Dielectronic recombination computations of Rh-, Pd- and Ag-like W with the FAC code

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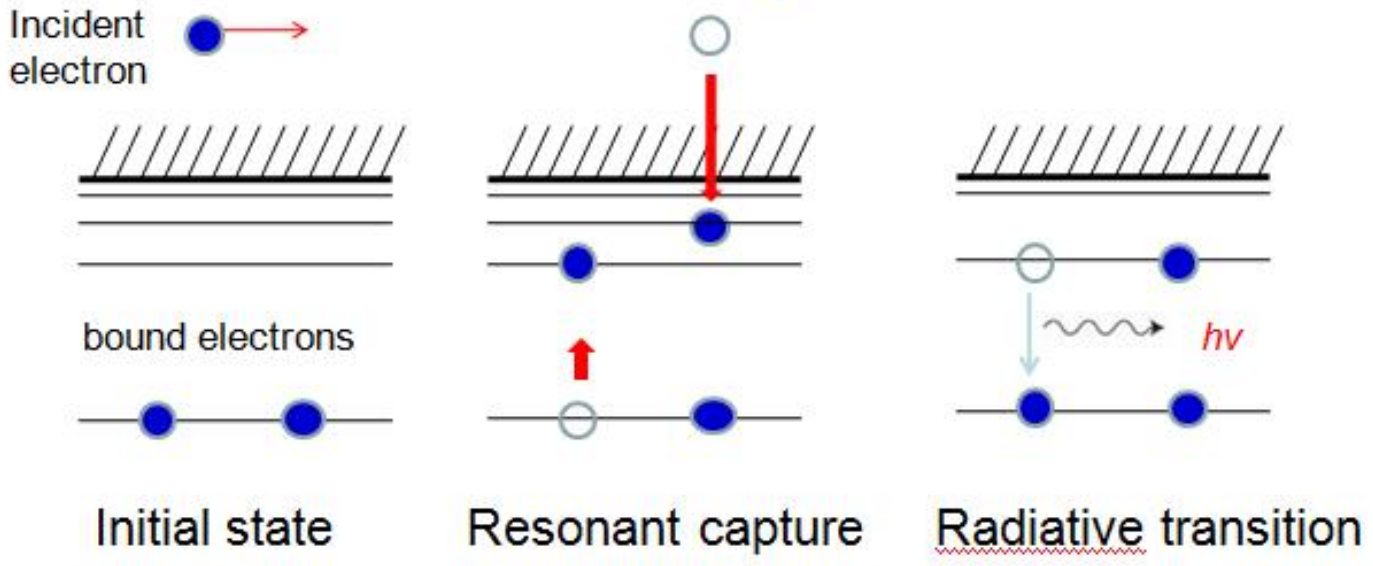
Contents

DR Process

What is DR process



$$e + A^{q+}(i) \rightarrow [A^{(q-1)+}]^{**}(j) \rightarrow [A^{(q-1)+}]^{*}(k) + h\nu$$

$$[Zn]\ 4p^6 4d^9 + e \rightarrow [Zn]\ 4p^6 4d^8 n'l'nl,\ n'l' = 4f, 5l, 6l,$$

$$+4p^5 4d^{10} nl + 4p^5 4d^9 n'l'nl,\ n'l' = 4f, 5l, 6l,$$

$$[Zn]\ 4p^6 4d^8 n'l'nl + 4p^5 4d^{10} nl + 4p^5 4d^9 n'l'nl,$$

$$\rightarrow [Zn]\ 4p^6 4d^9\ nl + 4p^6 4d^8\ n'l'n''l'' + h\nu,$$

RS NRS

$$\downarrow$$

$$[Zn]\ 4p^6 4d^9 + e$$

DR Process

DC strength:

$$S_{ij}^{DC} = \frac{\pi^2 \hbar^3}{m_e E_{ij}} \frac{g_j}{2g_i} A_{ji}^a$$

where g_j and g_i are the statistical weights of the doubly excited autoionization state j and initial state i, respectively, A_{ji}^a is the autoionization rate, and E_{ij} is resonant energy.

DR branch ratio:

$$B_j^r = \frac{\sum_f A_{jf}^r + \sum_{f'} A_{jf'}^r}{\sum_{i'} A_{di'}^a + \sum_f A_{jf}^r + \sum_{f'} A_{jf'}^r}$$

Here A^a and A^r are the Auger and radiative rates, respectively. f denotes singly excited final states, f' denotes doubly excited final states that lie below the ionization limit, d denotes doubly excited final states lying above the ionization threshold, and i' is the final state of the Auger decay.

DR rate coefficient:

$$\alpha_i^{DR}(T_e) = \frac{h^3}{(2\pi m_e T_e)^{3/2}} \sum_j \frac{Q_j}{2g_i} \exp\left(-\frac{E_{ij}}{kT_e}\right)$$

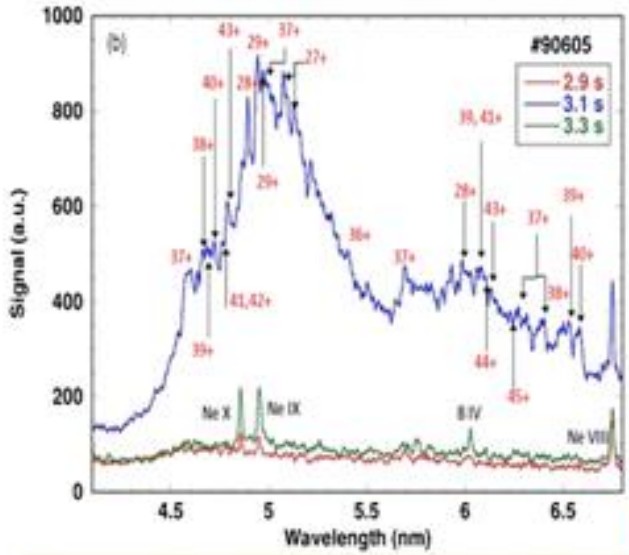
Intensity factor:

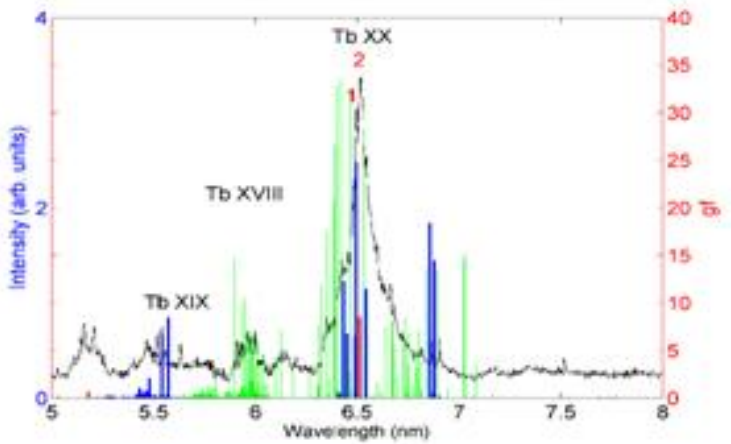
$$Q_j = g_j A_{ji}^a B_j^r$$

Important stages

IOP PUBLISHING JOURNAL OF PHYSICS B: ATOMIC, MOLECULAR AND OPTICAL PHYSICS
J. Phys. B: At. Mol. Opt. Phys. 43 (2010) 205004 (14pp) doi:10.1088/0953-4075/43/20/205004

Tungsten spectra recorded at the LHD and comparison with calculations





The most important transitions can be inferred from studies of W spectra.

