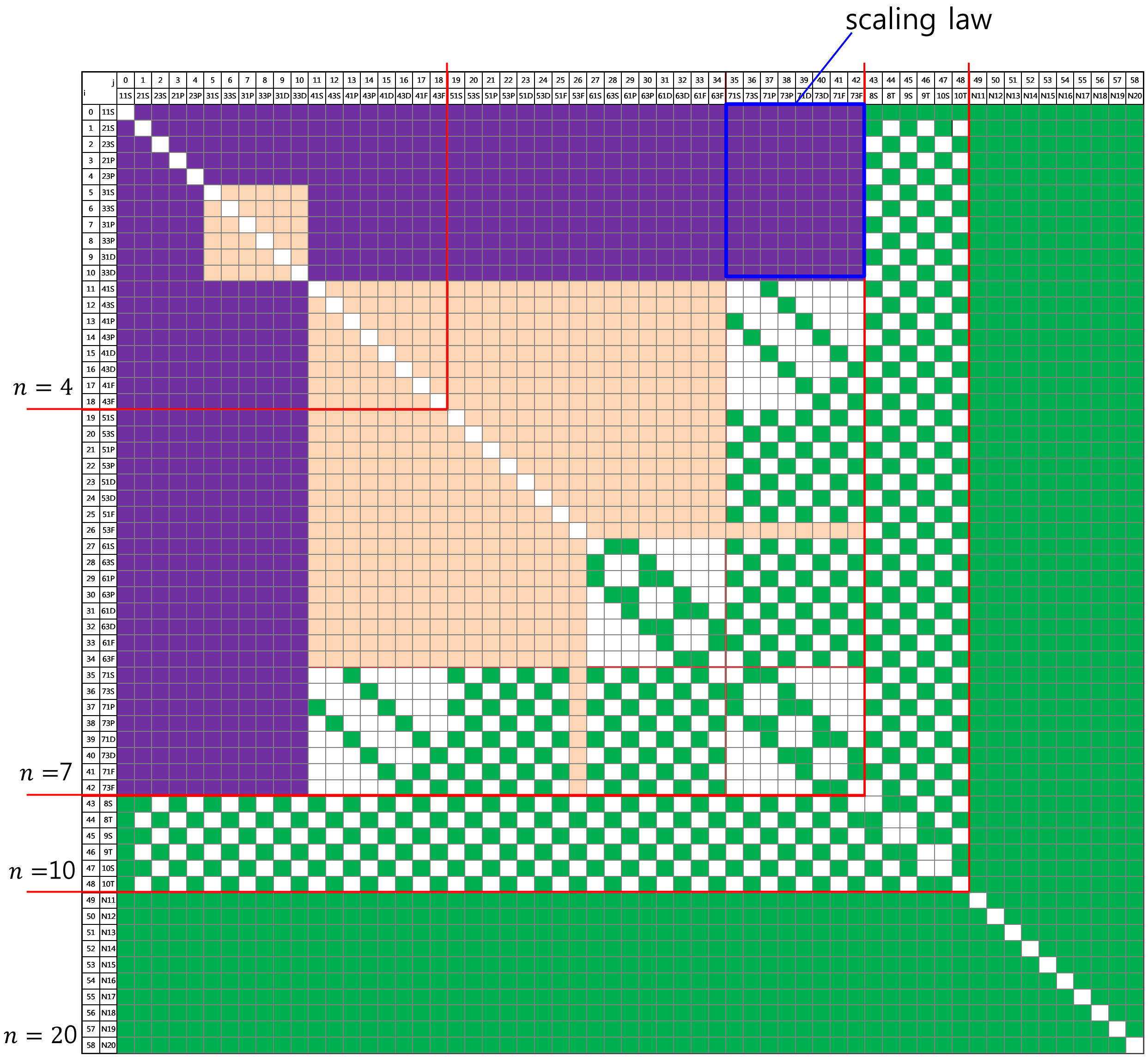
$$n(p)=r_0 n_e n^+ + r_1 n_e n(1^1S) + r_2 n_e n(2^1S) + r_3 n_e n(2^3S)$$

formulation II for Helium

$$n(p)=R_0 n_e n^+ + R_1 n_e n(1^1S)$$

He collisional radiative model has been developed by T. Fujimoto and M. Goto.
We analyzed plasma parameters (T_e, n_e) in low pressure and low temperature plasma with He CR-model based on Goto's paper. (M. Goto, J. Quant. Spectrosc. Radiat. Transfer 76, p331-344 (2003))

