Aspects and prospects of KAERI atomic data center

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Nuclear Data Center

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Outline

1. Research Activities (2015-2017)

2. KAERI Atomic Database Updates

3. Summary and Outlook

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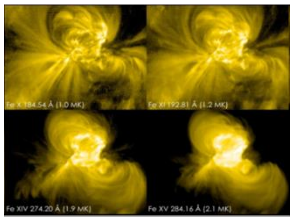
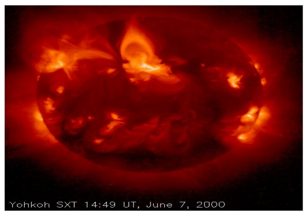
Research Activities

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

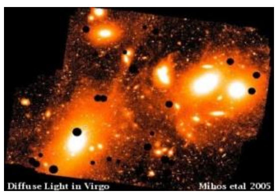


Sun

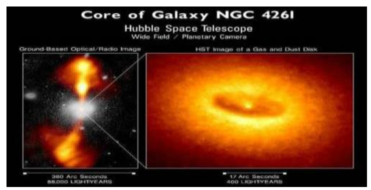


Star

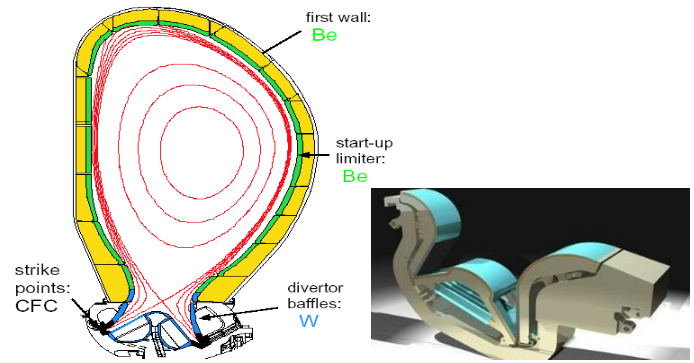
SNR



Galaxy

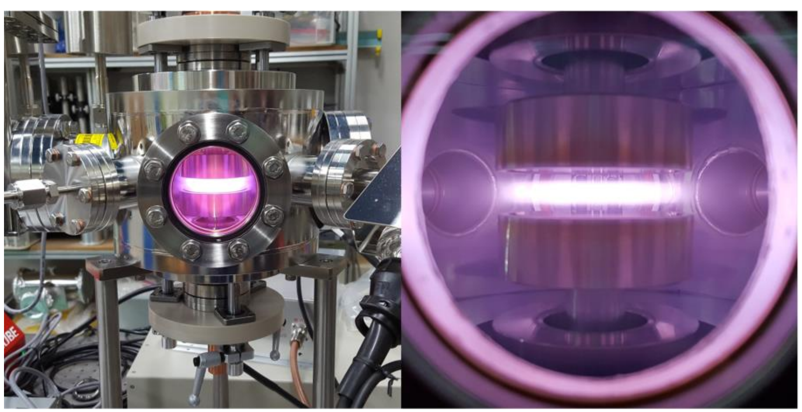


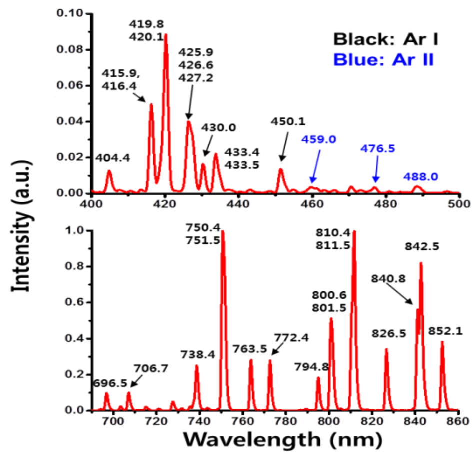
AGN



ITER wall design

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





Research Activities

1. Dielectronic recombination (DR)
   - **Highly charged W^{44+}~W^{46+}**
   - **Lowly charged W^{5+}~W^{11+}**

2. Photon emissivity coefficient (PEC)
   - **W^{5+}~W^{48+}**

3. Spectroscopic measurement & collisional-radiative (CR) modeling
   - **Ar**

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Spectroscopic Modeling

Emissivity ε_{ij} for line transition $i \rightarrow j$

$$\varepsilon_{ij} = n_Z(r,t)\, n_e(r,t)\, \mathrm{PEC}_{ij}(T_e, n_e)$$

→ Photon Emissivity Coefficient

Charge Z ion density from ***transport*** modeling

Electron density

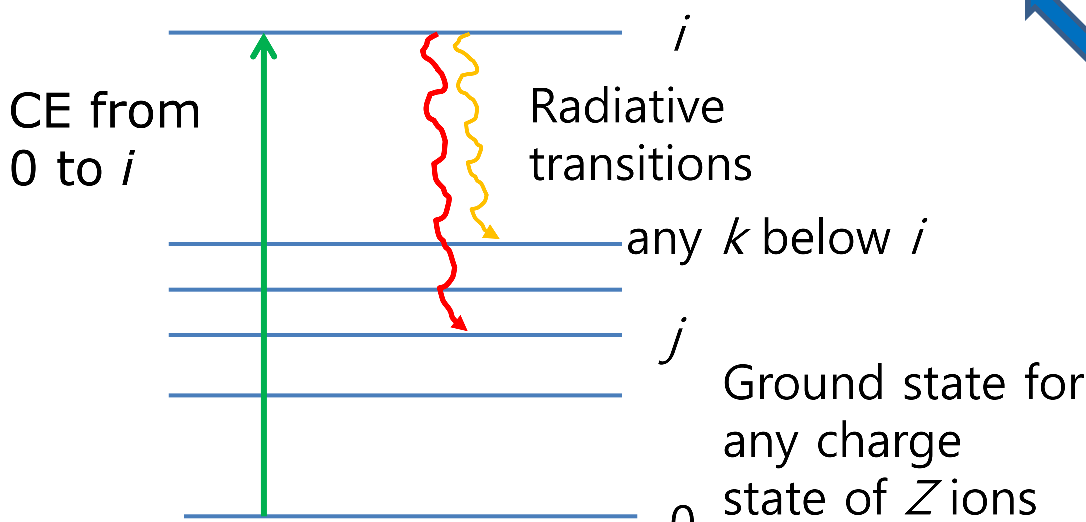
$$\mathrm{PEC}_{ij}(T_e) = X_{0i} \frac{A_{ij}}{\sum_{k<i} A_{ik}}$$

Collisional excitation (CE) rate

Radiative transition probability

Atomic Data

Simple **coronal** Model for state population density



$$I = \int_{LOS} \varepsilon_{ij}(r)\, dl$$

$$n_e\left[cm^{-3}\right] \le 5.6 \times 10^{8} (Z+1) \times T_e\left[eV\right]^{1/2} \exp\left[\frac{1.162 \times 10^{3} (Z+1)^2}{T_e}\right]$$

with **hydrogenic approximation**

Transport Modeling

Transport equation for charge Z ion

$$\frac{\partial n_Z(r,t)}{\partial t} = -\nabla \cdot \Gamma_Z(r,t) + S_Z(r,t)$$

Transport term $\Rightarrow$

$$\Gamma_Z(r,t) = -D(r)\frac{\partial n_Z(r,t)}{\partial r} + V(r)n_Z(r,t)$$

Diffusion coefficient　　Drift, convection coefficient

Source & sink term $\Rightarrow$

$$S_Z(r,t) = -n_e\left(\alpha_I^Z + \alpha_R^Z\right)\cdot n_z + n_e\alpha_I^{Z-1}\cdot n_{z-1} + n_e\alpha_R^{Z+1}\cdot n_{z+1}$$

Ionization rate coefficient　　Recombination coefficient

Atomic Data

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Photon Emissivity Coefficient (PEC)

W^{q+} (q=5) ground state $4d^{10}\ 4f^{14}\ 5s^2\ 5p^6\ 5d$, IE : 66.37 eV

$$4d^{10}\ 4f^{14}\ [5s^2\ 5p^6\ 5d]^{-1}\ n'l' \rightarrow 4d^{10}\ 4f^{14}\ [5s^2\ 5p^6\ 5d]^{-1}\ nl + h\nu$$

$$4d^{10}\ 4f^{13}\ 5s^2\ 5p^6\ 5d\ n'l' \rightarrow 4d^{10}\ 4f^{13}\ 5s^2\ 5p^6\ 5d\ nl + h\nu$$

$$\rightarrow 4d^{10}\ 4f^{14}\ 5s^2\ 5p^6\ 5d + h\nu$$

$$\rightarrow 4d^{10}\ 4f^{14}\ [5s^2\ 5p^6\ 5d]^{-1} + h\nu$$

$(n'=5,6,\ n \le n')$

W^{q+} (q=6-11) ground state $4d^{10}\ 4f^{26-q-m}\ 5s^2\ 5p^m$ (m=6-2), IE : 125.7 eV-234.2 eV

$$4d^{10}\ 4f^{26-q-m}\ [5s^2\ 5p^m]^{-1}\ n'l' \rightarrow 4d^{10}\ 4f^{26-q-m}\ [5s^2\ 5p^m]^{-1}\ nl + h\nu$$

$$\rightarrow 4d^{10}\ 4f^{26-q-m+1}\ [5s^2\ 5p^m]^{-1} + h\nu$$

$$\rightarrow 4d^{10}\ 4f^{26-q-m+1}\ [5s^2\ 5p^m]^{-2}\ n'l' + h\nu$$

$$4d^{10}\ 4f^{26-q-m-1}\ 5s^2 5p^m\ n'l' \rightarrow 4d^{10}\ 4f^{26-q-m-1}\ 5s^2 5p^m\ nl + h\nu$$

$$\rightarrow 4d^{10}\ 4f^{28-q-m}\ 5s^2 5p^m + h\nu$$

$$\rightarrow 4d^{10}\ 4f^{28-q-m}\ [5s^2 5p^m]^{-1} + h\nu$$

$(n'=5,6,\ n \le n')$

W^{q+} (q=12-16) ground state $4d^{10}\ 4f^{28-q-m}\ 5s^m$ (m=1 or 2), IE : 273.6 eV-390.2 eV

$$4d^{10}\ 4f^{28-q-m}\ 5s^{m-1}\ n'l' \rightarrow 4d^{10}\ 4f^{28-q-m}\ 5s^{m-1}\ nl + h\nu$$

$$\rightarrow 4d^{10}\ 4f^{28-q-m+1}\ 5s^{m-1} + h\nu$$

$$\rightarrow 4d^{10}\ 4f^{28-q-m+1}\ 5s^{m-2}\ n'l' + h\nu$$

$$4d^{10}\ 4f^{28-q-m-1}\ 5s^m\ n'l' \rightarrow 4d^{10}\ 4f^{28-q-m-1}\ 5s^m\ nl + h\nu$$

$$\rightarrow 4d^{10}\ 4f^{28-q-m}\ 5s^m + h\nu$$

$$\rightarrow 4d^{10}\ 4f^{28-q-m}\ 5s^{m-1}\ n'l' + h\nu$$

$(n'=5,6,\ n \le n')$

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Photon Emissivity Coefficient (PEC)

W^{q+} (q=17-27) ground state $4d^{10}\ 4f^{m}$ (m=14-1),
Ionization energy (IE) : 432.3 eV-885.7 eV

Upper state **Lower state**

$$4d^{10}\ 4f^{m-1}\ n'l' \rightarrow 4d^{10}\ 4f^{m-1}\ nl + h\nu$$
$$\rightarrow 4d^{10}\ 4f^{m} + h\nu \qquad (n'=n=5)$$

W^{q+} (q=28-37) ground state $4d^{m}$ (m=10-1),
Ionization energy (IE) : 1133.8 eV-1620.2 eV

$$4d^{m-1}\ n'l' \rightarrow 4d^{m-1}\ nl + h\nu \quad (n'=4,5,\ n \leq n')$$

W^{q+} (q=38-45) ground state $4s^{m}\ 4p^{46-q-m}$ (m=0-2),
Ionization energy (IE) : 1830.7 eV-2414.2 eV

$$[4s^{m}\ 4p^{46-q-m}]^{-1}\ n'l' \rightarrow [4s^{m}\ 4p^{46-q-m}]^{-1}\ nl + h\nu$$
$$(n'=4,5,\ n \leq n')$$

W^{q+} (q=46-48) ground state $3d^{m}$ (m=10-8),
Ionization energy (IE) : 4059.2 eV-4309.4 eV

$$3d^{m-1}\ n'l' \rightarrow 3d^{m-1}nl + h\nu \quad (n'=n=4)$$
$$\rightarrow 3d^{m} + h\nu$$

