Theoretical Electron Impact Ionization, Recombination, and Photon Emissivity Coefficient for Tungsten Ions

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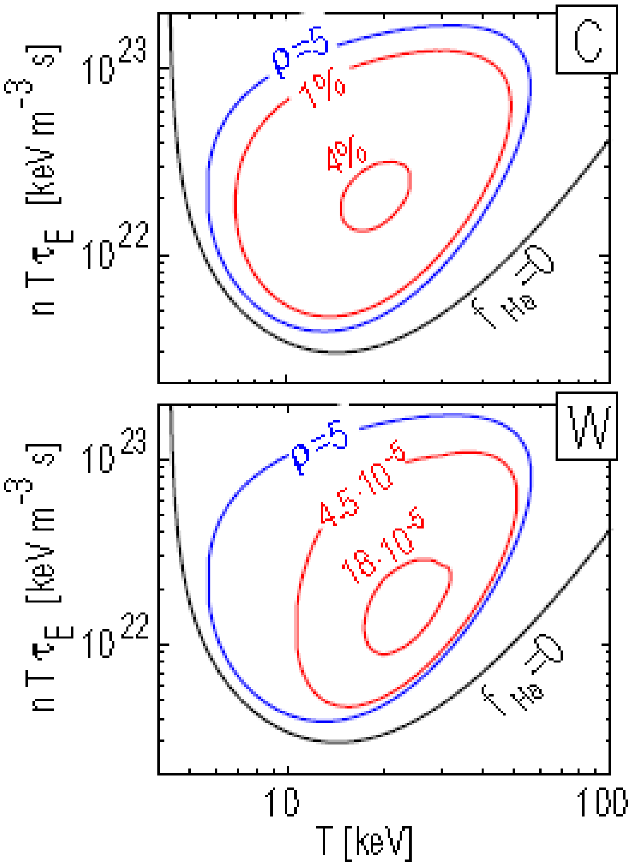
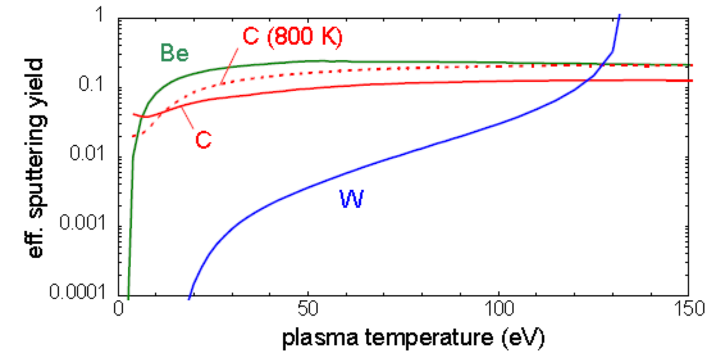
Introduction

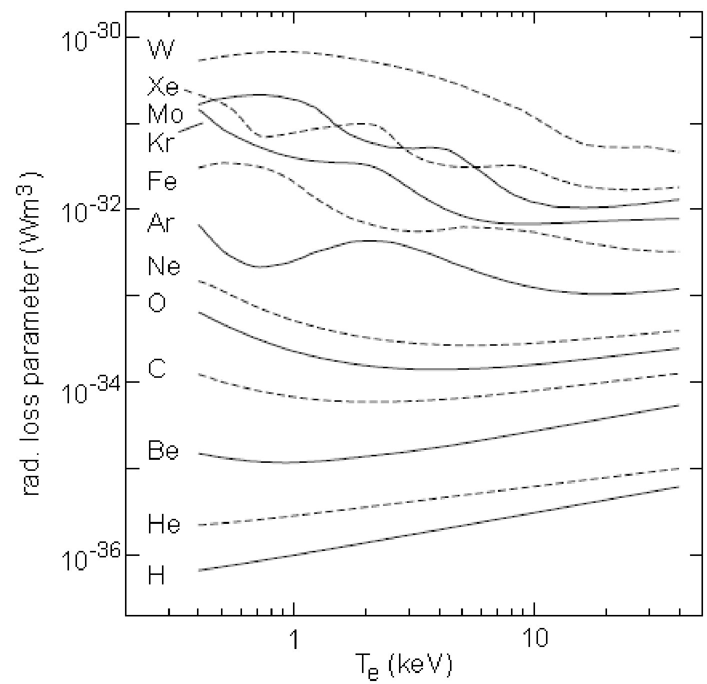
❖ Plasma wall interaction & impurities



$$\rho = \frac{\tau^*_{He}}{\tau_E},\; f_i = \frac{n_i}{n} = 1 - 2f_{He} - Zf_Z$$

T. Pütterich, IPP thesis report (2006)

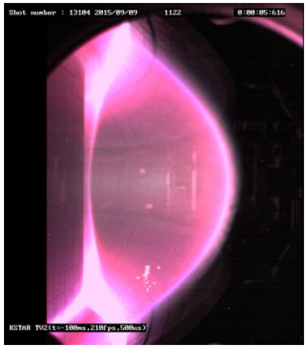




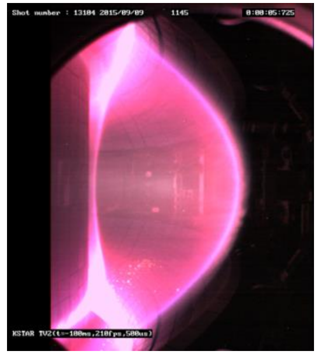
R. Neu, IPP report (2003)

Introduction

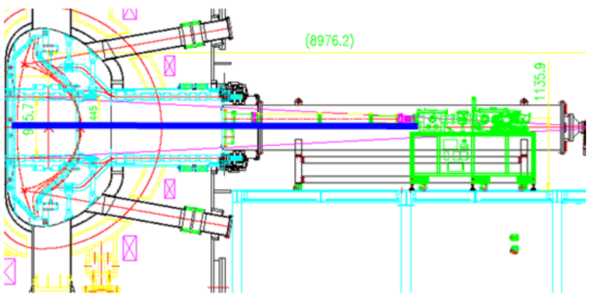
5.616 s



5.725 s

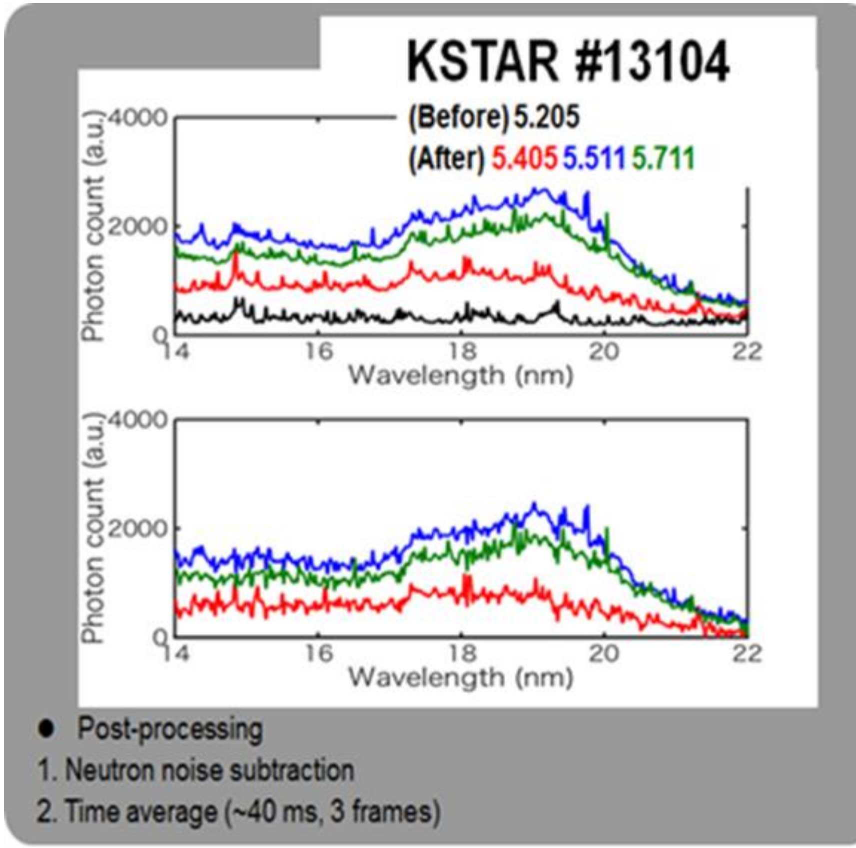


LOS of VUV



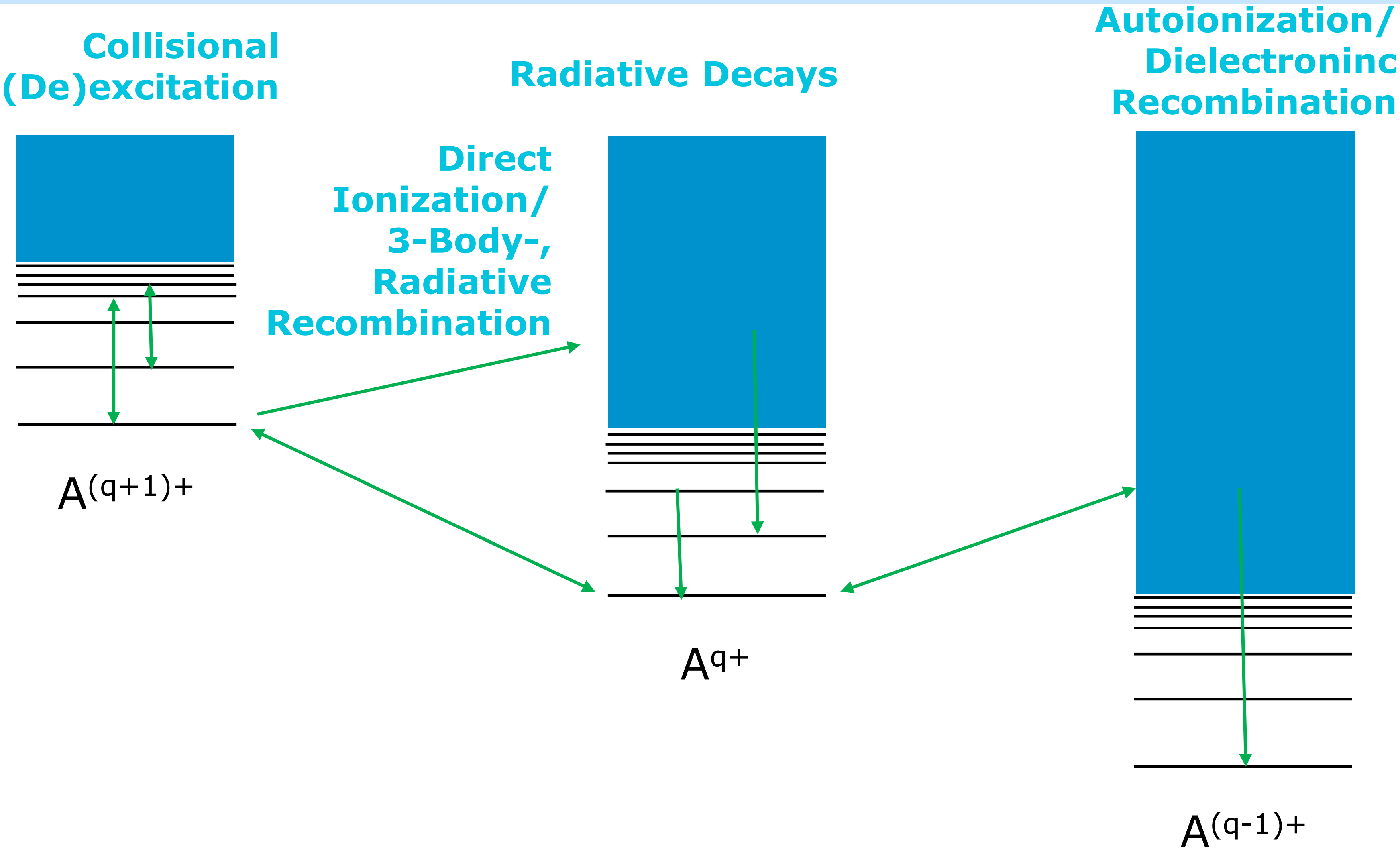
VUV @19.19 nm

KSTAR campaign 2015
W powder injection experiment
by KAIST and ITER Korea teams



- **A spectroscopic modeling for analysis of the experiment has been carried out being combined with a transport effect.**