Electron Impact Excitation Cross Sections



: Fitted Cross section by Y. Ralchenko

: Calculated Cross section by CCC89

: Fujimoto's semi-empirical Cross section

$n = 1\sim4 : n, L, S$

$n = 5\sim7 : n, L, S\ (L \leq 3)$

$n = 8\sim10 : n, S$

$n \geq 11$: Hydrogen-like

CCC89 cross sections are more stable than fitted cross sections for transition of n=3-3 and n=4-4.

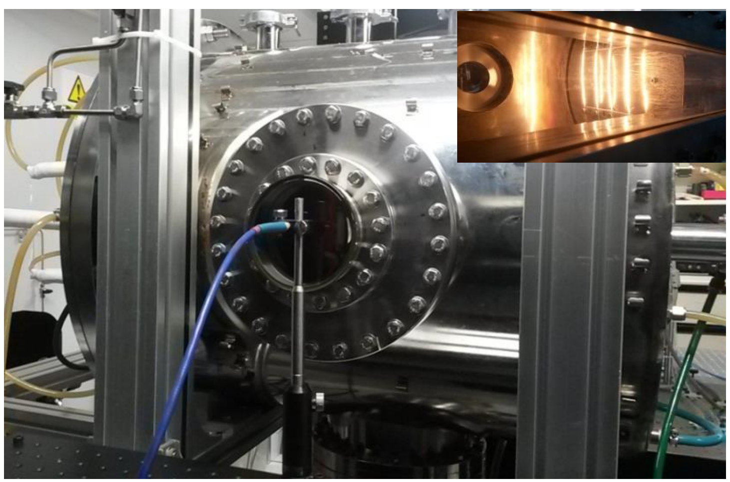
● Modified He CR-Model

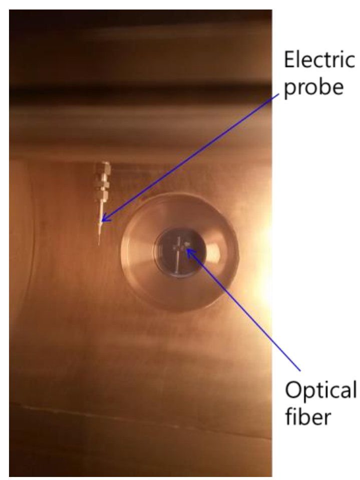
RTE (Radiation Trapping effect) is a non-local problem. The emission and induced absorption processes occur the different locations, and are related with each other.

$$n(p) = r_0 n_e n^+ + r_0 n_e n(1) + r_0 n_e n(2^1S) + r_0 n_e n(2^3S) \boxed{+ r_4 I_{2^1P} n(1) + r_4 I_{3^1P} n(1) + r_4 I_{4P} n(1)}$$

: radiation trapping effect *from ground state*

● Experiment (hot filament discharge)





