Dielectronic Recombination of W^{45+} and W^{44+} : Configuration Mixing and Channels

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Contents

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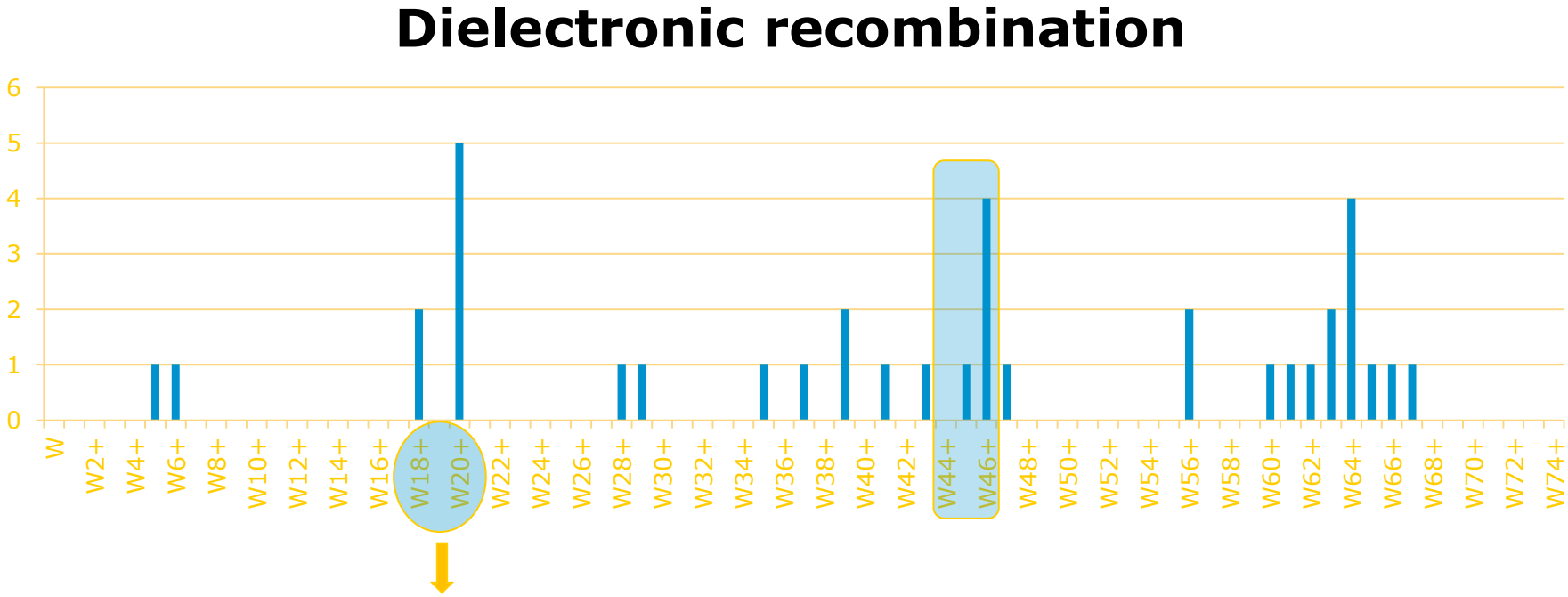
Introduction

- DR cross sections and rate coefficients have been calculated for W^{45+} and W^{44+} based on an IPIR-DW approximation using flexible atom code (fac).

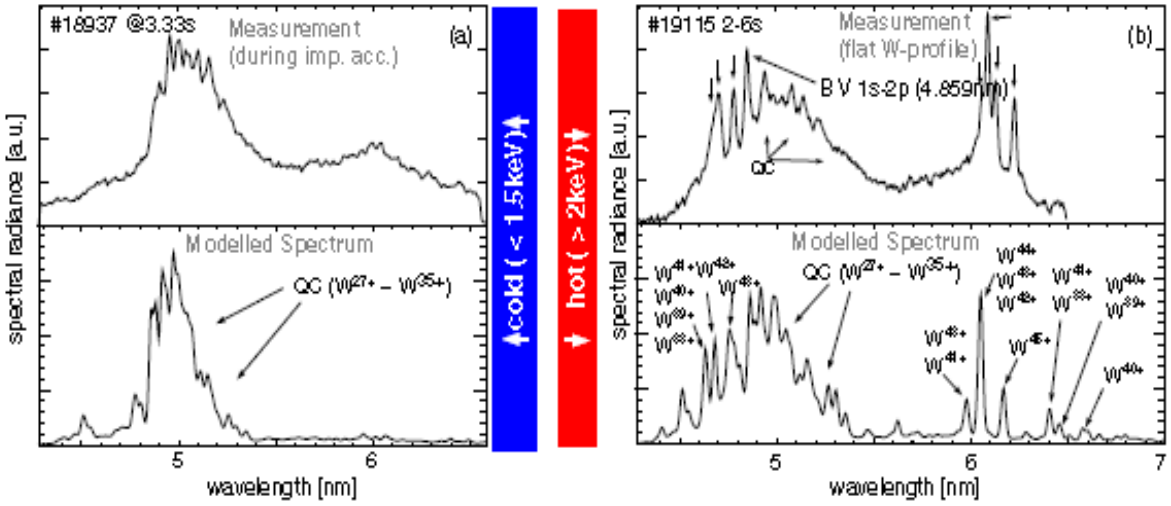
- Effects of configuration mixing (CM) involving double electron core excitation and non-resonant stabilizations + decay to autoionizing levels possibly followed by cascades (DAC) on DR are investigated.

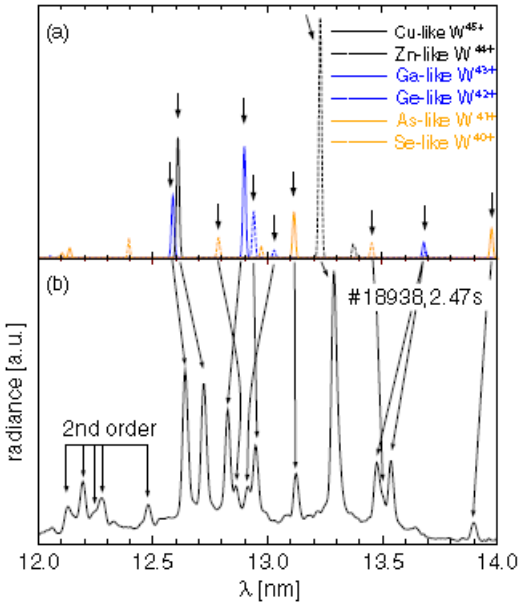
Introduction

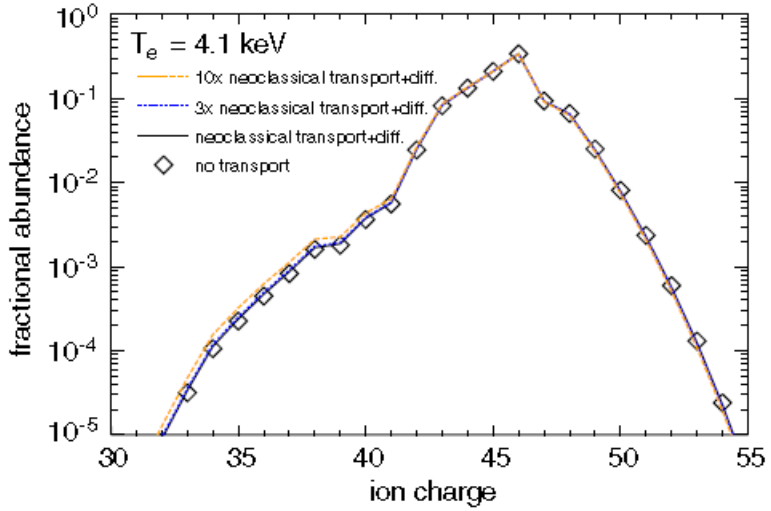


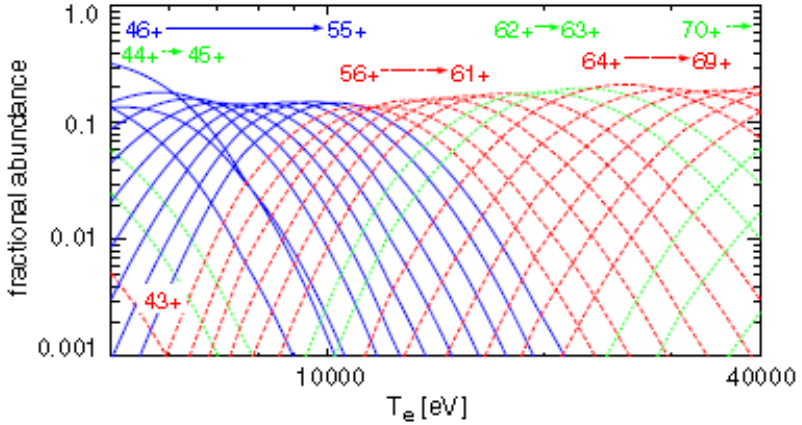
Experimental data is available only for these ions.