Atomic processes in plasma



Spectroscopic modeling

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

$$\varepsilon_{ij} = n_Z(r,t)\, n_e(r,t)\, PEC_{ij}(T_e, n_e)$$

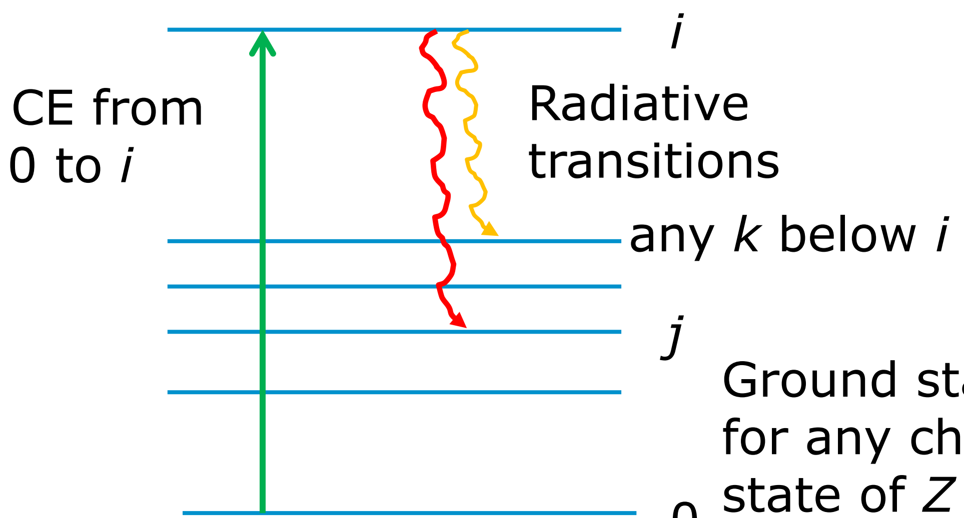
→ Photon Emissivity Coefficient

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

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

- Collisional excitation (CE) rate
- Radiative transition probability

Simple **coronal** Model for state population density



Ground state for any charge state of Z ions

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

Atomic Data

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

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 →

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

Diffusion coefficient   Drift, convection coefficient

Source & sink term →

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

Ionization rate coefficient	Recombination coefficient

Atomic Data

PEC calculation for W ions

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

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

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

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

$$4d^{10}\ 4f^{26-q-m}\ [5s^{2}\ 5p^{m}]^{-1}\ n'l' \rightarrow 4d^{10}\ 4f^{26-q-m}\ [5s^{2}\ 5p^{m}]^{-1}\ nl + h\nu$$
$$\rightarrow 4d^{10}\ 4f^{26-q-m+1}\ [5s^{2}\ 5p^{m}]^{-1} + h\nu$$
$$\rightarrow 4d^{10}\ 4f^{26-q-m+1}\ [5s^{2}\ 5p^{m}]^{-2}\ n'l' + h\nu$$
$$4d^{10}\ 4f^{26-q-m-1}\ 5s^{2}5p^{m}\ n'l' \rightarrow 4d^{10}\ 4f^{26-q-m-1}\ 5s^{2}5p^{m}\ nl + h\nu$$
$$\rightarrow 4d^{10}\ 4f^{28-q-m}\ 5s^{2}5p^{m} + h\nu$$
$$\rightarrow 4d^{10}\ 4f^{28-q-m}\ [5s^{2}5p^{m}]^{-1} + h\nu$$

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

PEC calculation for W ions

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

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

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

$$\rightarrow 4d^{10}\ 4f^{14}\ 5s^2\ 5p^6\ 5d + h\nu \quad (n'=5,6,$$

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

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

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

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

$$[4s^m\ 4p^{46-q-m}]^{-1}\ n'l' \rightarrow [4s^m\ 4p^{46-q-m}]^{-1}\ nl + h\nu$$

$$(n'=4,5,\ n \le n')$$

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

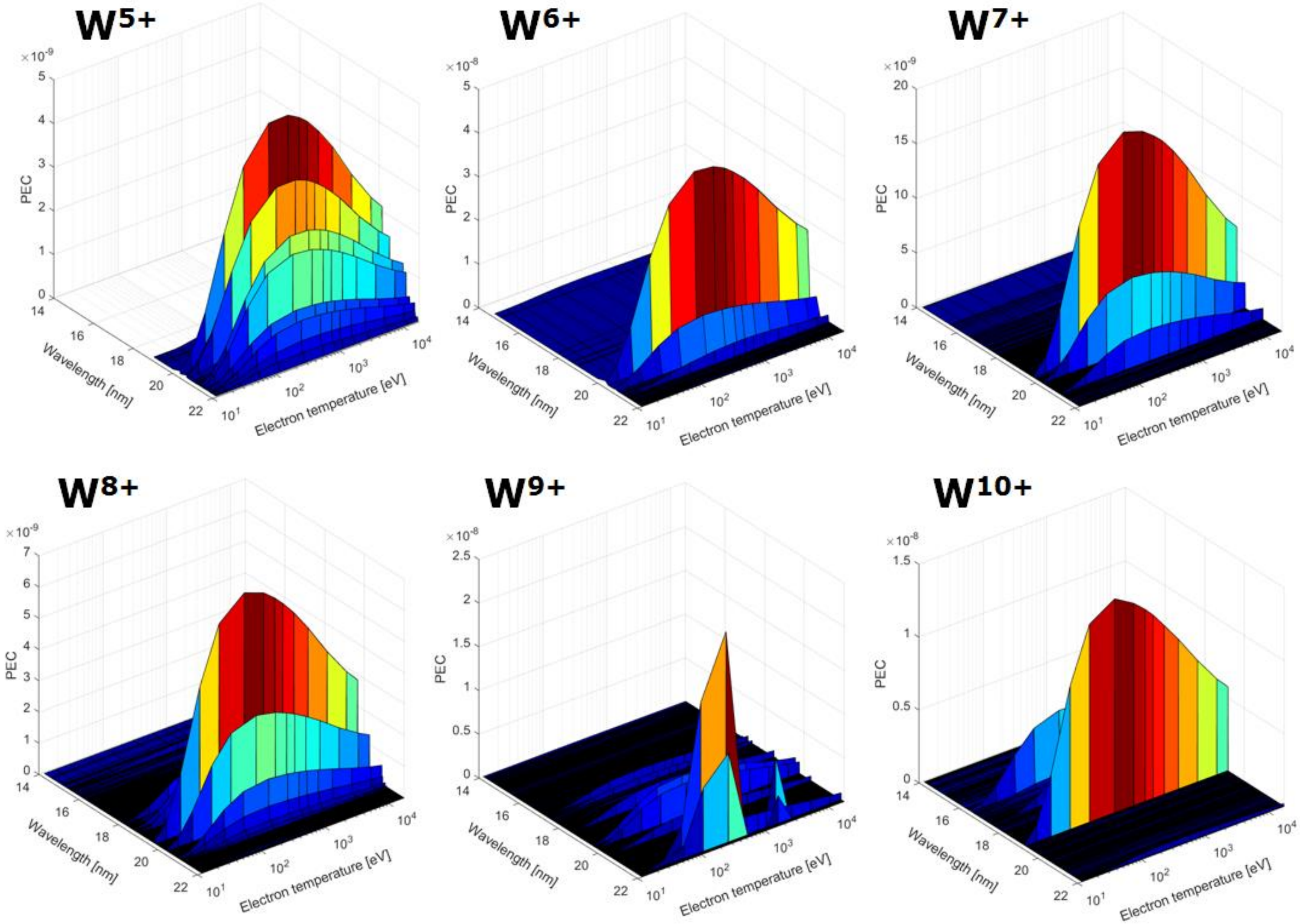
$$3d^{m-1}\ n'l' \rightarrow 3d^{m-1} nl + h\nu \quad (n'=n=4)$$

$$\rightarrow 3d^m + h\nu$$

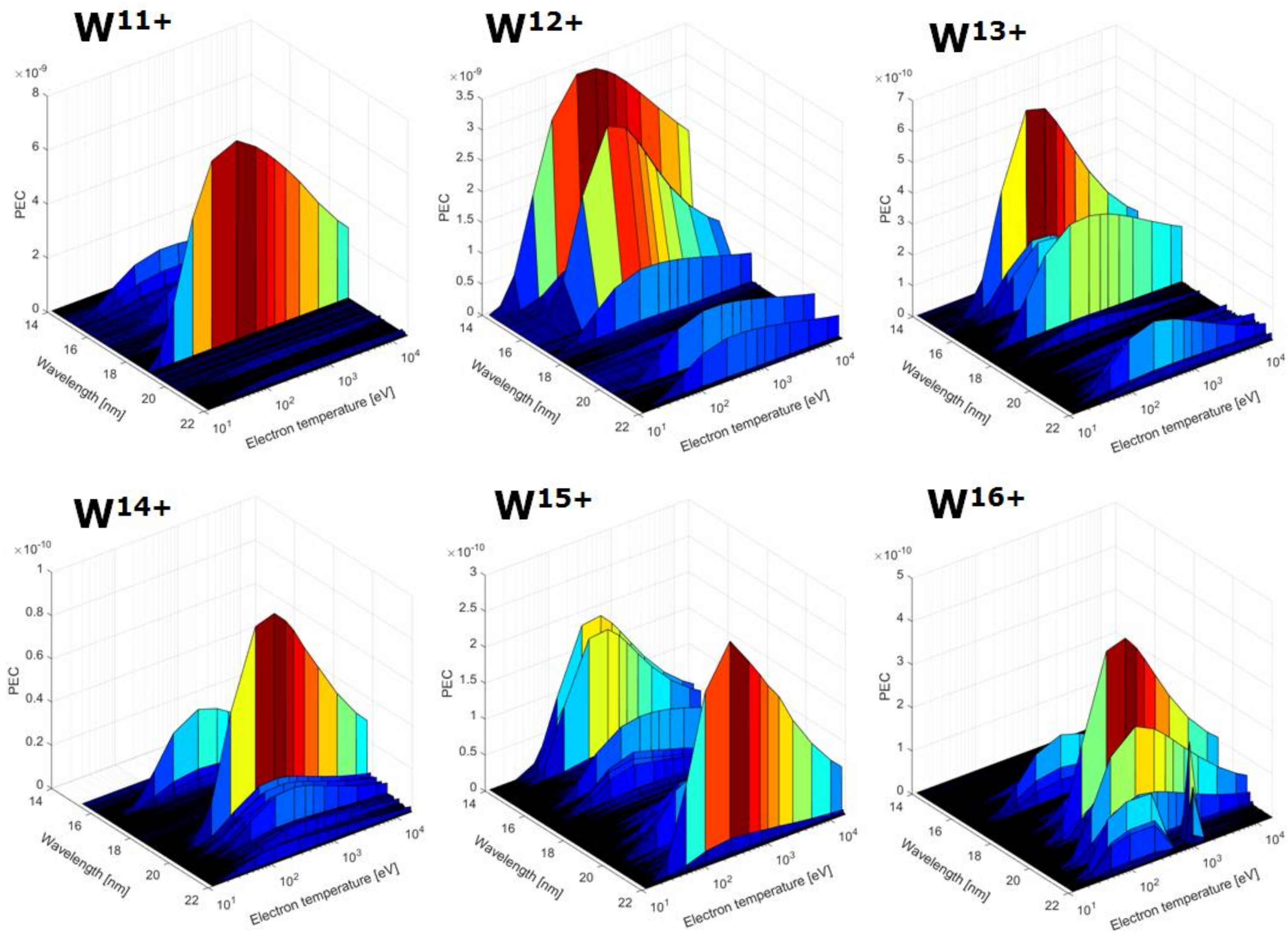
FAC data *vs.* ADAS data

Full J-J coupled level resolved scheme	Configuration average scheme
For eg. W^{25+} Total 9+496 levels	1+28 states