They occur in Ag-like, Pd-like and Rh- like W^{27+}- W^{30+}. *Sugar et al JOSA 10, 1321 (1993)*

In all reported studies the emission is dominated by Ag and Pd-like lines i.e the spectra containing fewest lines where the emission is not divided amongst many transitions.

1. DR of Rh-like W

Published work

PHYSICAL REVIEW A **85**, 052706 (2012)

Dielectronic recombination of Rh-like Gd and W

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(Received 17 April 2012; published 15 May 2012)

Ab initio calculations of dielectronic recombination rate coefficients of Rh-like gadolinium and tungsten have been performed. Energy levels, radiative transition probabilities, and autoionization rates of Pd-like gadolinium and tungsten for $[\mathrm{Zn}]4p^6 4d^8 4fnl$, $[\mathrm{Zn}]4p^6 4d^8 5l'nl$, $[\mathrm{Zn}]4p^6 4d^8 6l'nl$ and $[\mathrm{Zn}]4p^5 4d^{10} nl$, $[\mathrm{Zn}]4p^5 4d^9 4fnl$, $[\mathrm{Zn}]4p^5 4d^9 5l'nl$, $[\mathrm{Zn}]4p^5 4d^9 6l'nl$ ($n \leqslant 18$) complexes were calculated using the flexible atomic code. The contributions from resonant and nonresonant radiative stabilizing transitions to the total rate coefficients are discussed. Results show that the contributions from nonresonant radiative stabilizing transitions are significantly enchanced for W when compared with Gd as a result of lowering of energy levels relative to the ionization limit. In addition, the widely used Burgess-Merts semiempirical formula may underestimate the dielectronic recombination rate coefficients in the temperature regions of interest. The present calculated rate coefficients are fitted to a semiemperical formula. The data obtained are expected to be useful for modelling plasmas both for extreme ultraviolet lithography source development and for fusion applications.

Energy level

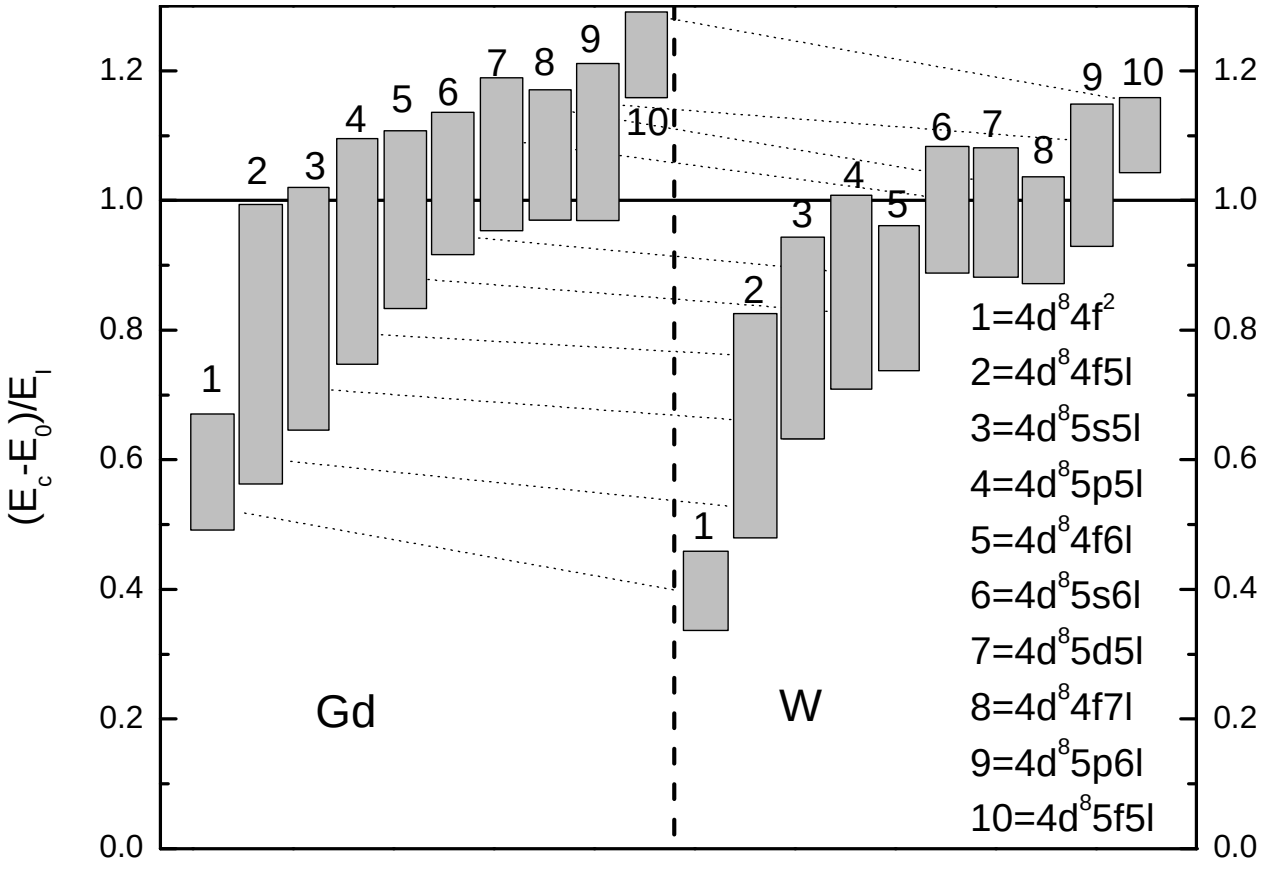


Figure: Energy levels of doubly excited configurations within the 4d complexes relative to the first ionization limit E_I (565 eV for Gd and 1128 eV for W) which is indicated by the dashed line. E_0 is the gound states energy of Pd-like Gd and W.