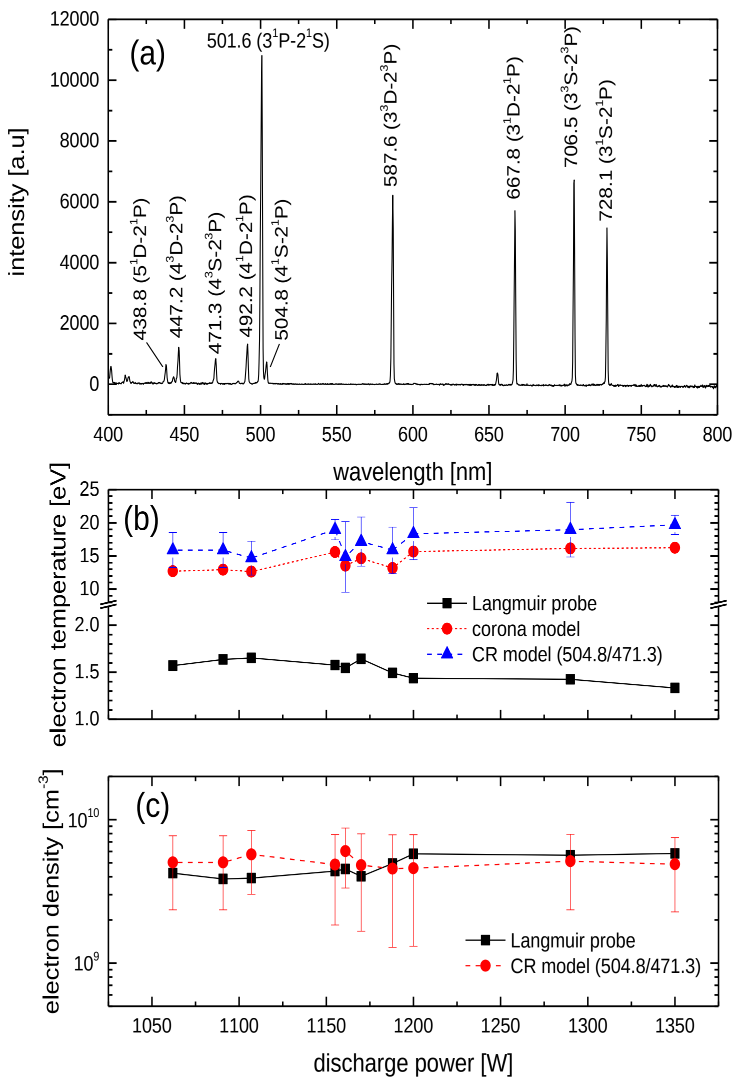
Experiment condition

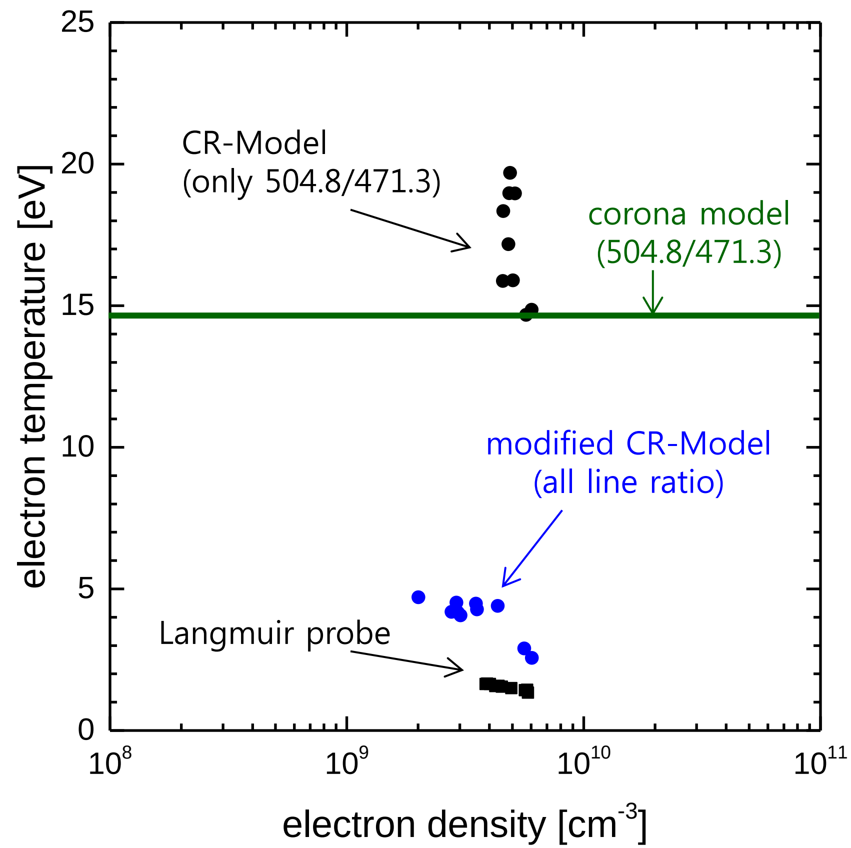
- base pressure : 0.05 mtorr,
- operating pressure : 7 mtorr
- discharge power : 118V / 9A