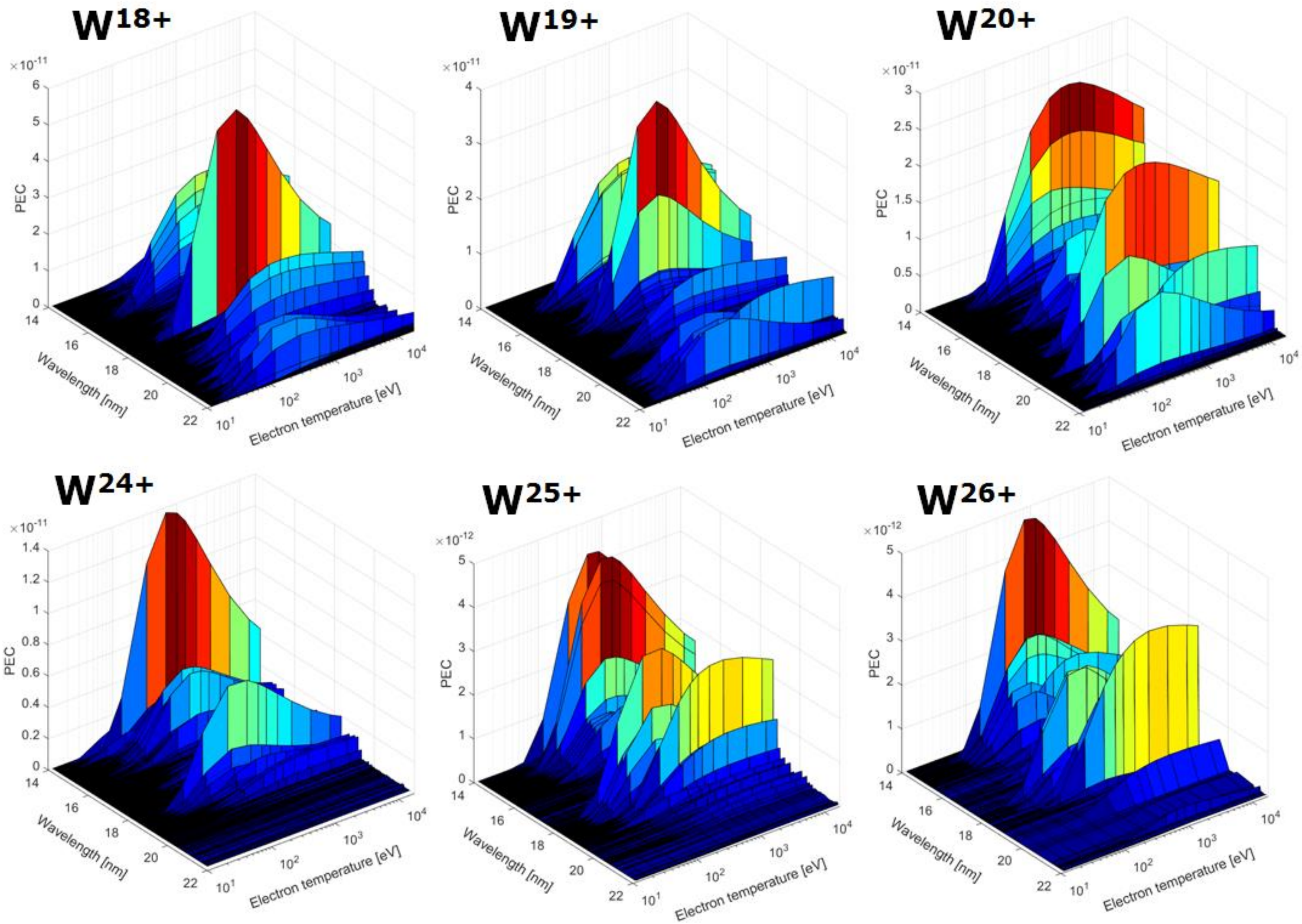
PEC calculation for W ions



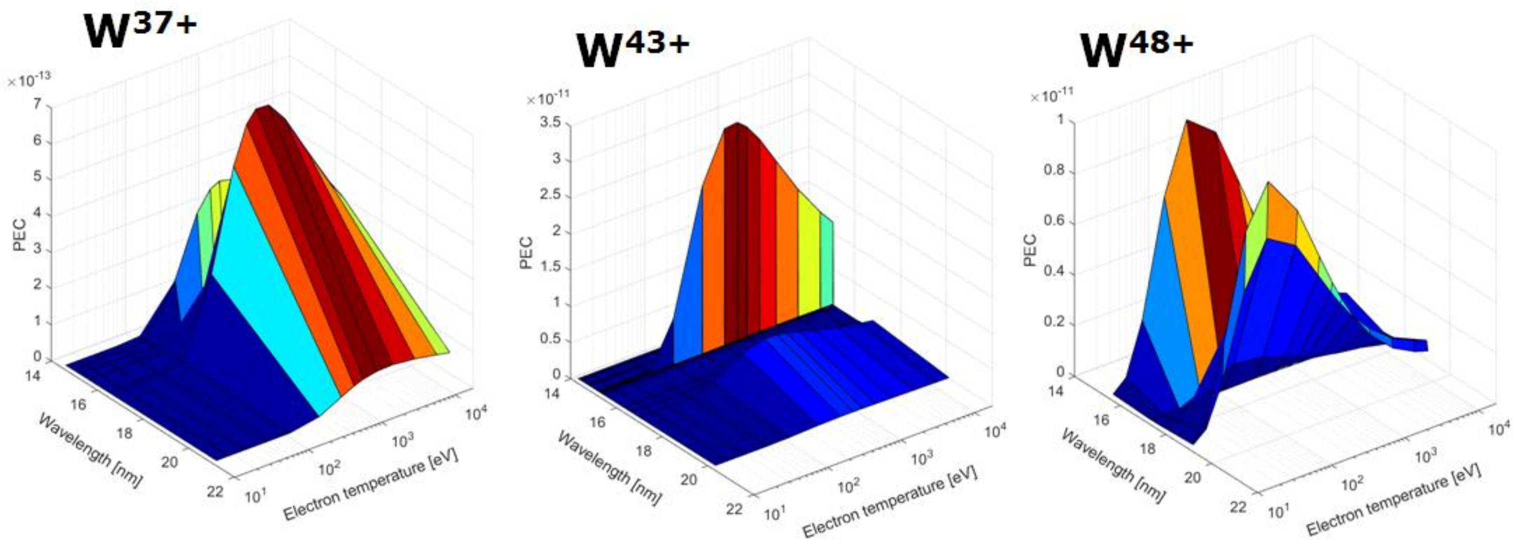
PEC calculation for W ions



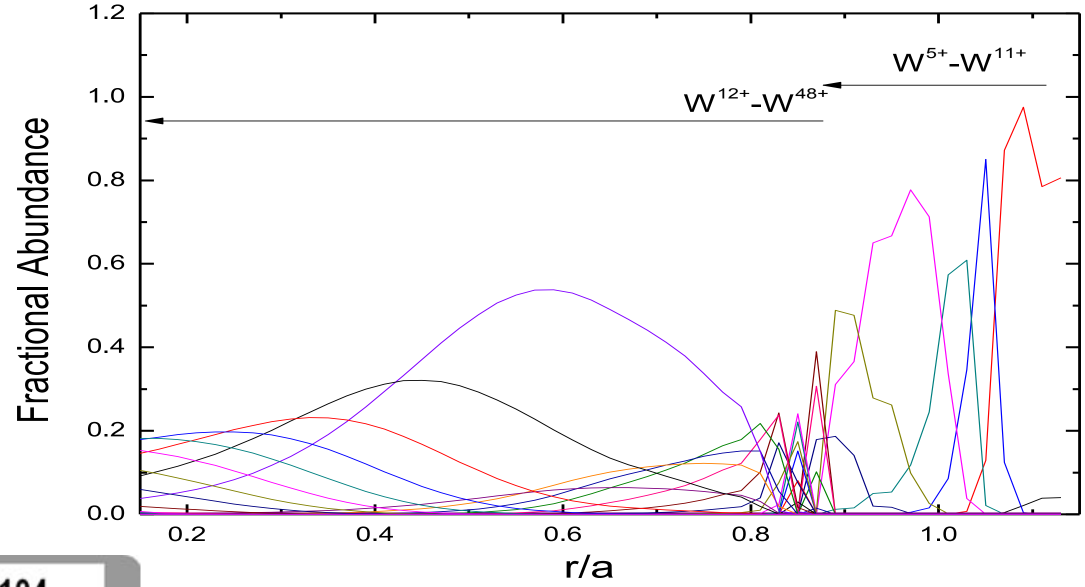
PEC calculation for W ions

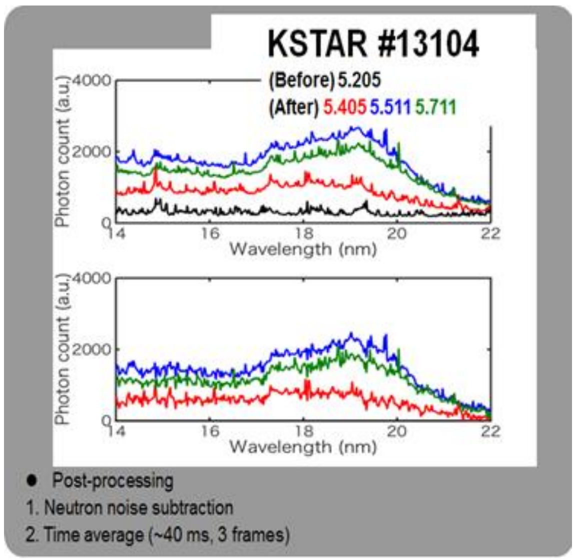


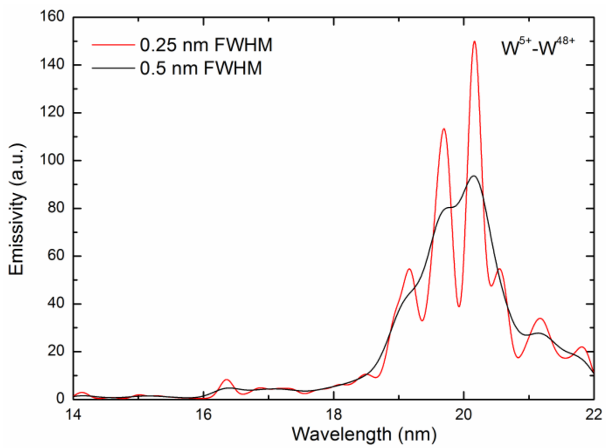
PEC calculation for W ions

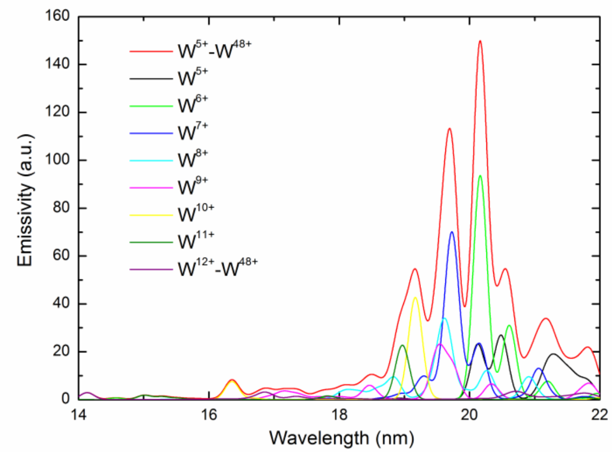


Transport free equilibrium state





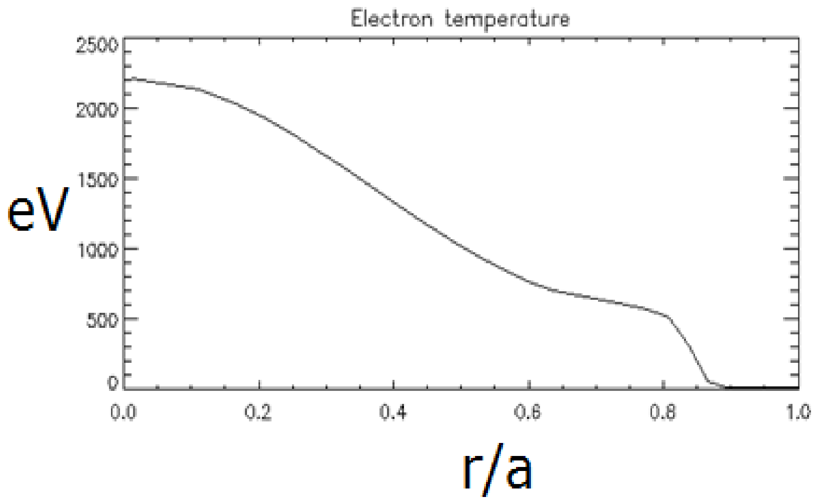


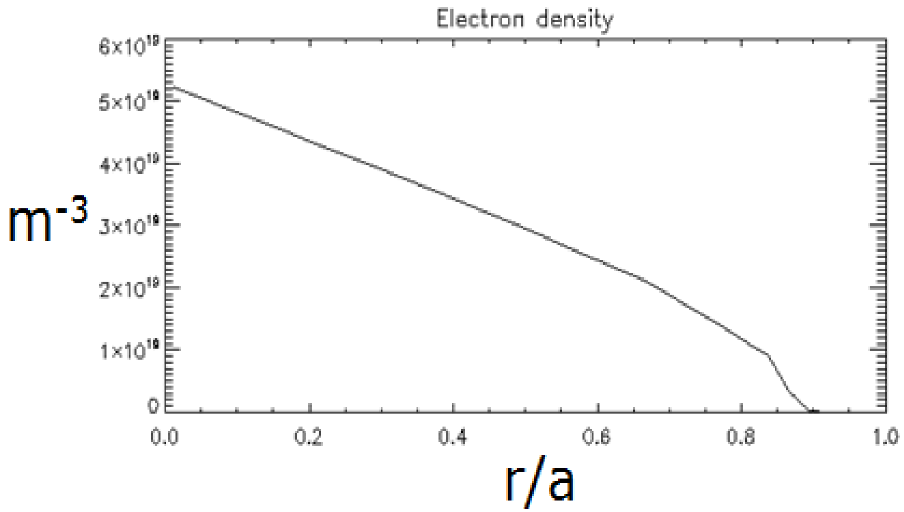


KAERI

Transport modeling for W ions

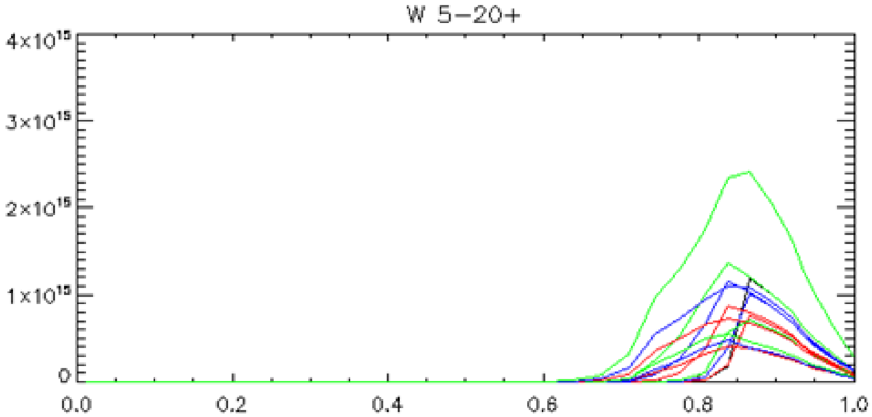
Electron temperature and density profile used for modeling