Energy level

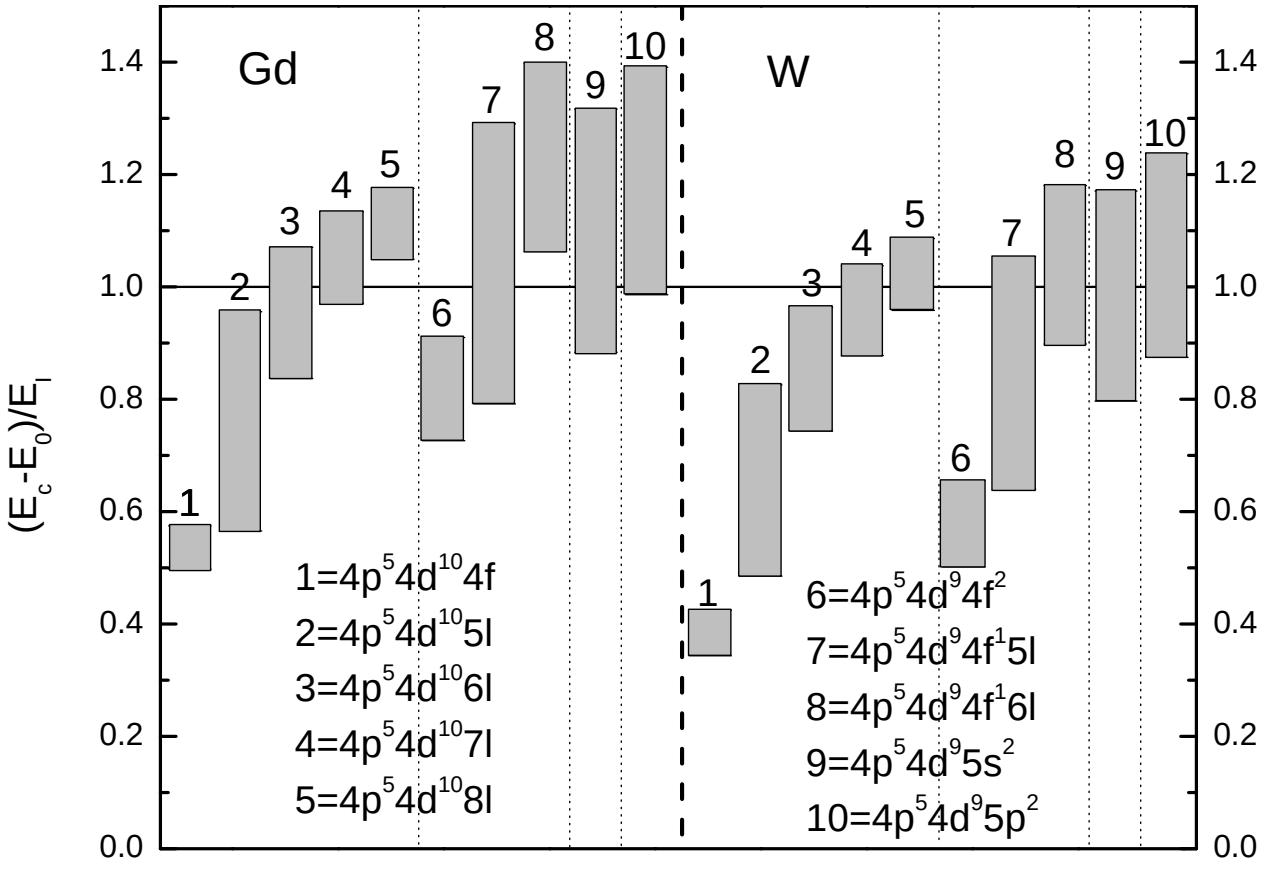


Figure: Energy levels of doubly excited configurations within the 4p complexes relative to the first ionization limit E_I (565 eV for Gd and 1128 eV for W) which is indicated by the dashed line. E_0 is the gound states energy of Pd-like Gd and W.