Hot filament discharge (C. H. Oh, HYU)

Experiment (hot-filament discharge)

● Diagnostics of plasma parameters (T_e, n_e)

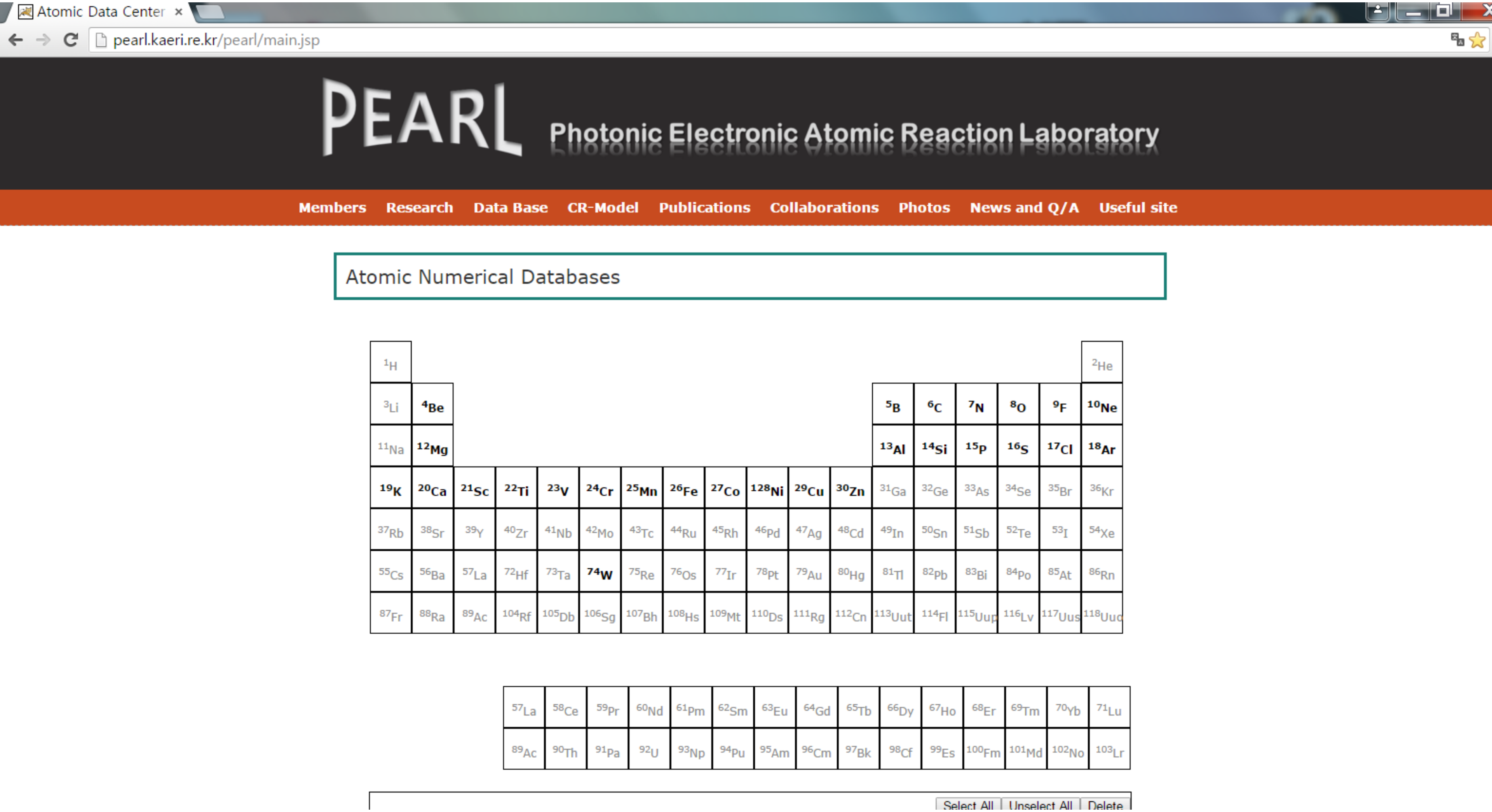




In low pressure helium plasma ($n_e < 10^{10}\ cm^{-3}$), radiation trapping effect was not negligible.