FAC data *vs.* ADAS data

FAC	ADAS
Full J-J coupled level resolved scheme	**Configuration average scheme**

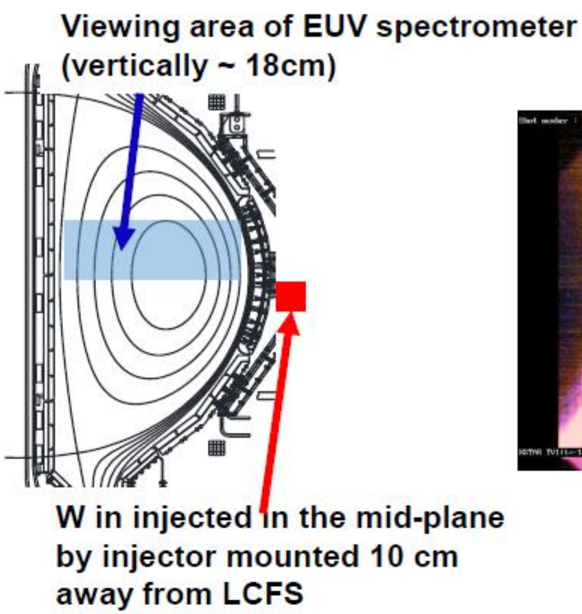
For eg. W^{25+}

Total 9+496 levels 1+28 states

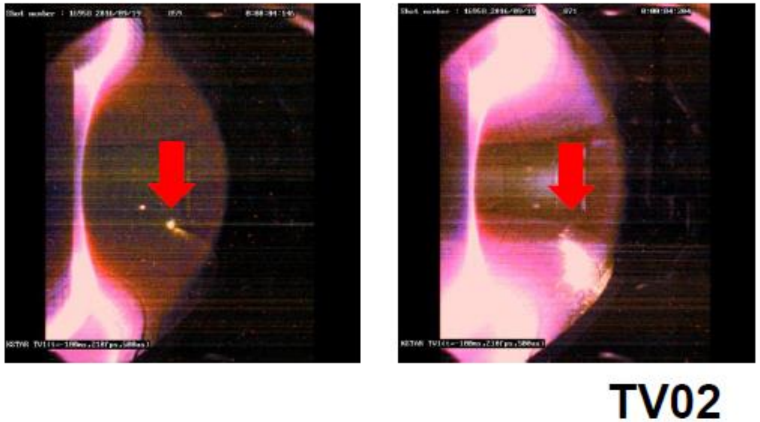
Impurity injection experiment in KSTAR

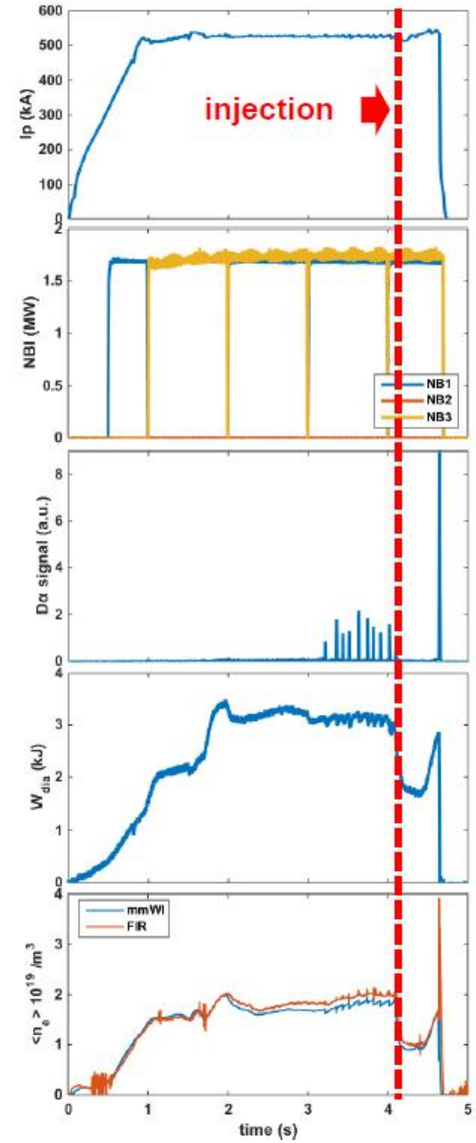
◆ **Shot information**

- **#16958**: B_T **= 2.5 T** with **NBI power = 2.8 MW**
- 2 – 3 mg of 12 μm W powder was injected at around 4.03 sec (# of W atoms in 1 mg: ~4.6 x 10^{18})
- Tungsten spectra were measured after the injection by compact advanced EUV spectrometer system (CAES).



#16958 Visible camera images



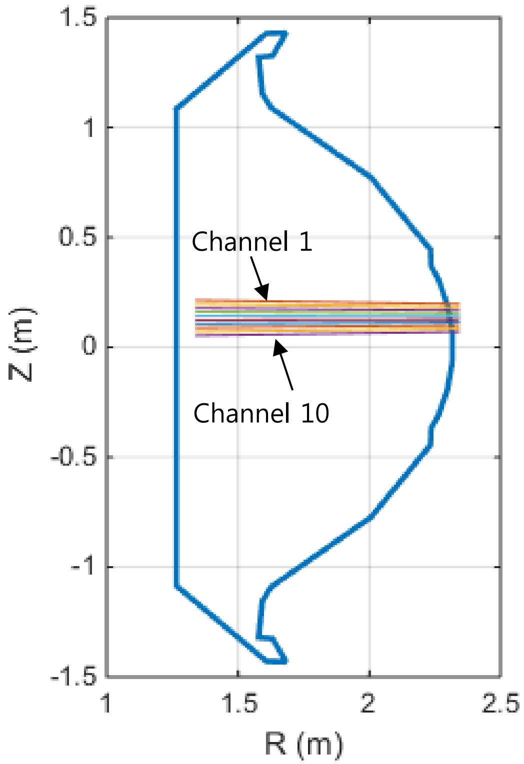


On the courtesy of In Woo Song in KAIST and KSTAR team

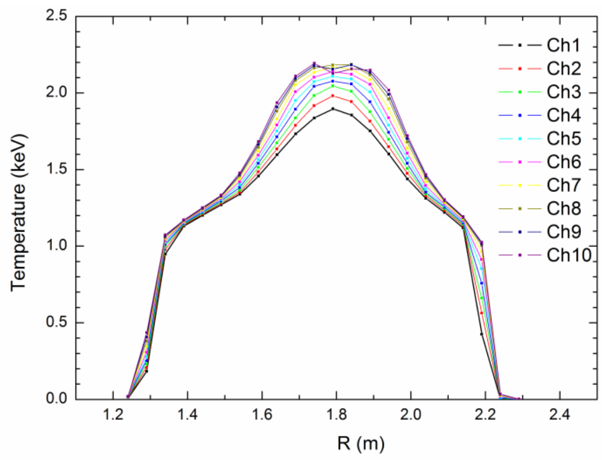
Measured spectra in KSTAR

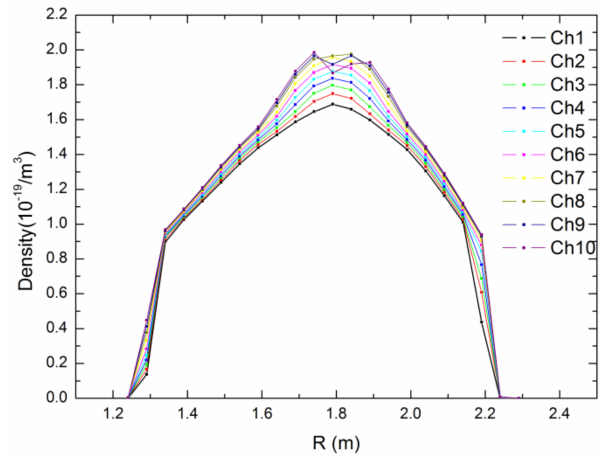
◆ Lines of sight, Thomson T_e & n_e profiles

LoS for CAES on KSTAR



- Simple 2-D configuration
  (only the pinhole position and the detector position are considered)
- 10 lines of sight (corresponding to 10 channels during #16958)
- Sample points are generated on the LoS with equal distance apart

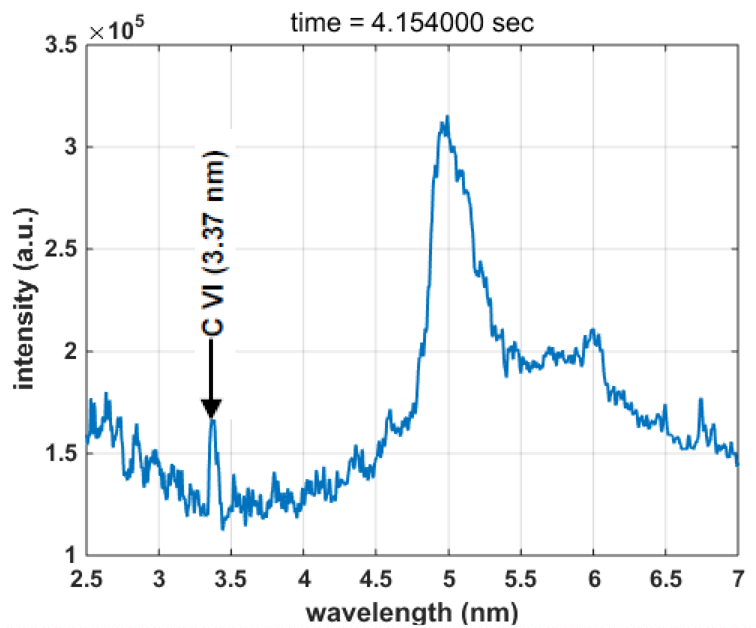


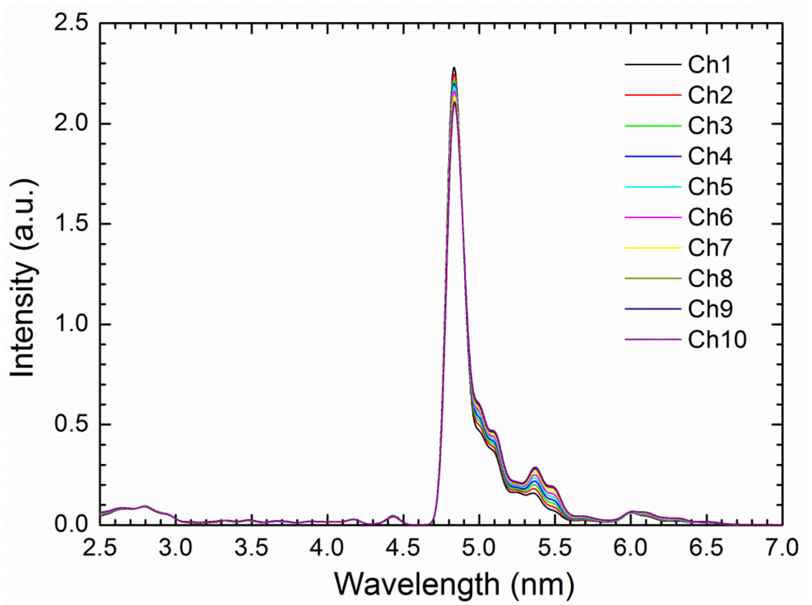


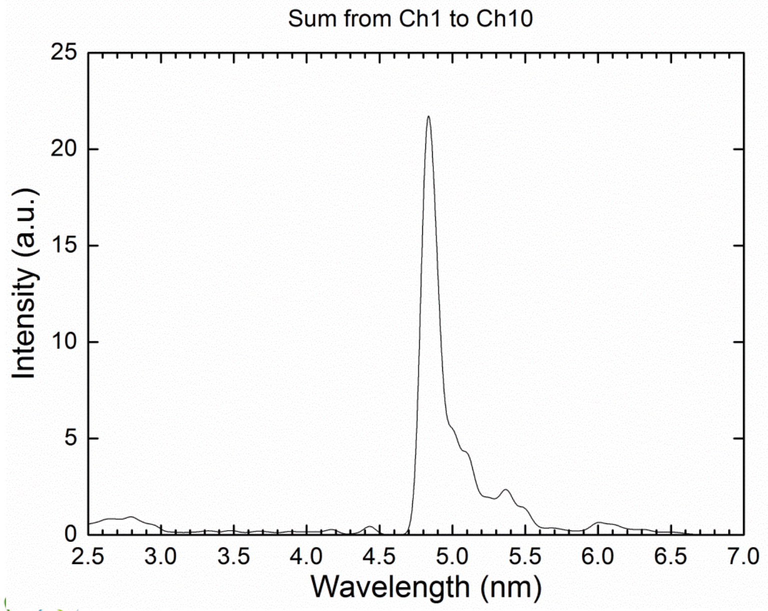
- Thomson data at 4.15 s (100 ms averaged) are used
- Fitted by using tanh function

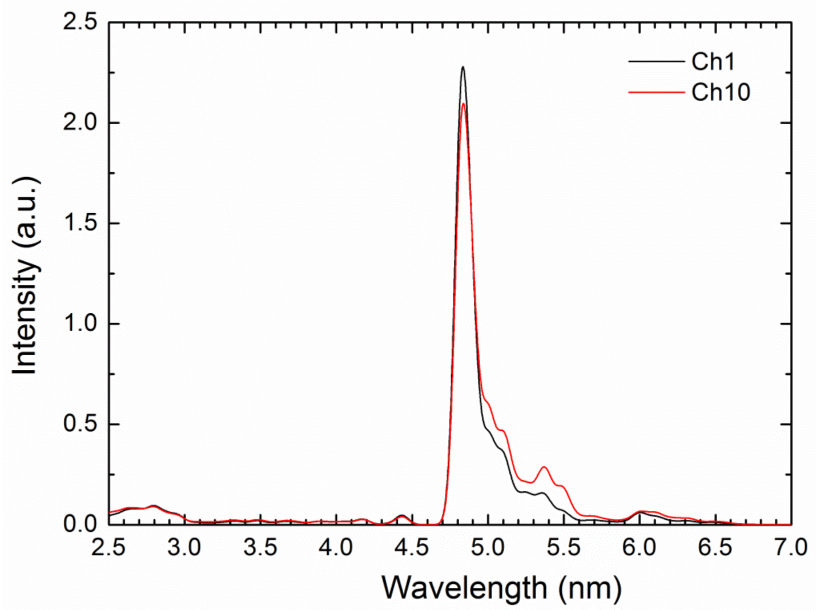
On the courtesy of In Woo Song in KAIST and KSTAR team

