

**A consistent set of atomic data  
for various elements in a fusion  
reactor  
(passive emissions / radiative  
losses)**

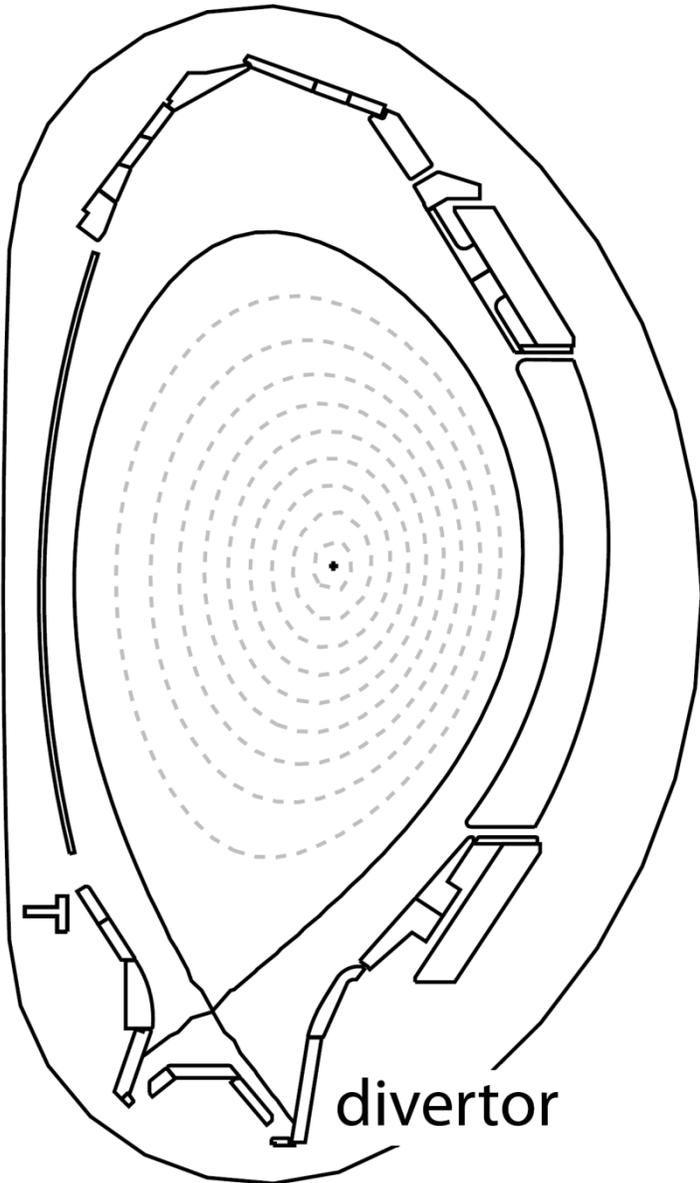
T. Pütterich

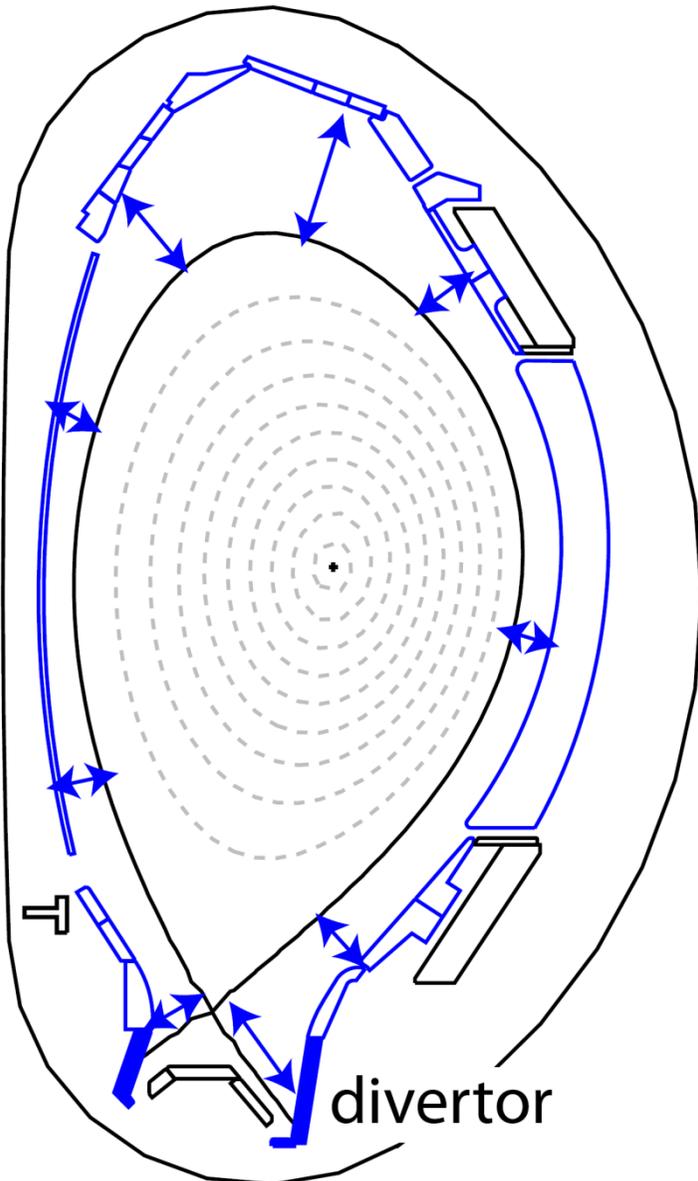