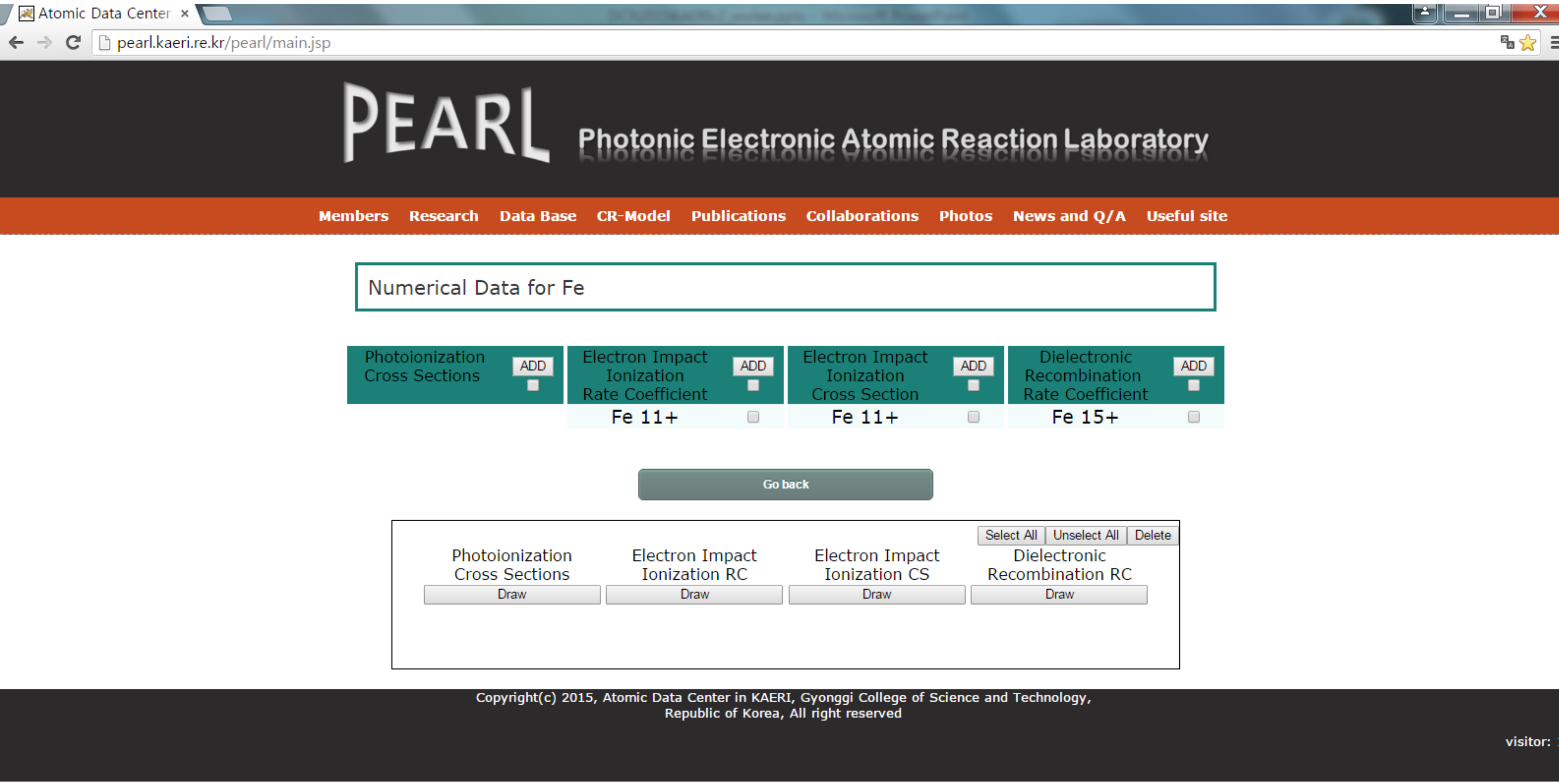
Database Updates (Atomic Data)

http://pearl.kaeri.re.kr



Database Updates (Atomic Data)