Measured vs. modeled spectra



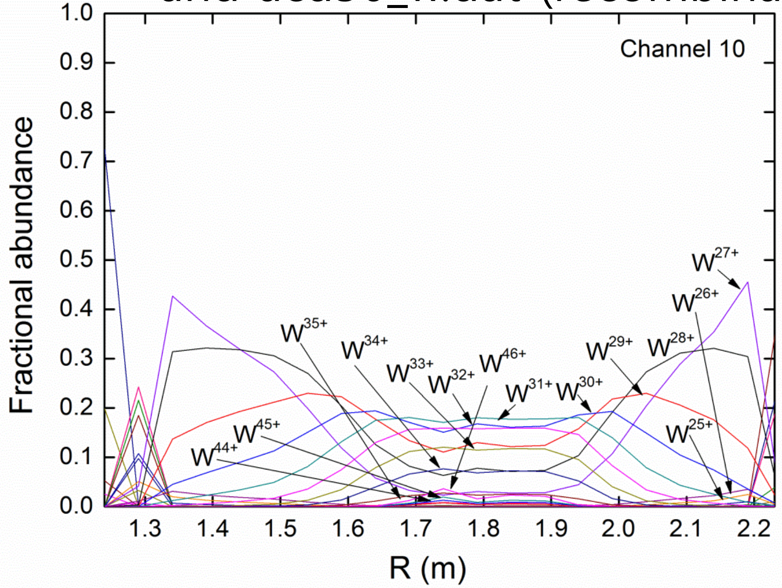


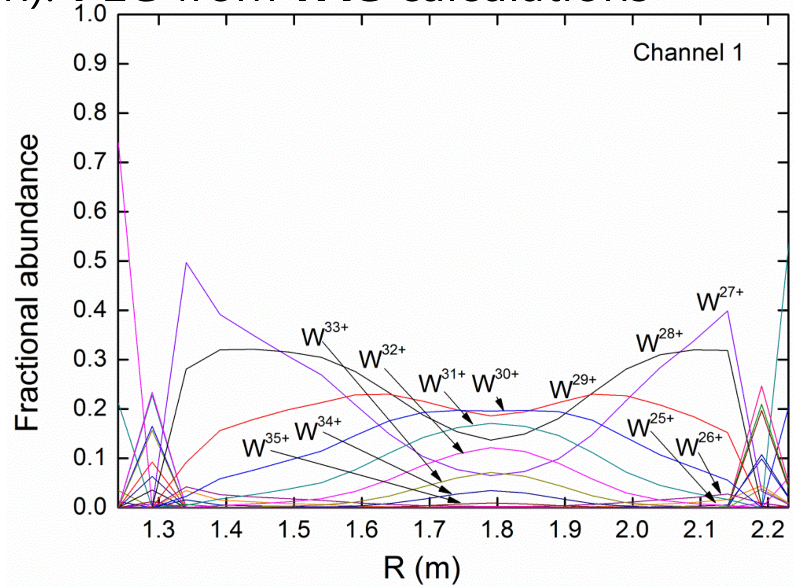


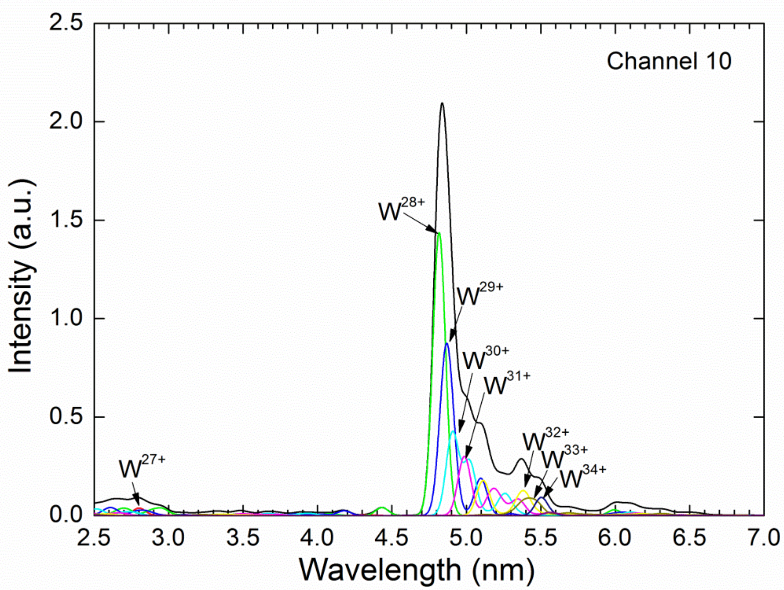


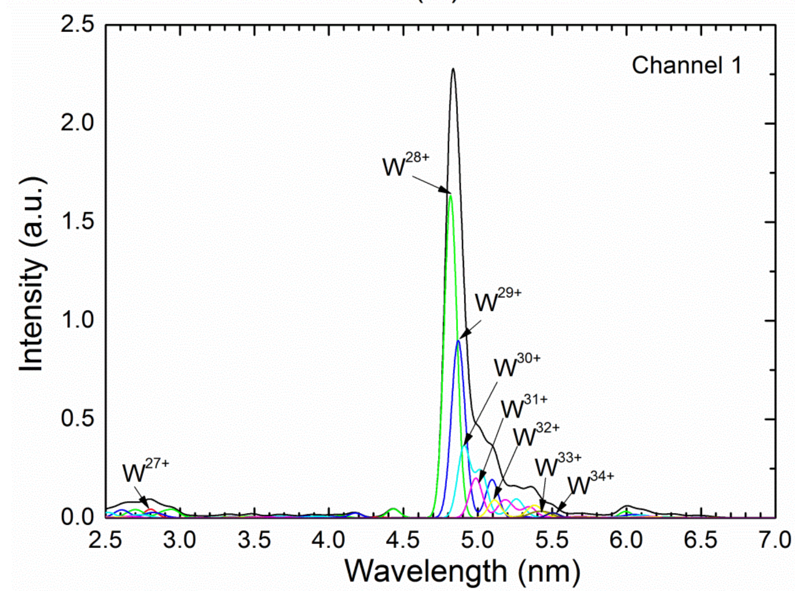
Transport free modeled spectra

Fractional abundance from **ADAS** ca09_w.dat (ionization) and acd50_w.dat (recombination). **PEC** from **FAC** calculations



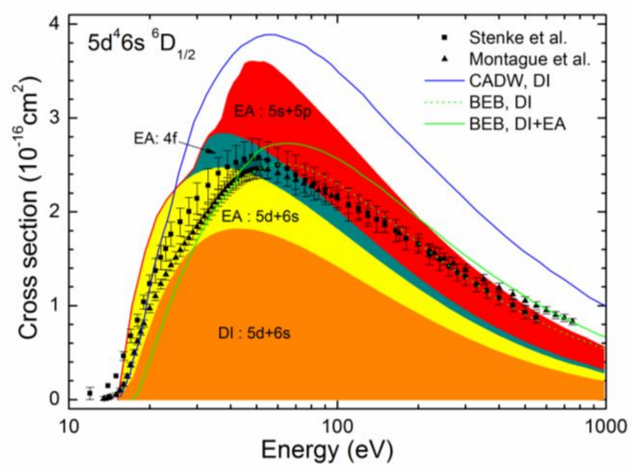




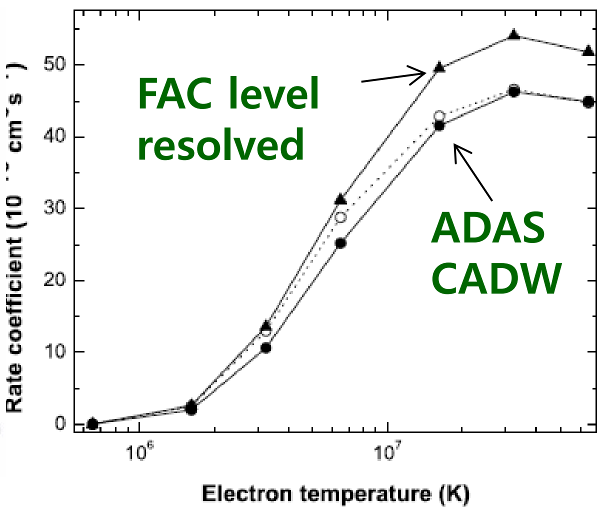


Ionization data for W

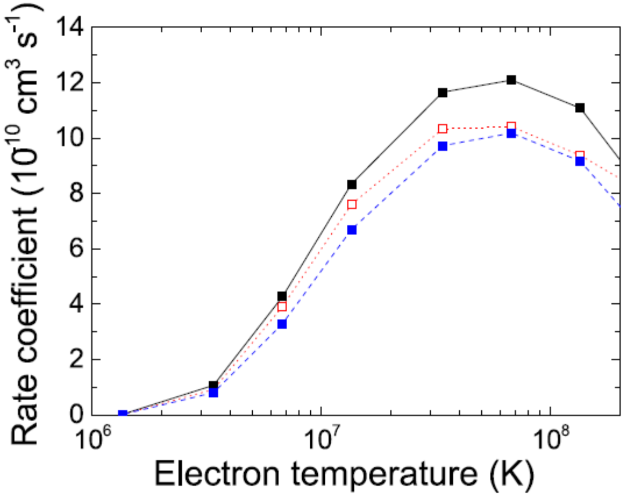
W^{+} **W^{17+}** **W^{25+}**



D.-H. Kwon, Y. S. Cho, and Y. O. Lee, IJMS **356**, 7 (2013)



D.-H. Zhang and D.-H. Kwon, JPB **47**, 075202 (2014)



A. Kyniene, S. Pakalka, S. Masys, and V. Jonauskas, JPB **49**, 185001 (2016)

ADAS ionization data by CADW ab-initio calculation for W ions is reliable within 30-50% accuracy being compared with other ab-initio calculations and the data set is available for all ionization stages.