*MPI für Plasmaphysik, Boltzmannstr. 2, 85748 Garching, Germany*

**Thanks to:** M. O'Mullane, R. Dux, A. Foster

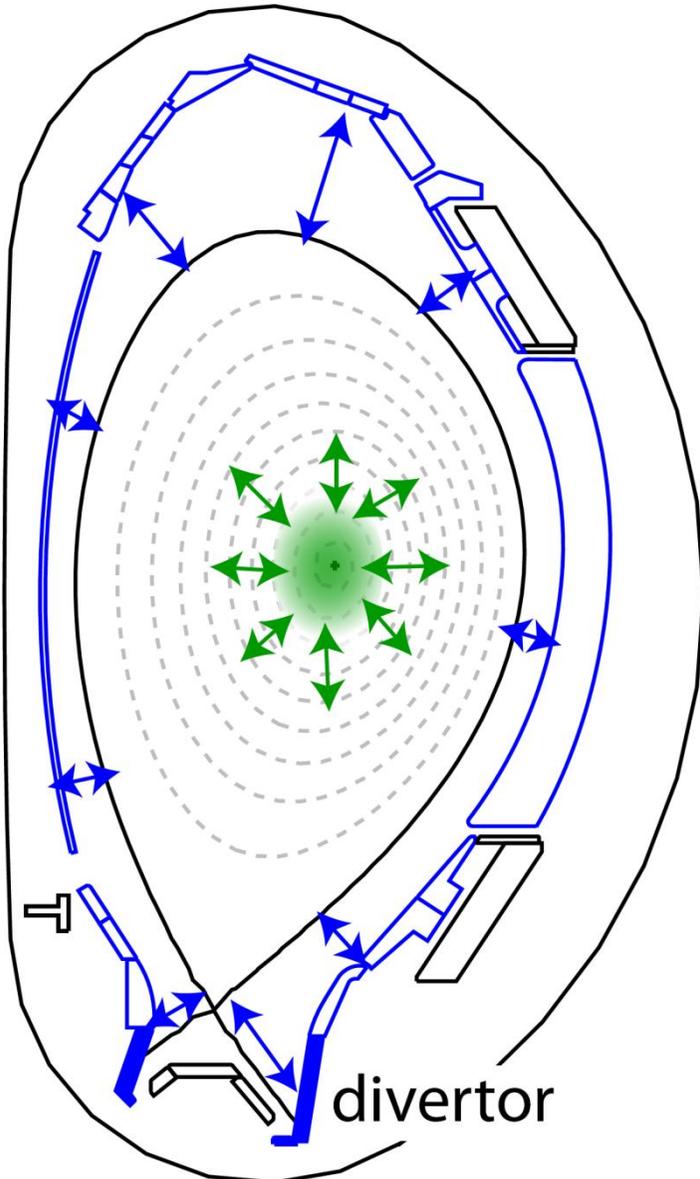
- Motivation
  - ⇒ Impurities in Fusion Plasmas
  - ⇒ Issues with existing data
  