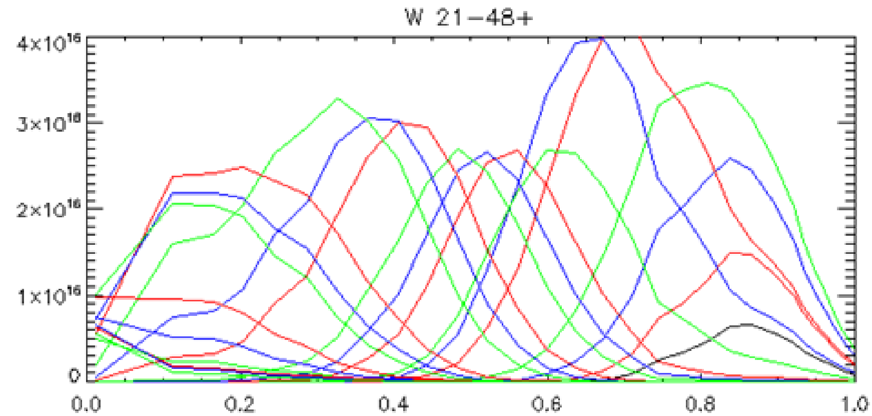


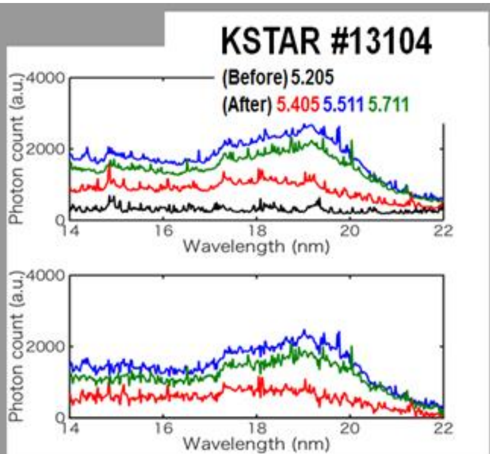


ASDEX-U D & V (assumed)
Ionization & recombination data (ADAS)
Transport equation (SANCO code)
by KAIST team

Transport effect



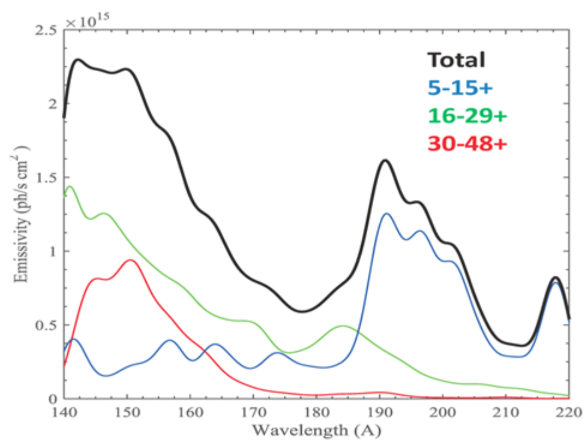


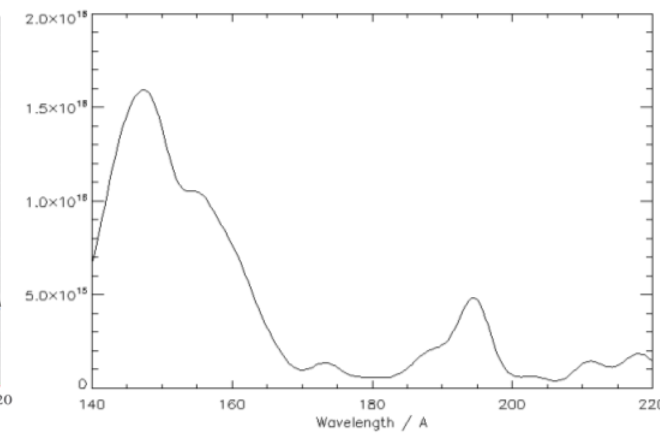


- Post-processing

1. Neutron noise subtraction
2. Time average (~40 ms, 3 frames)

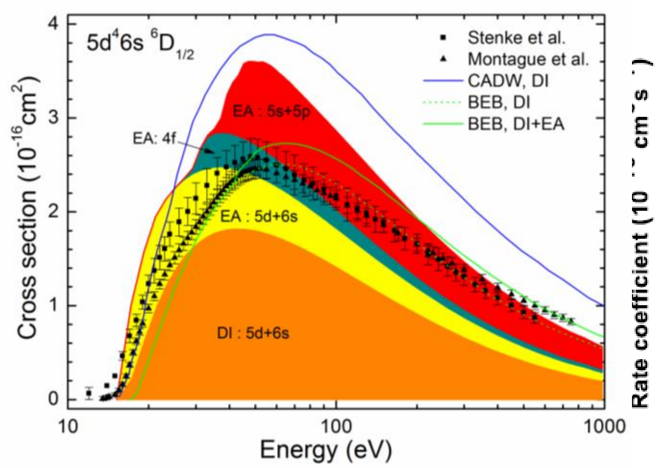
FAC PEC data *vs.* ADAS PEC data





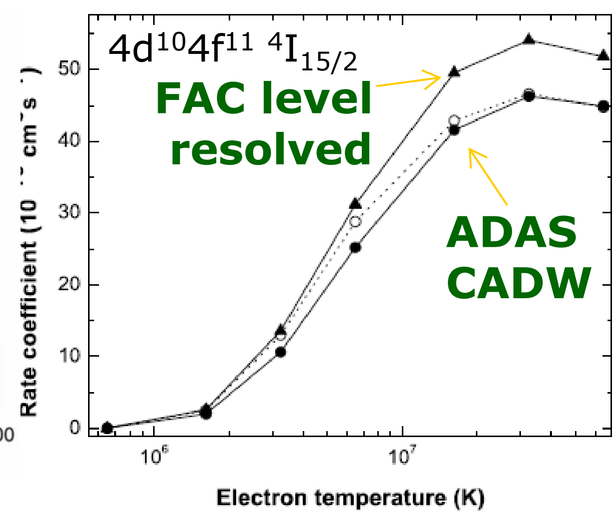
Ionization data for W spectroscopic modeling

W^{+}



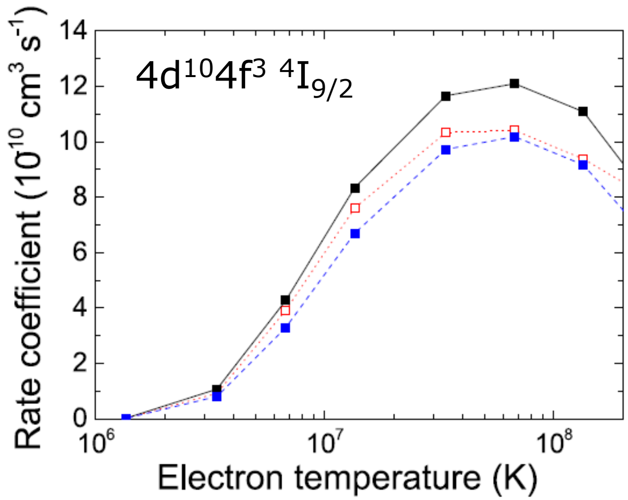
D.-H. Kwon, Y. S. Cho, and Y. O. Lee, IJMS **356**, 7 (2013)

W^{17+}



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

W^{25+}



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 by S. D. Loch et al. (Phys. Rev. A **72** 052716 2005).

R-Matrix *vs*. DW for CE

Channels :

$$S = S_i + s, \quad L = L_i + l, \quad \pi = (-1)^{\pi_i + \ell}$$

$$E = E_i + k_i^2$$

$$\psi_k = \sum_{ij}^{n_f} c_{ijk} A[\Phi_i, \phi_{ij}] + \sum_m d_{jk} \theta_m \ , \quad H = \sum_{i=1} H_D + \sum_{I<J} \frac{1}{r_{ij}}$$

$$H(N+1)\psi_k = E_k^{N+1} \psi_k \ , \ \psi_E = \sum_k A_{EK} \psi_k$$

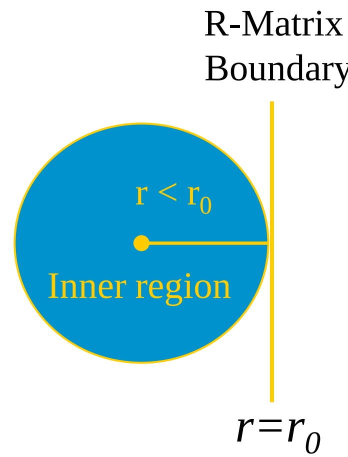
Wavefunction of the scattered electron in channel *i*

$$\begin{pmatrix} P_i(r) \\ Q_i(r) \end{pmatrix} = \sum_k A_{EK} \begin{pmatrix} w_{ik}(r) \\ v_{ik}(r) \end{pmatrix}$$

$$\frac{Q_i(r_0)}{P_i(r_0)} = \frac{b + \kappa}{2 r_0 c}$$

$$P_i(r_0) = \sum_j R_{ij} \left[2 r_0 c Q_j(r_0) - (b + \kappa_j) P_j(r_0) \right]$$

$$R_{ij} = \frac{1}{2 r_0} \sum_k \frac{w_{ik}(r_0) w_{jk}(r_0)}{E_k^{N+1} - E}$$



$r_0 < r < r_{max}$

Outer region

Exchange potential between scattered electron and bound electron is neglected.

Scattering matrices :

$$\mathrm{S} = (1 + \mathrm{K})(1 - \mathrm{K})^{-1}$$, S†S = I : Unitary condition is satisfied.

$$\mathrm{T} = 1 - \mathrm{S}$$

$$\Omega_{ab} = \frac{1}{2} \sum_{J\pi} (2J+1) \sum_{\kappa_a \kappa_b} \left| T_{ab}^{\kappa_a \kappa_b} \right|^2$$

DW approximation

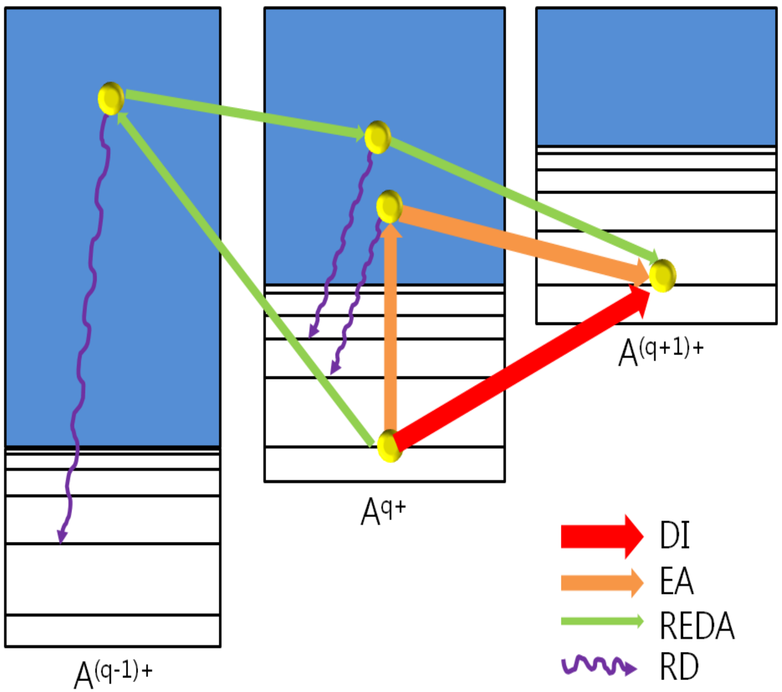
$$\mathbf{T} = \mathbf{I} - \mathbf{S} = \mathbf{I} - \frac{\mathbf{I} + i\mathbf{K}}{\mathbf{I} - i\mathbf{K}} = -\frac{2i\mathbf{K}}{\mathbf{I} - i\mathbf{K}} \simeq -2i\mathbf{K},$$

$$\Omega_{01}^{\mathrm{CE}} = 2 \sum_{\kappa_0 \kappa_1} \sum_{J_T} [J_T] \sum_{j_0 j_1} \left| K(j_0 \kappa_0, j_1 \kappa_1; J_T) \right|^2$$

$$= 2 \sum_{\kappa_0 \kappa_1} \sum_{J_T} [J_T] \left| \langle \Psi_{0\kappa_0}, J_T M_T | \sum_{i<j} \frac{1}{r_{ij}} | \Psi_{1\kappa_1}, J_T M_T \rangle \right|^2 .$$

➡ Channels are not coupled.
Unitarity is not satisfied.
Target state description is more expandable.