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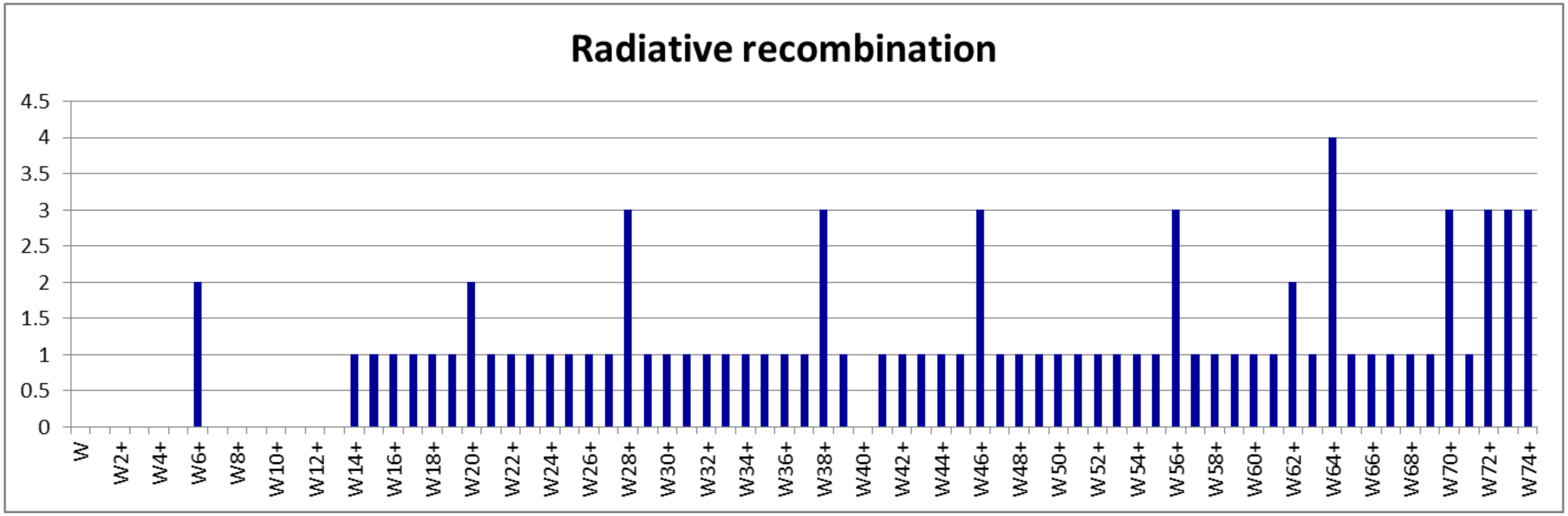
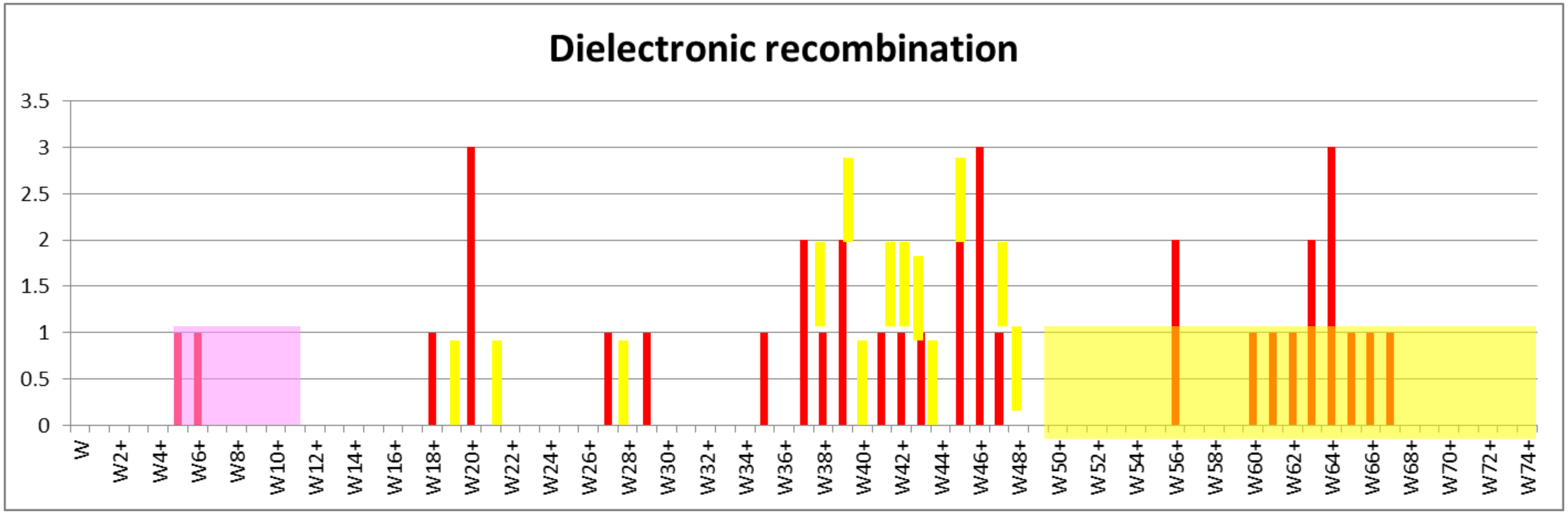
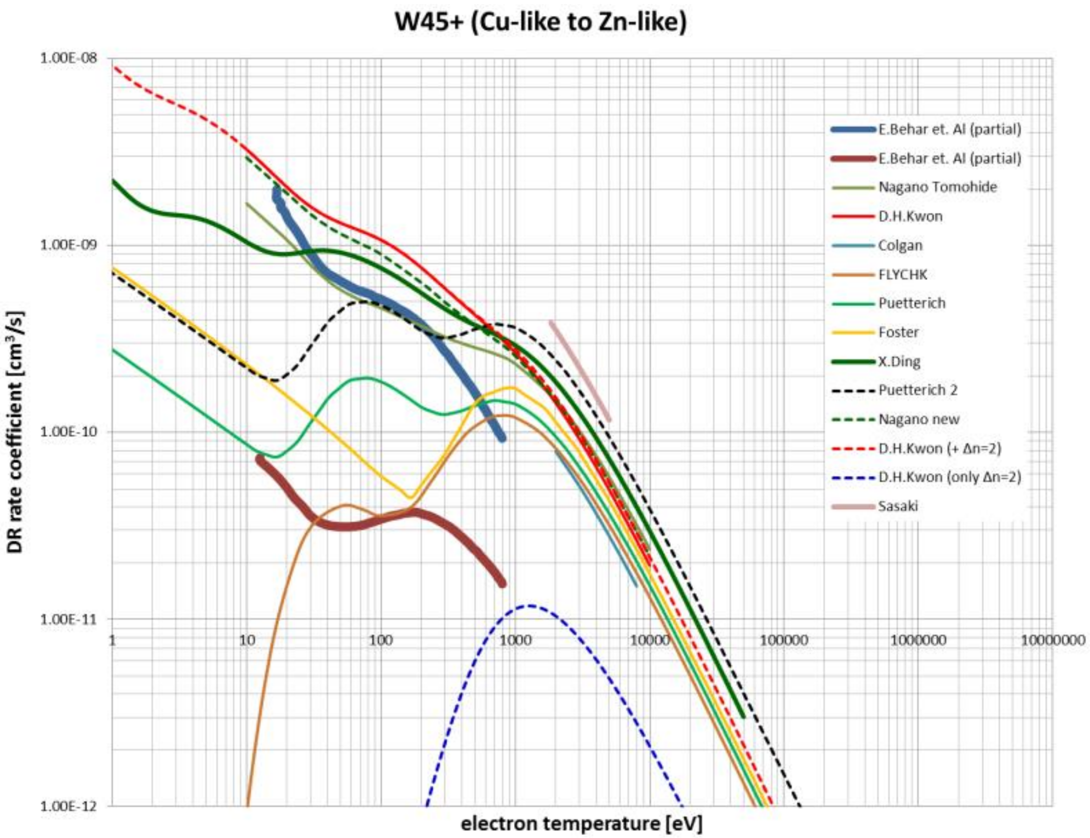
Recombination data for W





DR data for W



ab-initio calculation

$$\alpha_i(T) = \frac{1}{2g_i}\left(\frac{4\pi a_0^2 Ry}{k_B T}\right)^{3/2} \times$$

$$\sum_j g_j A_{ji}^a B_j \exp\left(-\frac{E_{ij}}{k_B T}\right)$$

$$B_j = \frac{\sum_t A_{jt}^r + \sum_{t'} A_{jt'}^r B_{t'}}{\sum_k A_{jk}^a + \sum_f A_{jf}^r}$$

Burgess formula

$$\alpha_i(T) = 7.59\times10^{-14} n_e n_Z \frac{B(q)D(q,T)}{T^{3/2}}$$

$$\times \sum_j f_{ji} A(y) \exp\left(-\frac{\bar{E}}{T}\right)$$

IAEA&KAERI Joint CM on DR for W (Sept. 2015)

ADAS recombination data based on a simple Burgess formula for W ions quite differ from other ab-initio calculations and the data is not available for many ionization stages.

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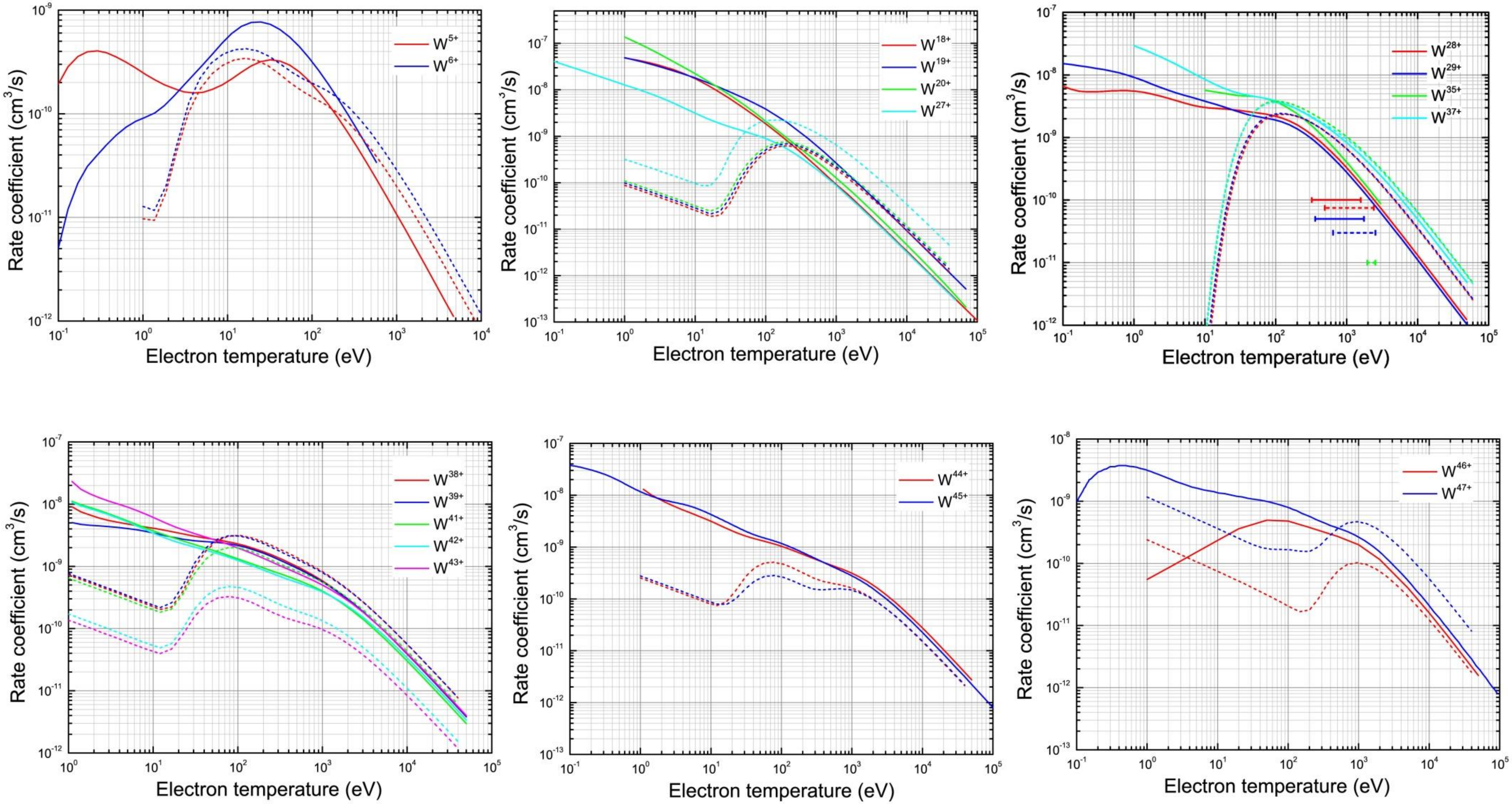
IAEA-KAERI joint CM on DR for W

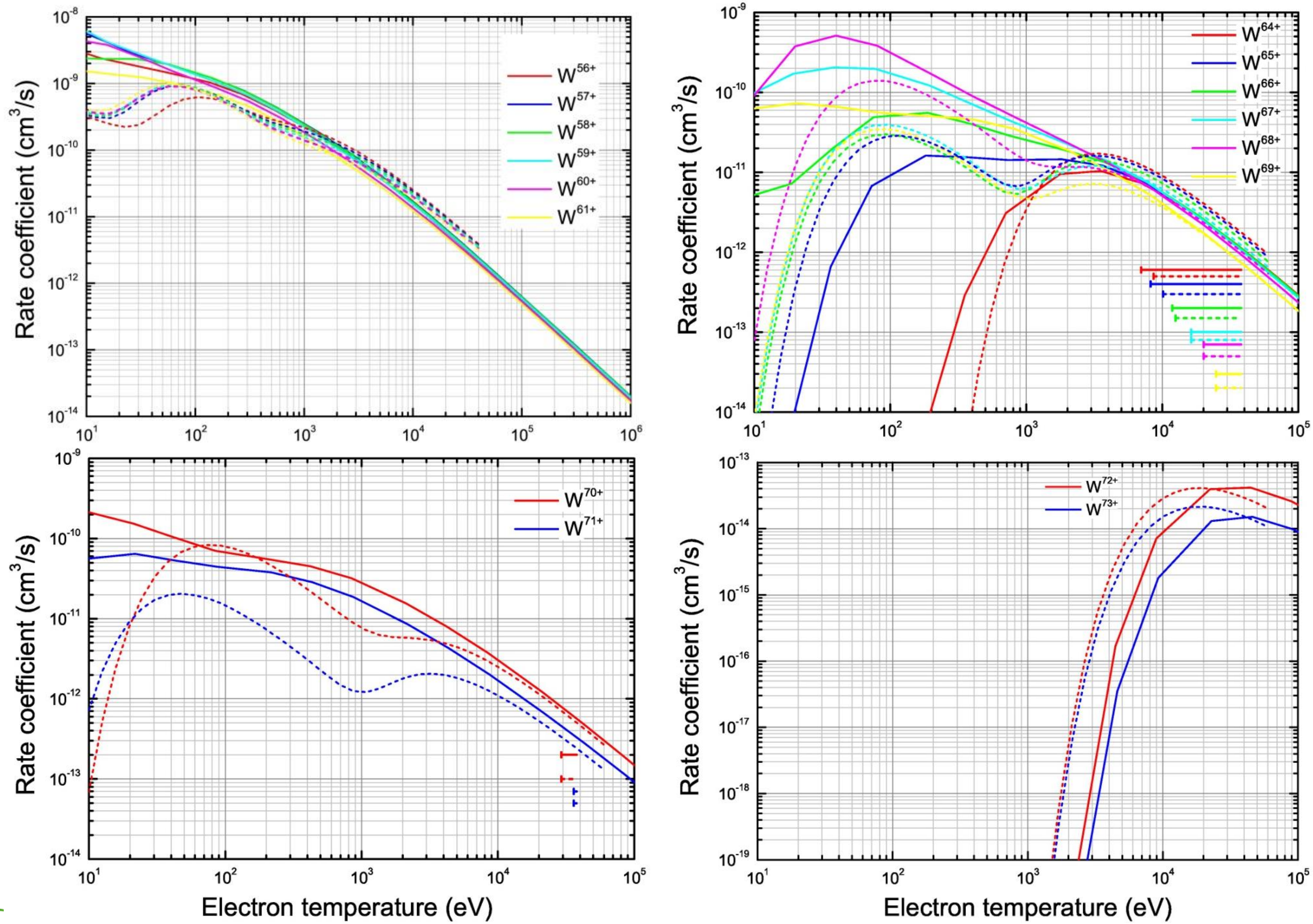
At KAERI (Sept. 2015)