4d and 4p complex

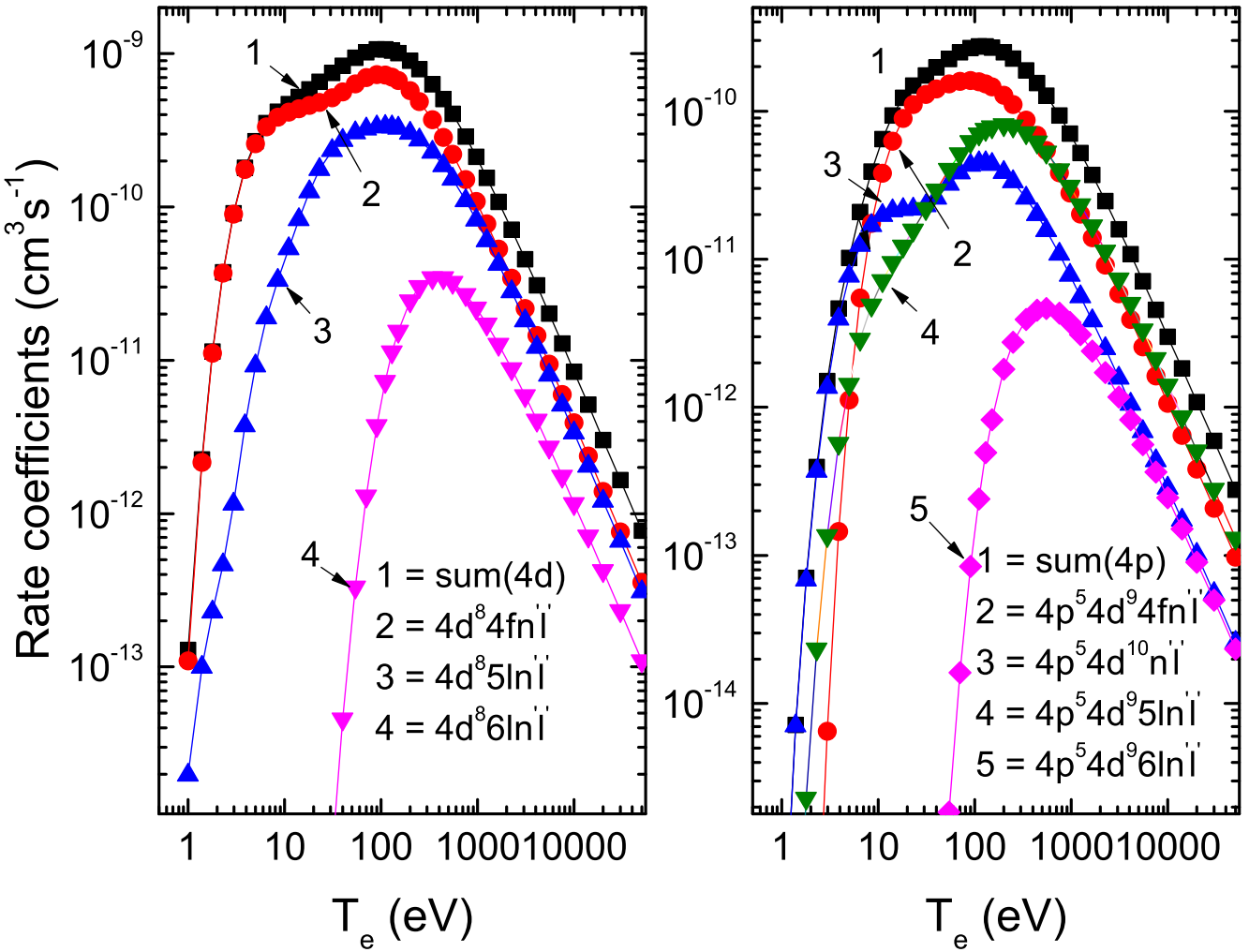


Figure: Partial DR rate coefficients for 4d and 4p core excited complexes

n dependence

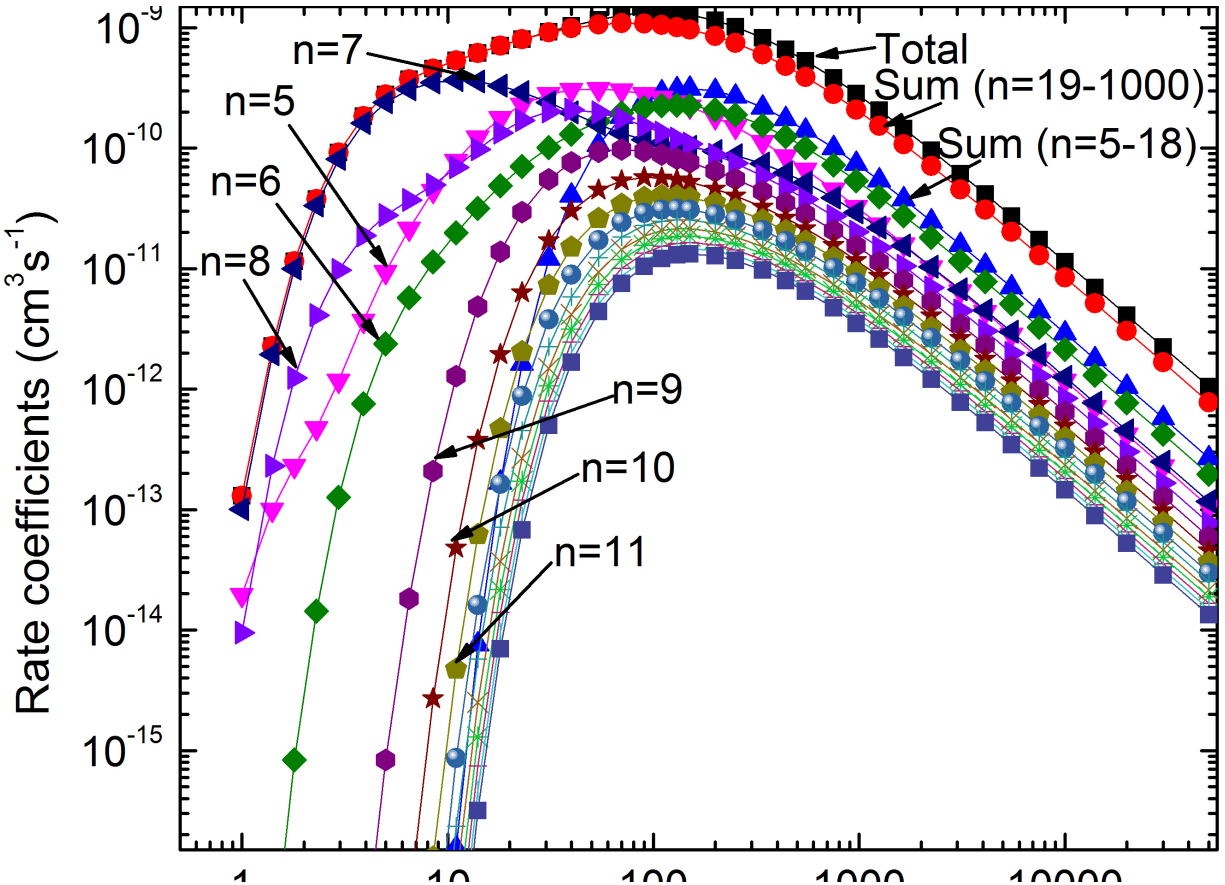


Figure: The DR rate coefficients where an incident electron is captured to the different orbitals of W.

DR rate

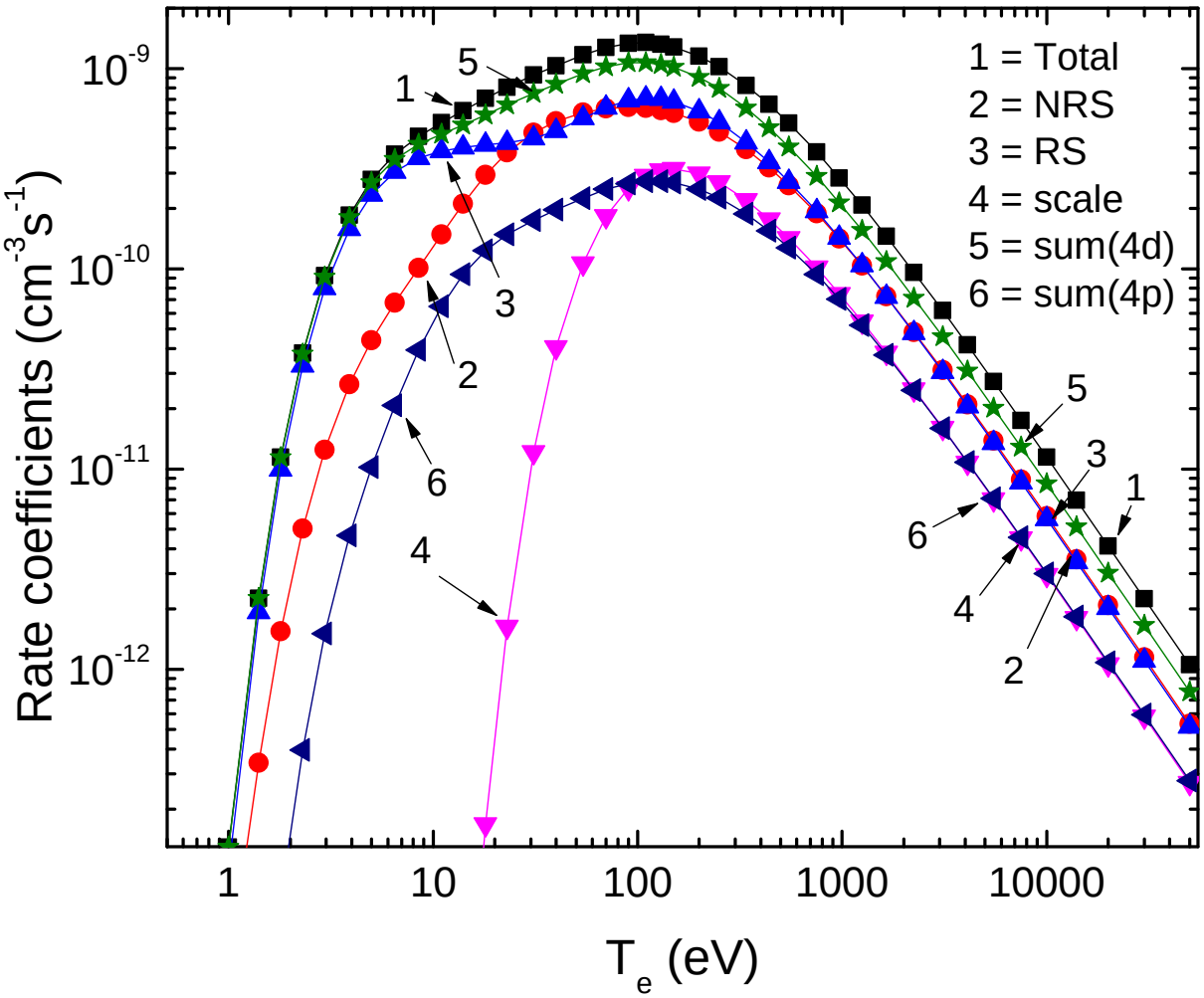
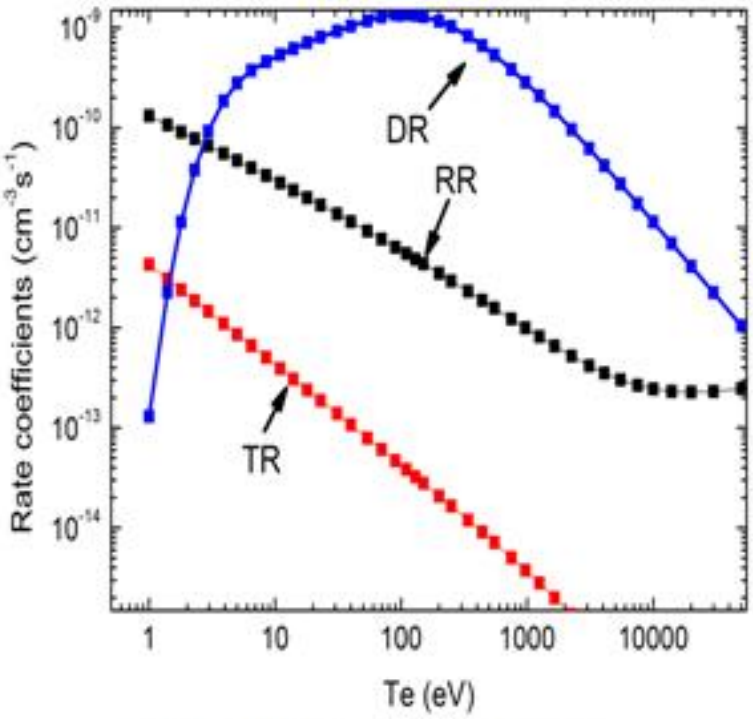
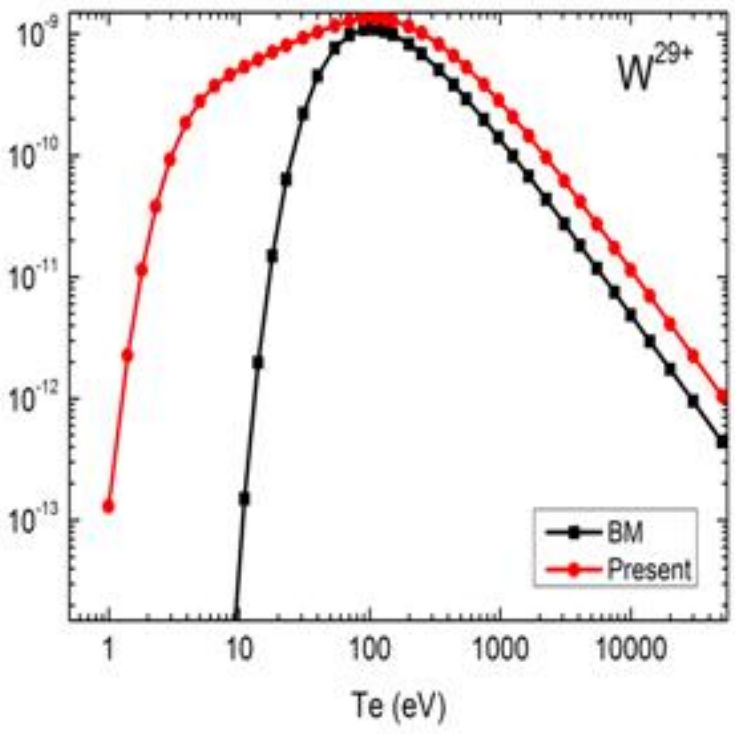