Introduction









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DR cross section and rate coefficient

$$e^- + A_i^{q+} \leftrightarrow \left[A_j^{(q-1)+}\right]^{**} \rightarrow \left[A_f^{(q-1)+}\right]^{*} + h\nu.$$

$$\bar{\sigma}_{ij} = \frac{\pi^2}{E_{ij}\Delta E}\frac{g_j}{2g_i}A^a_{ji}\frac{\sum_t A^r_{jt} + \sum_{t'} A^r_{jt'}B_{t'}}{\sum_k A^a_{jk} + \sum_f A^r_{jf}},$$

$$\bar{\sigma}^{\mathrm{DC}}_{ij} = \frac{\pi^2}{E_{ij}}\frac{g_j}{2g_i}A^a_{ji}\frac{\Gamma_j/2\pi}{(E-E_{ij})^2 + {\Gamma_j}^2/4} \cong \frac{\pi^2}{E_{ij}}\frac{g_j}{2g_i}A^a_{ji}\delta(E-E_{ij}).$$

$$\Gamma_j = \sum_k A^a_{jk} + \sum_f A^r_{jf}$$

$$\alpha_{ij}(T_\mathrm{e}) = \frac{1}{\pi^{1/2}}\left(\frac{2}{\mathrm{k_B}T_\mathrm{e}}\right)^{3/2}\int_0^\infty \sigma_{ij}(E)\exp\left(-\frac{E}{\mathrm{k_B}T_\mathrm{e}}\right)\mathrm{d}E$$

$$\cong \frac{1}{2g_i}\left(\frac{4\pi a_0^2 Ry}{k_\mathrm{B}T_\mathrm{e}}\right)^{3/2} g_j A^a_{ji}B_j \exp\left(-\frac{E_{ij}}{k_\mathrm{B}T_\mathrm{e}}\right),$$

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Calculated energies for W^{45+} and W^{44+}

Term	Present	NIST	% Diff.
$3d^{10}4s\ ^2S_{1/2}$	0	0	
$3d^{10}4p\ ^2P_{1/2}$	97.529	97.626	0.1
$3d^{10}4p\ ^2P_{3/2}$	198.930	198.897	0.02
$3d^{10}4d\ ^2D_{3/2}$	349.326	349.59	0.08
$3d^{10}4d\ ^2D_{5/2}$	370.857	371.153	0.08
$3d^{10}4f\ ^2F_{5/2}$	532.304	532.31	0.001
$3d^{10}4f\ ^2F_{7/2}$	537.749	537.74	0.002
$3d^{10}5s\ ^2S_{1/2}$	967.7	967.6	0.01
$3d^{10}5p\ ^2P_{1/2}$	1015.1	1014.9	0.02
$3d^{10}5d\ ^2D_{3/2}$	1134.4	1136.2	0.16
$3d^{10}5f\ ^2F_{5/2}$	1216.4	1216.7	0.02
$3d^{10}5g\ ^2G_{7/2}$	1256.4	1256.1	0.02
$3d^{10}6f\ ^2F_{5/2}$	1586.7	1587.4	0.04
$3d^{10}6g\ ^2G_{7/2}$	1609.5	1609.4	0.004
$3d^{9}4s^2\ ^2D_{5/2}$	1554.0	1547.6	0.4
$3d^9(^2D_{3/2})(4s_{1/2}4p_{1/2})^o_1$	1713.6	1707.3	0.4
$3d^9(^2D_{3/2})(4p^2_{1/2})_0$	1816.6	1809.7	0.4
$3p^53d^{10}4s^2\ ^2P^o_{3/2}$	2010.0	2000.1	0.5
$3p^5(^2P^o_{3/2})3d^{10}(4s_{1/2}4p_{1/2})^0_1$	2090.0	2092.2	0.1
$3d^94s(5/2,1/2)_24f_{7/2}$	2090.0	2095.5	0.4
$3p^5(^2P^o_{3/2})3d^{10}(4s_{1/2}4d_{5/2})_3$	2360.0	2367.1	0.3

Term	Present	NIST	% Diff.
$3d^{10}4s^2\ ^1S_0$	0	0	
$3d^{10}4s4p\ ^3P_0$	85.9	86.2	0.4
$3d^{10}4s4p\ ^3P_1$	93.105	93.306	0.2
$3d^{10}4s4p\ ^3P_2$	185.927	185.282	0.08
$3d^{10}4p^2\ ^3P_0$	197.5	196.9	0.2
$3d^{10}4s4p\ ^1P_1$	203.958	203.487	0.08
$3d^{10}4p^2\ ^3P_0$	291.11	290.83	0.1
$3d^{10}4p^2\ ^1D_2$	292.37	292.94	0.2
$3d^{10}4s4d\ ^3D_1$	344.86	345.01	0.05
$3d^{10}4s4d\ ^3D_2$	348.33	348.33	0.00
$3d^{10}4s4d\ ^3D_3$	365.86	364.98	0.24
$3d^{10}4s4d\ ^1D_2$	371.51	370.53	0.26
$3d^{10}4p^2\ ^3P_2$	398.61	398.1	0.13
$3d^{10}4p^2\ ^1S_0$	403.3	402.8	0.12
$3d^{10}4p4d\ ^3D_2$	543.7	543.4	0.05
$3d^{10}4p4d\ ^3D_3$	553.5	552.7	0.14
$3d^{10}4p4d\ ^3F_4$	558.85	558.59	0.05
$3d^{10}4p4d\ ^1F_3$	580.1	578.6	0.27
$3d^94s^24p$	1623	1614	0.56
$3d^94s4p^2(^3P_0)(1/2,0)_{1/2}$	1786	1782	0.2
$3d^9(\ ^2D_{5/2})4s^24f$	2087.8	2082.2	0.27
$3d^9(\ ^2D_{3/2})4s4p4d$	2155.34	2154.81	0.02
$3p^5(^2P^o_{3/2})3d^{10}4s^24d$	2355.3	2350.7	0.19
$3d^9(\ ^2D_{5/2})4s^25f$	2741.9	2750.3	0.31
$3d^9(\ ^2D_{5/2})4s^26f$	3106.6	3107.8	0.04
$3p^5(^2P^o_{3/2})3d^{10}4s^25d$	3124.4	3121	0.11
$3d^9(\ ^2D_{5/2})4s^27f$	3323.2	3315	0.25

Excellent agreement with the recommanded NIST data (0.001 ~ 0.5 %)