EII pathways and cross sections



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)

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

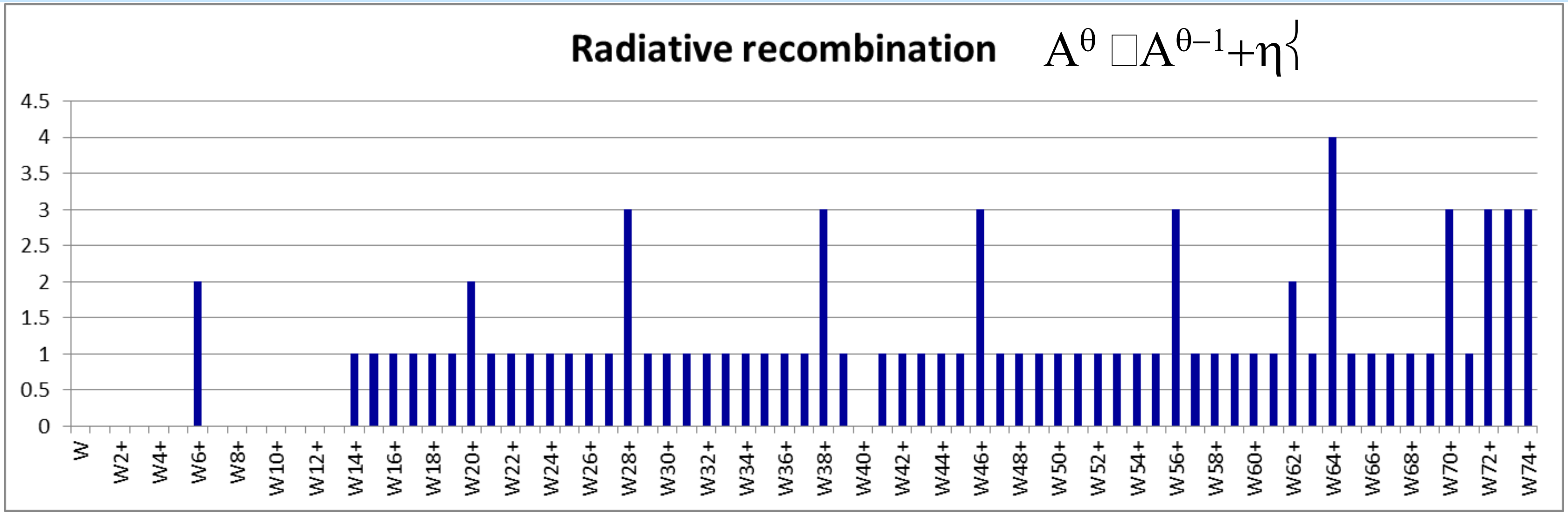
Total EII cross section in an Independent Process-Isolated Resonance (IP-IR) approximation

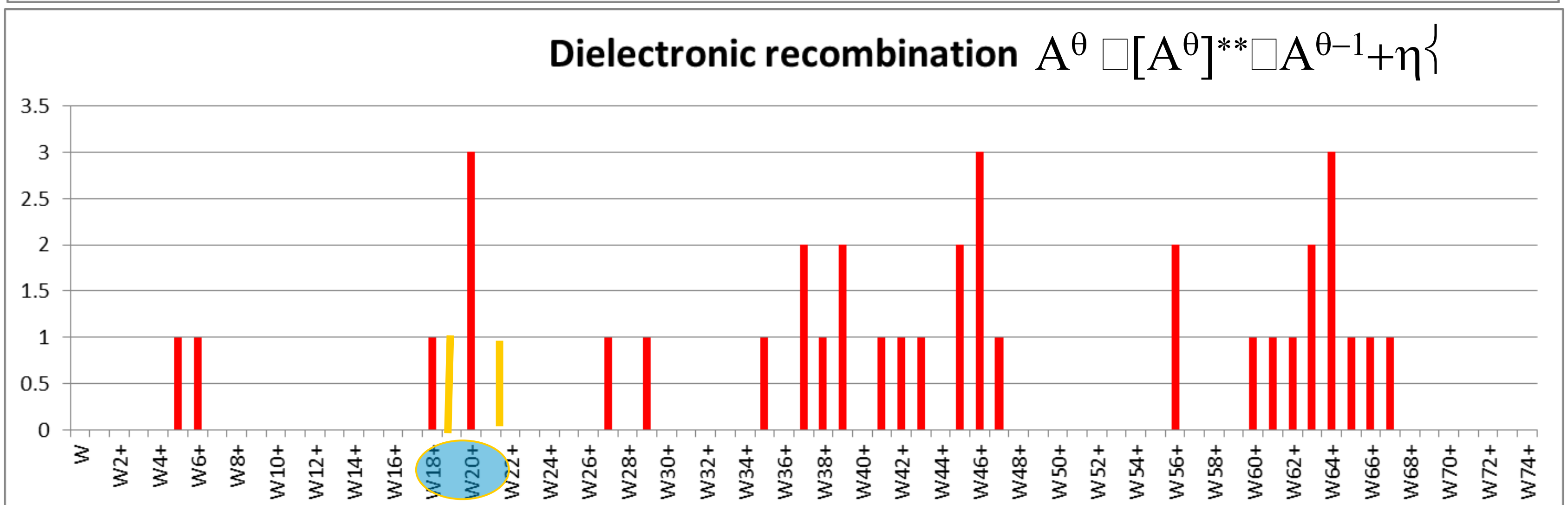
$$\sigma_{tot} = \sum_f \sigma_f^{DI} + \sum_j \sigma_j^{CE} B_j^{a} + \sum_k \bar{\sigma}_k^{DC} B_k^{da}$$

Autoionization (AI) branching ratio (BR) and double AI-BR

$$B_j^{a} = \frac{\sum_s A^{a}_{js} B^{r}_{s} + \sum_t A^{r}_{jt} B^{a}_{t}}{\sum_s A^{a}_{js} + \sum_t A^{r}_{jt}}, \quad B_k^{da} = \frac{\sum_{j'} A^{a}_{kj'} B^{a}_{j'}}{\sum_{j'} A^{a}_{kj'} + \sum_{t'} A^{r}_{j't}}$$

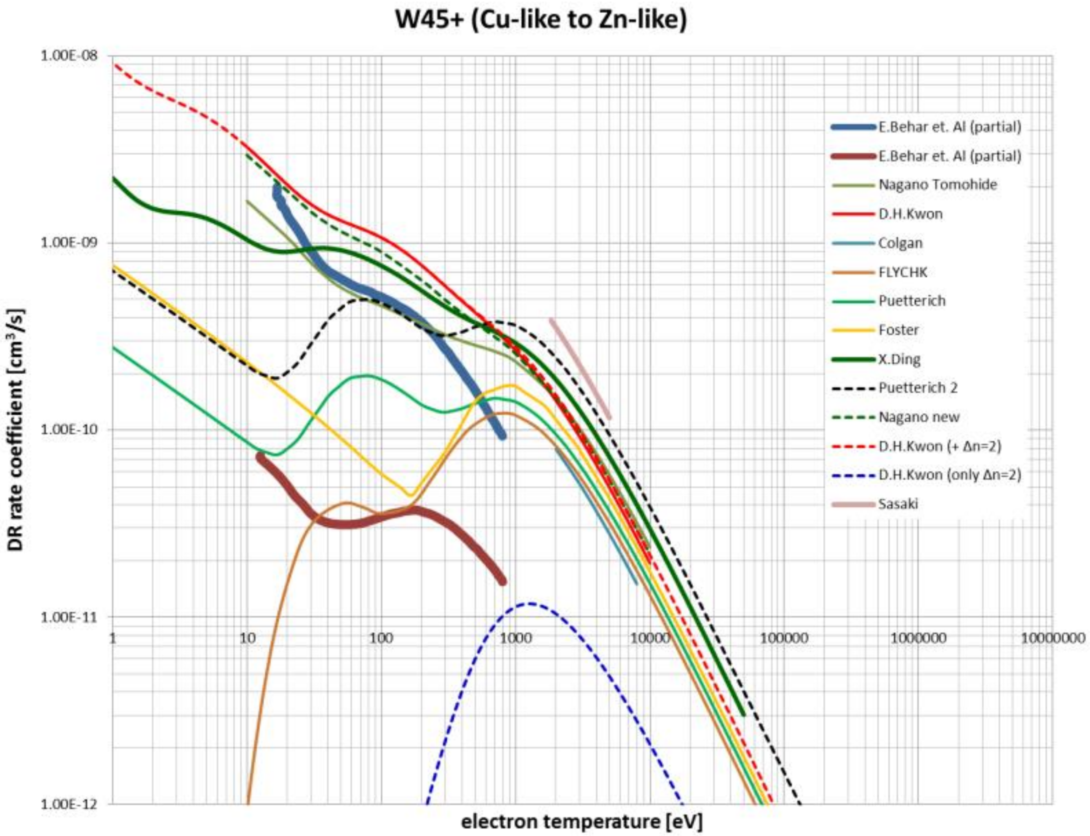
Compilation of recombination data





4f open shell, benchmark experimental data by measurement in TSR is available.

DR data for W spectroscopic modeling



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

ab-initio calculation

$$\alpha_i(T) = \frac{1}{2g_i}\left(\frac{4\pi a_0^2 \mathrm{Ry}}{k_B T}\right)^{3/2} \times \sum_j g_j A^a_{ji} B_j \exp\left(-\frac{E_{ij}}{k_B T}\right)$$

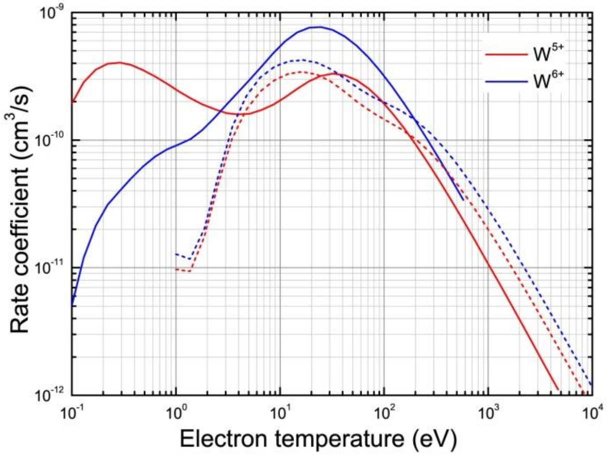
$$B_j = \frac{\sum_t A^r_{jt} + \sum_{t'} A^r_{jt'} B_{t'}}{\sum_k A^a_{jk} + \sum_f A^r_{jf}}$$

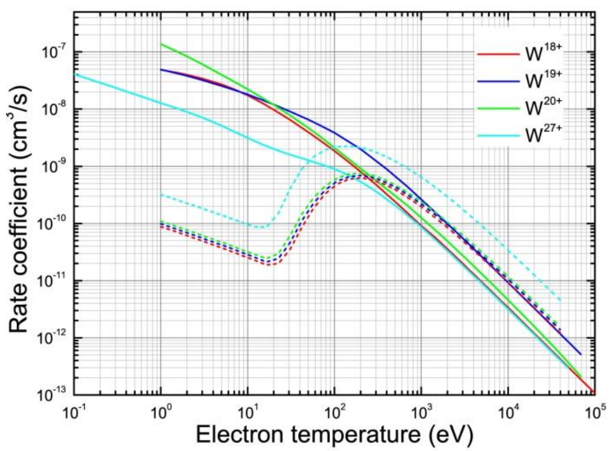
Burgess formula

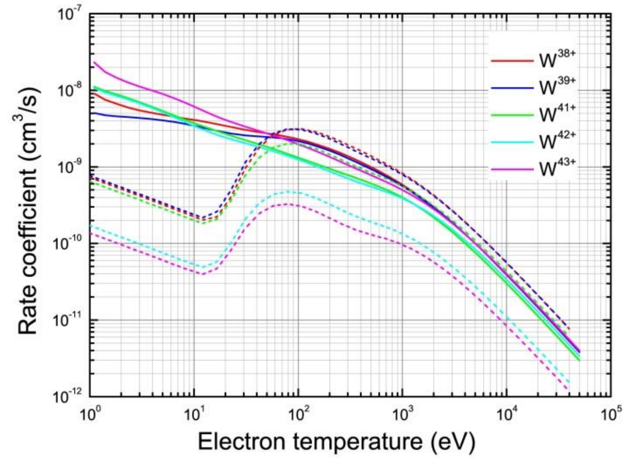
$$\alpha_i(T) = 7.59 \times 10^{-14} n_e n_Z \frac{B(q)D(q,T)}{T^{3/2}} \times \sum_j f_{ji} A(y) \exp\left(-\frac{\overline{E}}{T}\right)$$

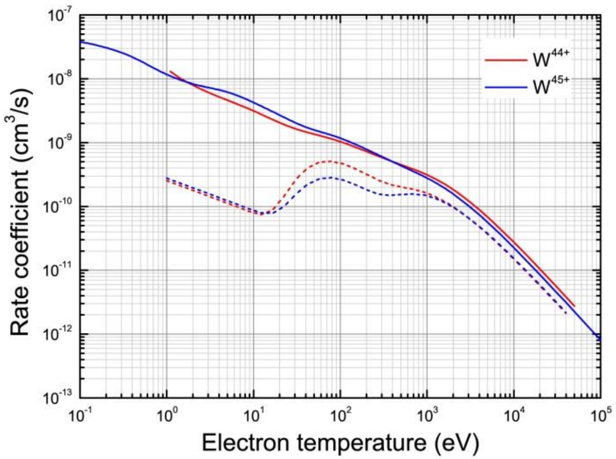
➡ ADAS recombination data based on a simple Burgess formula for W ions quite differ from other ab-initio calculations and the data is not available for many ionization stages.