New recommended DR data for W ions



ADNDT in press, available online 5 June 2017

New recommended DR data for W ions



ADNDT *in press, available online 5 June 2017*

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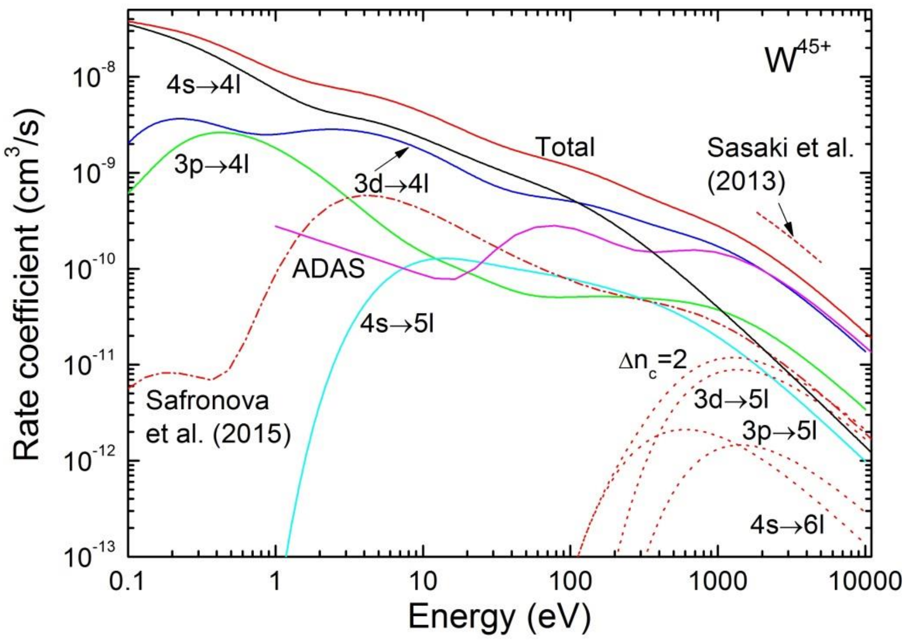
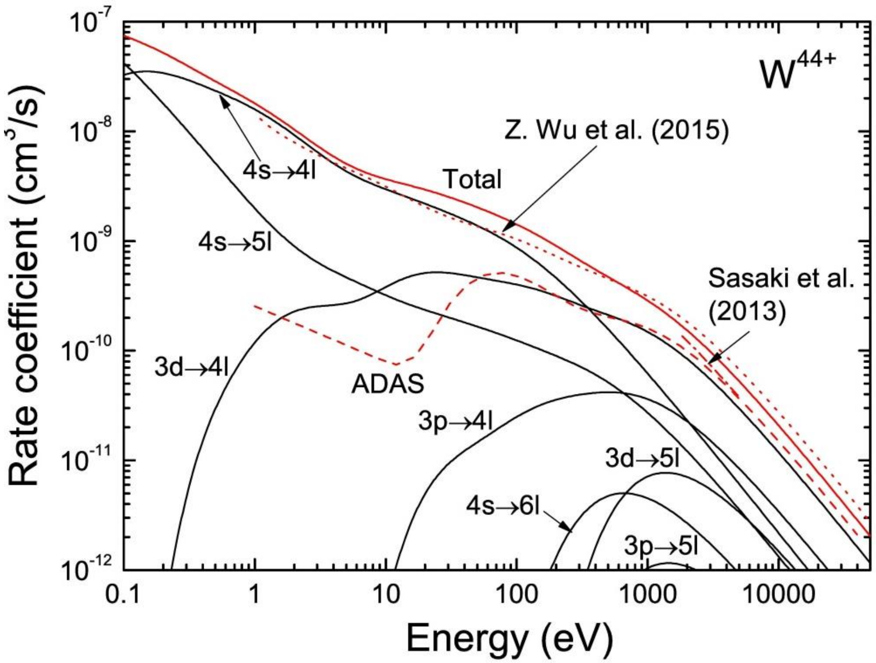
DR data for W ions (Our calculations)

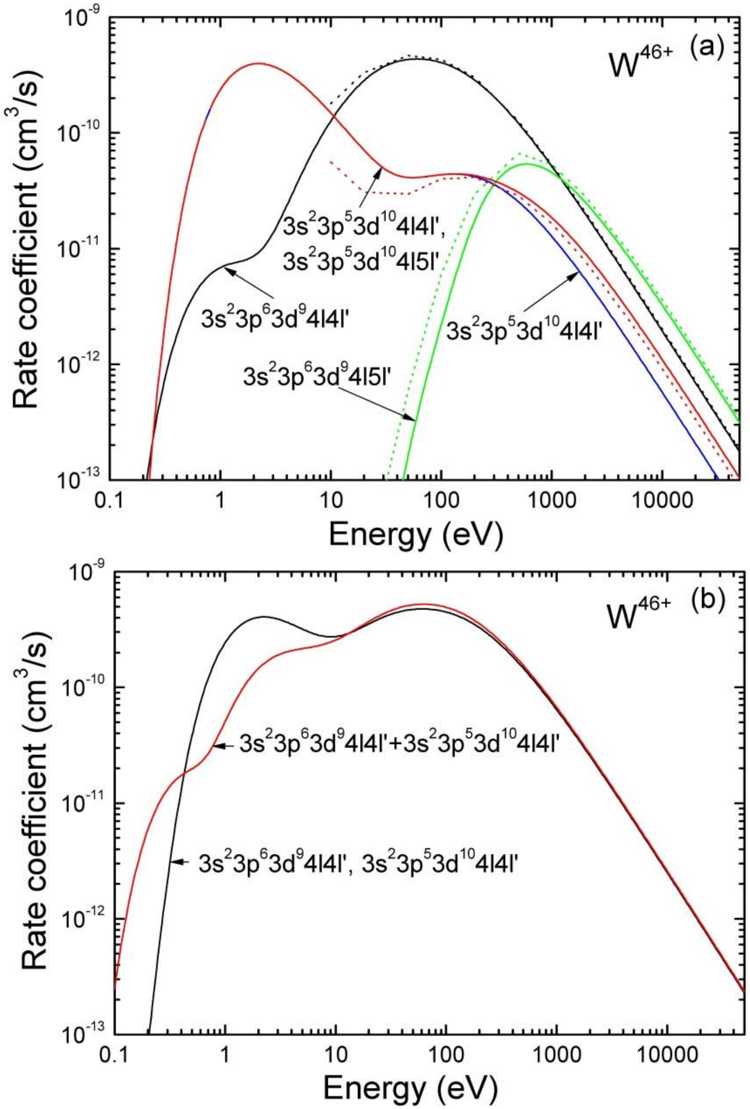


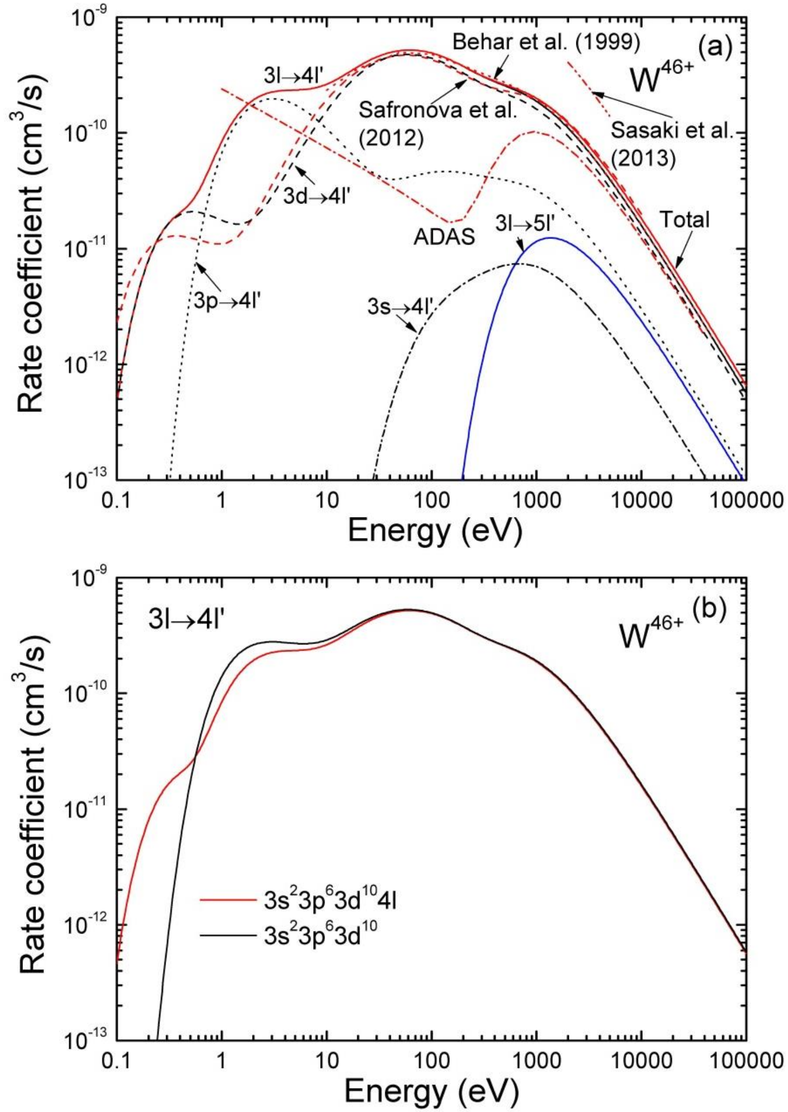


D.-H. Kwon and W. Lee, JQSRT **170**, 182 (2016); ibid., **179**, 98 (2016)

D.-H. Kwon and W. Lee, JQSRT, **179**, 98 (2016)

DR data for W ions (Our calculations)





DR data for W ions (Our calculations)

Threshold energy of resonance for DR of W^{q+} (q = 5-11)

Ion	Ground configuration	FAC (eV)	NIST (eV)	% Error
W^{4+}	$4f^{14}5s^25p^65d^2$	51.62	51.6	0.04
W^{5+}	$4f^{14}5s^25p^65d$	65.20	64.77	0.66
W^{6+}	$4f^{14}5s^25p^6$	116.92	122.01	4.17
W^{7+}	$4f^{14}5s^25p^5$ or $4f^{13}5s^25p^6$	140.53	141.2	0.47
W^{8+}	$4f^{14}5s^25p^4$	162.17	160.2	1.35
W^{9+}	$4f^{14}5s^25p^3$	180.9	179.0	1.06
W^{10+}	$4f^{14}5s^25p^2$	203.93	208.9	2.38
W^{11+}	$4f^{14}5s^25p$ $4f^{13}5s^25p^2$		231.6	

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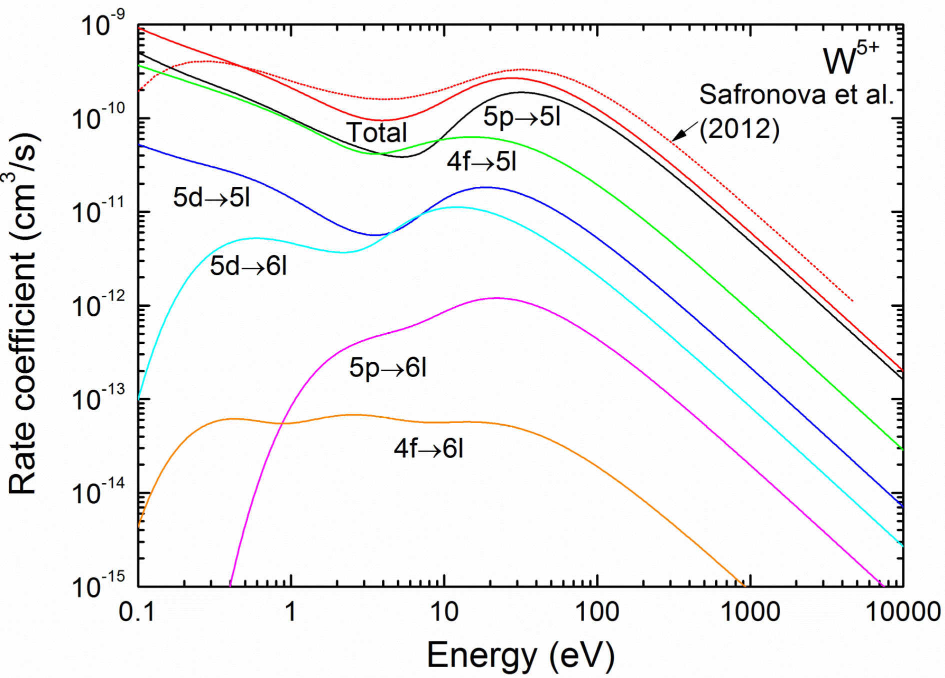
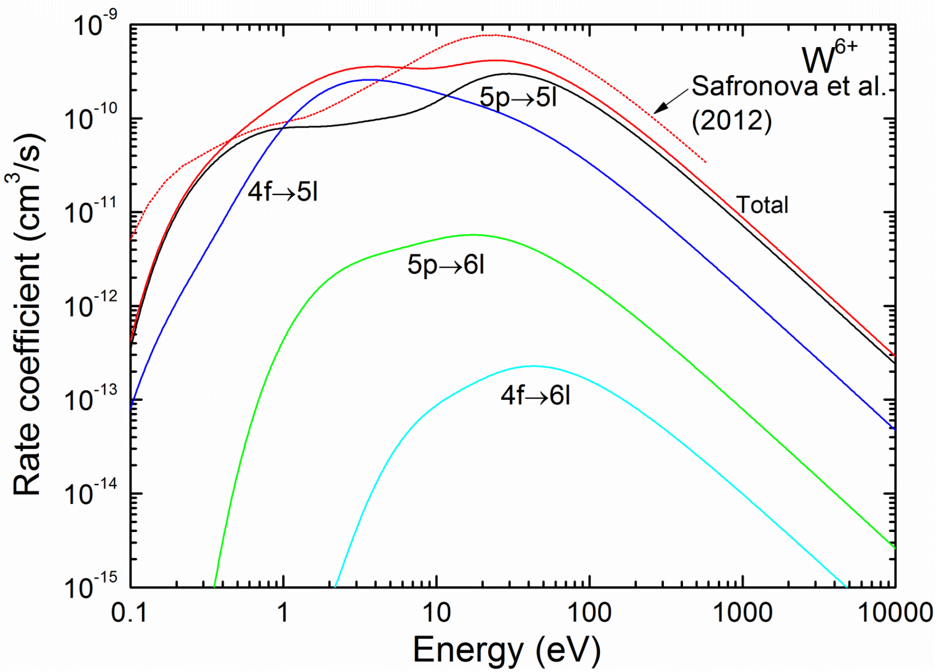
DR data for W ions (Our calculations)