- New Calculations using ADAS codes
  - ⇒ What quality has the new data?
  - ⇒ First tests with the new data
  
- First Applications of the new data
- Course of Action?

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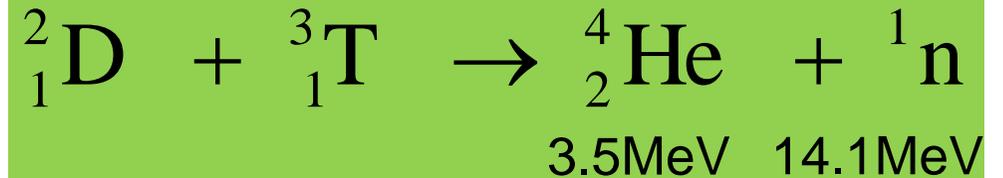


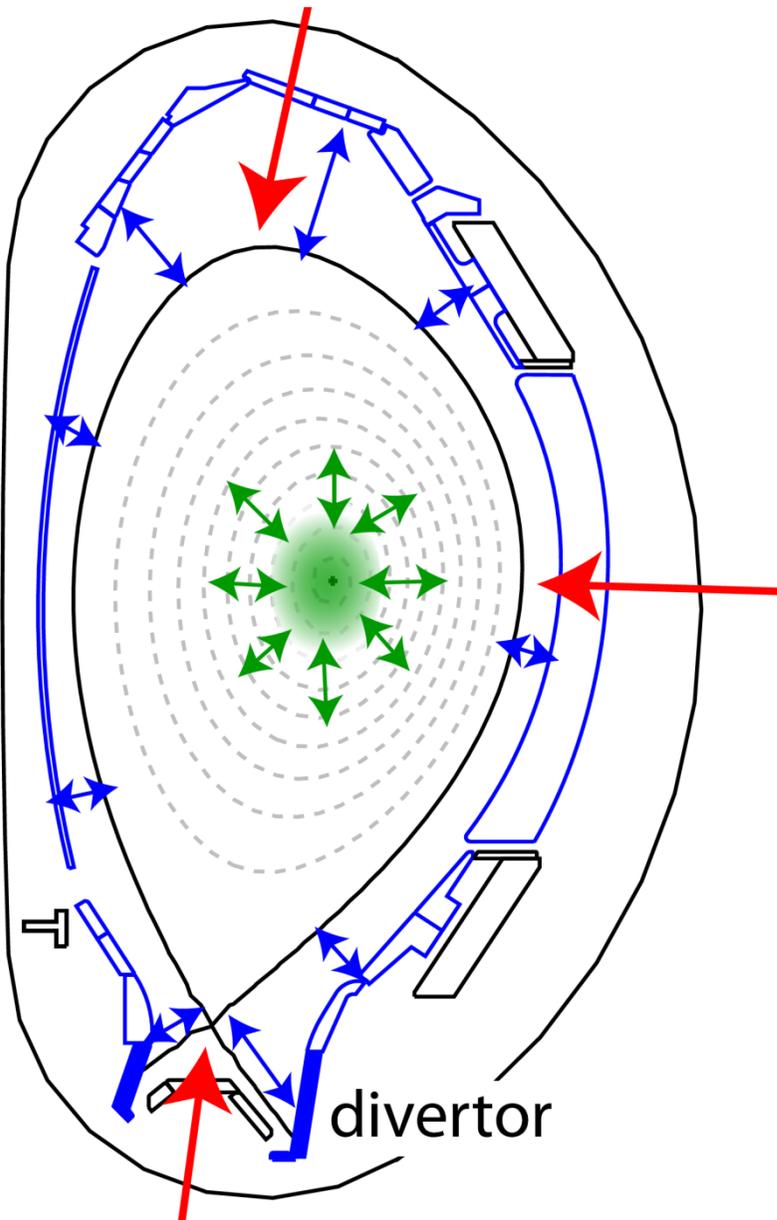
- Erosion from first wall  
(e.g. W, Be, C.....)