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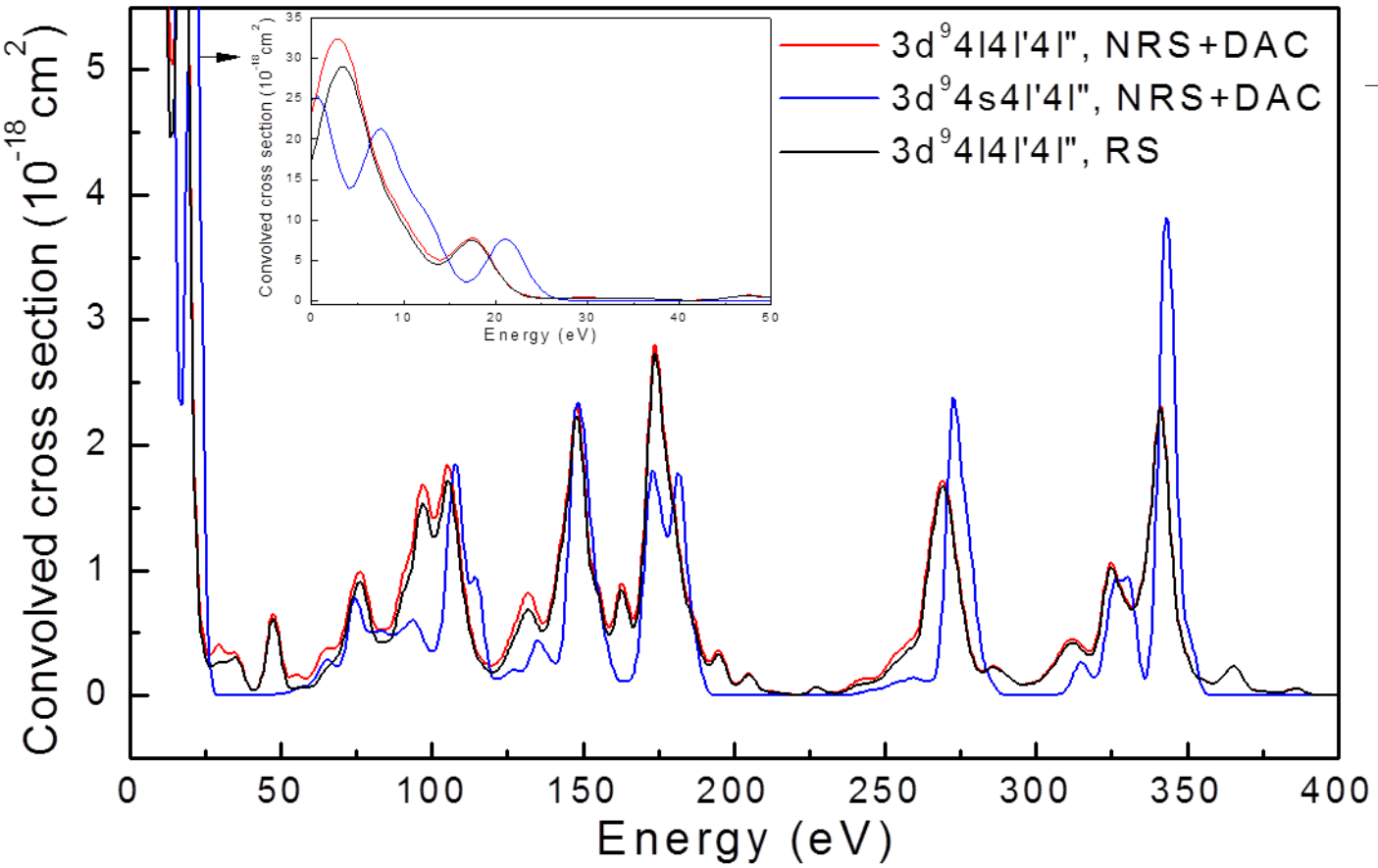
W^{45+} : $3d+e^- \rightarrow 4l4l'$ (CM & NRS+DAC)

$$3s^2 3p^6 3d^{10} 4s + e^- \rightarrow 3d^9 4l4l'nl'' \rightarrow \left\{ \begin{array}{c} 3d^{10}4l \\ 3d^{10}nl''(n>4) \\ 3d^9 4l4l'(n>4) \end{array} \right\} + e^- \rightarrow \left\{ \begin{array}{c} 3d^{10}4l4l' \\ 3d^{10}4lnl''(n>4) \\ 3d^9 4l4l'nl''(n=4) \end{array} \right\} + \omega$$



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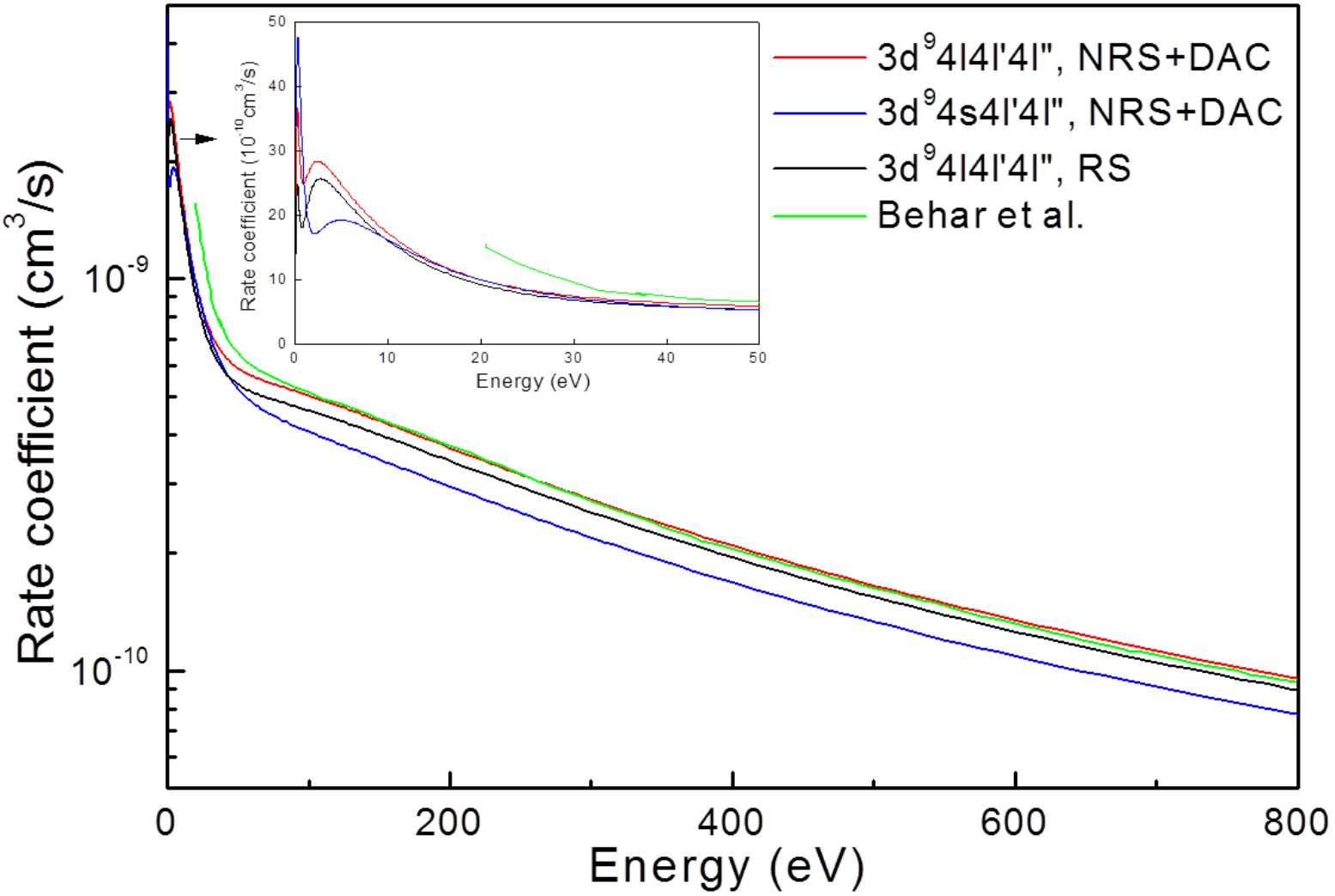

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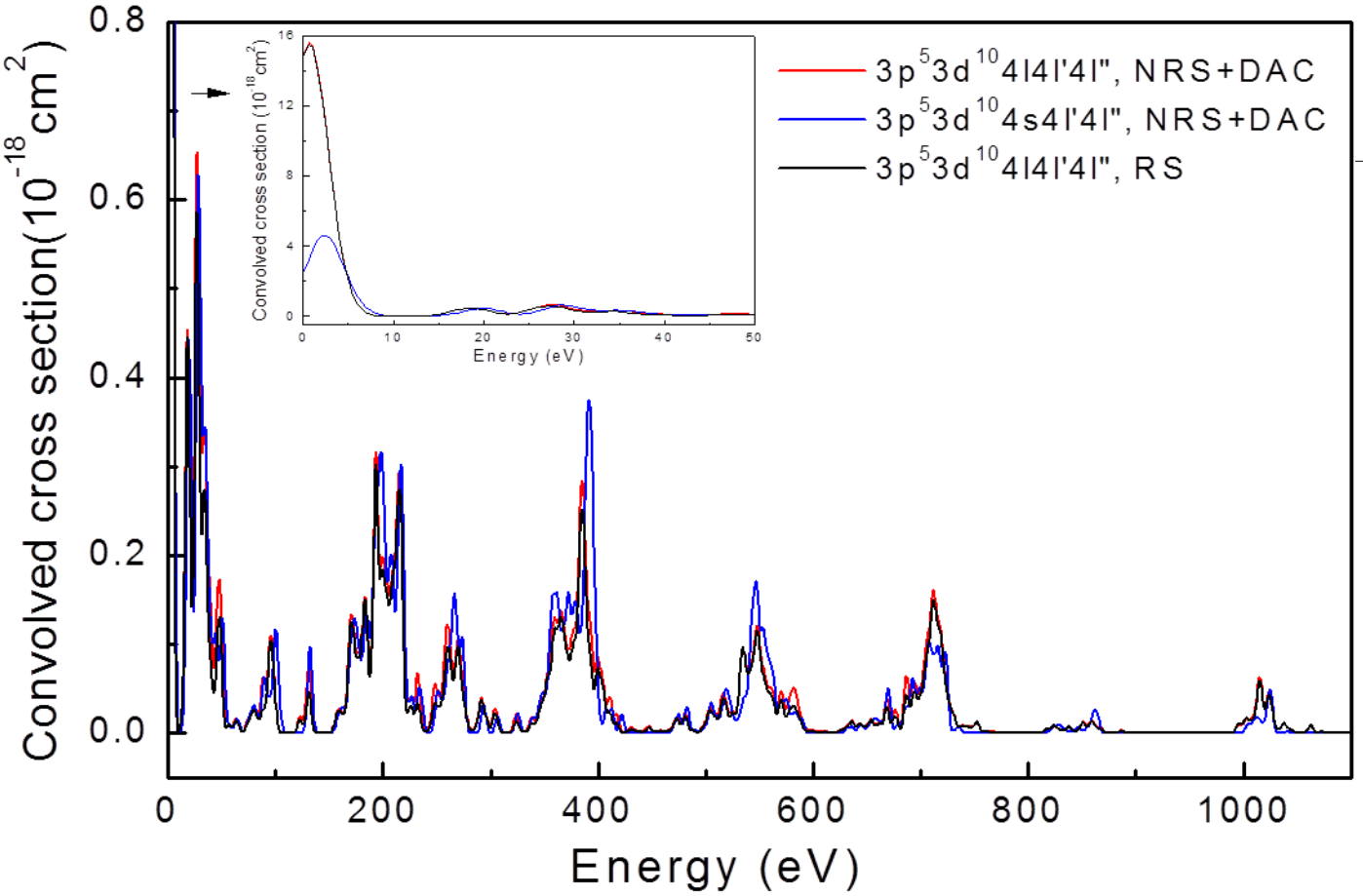
W^{45+} : $3p+e^- \rightarrow 4l4l'$ (CM & NRS+DAC)