Figure: Contributions from the RS and NRS transition as well as different core excitations to total DR rate coefficients as a function of Te in Rh-like W.

Recombination process

Influence of DR process





$$\alpha_{RR} = 5.2 \times 10^{-14}(\phi_Z/T_e)^{1/2} Z[0.429 + \tfrac{1}{2}\log_{10}(\phi_Z/T_e) + 0.469(T_e/\phi_Z)^{1/2}]$$

$$\alpha_{3b} = 2.97 \times 10^{-27}\xi_Z/T_e\phi_Z^2(4.88 + T_e/\phi_Z)$$

J. Appl. Phys. **44**, 3524 (1973)

$$R^{DR} = 4.8 \times 10^{-11}(\frac{E_H}{T})^{3/2}/B(z)$$

Burgess-Merts (BM) approximation

A. Burgess, Astrophys. J **141**, 1588 (1965).

A. Merts, R. D. Cowan, N. H. J. Magee, Los Almos Scientific Laboratory Report No. LA-6220-MS, 1976 (unpublished).

Section conclusions

- Dielectronic recombination process is important.
- The 4p complexes contribute is aroud 25% to the total DR rate coefficients.
- The contributions from NRS transitions are significantly enhanced for W when compared with Gd as a result of lowering of energy levles relative to the ionization limit.

2. DR of Pd-like W

[†]Bowen Li *et al.* in preparing

Earlier work

IOP Publishing Journal of Physics B: Atomic, Molecular and Optical Physics

J. Phys. B: At. Mol. Opt. Phys. **44** (2011) 035005 (15pp) doi:10.1088/0953-4075/44/3/035005

Excitation energies, radiative and autoionization rates, dielectronic satellite lines and dielectronic recombination rates for excited states of Ag-like W from Pd-like W

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Abstract

Energy levels, radiative transition probabilities and autoionization rates for [Kr]$4d^9 4f nl$ ($n = 4$–9), [Kr]$4d^9 5l' nl$ ($n = 5$–9) and [Kr]$4d^9 6l' nl$ ($n = 6$–7) states in Ag-like tungsten (W^{27+}) are calculated using the relativistic many-body perturbation theory method, the multiconfiguration relativistic Hebrew University Lawrence Livermore Atomic Code and the Hartree–Fock-relativistic method. Branching ratios relative to the first threshold and intensity factors are calculated for satellite lines, and dielectronic recombination (DR) rate coefficients are determined for the singly excited [Kr]$4d^{10} nl$ ($n = 4$–9) states. The total DR rate coefficient is derived as a function of electron temperature. These atomic data are important in the modelling of N-shell radiation spectra of heavy ions generated in various collision as well as plasma experiments. The tungsten data are particularly important for fusion application.