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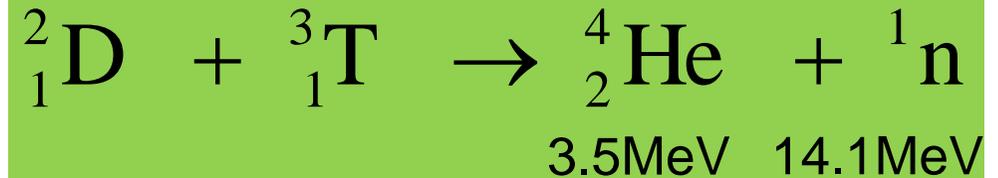
- Production of He in reactor core





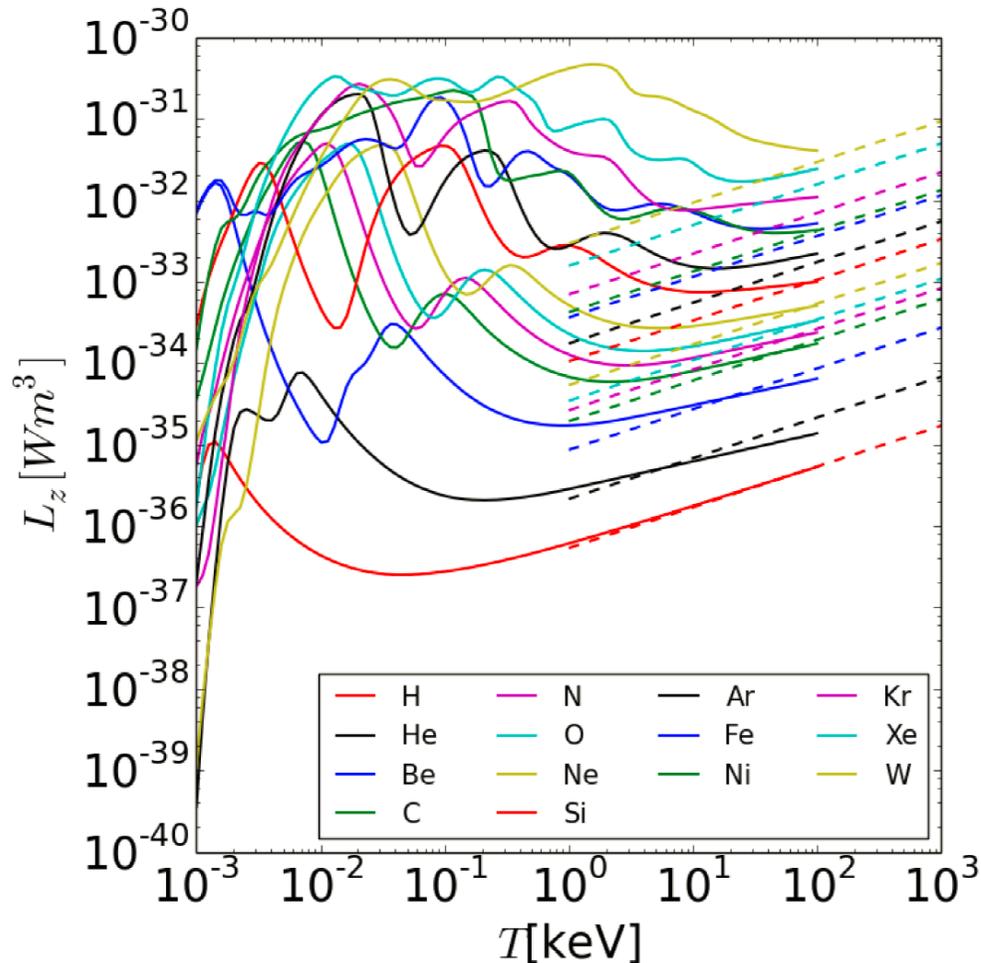
- Erosion from first wall  
(e.g. W, Be, C.....)