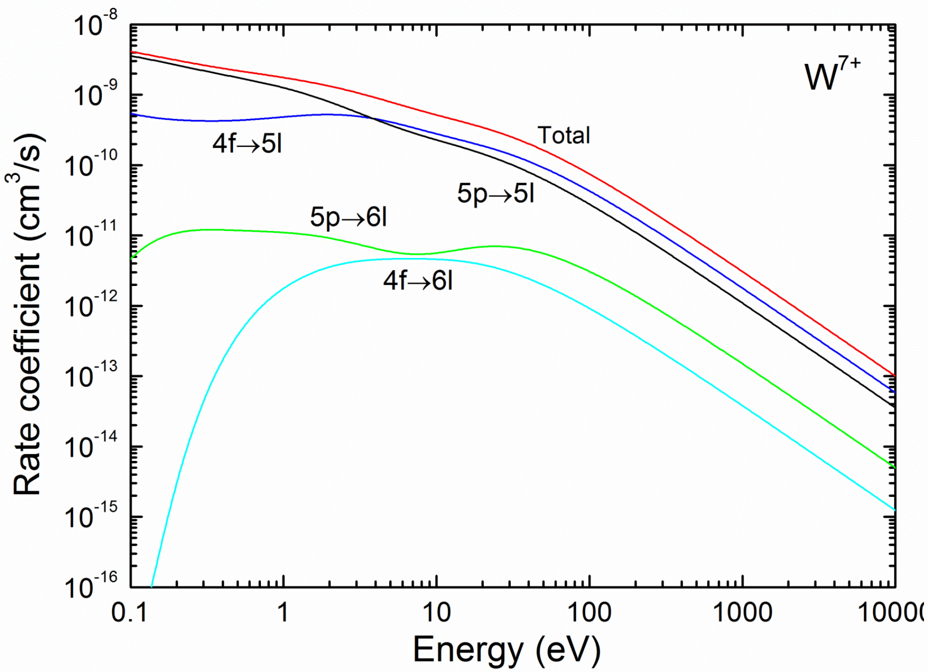




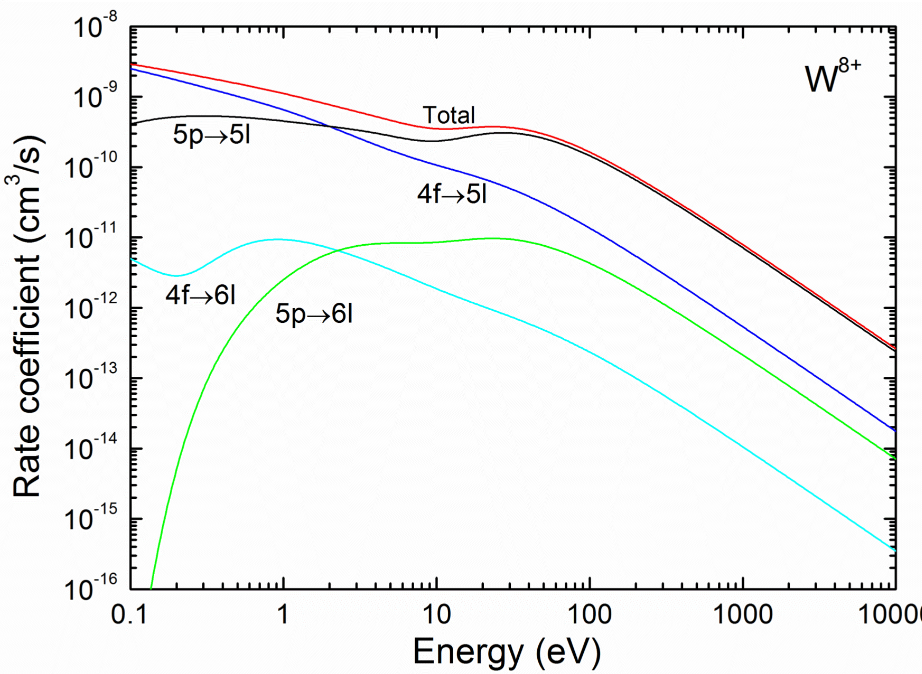
$4f^{14}5s^25p^65d$
Ground level

$4f^{14}5s^25p^6$
Ground level

DR data for W ions (Our calculations)



4f145s25p5
Ground level



4f145s25p4
Ground level

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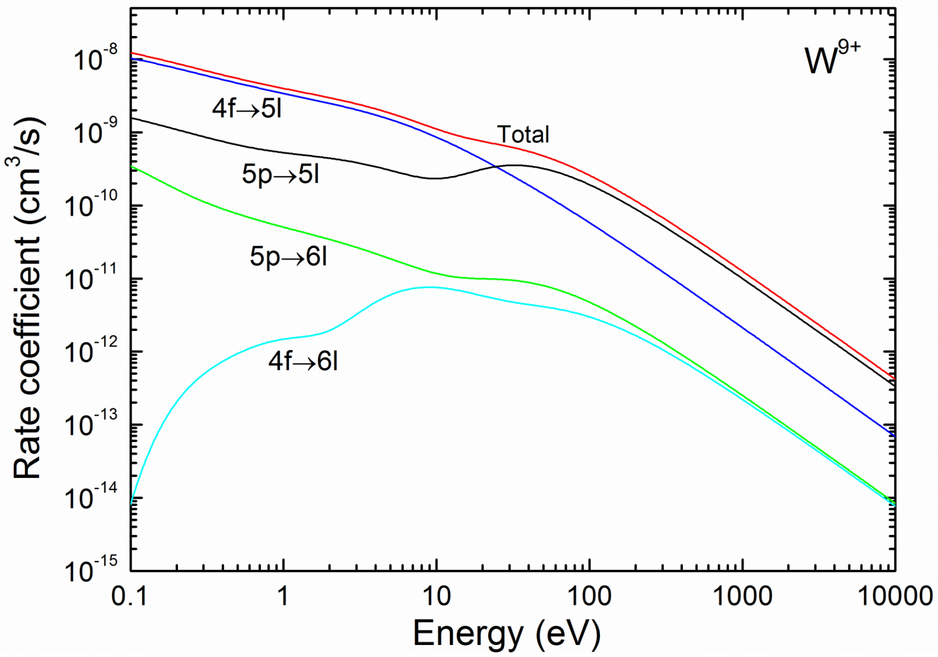
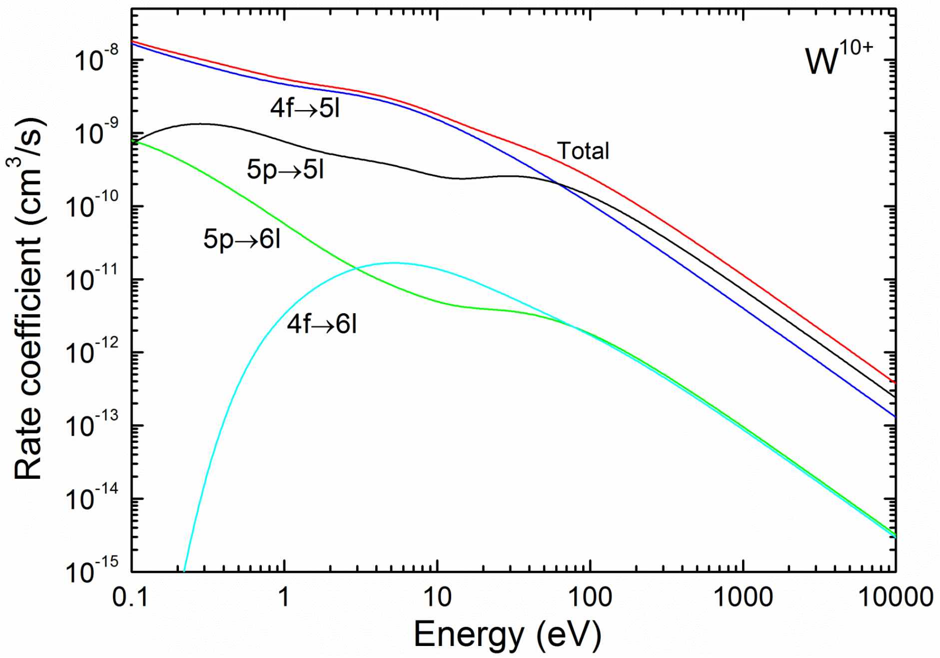
DR data for W ions (Our calculations)



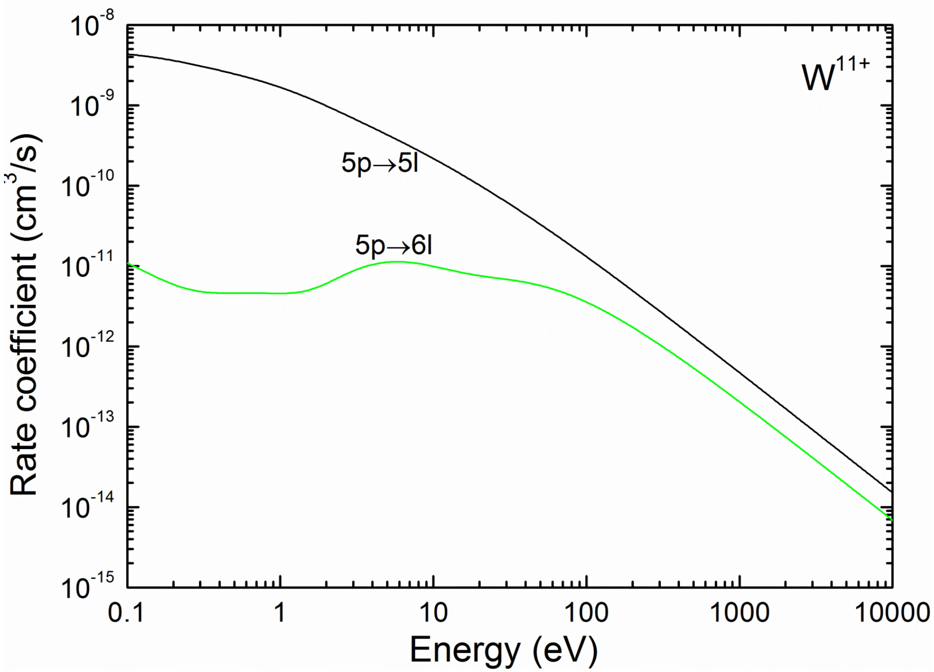
$4f^{14}5s^{2}5p^{3}$
Ground level



$4f^{14}5s^{2}5p^{2}$
Ground level

To be submitted.

DR data for W ions (Our calculations)



$4f^{13}5s^{2}5p^{2}$
Ground level

Due to so many resonances of 4f core excitation, DR via 4f transition has been still run.