4d and 4p complex

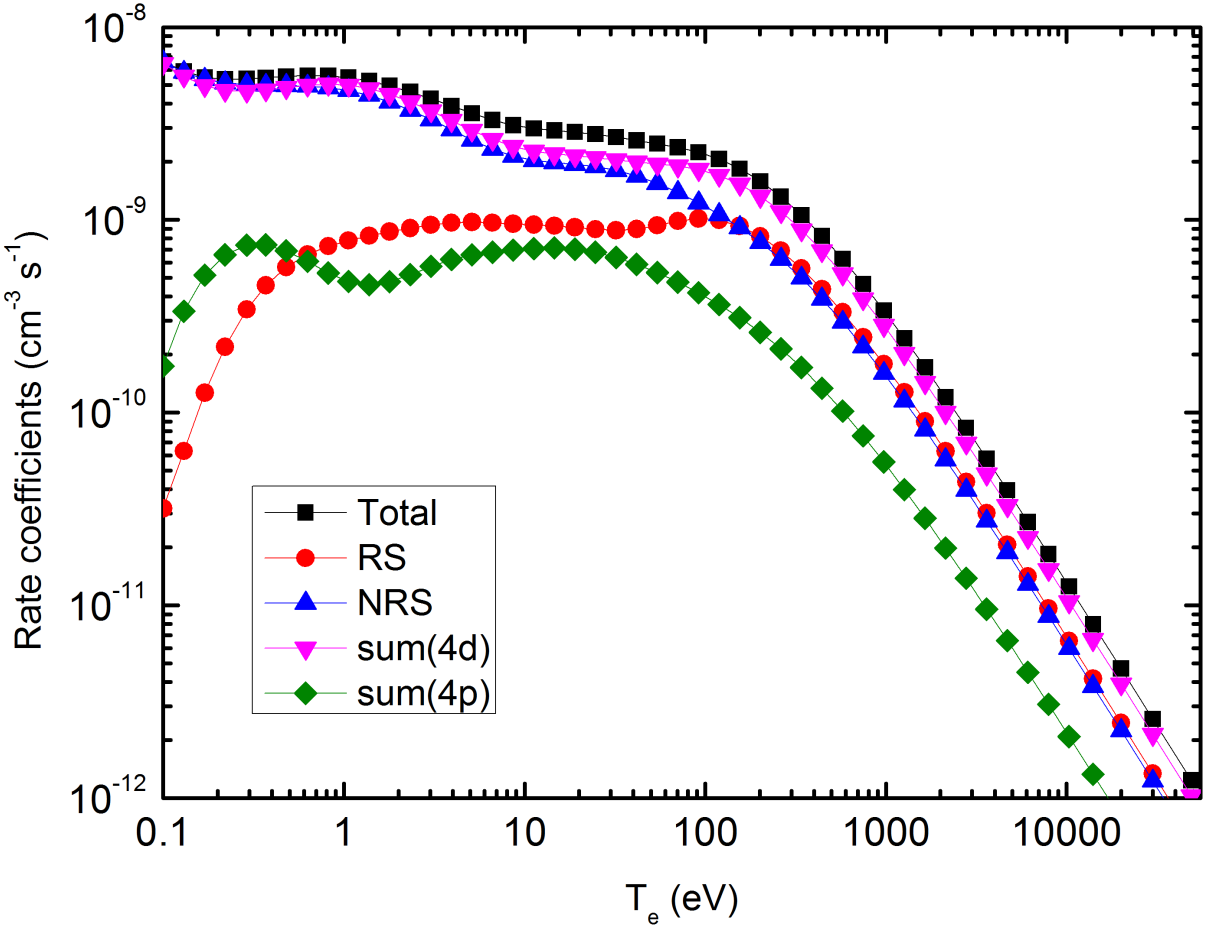


Figure: Contributions from the RS and NRS transition as well as different core excitations to total DR rate coefficients as a function of Te in Pd-like W.

DR rate

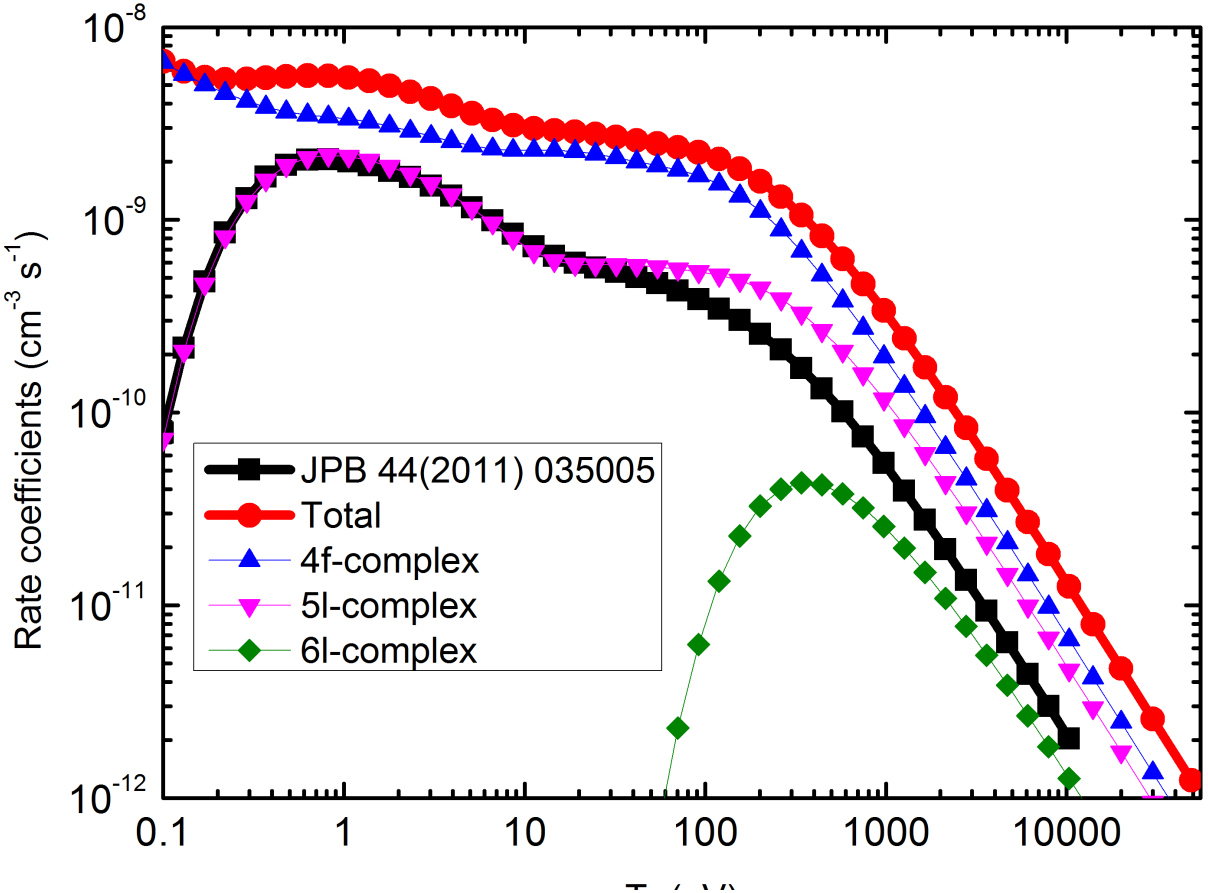


Figure: Contributions from the RS and NRS transition as well as different core excitations to total DR rate coefficients as a function of Te in Pd-like W.