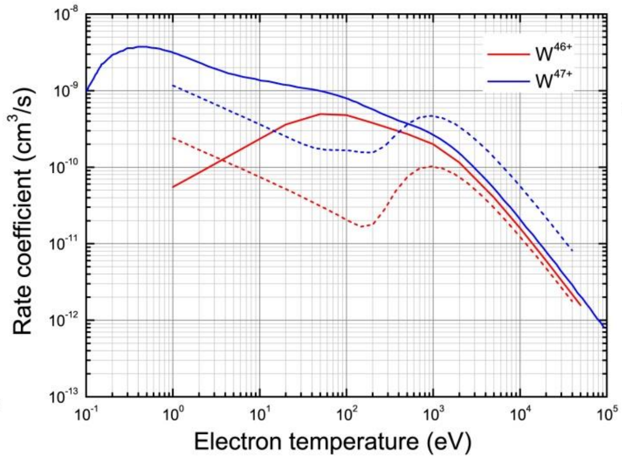
New recommended DR data for W ions

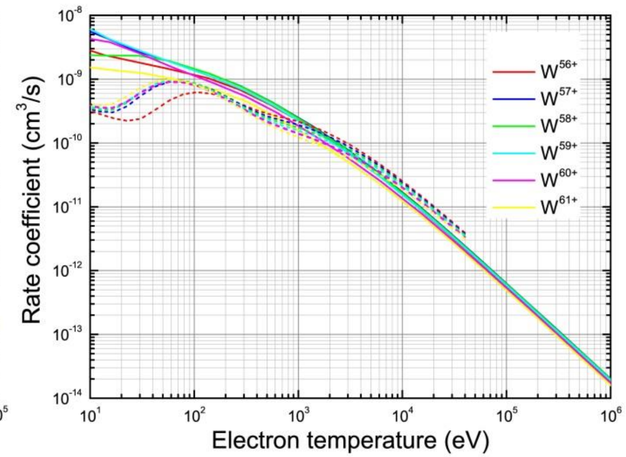












Fractional abundance

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

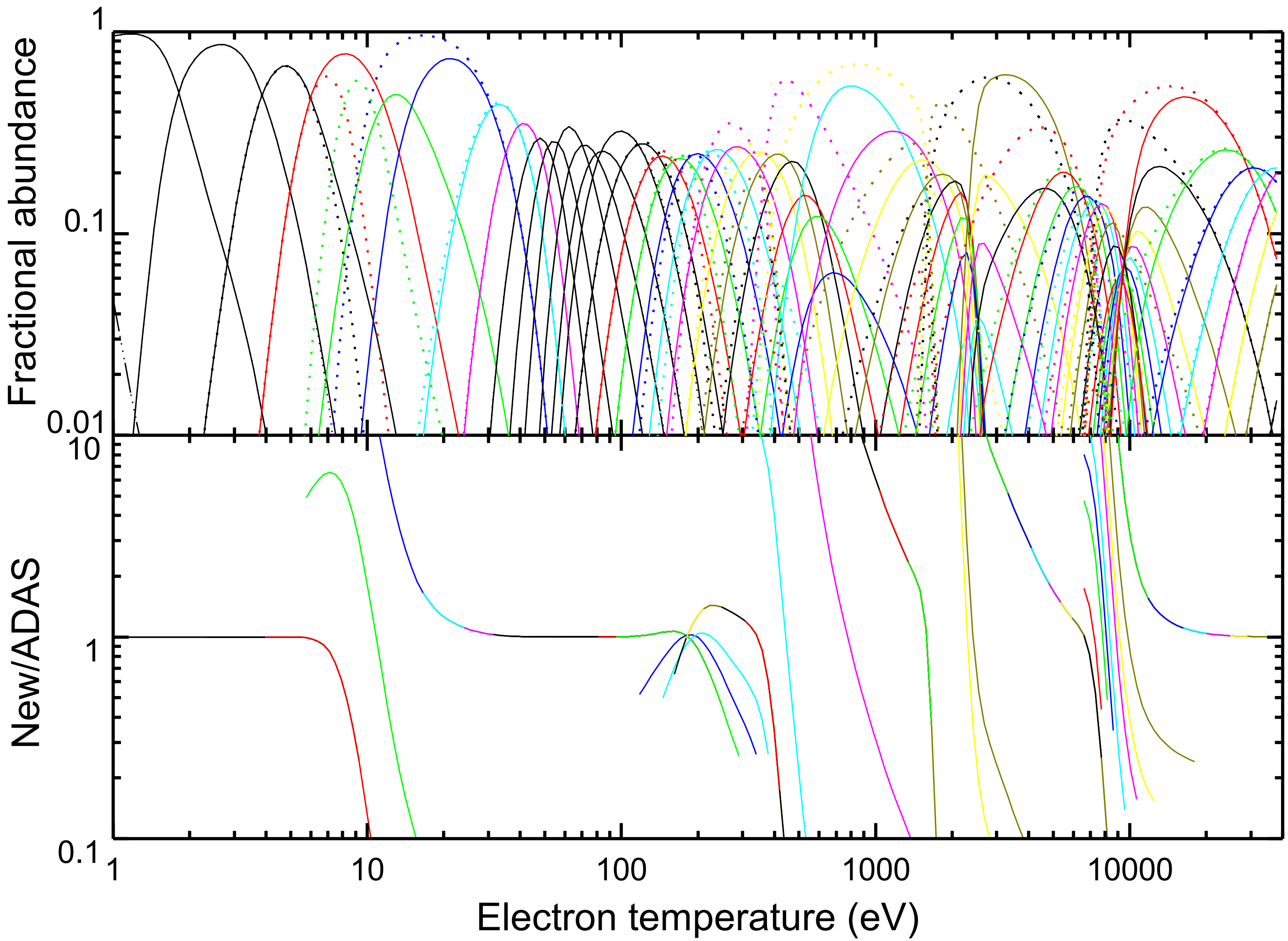
$$N_{\text{tot}} \frac{d}{dt} \begin{bmatrix} f^0 \\ f^1 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \end{bmatrix}$$ ⬅ Collisional Ionization Equilibrium