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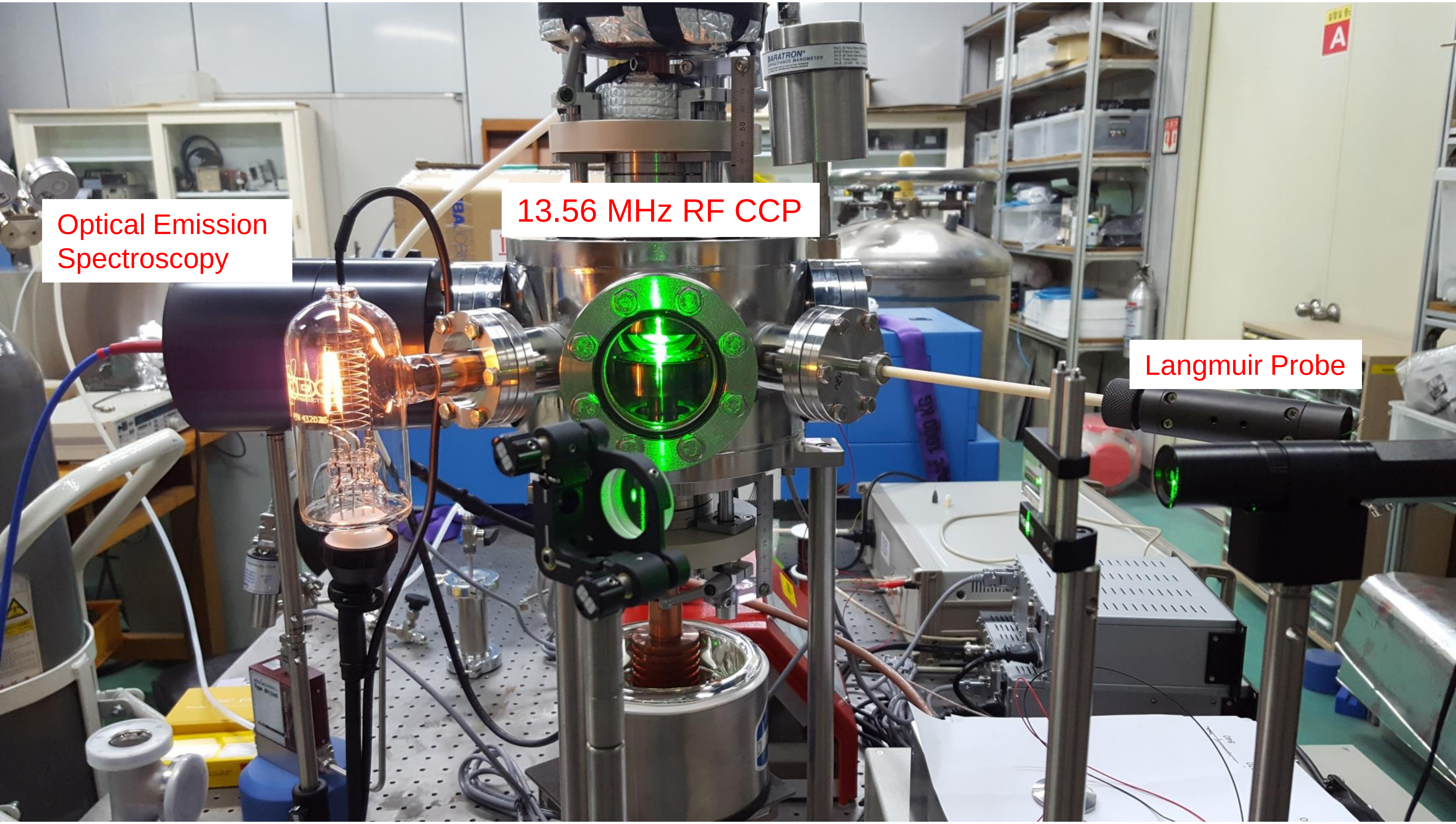
Spectroscopy in CCP device

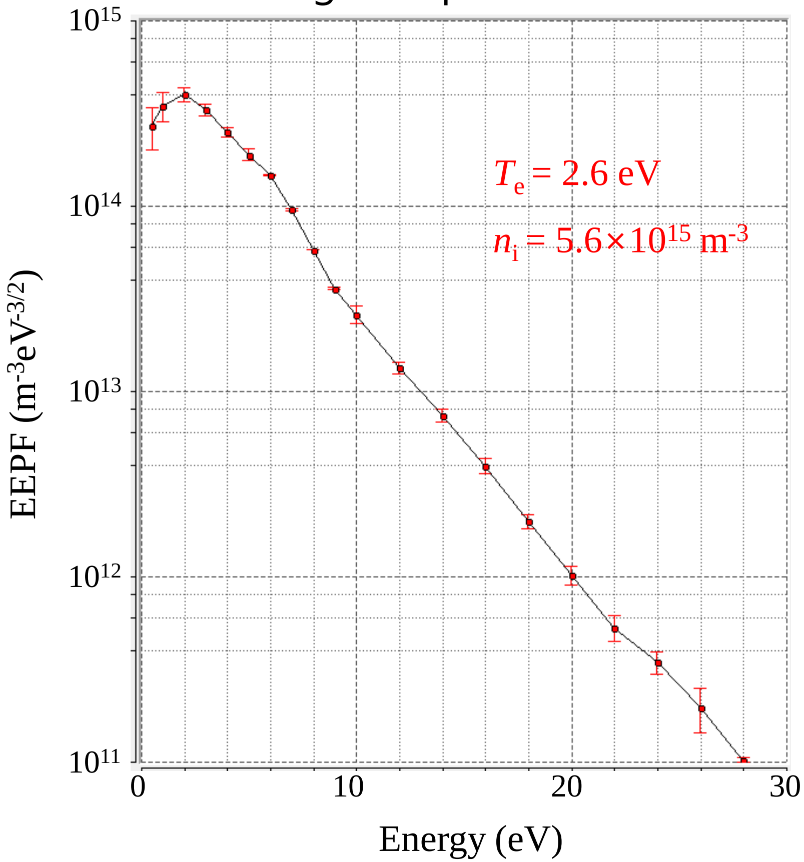
Experimental setup



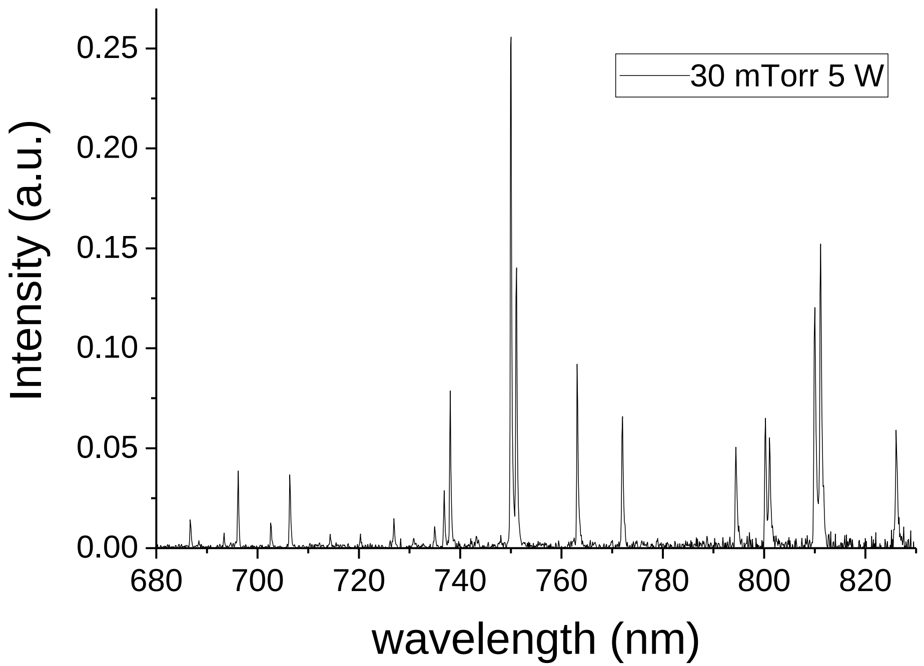
Spectroscopy in CCP device

Langmuir probe diagnostics and OES

Langmuir probe data



OES data



Spectra measured by Ocean Optics HR4000 (calibrated)

EEPF: measured by Impedans Ltd. Langmuir probe

CR modeling for Ar

$$\sum_{\substack{j=0\\ j\neq 1}}^{4} = \alpha_{j1}N_j n_e + \sum_{\substack{m=5\\ m\neq 10}}^{13} A_{m1}N_m + \sum_{m=5}^{14}\alpha_{m1}N_m n_e$$
$$= \left[\left(\alpha_{1i} + \sum_{\substack{k=0\\ k\neq 1}}^{14}\alpha_{1k}\right)n_e + \tau_1^{-1} + \sum_{j=1}^{4}\alpha_{1j}N_j\right]N_1$$

$$\sum_{\substack{j=0\\ j\neq 2}}^{4}\alpha_{j2}N_j n_e + \sum_{\substack{m=5\\ m\neq 6}}^{14} A_{m2}N_m$$
$$= \left[\left(\alpha_{2i} + \sum_{\substack{k=0\\ k\neq 2}}^{4}\alpha_{2k}\right)n_e + A_2^{\mathrm{eff}} + \sum_{j=1}^{4}\alpha_{2j}N_j\right]N_2$$

$$\sum_{\substack{j=0\\ j\neq 3}}^{4}\alpha_{j3}N_j n_e + \sum_{m=5,8,11,13} A_{m3}N_m + \sum_{m=5}^{14}\alpha_{m3}N_m n_e$$
$$= \left[\left(\alpha_{3i} + \sum_{\substack{k=0\\ k\neq 3}}^{14}\alpha_{1k}\right)n_e + \tau_3^{-1} + \sum_{j=1}^{4}\alpha_{3j}N_j\right]N_3$$

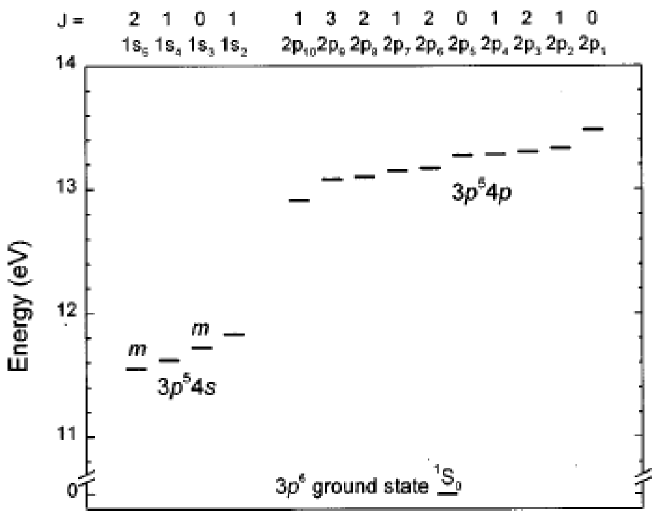
$$\sum_{\substack{j=0\\ j\neq 4}}^{4}\alpha_{j4}N_j n_e + \sum_{\substack{m=5\\ m\neq 6,10}}^{14} A_{m4}N_m$$
$$= \left[\left(\alpha_{4i} + \sum_{k=0}^{3}\alpha_{4k}\right)n_e + A_4^{\mathrm{eff}} + \sum_{j=1}^{4}\alpha_{4j}N_j\right]N_4$$

$$\sum_{j=0,1,3}\alpha_{jm}N_j n_e = \sum_{k<m} A_{mk}^{(\mathrm{eff})}N_m + \left(\alpha_{mi} + \sum_{k=0,1,3}\alpha_{mk}\right)N_m n_e$$

N_0 : Ground state $3p^6\ {}^1S_0$

$N_{j=1-4}$: Metastable $(j = 1, 3)$ and resonance $(j = 2,4)$ states $1s_{5\text{-}2}$, $3p^5 4s\ {}^{2S+1}P_J$

$N_{m=5-14}$: Excited states $2p_{10\text{-}1}$, $3p^5 4p\ {}^{2S+1}L_J$



Under construction !

Database updates

Our website for atomic data and CR modeling

http://pearl.kaeri.re.kr

KAERI

Summary & Outlook

1. We have calculated PEC for tungsten (W) ions W^{q+} ($q = 5\text{-}48$) by parallelizing radiative transition routine of FAC.
2. We had compiled available DR data for W ions and gave the recommended data through IAEA and KAERI joint CM.
3. We have calculated DR for W^{q+} ($q = 5\text{-}11, 44\text{-}46$) and will calculate DR for W^{q+} ($q = 30\text{-}34$).
4. We have installed a CCP device and measured plasma temperature and density for Ar with a Langmoir probe. OES for Ar has also been carried out. CR modeling including detailed collision and radiative processes will be constructed.
5. We have updated the calculated atomic data and implemented the previous CR modeling for He I on our Web DB (http://pearl.kaeri.re.kr).
6. Parallelization for FAC was done for AI routine will be performed.
7. Unitary correction for collisional excitation routine based on distorted wave approximation of FAC will be tried.