$$3s^2 3p^6 3d^{10} 4s + e^- \rightarrow 3p^5 3d^{10} 4l4l'nl'' \rightarrow \left\{ \begin{array}{c} 3d^{10}4l \\ 3d^{10}nl''(n>4) \\ 3d^9 4l4l' \\ 3p^5 3d^{10} 4l4l'(n>4) \end{array} \right\} + e^- \rightarrow \left\{ \begin{array}{c} 3d^{10}4l4l' \\ 3d^{10}4lnl''(n>4) \\ 3d^9 4l4l'nl''(n=4) \end{array} \right\} + \omega$$



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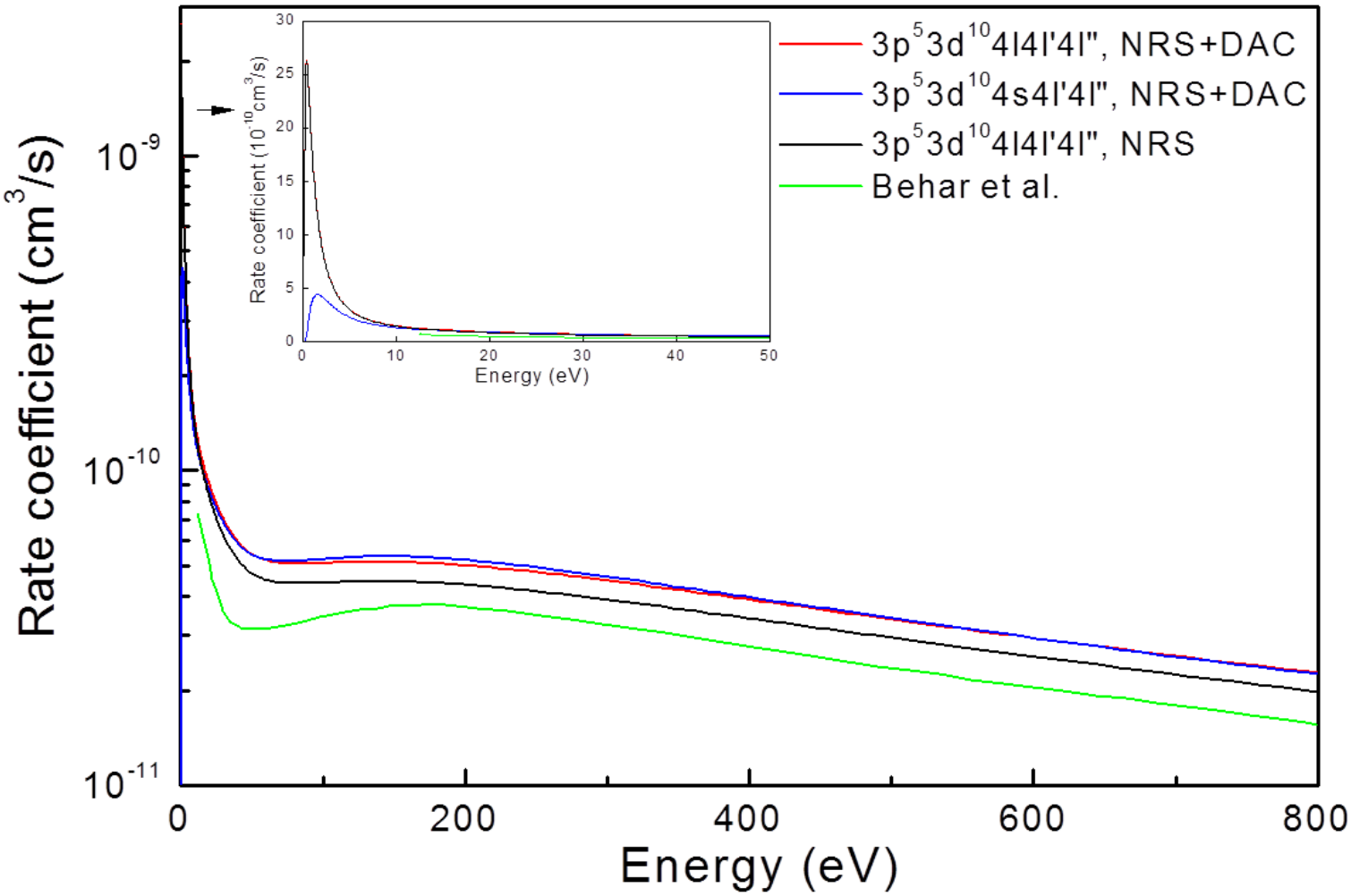
W^{45+} : $3p+e^{-} \rightarrow 4l4l'$ (CM & NRS+DAC)



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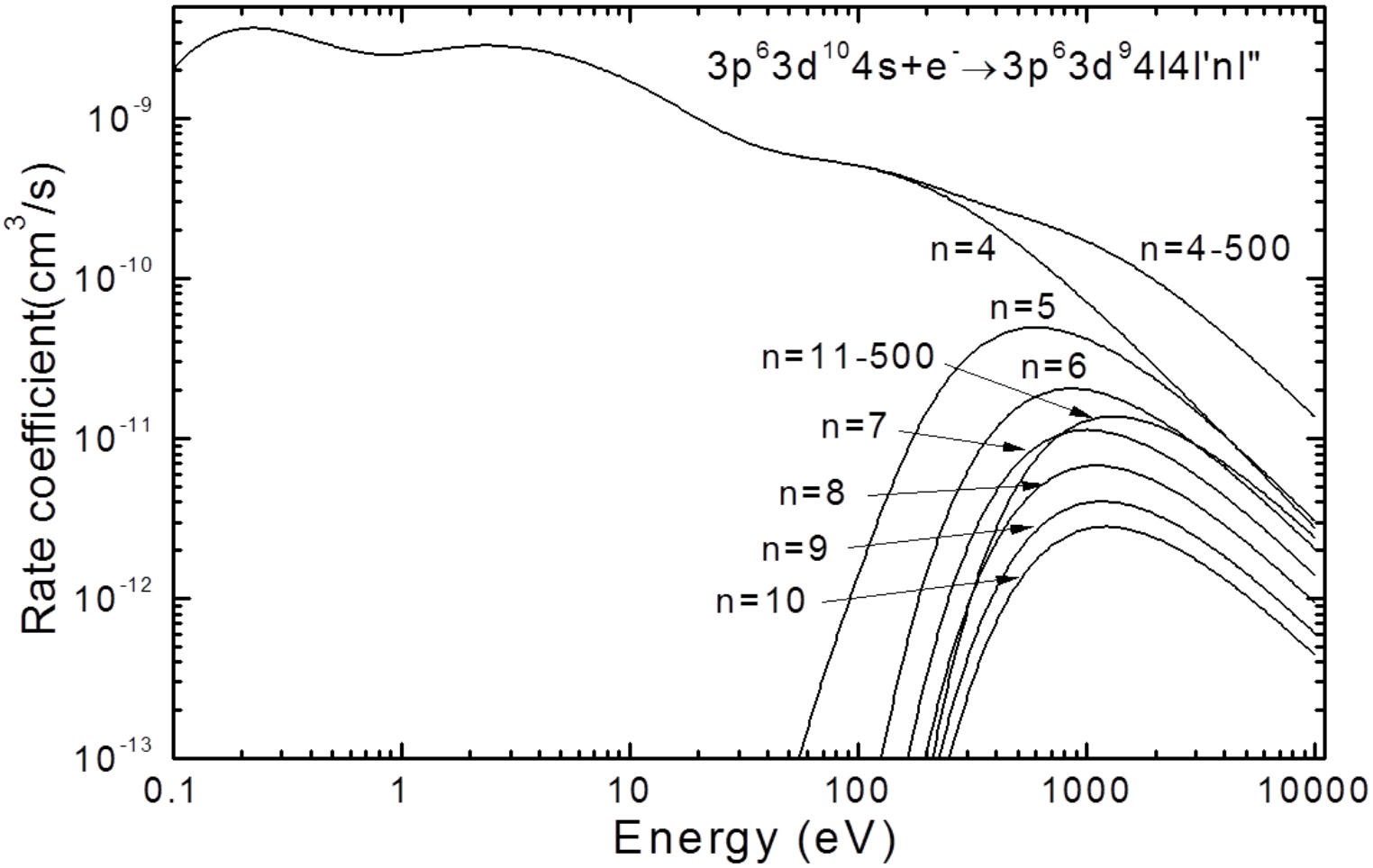
W^{45+} : 3d → 4l core excitation rate coeff.