- Production of He in reactor core



- Intentionally injected impurities  
(e.g. N, Ne, Ar, Kr...)

## Cooling Factors (H. Lux, ADAS WS 2014)



### ■ Strategy:

Take what is available

⇒ Various calculation qualities

⇒ Systematic trends might be hidden

⇒ Not all data optimized for application in a reactor

- Motivation
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# What data was calculated I – What elements?

**PERIODIC TABLE**  
**Atomic Properties of the Elements**

**NIST**  
National Institute of Standards and Technology  
U.S. Department of Commerce

**Frequently used fundamental physical constants**

For the most accurate values of these and other constants, visit [physics.nist.gov/constants](http://physics.nist.gov/constants)  
1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of <sup>133</sup>Cs

speed of light in vacuum	<i>c</i>	299 792 458	m s <sup>-1</sup>	(exact)
Planck constant	<i>h</i>	6,626 07 × 10 <sup>-34</sup>	J s	( <i>h</i> = <i>h</i> /2π)
elementary charge	<i>e</i>	1.602 177 × 10 <sup>-19</sup>	C	
electron mass	<i>m<sub>e</sub></i>	9.109 38 × 10 <sup>-31</sup>	kg	
	<i>m<sub>e</sub>c<sup>2</sup></i>	0.510 999	MeV	
proton mass	<i>m<sub>p</sub></i>	1.672 622 × 10 <sup>-27</sup>	kg	
fine-structure constant	<i>α</i>	1/137.035 999		
Rydberg constant	<i>R<sub>∞</sub></i>	10 973 731.569	m <sup>-1</sup>	
	<i>R<sub>∞</sub>c</i>	3.289 841 960 × 10 <sup>15</sup>	Hz	
	<i>R<sub>∞</sub>hc</i>	13.605 69	eV	
Boltzmann constant	<i>k</i>	1,380 6 × 10 <sup>-23</sup>	J K <sup>-1</sup>	