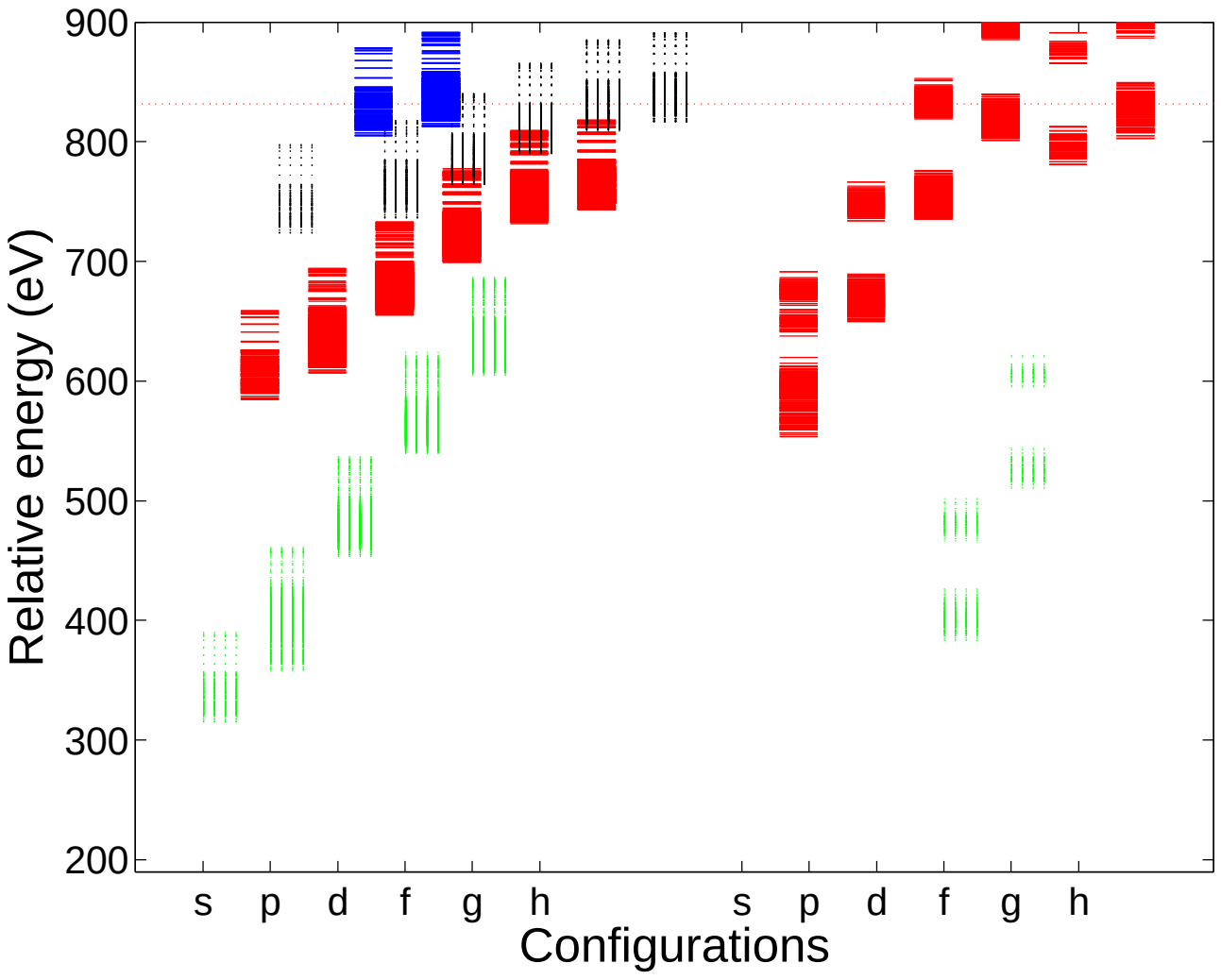
Section conclusions

- Very big discrepancy with Safronova *et al.*.
- Need new experiment or other calculations.
- $\Delta n = 0$ and $\Delta n = 1$ are important.