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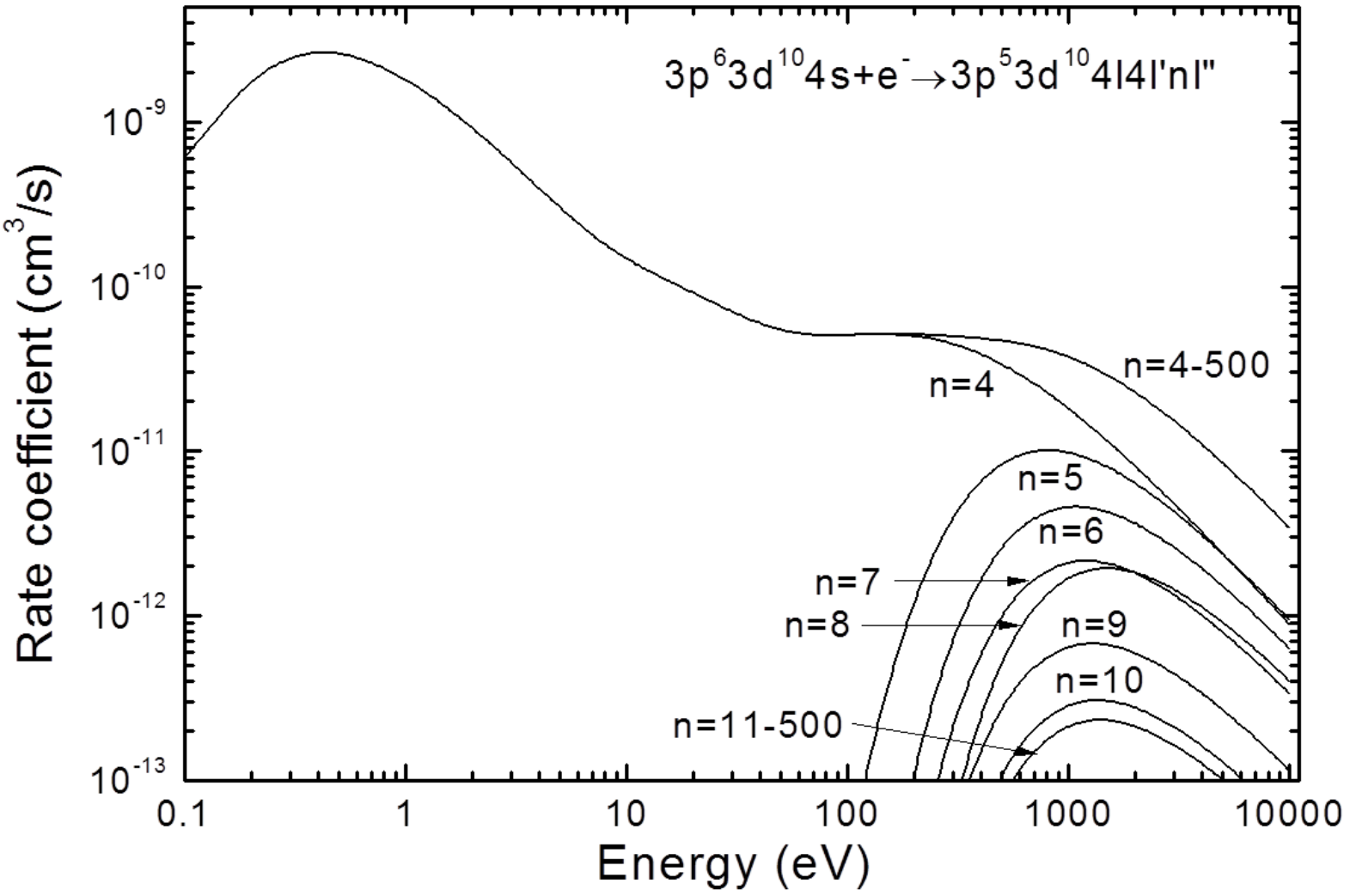
W^{45+} : 3p → 4l core excitation rate coeff.



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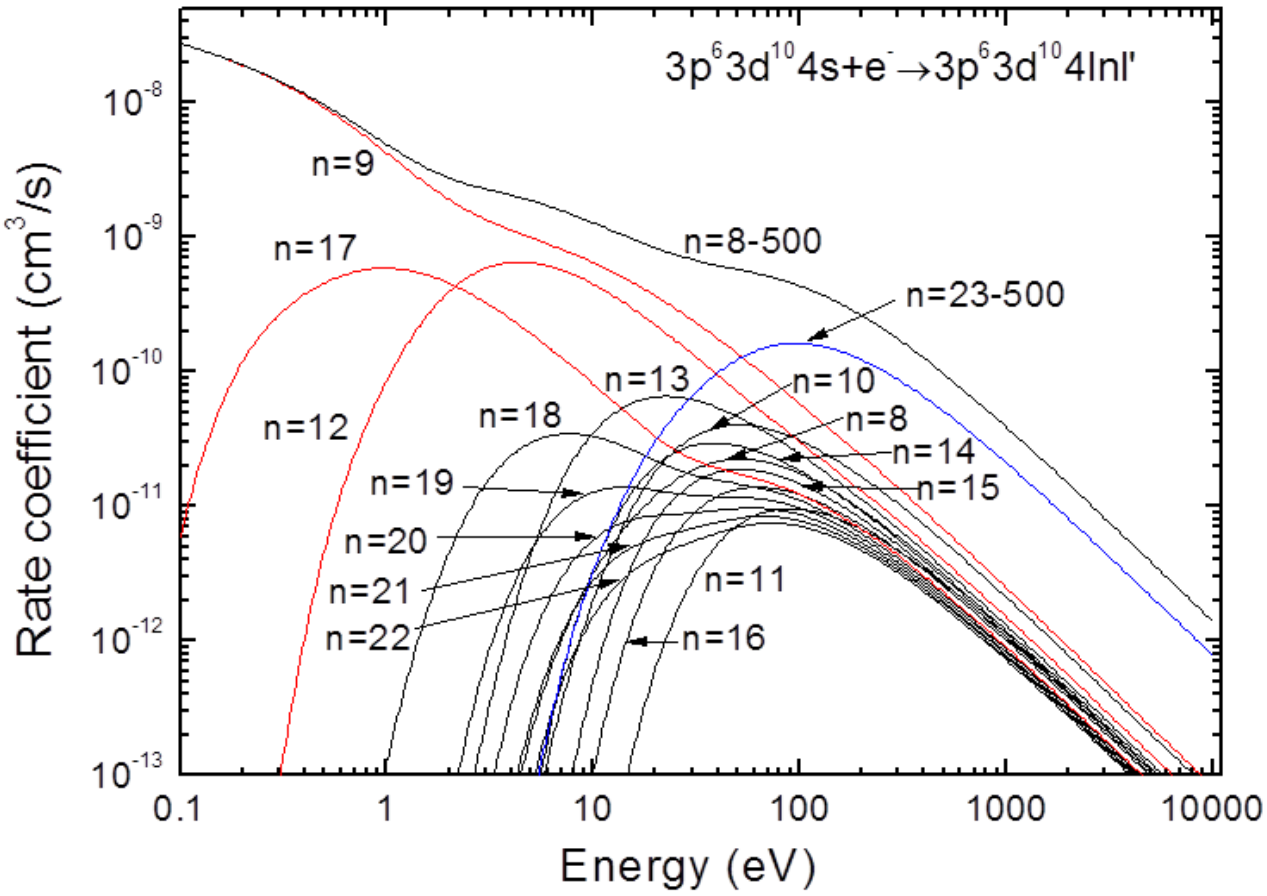
W^{45+} : 4s → 4l core excitation