Selection of Reactions for various ion stages

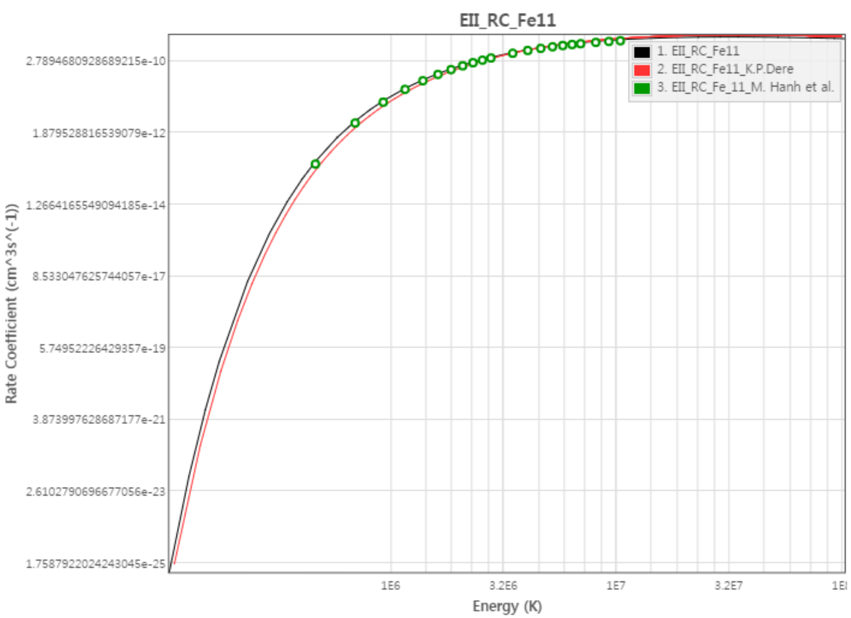


Flexible and comparable plots for selected ion and reaction

Atomic Data Center × | Electron Impact Ioni ×

pearl.kaeri.re.kr/pearl/graphEIIRC.jsp?reaction=EII_RC_Fe11&element=Fe&ref=undefined

Electron Impact Ionization Rate Coefficient for Fe



X-axis : Logarithmic from 104440.5 to 1.044405E8

Y-axis : Logarithmic from 9.0628E-26 to 1.6648237E-9

Legend position : Top Right

Update | Reset | Get Data

Close

Data list

- 1. EII_RC_Fe11 : Data
- 2. EII_RC_Fe11_K.P.Dere : Data
- 3. EII_RC_Fe_11_M. Hanh et al. : Data

Reference

1. EII_RC_Fe11	D.-H. Kwon and D.W.Savin, Astrophysical Journal.784,13 (2014)
2. EII_RC_Fe11_K.P.Dere	K.P.Dere, A&A 466, 771-792 (2007)
3. EII_RC_Fe_11_M. Hanh et al.	M. Hahn et al., Astrophys. J. 729, 76 (2011).