Total recombination rate coefficient

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

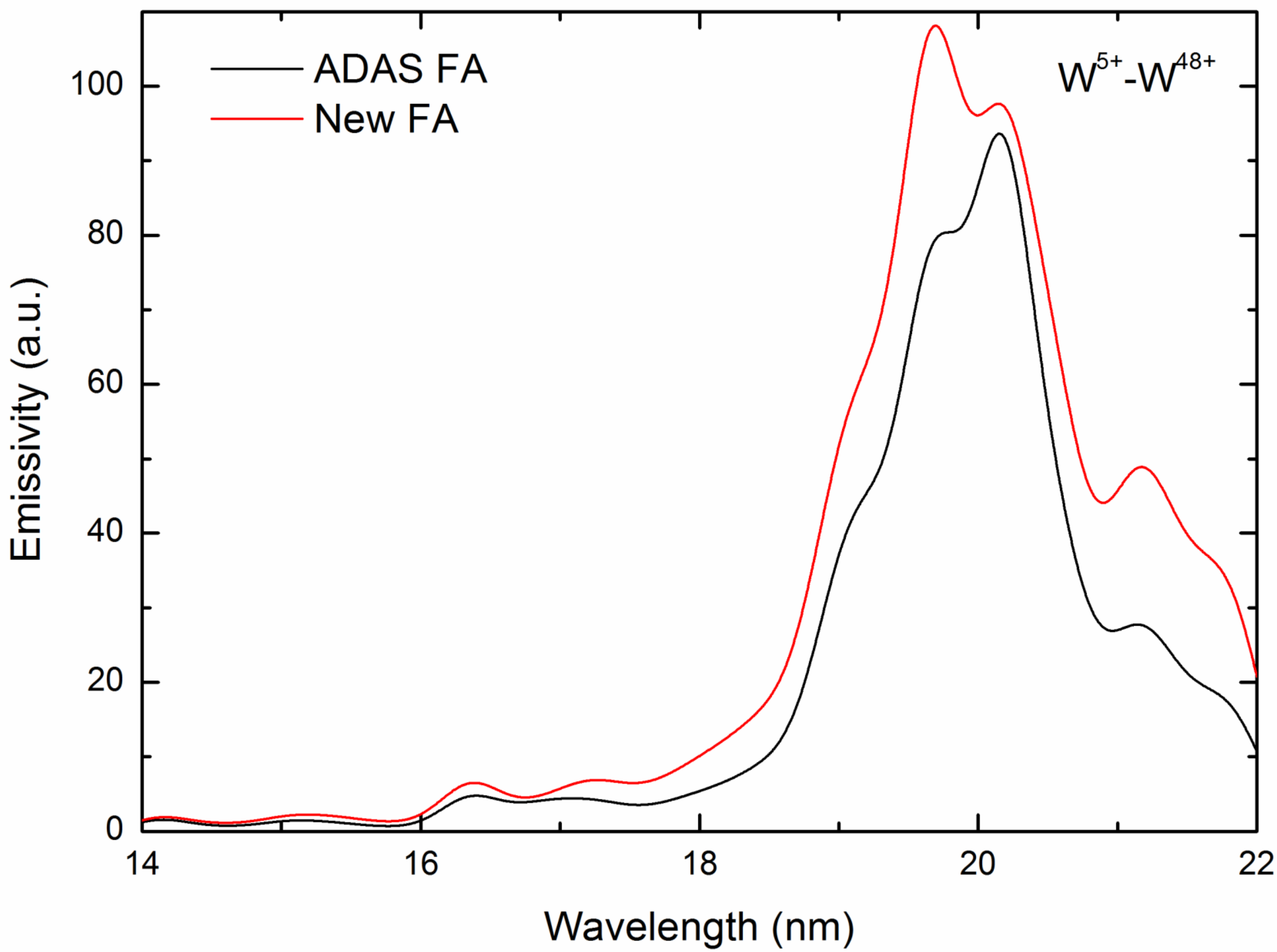
Total ionization rate coefficient

Fractional abundance difference



Submitted to Nuclear Fusion

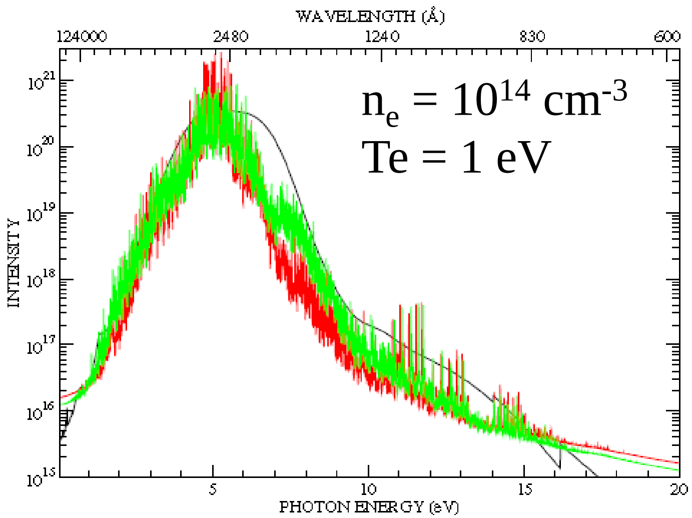
Spectra sensitivity

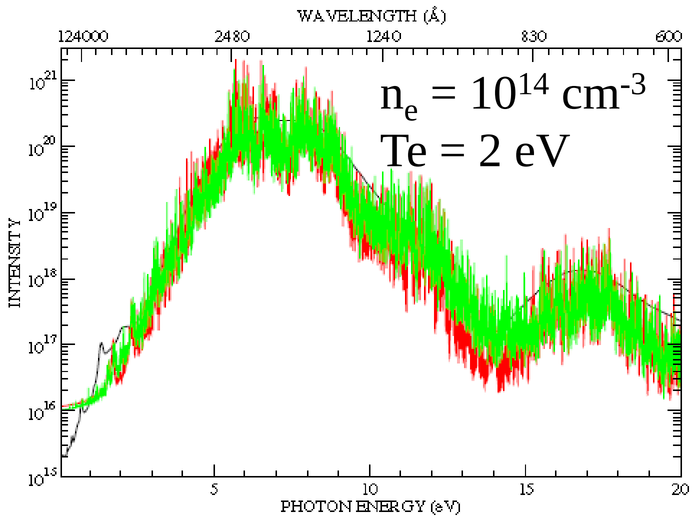


Modeling uncertainties

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

CR modeling for lowly charged W ions





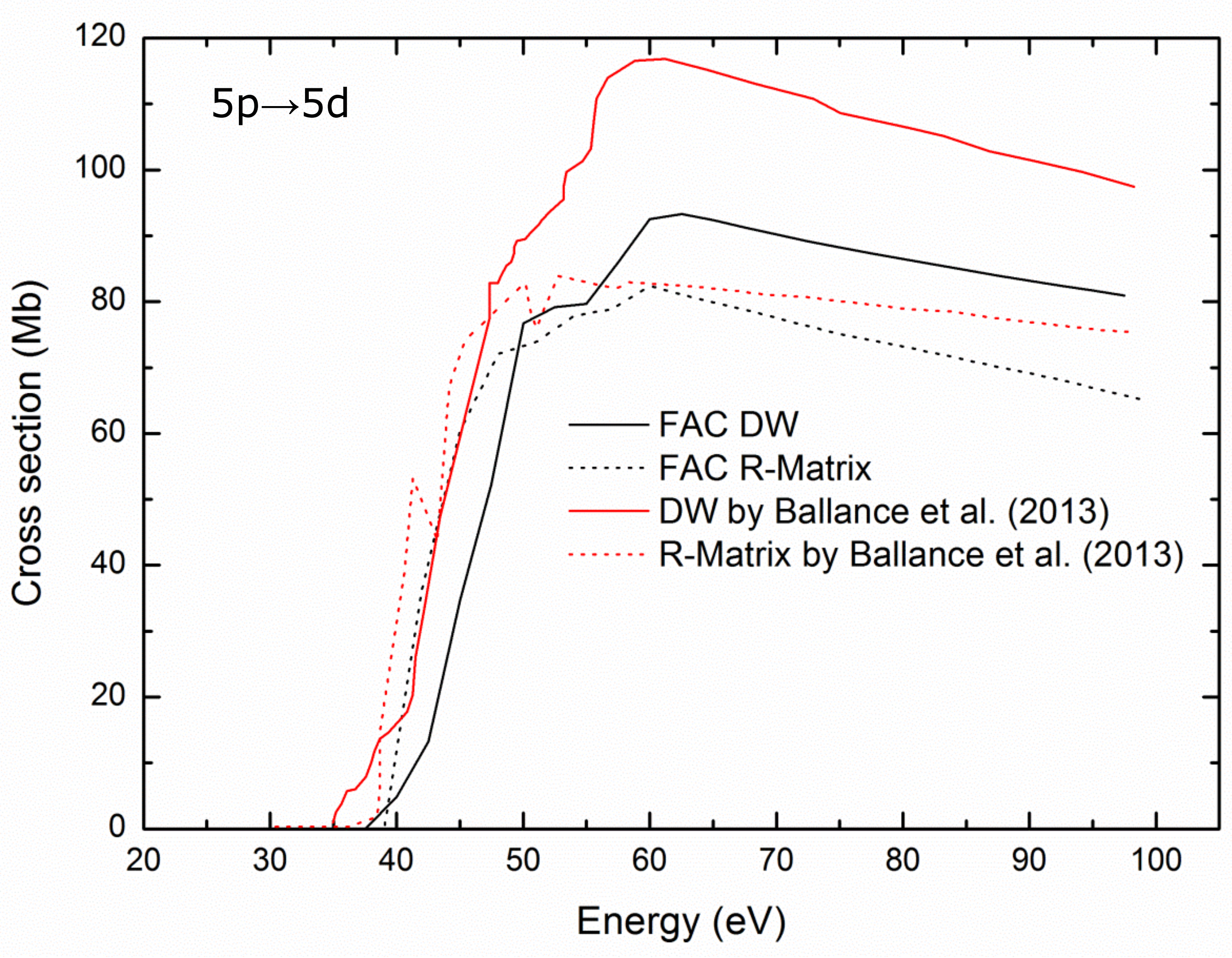
$$
\begin{aligned}
\frac{\mathrm{d}N_{l,j}}{\mathrm{d}t} = N_e \Bigg\{ & \sum_{i(i\neq j)} [N_{l,i} q_{i\to j}(T_e) - N_{l,j} q_{j\to i}(T_e)] \\
& + \sum_i N_{l+1,i} C_{l+1,i\to l,j}(T_e) - N_{l,j} \sum_i C_{l,j\to l-1,i}(T_e) \\
& + \sum_i N_{l-1,i} D^{\mathrm{DC}}_{l-1,i\to l,j}(T_e) - N_{l,j} \sum_i D^{\mathrm{DC}}_{l,j\to l+1,i}(T_e) \\
& + \sum_i N_{l-1,i} \alpha^{\mathrm{RR}}_{l-1,i\to l,j}(T_e) - N_{l,j} \sum_i \alpha^{\mathrm{RR}}_{l,j\to l+1,i}(T_e) \Bigg\} \\
& + N_e^2 \left[\sum_i N_{l-1,i} \beta_{l-1,i\to l,j}(T_e) - N_{l,j} \sum_i \beta_{l,j\to l+1,i}(T_e) \right] \\
& + \sum_{i(i>j)} N_{l,i} A_{i\to j} - N_{l,j} \sum_{i(i<j)} A_{j\to i} \\
& + \sum_i N_{l+1,i} R^{\mathrm{AI}}_{l+1,i\to l,j} - N_{l,j} \sum_i R^{\mathrm{AI}}_{l,j\to l-1,i}\,, \qquad (1)
\end{aligned}
$$

ATOMIC non-LTE calculation

J. Abdallah Jr, J. Colgan, R. E. H. Clark, C. J. Fontes and H. L. Zhang, J. Phys. B **44** 075701 (2011)

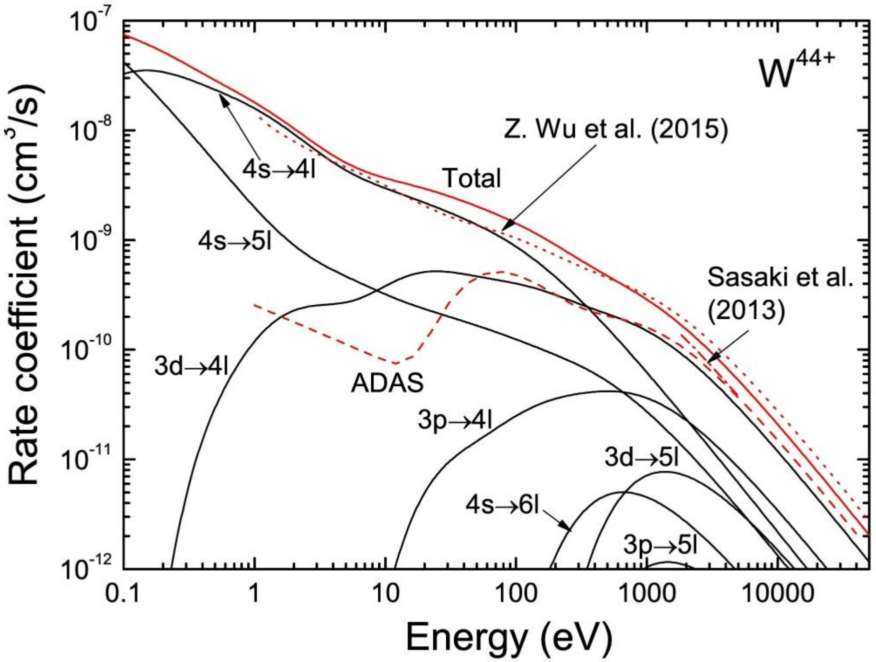
CE for lowly charged W ions

Collisional excitation of W^{3+} $(5d^3\ ^4F_{3/2})$



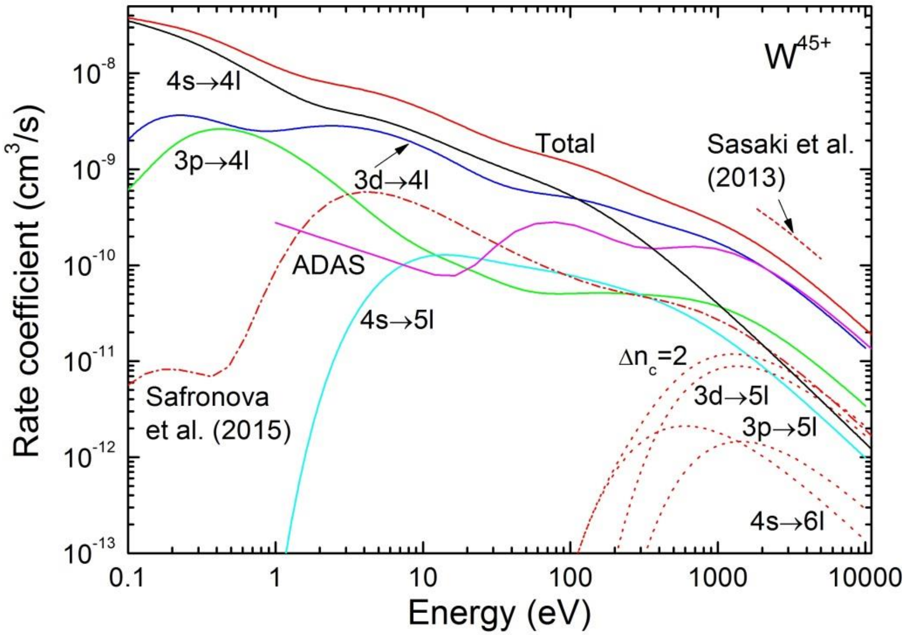
DR data of W ions

Zn-like $3d^{10}4s^2$



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

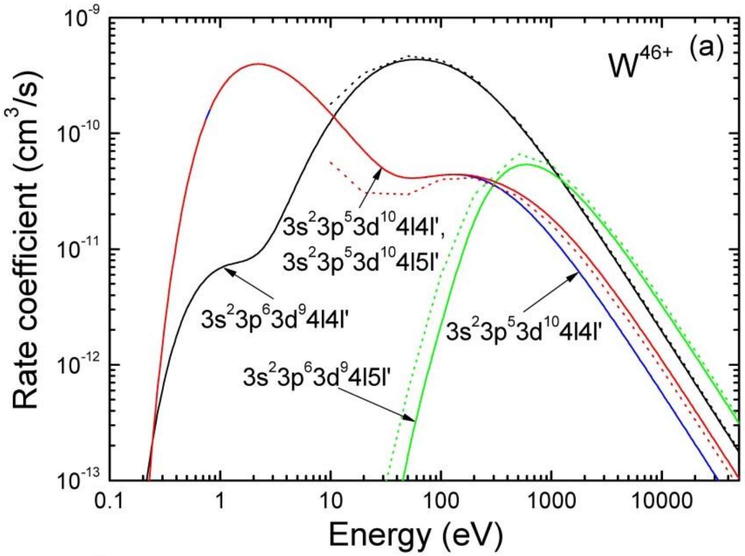
Cu-like $3d^{10}4s$

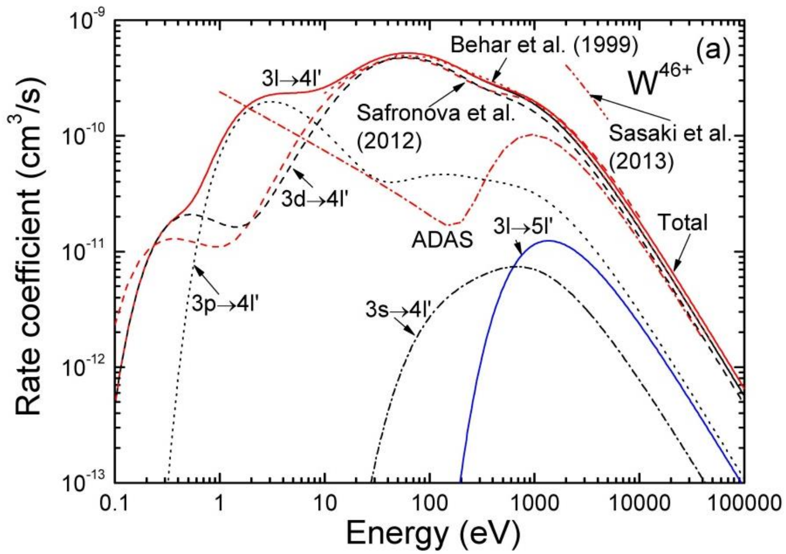


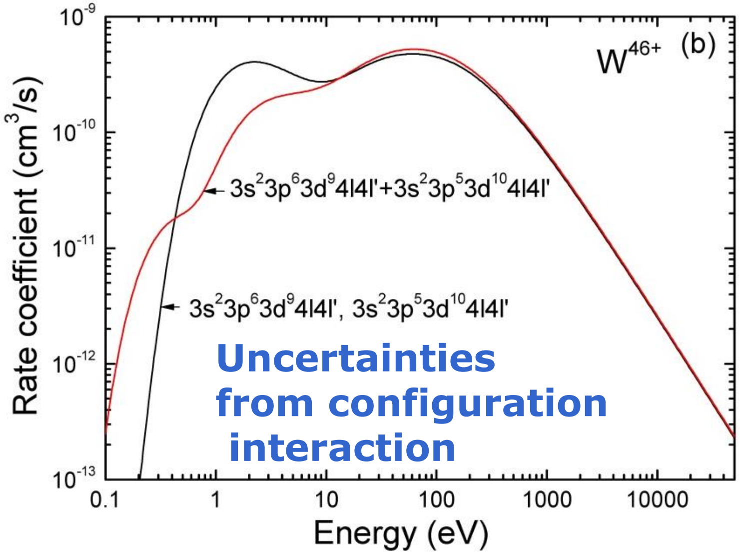
D.-H. Kwon and W. Lee, JQSRT **170**, 182 (2016); ibid., **179**, 98 (2016)