$$3s^2 3p^6 3d^{10} 4s + e^- \rightarrow 3d^{10} 4l n l' \rightarrow 3d^{10} 4l + e^-$$

$$\rightarrow 3d^{10} 4l 4l' + \omega$$



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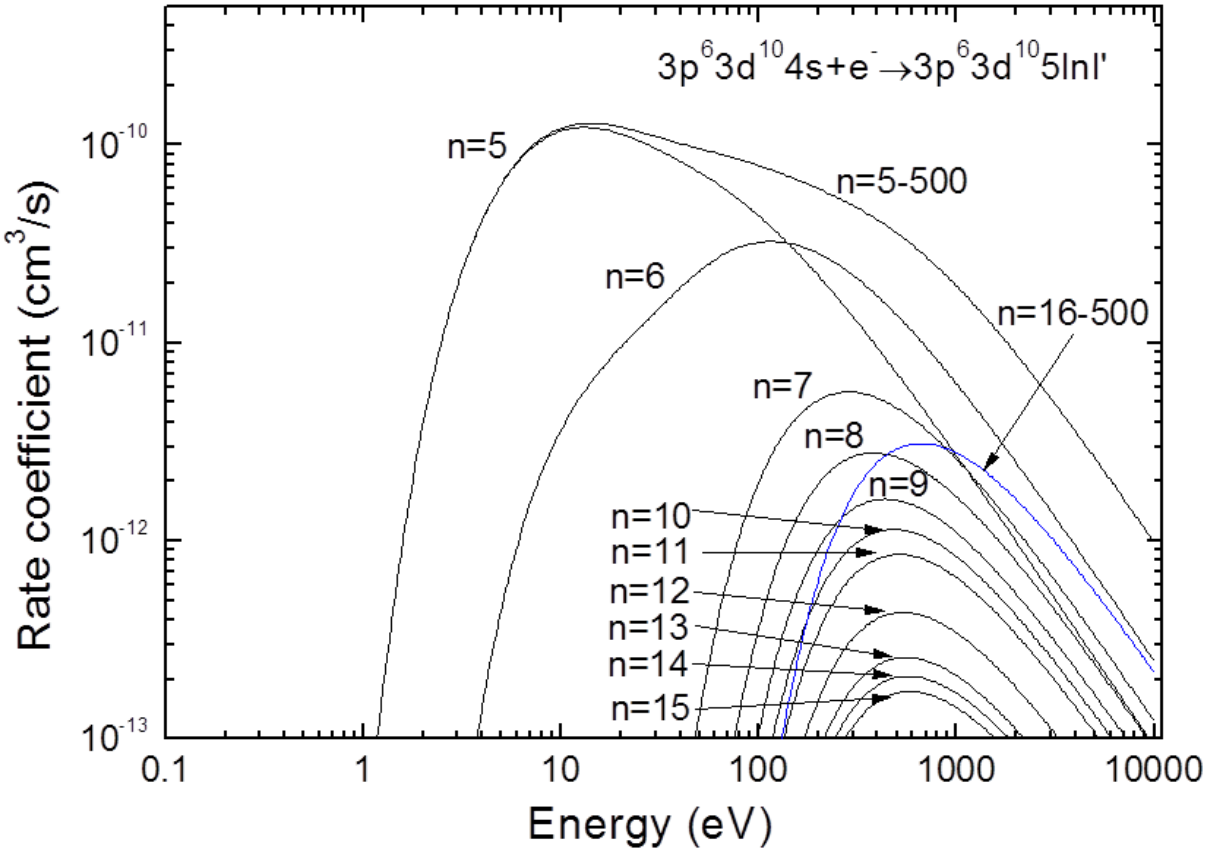
W^{45+} : 4s → 5l core excitation

$$3s^2 3p^6 3d^{10} 4s + \mathrm{e}^- \rightarrow 3d^{10} 5lnl' \rightarrow \left\{ \begin{array}{c} 3d^{10} 4l \\ 3d^{10} 5l (n \geq 10) \end{array} \right\} + \mathrm{e}^-$$

$$\rightarrow \left\{ \begin{array}{c} 3d^{10} 4l5l' \\ 3d^{10} 5l5l' \\ 3d^{10} 4lnl'' (n > 5) \end{array} \right\} + \omega$$



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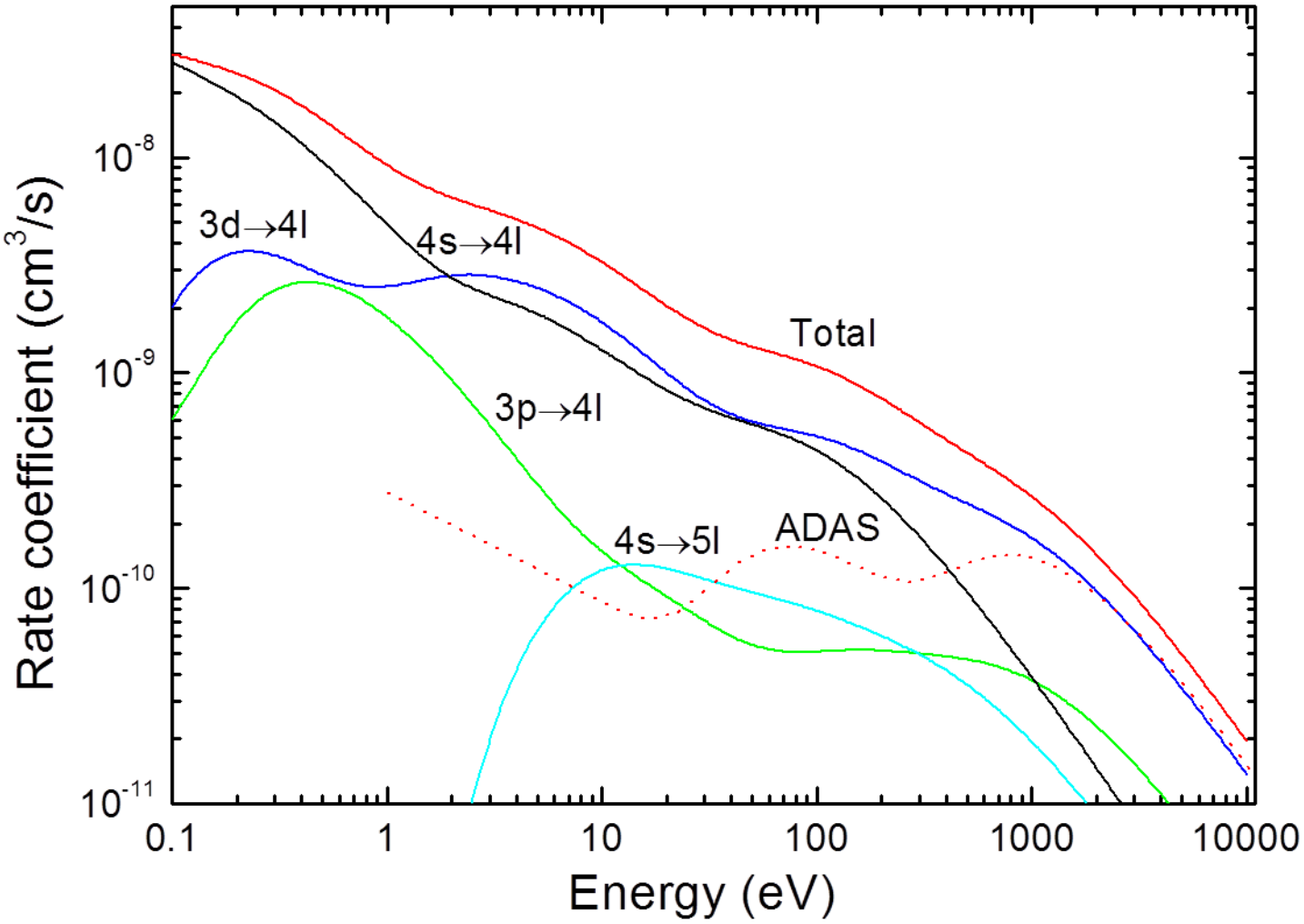
W^{45+} : Total Rate Coefficient