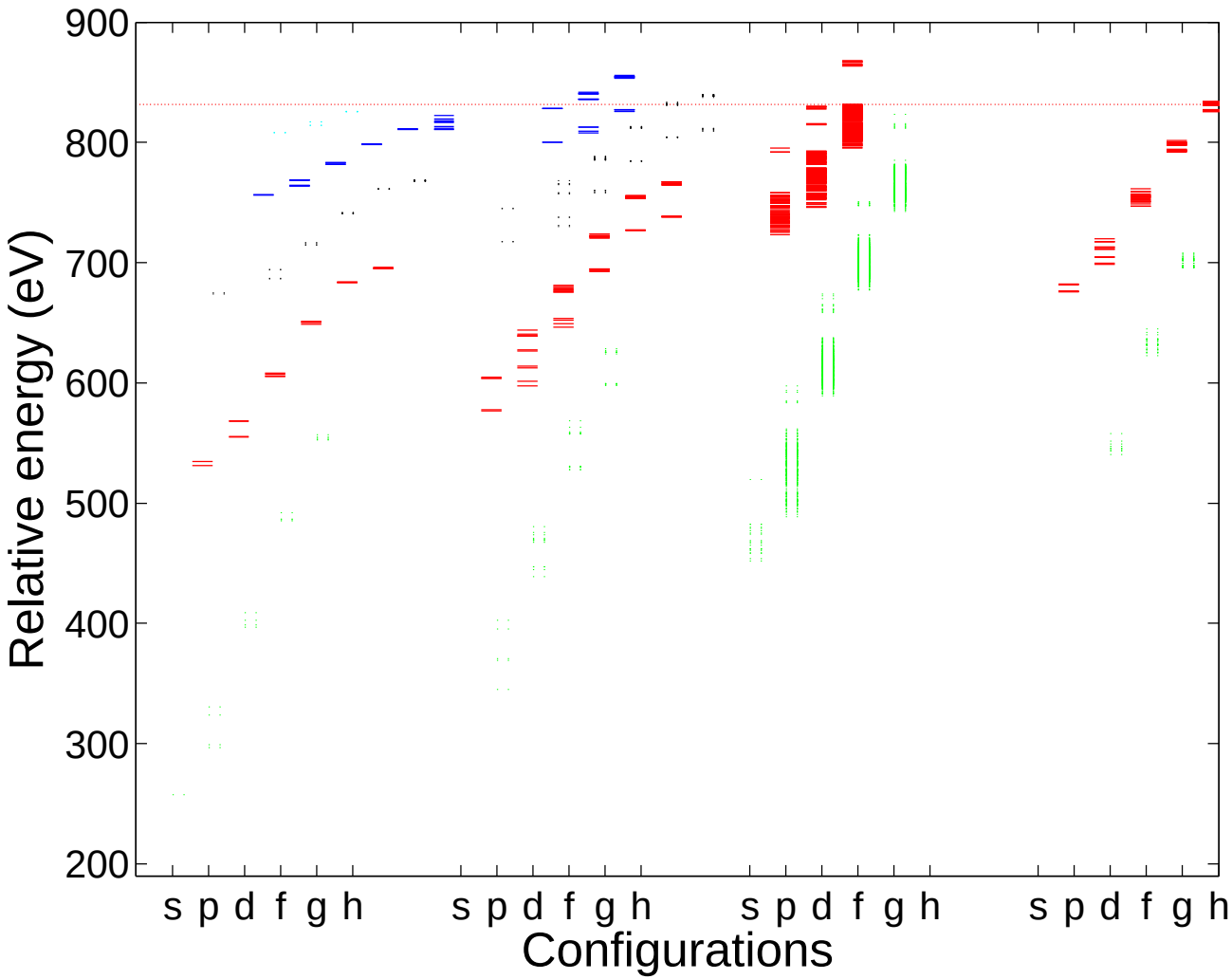
3. DR of Ag-like W

[†]Bowen Li *et al.* in preparing, without extrapolation

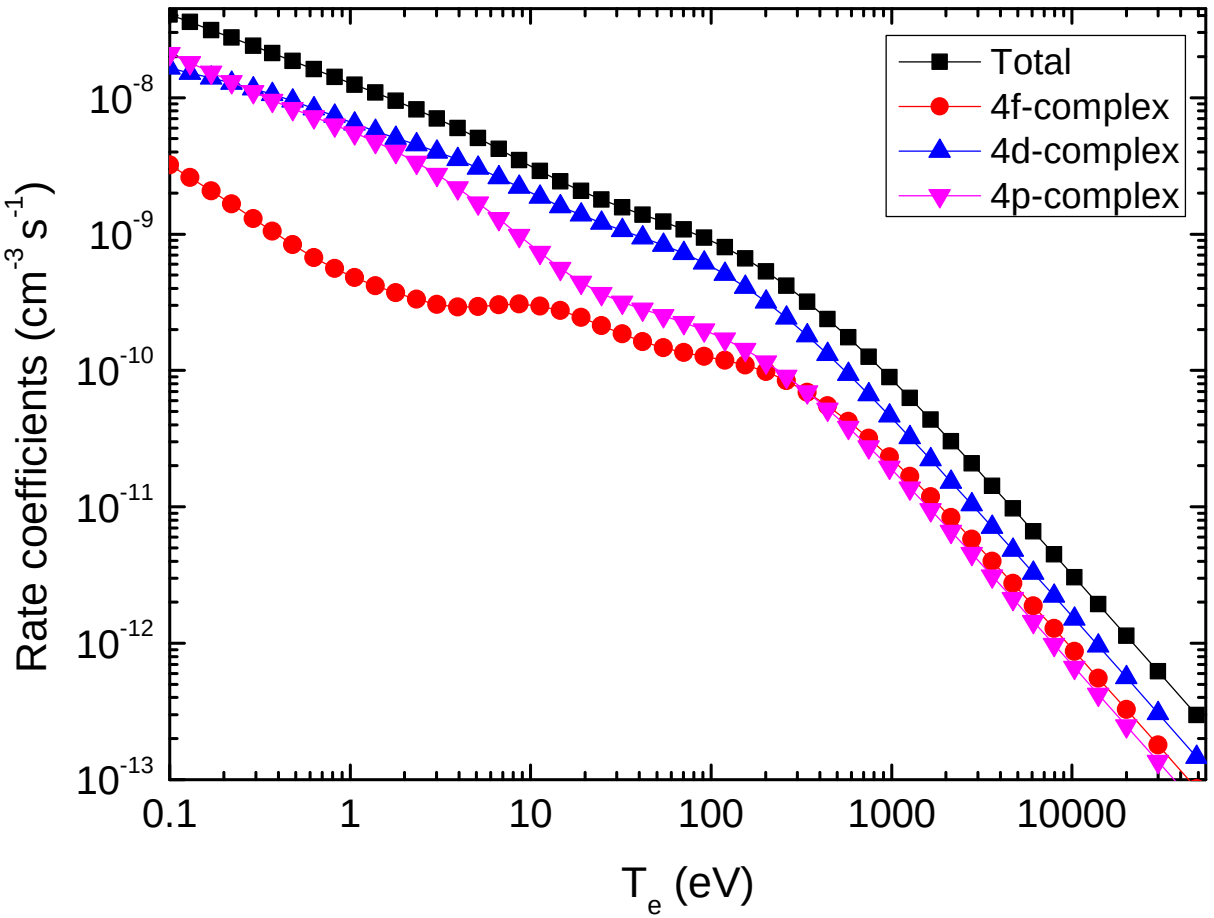
Energy level



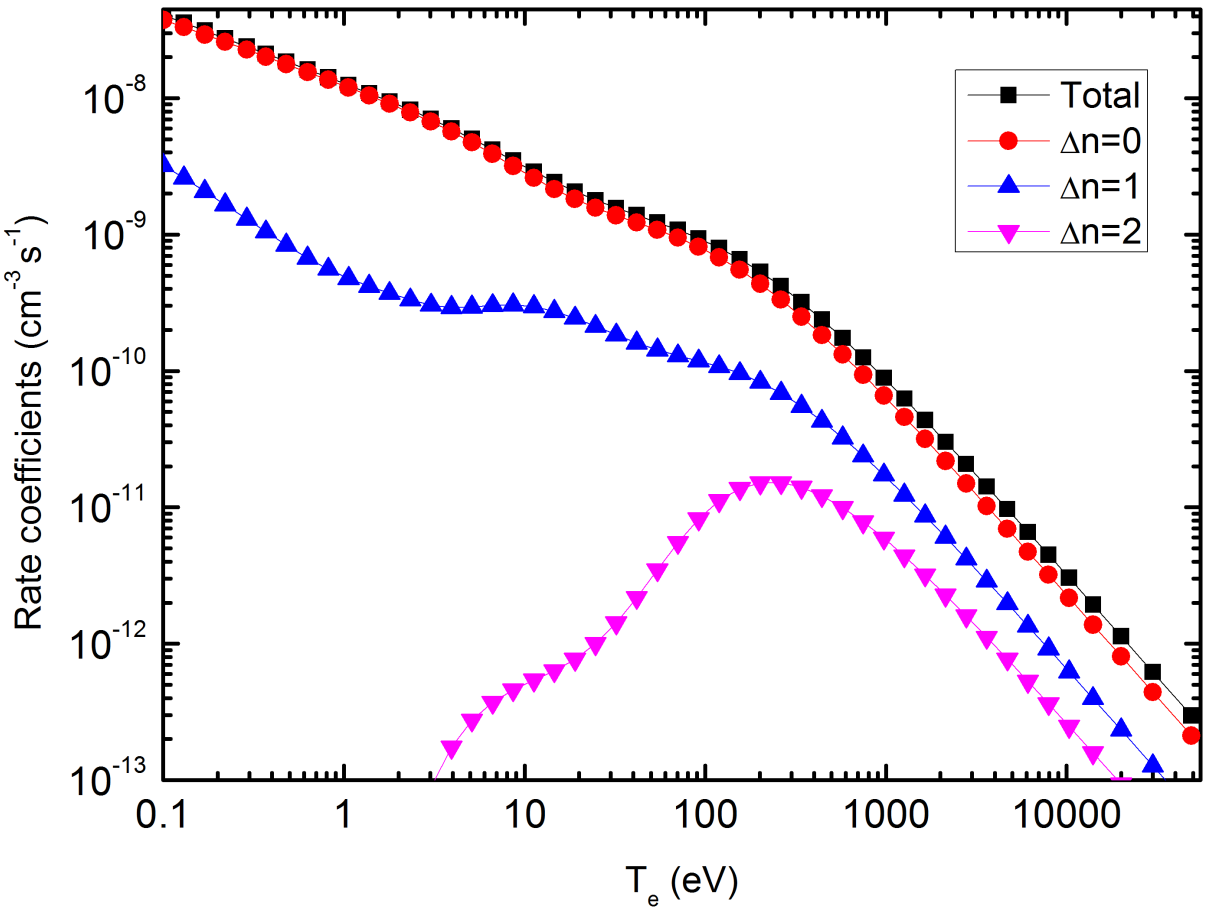
Energy level



Complex


Total
4f-complex
4d-complex
4p-complex
Rate coefficients (cm^{-3} s^{-1})
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
0.1
1
10
100
1000
10000
T_e (eV)

DR rate


Total
Δn=0
Δn=1
Δn=2
Rate coefficients (cm^{-3} s^{-1})
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
0.1
1
10
100
1000
10000
T_e (eV)

Future work

- Check the Pd-like W data.
- Finish the calculations on Ag-like W.
- ...

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Thank you for your attention!