Ionization potential of the ion = 326.324

f = 1.49

Scaled Rate Coefficient

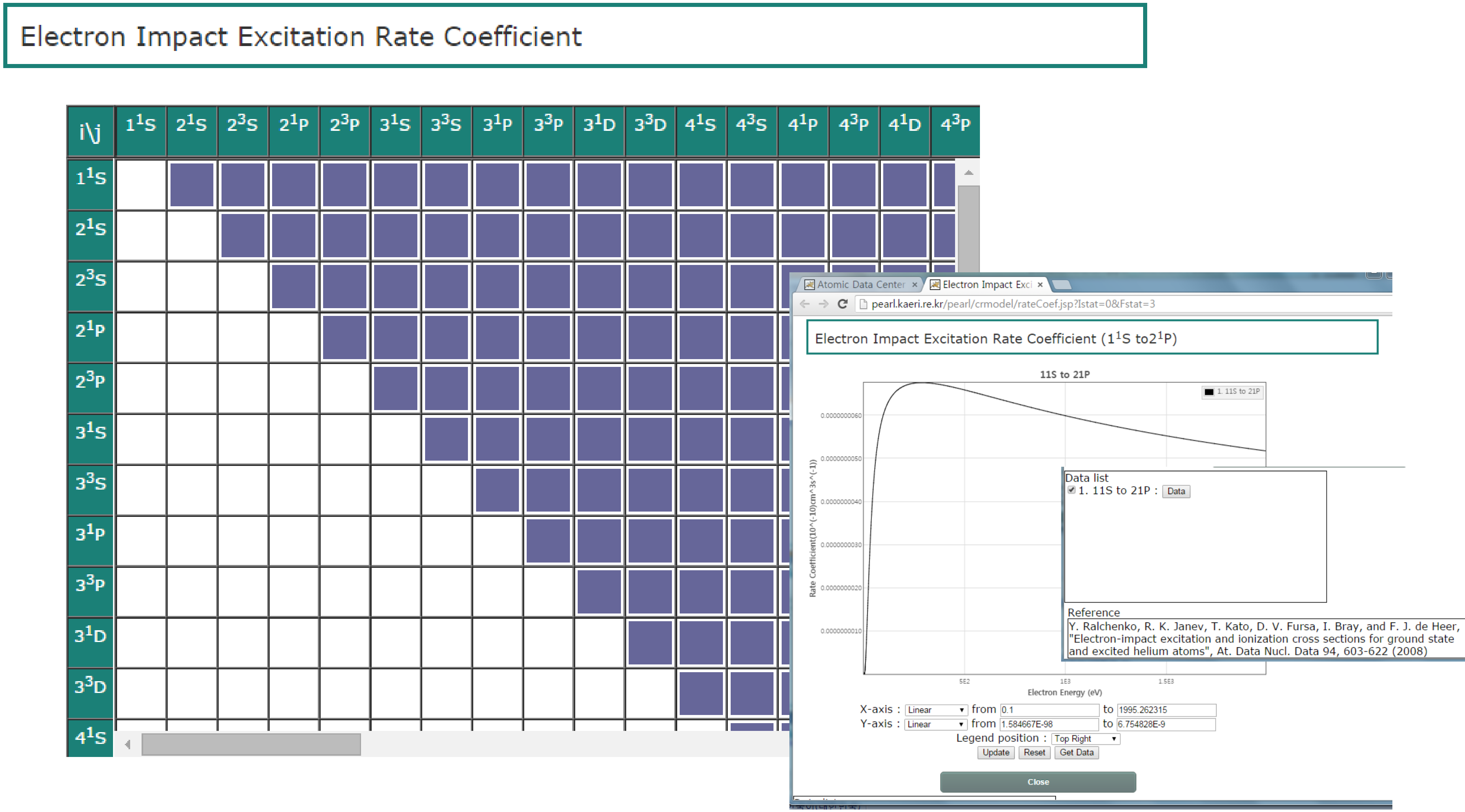
a_i	a_0	a_1	a_2	a_3
1. EII_RC_Fe11	1.923653E-5	-1.4983809999979947E-5	-7.185951999999496E-5	3.23617599999999 4
2. EII_RC_Fe11_K.P.Dere				
3. EII_RC_Fe_11_M. Hanh et al.				

Database Updates (Atomic Data)

State selected photoionization data

Database Updates (CR modeling on Web)

Atomic data used for CR modeling (for eg. He I case)



Database Updates (CR modeling on Web)