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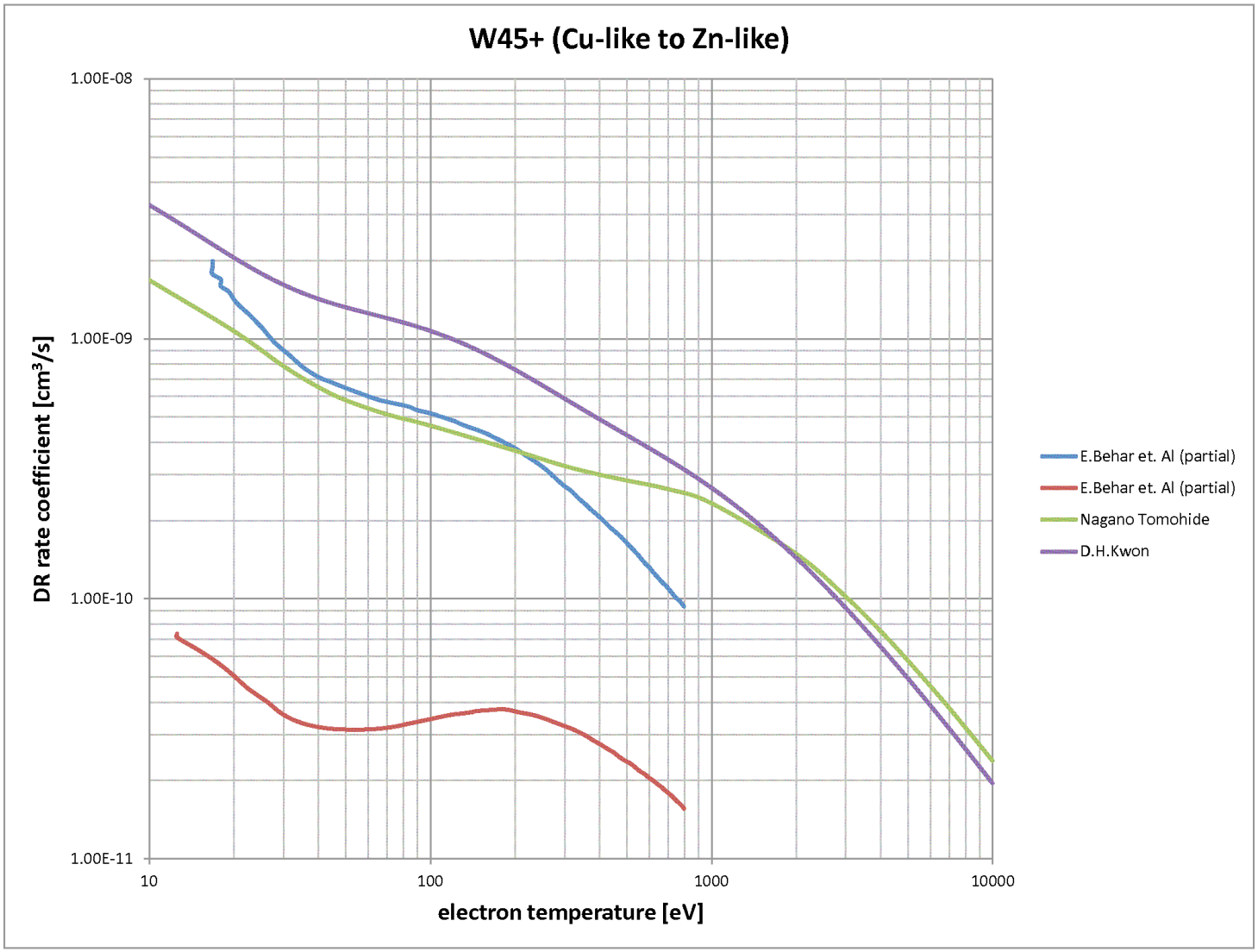
W^{45+} : Total Rate Coefficient

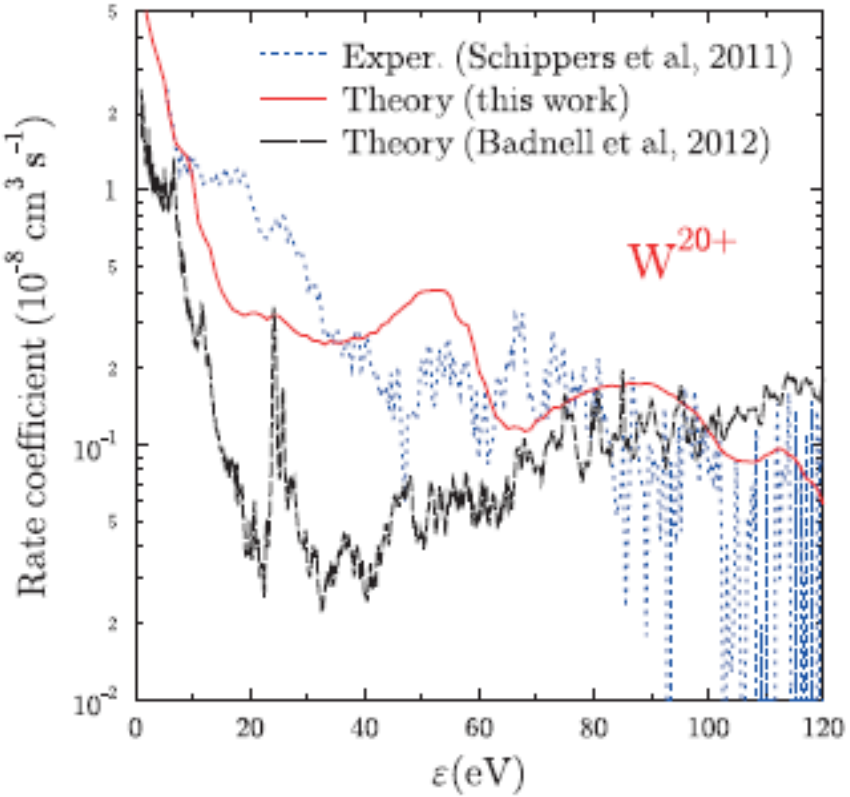


Resonance profile (dense states)

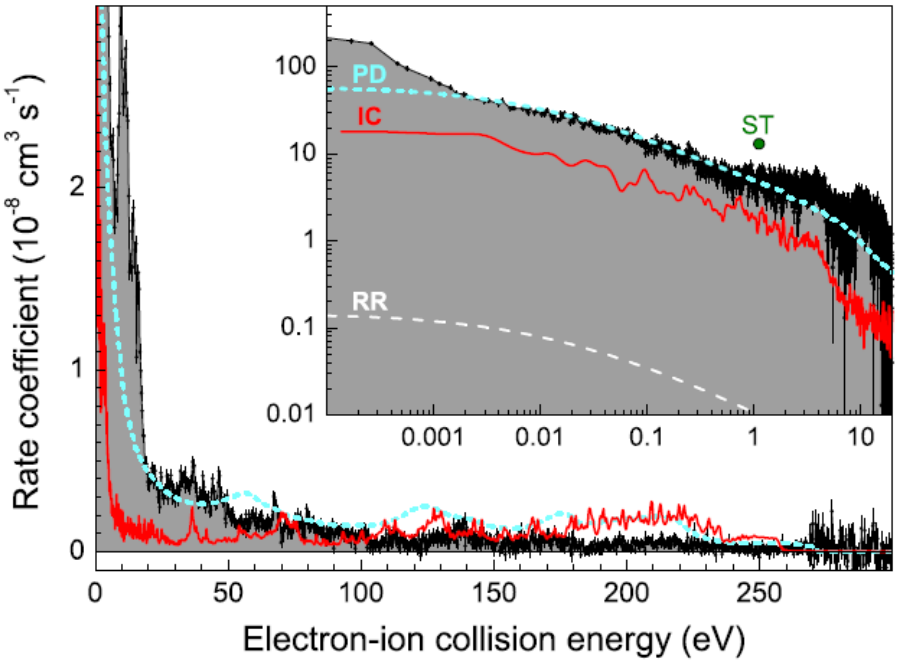
$$\bar{\sigma}_{ij}^{\mathrm{DC}} = \frac{\pi^2}{E_{ij}} \frac{g_j}{2g_i} A_{ji}^a \frac{\Gamma_j/2\pi}{(E-E_{ij})^2 + \Gamma_j{}^2/4} \cong \frac{\pi^2}{E_{ij}} \frac{g_j}{2g_i} A_{ji}^a \delta(E-E_{ij}).$$

$$\Gamma_j = \sum_k A_{jk}^a + \sum_f A_{jf}^r$$

$$\Gamma_j \rightarrow \Gamma_{sp} = 10 \text{ eV}$$



RECOMBINATION OF W^{18+} IONS WITH ELECTRONS: ...