Collaborations

KAIST Dept. of Physics, Fusion Plasma Transport Research Center

NFRI ITER Korea VUV Diagnostic Team, KSTAR Team

KRISS Physical Metrology team: Absolute calibration for spectrometer

Fractional abundance

$$N_{\rm tot} = \sum_{i=0}^{Z} N^i, \quad f^q = \frac{N^q}{N_{\rm tot}} \Rightarrow \text{Fractional Abundance} \quad \sum_{i=0}^{Z} f^i = 1.$$

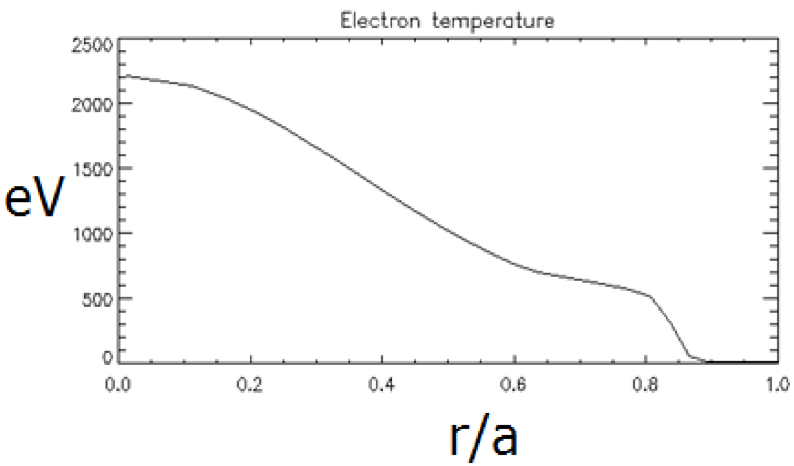
$$N_{\rm tot}\frac{d}{dt}\begin{bmatrix} f^0 \\ f^1 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \end{bmatrix} \Leftarrow \text{Collisional Ionization Equilibrium}$$

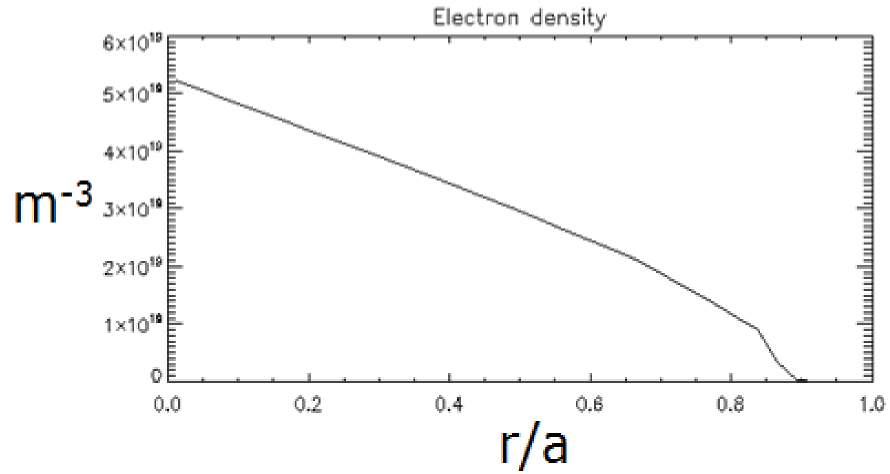
Total recombination rate coefficient

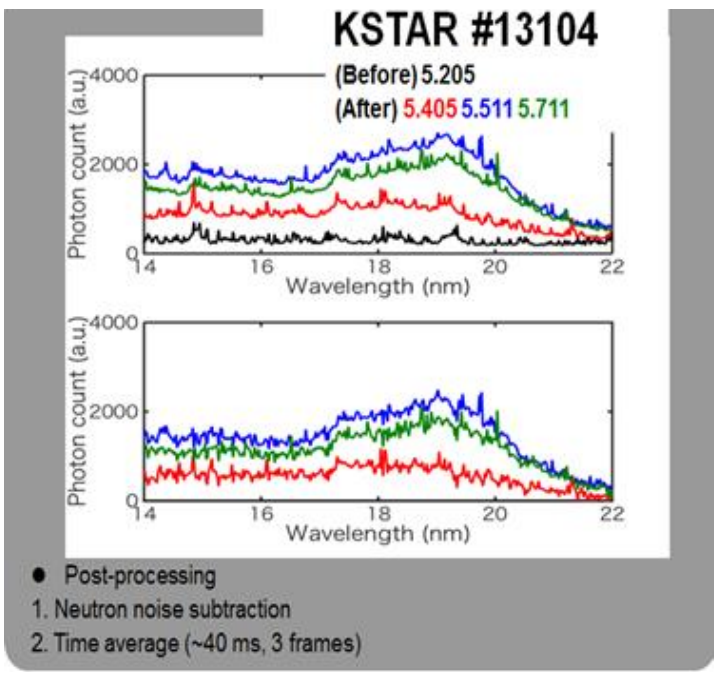
$$N_{\rm tot} n_e \begin{bmatrix} -S_{\rm tot}^{0\to1} & \alpha_{\rm tot}^{1\to0} & 0 \\ S_{\rm tot}^{0\to1} & -\alpha_{\rm tot}^{1\to0} - S_{\rm tot}^{1\to2} & \alpha_{\rm tot}^{2\to1} \\ 0 & S_{\rm tot}^{1\to2} & \ddots \end{bmatrix} \begin{bmatrix} f^0 \\ f^1 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \end{bmatrix}$$

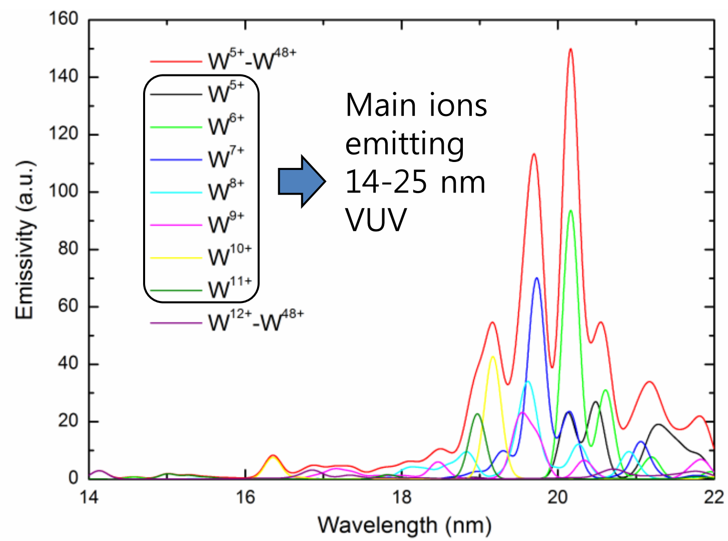
Total ionization rate coefficient

W VUV Spectra measured in KSTAR



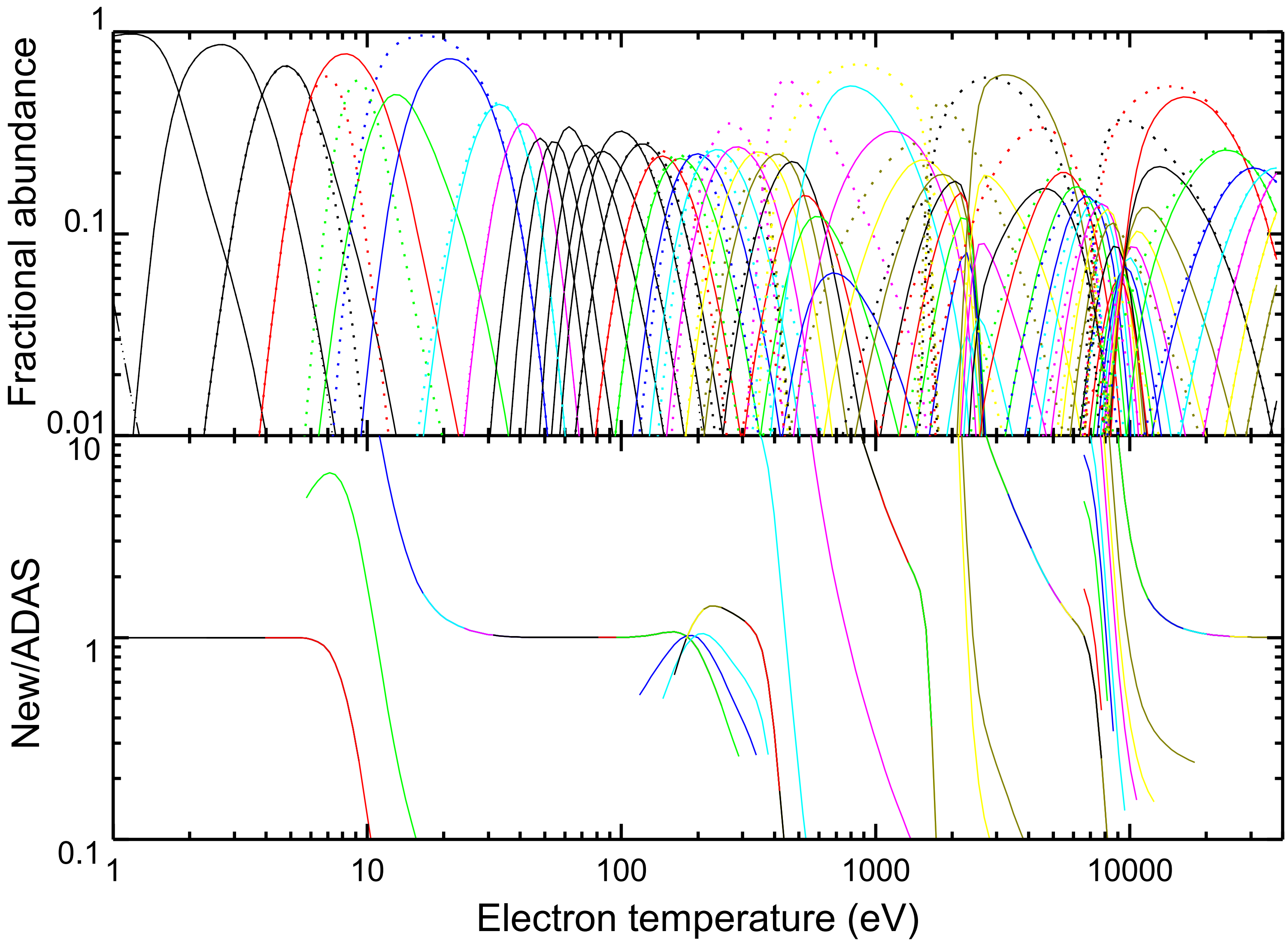




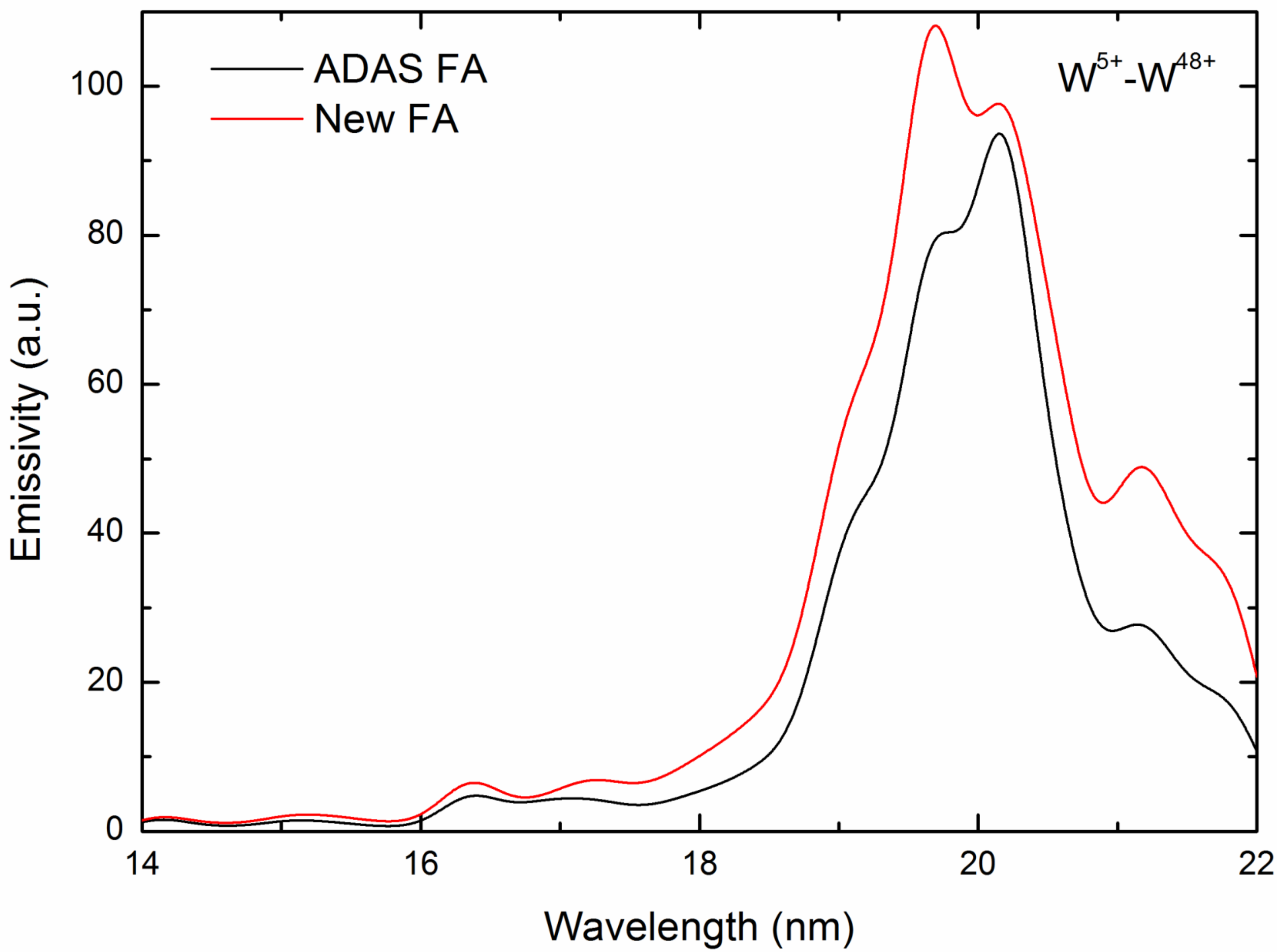


Transport free spectrum

Fractional abundance difference



Spectra sensitivity



Modeling uncertainties

- Electron temperature & density profiles
- Transport D & V coefficients
- Time evolution of impurity
- Atomic data for ionization and recombination
- PEC beyond coronal model