Input of plasma and atomic parameters

Line Ratio as a Function of T_e/n_e

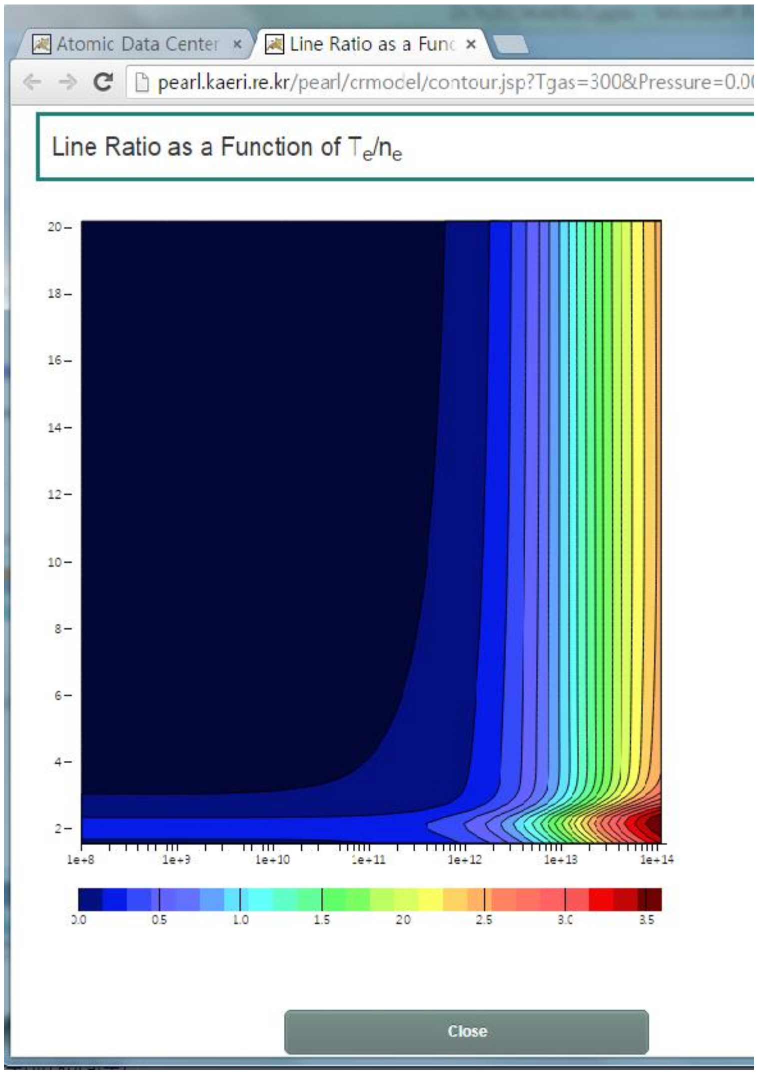
You can find a figure for relation between line intensity ratio and plasma parameters (Te, Ne). The figure was calculated by the formulation I of He CR-Model. The plasma was assumed as ionizing plasma (R_0=0).

Enter some parameters at below box and press button.

Gas Temperature(K) :	300	(250~500 K)
Pressure (mTorr) :	5	(0.5~50 mTorr)
Magnetic Field (T) :	0	(0~0.1 T)
2^1S state population density (cm^{-3}):	1e6	(1E1~1E9 cm^{-3})
2^3S state population density (cm^{-3}):	3e8	(1E1~1E9 cm^{-3})

Submit

Contour plot for various line ratios as a function of plasma density and temperature



Gas Temperature(K)	300
Pressure (mTorr)	5.0
Magnetic Field (T)	0
2^1S state population density (cm^{-3})	1e6
2^3S state population density (cm^{-3})	3e8

Intensity I

3^1S-2^1P	3^3S-2^3P	3^1P-2^1S	3^3P-2^3S
3^1D-2^1P	3^3D-2^3P	4^1S-2^1P	4^3S-2^3P
4^1P-2^1S	4^3P-2^3S	4^1D-2^1P	4^3D-2^3P

Intensity II

3^1S-2^1P	3^3S-2^3P	3^1P-2^1S	3^3P-2^3S
3^1D-2^1P	3^3D-2^3P	4^1S-2^1P	4^3S-2^3P
4^1P-2^1S	4^3P-2^3S	4^1D-2^1P	4^3D-2^3P

Draw Graph

Summary & Outlook

1. We have carried out calcultions for EII and DR by FAC and photoionization by non-iterative eigenchannel R-Matrix method.

2. Spectroscopic measurements in various plasma devices and CR modeling have been performed for He I.

3. We have updated the calculated atomic data and implemented CR modeling on our Web DB (http://pearl.kaeri.re.kr).

4. Parallelization for FAC DR calculation will be done.

5. Improving accuracy of FAC collisional excitation calculation for neural atom will be sought.

6. Validation for atomic data and CR modeling will be going on by spectroscopic measurements.