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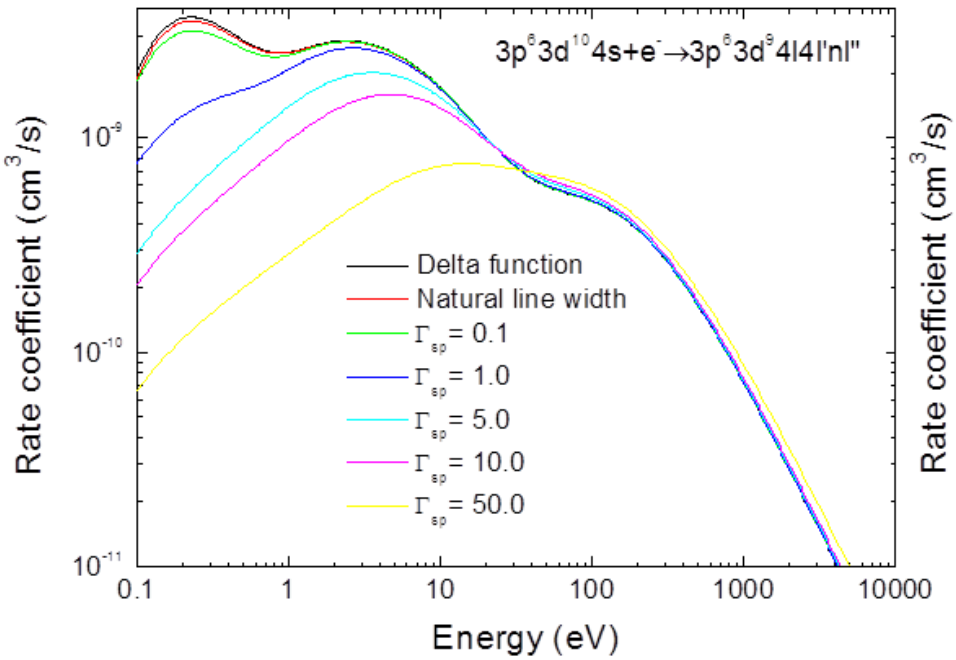
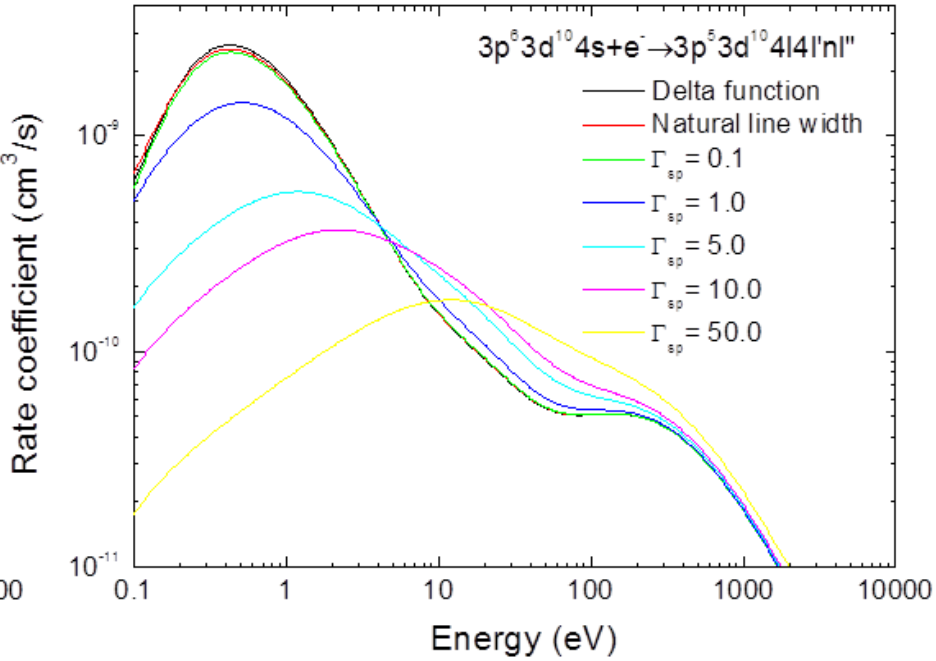
W^{45+}:Resonance profile (dense states)





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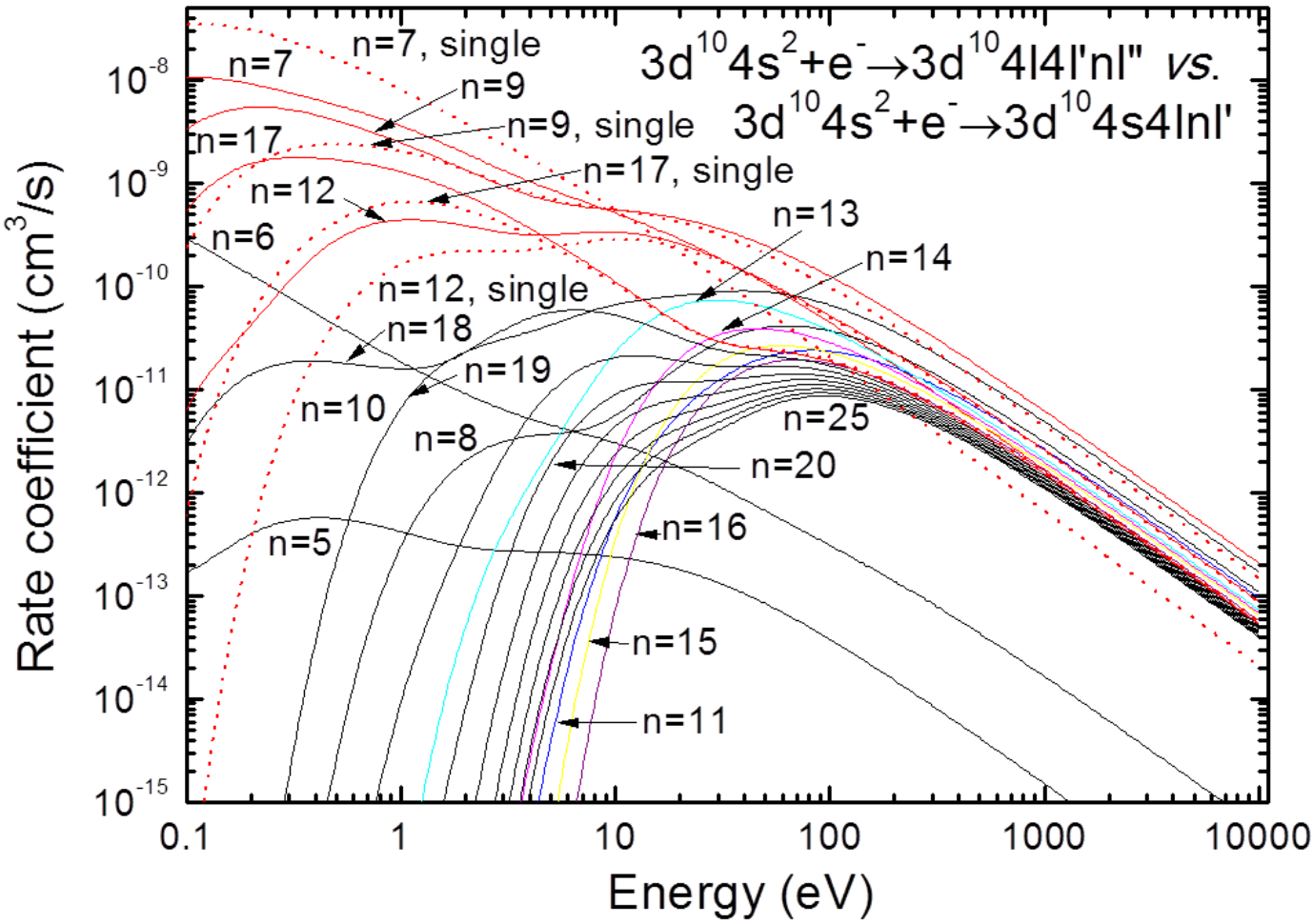
W^{44+} : 4s → 4l core excitation



DR computation challenges

- **Long running time for branching ratio calculation due to so many resonance levels or NRS+DAC consideration as more CM is considered or ion stage with complex configuration structure is treated.**

- **Parallel algorithms are needed for the AI or RD transition rate calculation.**

Summary & Outlook

- Our calculated energies for W^{45+} and W^{44+} are in excellent agreement with the recommended NIST data. (0.001 ~ 0.5 %)
- CM affects on DR rate coefficient significantly specially at low energies near threshold due to appearance of new resonances or resonance energy shift.
- Accurate DR rate coefficient of W^{45+} counting all contributable resonances was provided.
- Density effect , GCR and state resolved DR are our future works.