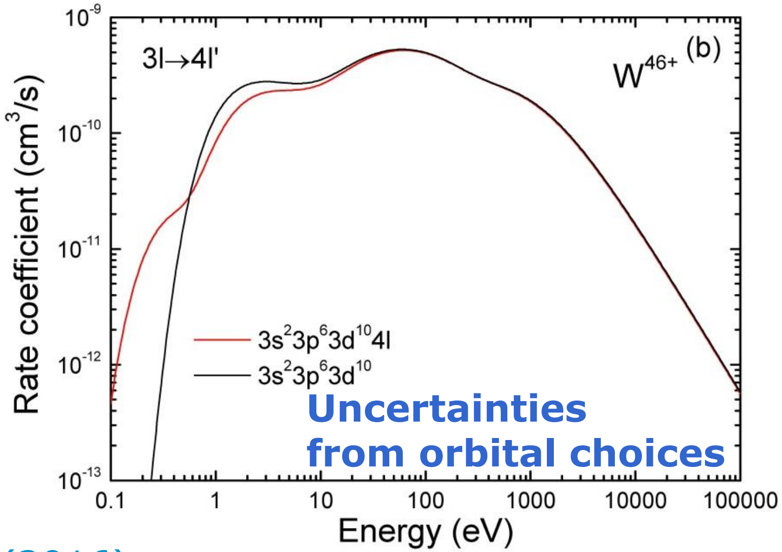
DR data of W ions

Ni-like $3d^{10}4s$



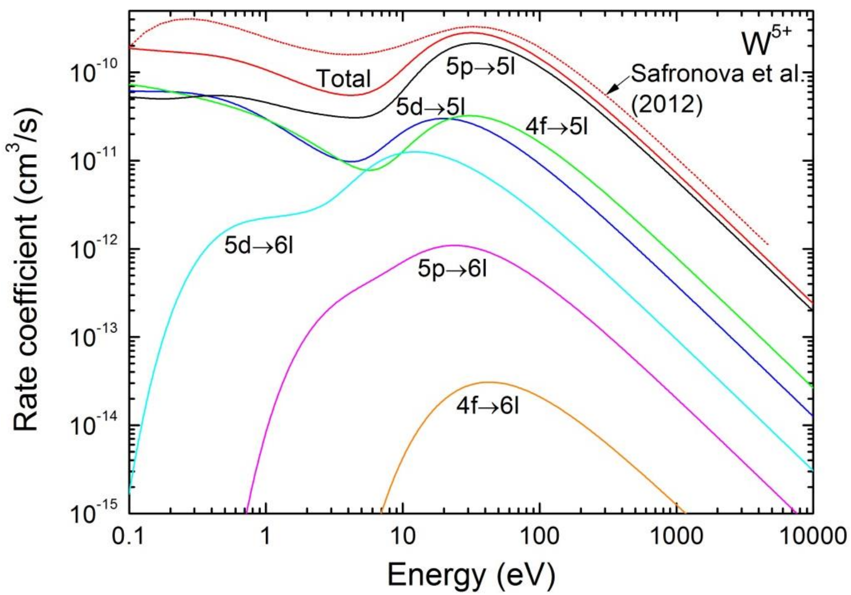


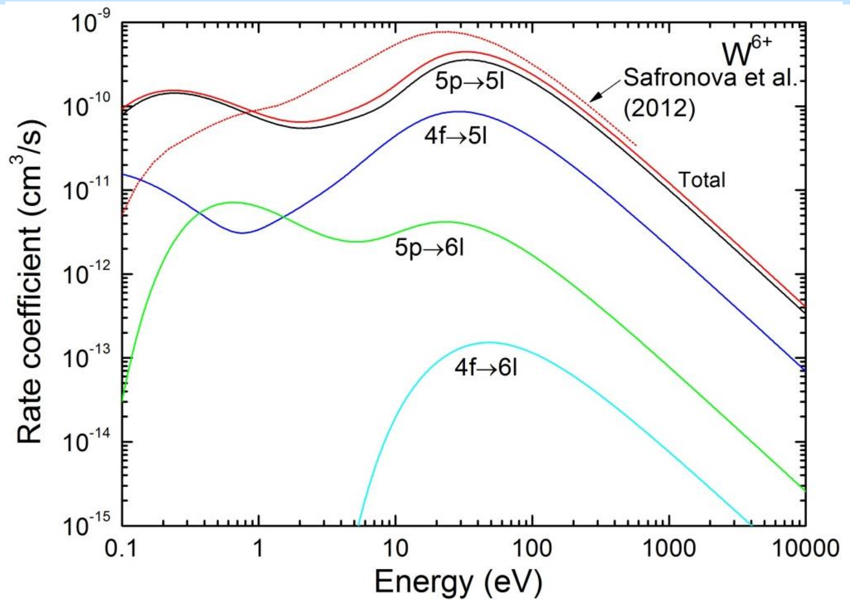


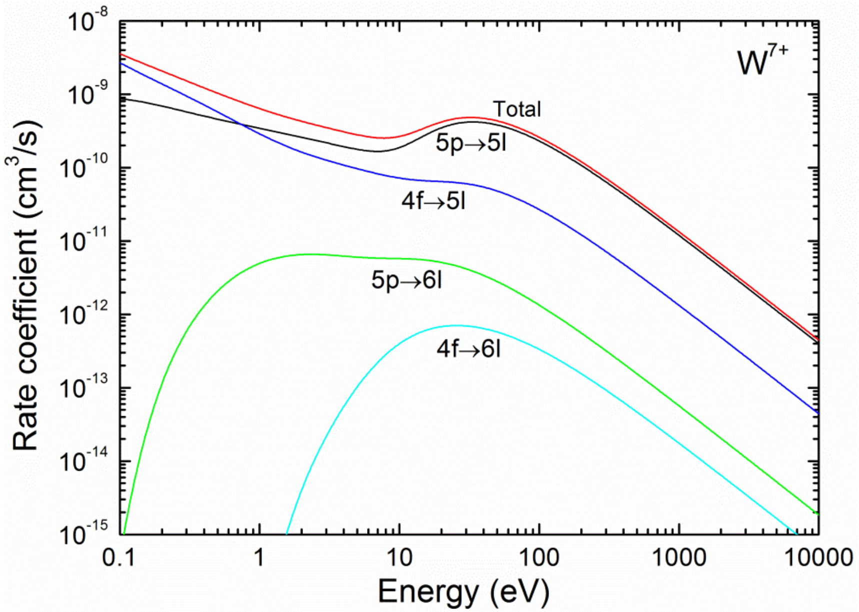


D.-H. Kwon and W. Lee, JQSRT **179**, 98 (2016)

DR data of W ions





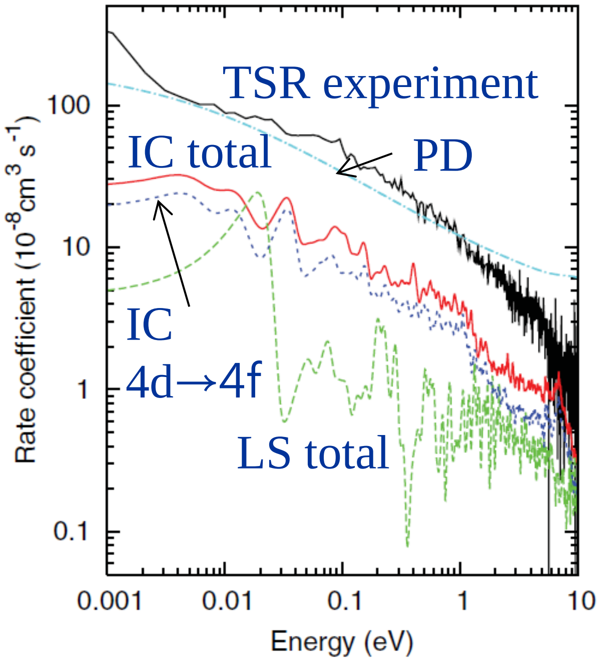


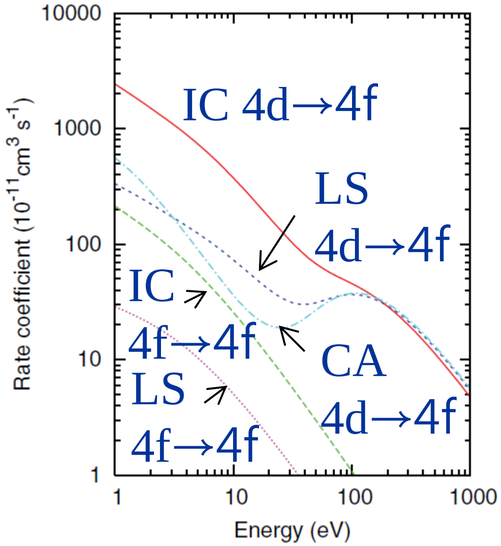
Ground configuration

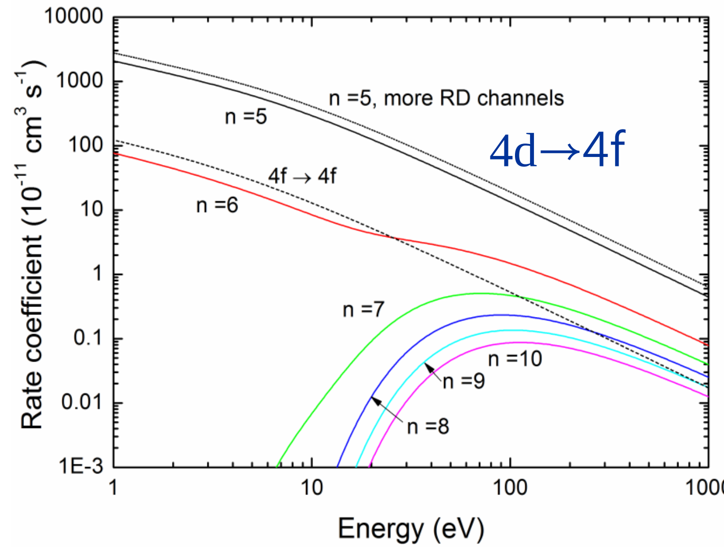
W^{5+}	$4f^{14}5s^25p^65d$
W^{6+}	$4f^{14}5s^25p^6$
W^{7+}	$4f^{14}5s^25p^5$ or $4f^{13}5s^25p^6$

DR data of W ions

W^{20+} ($4d^{10}4f^{8}$)







N. R. Badnell et al., PRA **85**, 052716 (2012)

Δn =0, 4d→4f, 4f→4f
Δn=1, 4d→5l, 4f→5l

Our calculation

4d→4f resonances
: 84223-188900

4f→4f resonances
: 28944-40689

FAC radiative decay
routine was parallelized.

Nuclear Data Center

Summary and outlook

- We have calculated DR and PEC of W ions for spectroscopic modeling.

- Recently recommended DR rate coefficients for W ions have been used for a spectroscopic modeling and the sensitivities of the line intensities to DR rate coefficient have been investigated.

- DR for W^{q+} (q=8-12, $[Kr]4d^{10}4f^{m}5s^{2}5p^{n}$) will be calculated.

Collaborations

KAIST — Dept. of Physics, Fusion Plasma Transport Research Center (Prof. W. Choe)

NFRI — ITER Korea VUV Diagnostic Team (Dr. C. R. Seon), KSTAR Team

Our website for atomic data and modeling

http://pearl.kaeri.re.kr