**Physical Measurement Laboratory** [www.nist.gov/pml](http://www.nist.gov/pml)

**Standard Reference Data** [www.nist.gov/srd](http://www.nist.gov/srd)

Period	Group 1 IA		Group 2 IIA		Groups IIIA to VIIIA										Group 18 VIIIA				
	1	2	3	4	5	6	7	8	9	10	11	12	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18	
1	<sup>1</sup> H Hydrogen 1.008 1s																		<sup>2</sup> He Helium 4.002602 1s <sup>2</sup>
2	<sup>3</sup> Li Lithium 6.94 1s <sup>2</sup> 2s <sup>1</sup>	<sup>4</sup> Be Beryllium 9.0121831 1s <sup>2</sup> 2s <sup>2</sup>											<sup>5</sup> B Boron 10.81 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>1</sup>	<sup>6</sup> C Carbon 12.011 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>2</sup>	<sup>7</sup> N Nitrogen 14.007 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>3</sup>	<sup>8</sup> O Oxygen 15.999 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>4</sup>	<sup>9</sup> F Fluorine 18.99840316 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>5</sup>	<sup>10</sup> Ne Neon 20.1797 1s <sup>2</sup> 2s <sup>2</sup> 2p <sup>6</sup>	
3	<sup>11</sup> Na Sodium 22.98976928 [Ne]3s <sup>1</sup>	<sup>12</sup> Mg Magnesium 24.305 [Ne]3s <sup>2</sup>											<sup>13</sup> Al Aluminum 26.9815385 [Ne]3s <sup>2</sup> 3p <sup>1</sup>	<sup>14</sup> Si Silicon 28.085 [Ne]3s <sup>2</sup> 3p <sup>2</sup>	<sup>15</sup> P Phosphorus 30.97376200 [Ne]3s <sup>2</sup> 3p <sup>3</sup>	<sup>16</sup> S Sulfur 32.06 [Ne]3s <sup>2</sup> 3p <sup>4</sup>	<sup>17</sup> Cl Chlorine 35.45 [Ne]3s <sup>2</sup> 3p <sup>5</sup>	<sup>18</sup> Ar Argon 39.948 [Ne]3s <sup>2</sup> 3p <sup>6</sup>	
4	<sup>19</sup> K Potassium 39.0983 [Ar]4s <sup>1</sup>	<sup>20</sup> Ca Calcium 40.078 [Ar]4s <sup>2</sup>	<sup>21</sup> Sc Scandium 44.955908 [Ar]3d <sup>1</sup> 4s <sup>2</sup>	<sup>22</sup> Ti Titanium 47.867 [Ar]3d <sup>2</sup> 4s <sup>2</sup>	<sup>23</sup> V Vanadium 50.9415 [Ar]3d <sup>3</sup> 4s <sup>2</sup>	<sup>24</sup> Cr Chromium 51.9961 [Ar]3d <sup>5</sup> 4s <sup>1</sup>	<sup>25</sup> Mn Manganese 54.938044 [Ar]3d <sup>5</sup> 4s <sup>2</sup>	<sup>26</sup> Fe Iron 55.845 [Ar]3d <sup>6</sup> 4s <sup>2</sup>	<sup>27</sup> Co Cobalt 58.933194 [Ar]3d <sup>7</sup> 4s <sup>2</sup>	<sup>28</sup> Ni Nickel 58.6934 [Ar]3d <sup>8</sup> 4s <sup>2</sup>	<sup>29</sup> Cu Copper 63.546 [Ar]3d <sup>10</sup> 4s <sup>1</sup>	<sup>30</sup> Zn Zinc 65.38 [Ar]3d <sup>10</sup> 4s <sup>2</sup>	<sup>31</sup> Ga Gallium 69.723 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>1</sup>	<sup>32</sup> Ge Germanium 72.630 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>2</sup>	<sup>33</sup> As Arsenic 74.921595 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>3</sup>	<sup>34</sup> Se Selenium 78.971 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>4</sup>	<sup>35</sup> Br Bromine 79.904 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>5</sup>	<sup>36</sup> Kr Krypton 83.798 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>6</sup>	
5	<sup>37</sup> Rb Rubidium 85.4678 [Kr]5s <sup>1</sup>	<sup>38</sup> Sr Strontium 87.62 [Kr]5s <sup>2</sup>	<sup>39</sup> Y Yttrium 88.90584 [Kr]4d <sup>1</sup> 5s <sup>2</sup>	<sup>40</sup> Zr Zirconium 91.224 [Kr]4d <sup>2</sup> 5s <sup>2</sup>	<sup>41</sup> Nb Niobium 92.90637 [Kr]4d <sup>4</sup> 5s <sup>1</sup>	<sup>42</sup> Mo Molybdenum 95.95 [Kr]4d <sup>5</sup> 5s <sup>1</sup>	<sup>43</sup> Tc Technetium (98) [Kr]4d <sup>5</sup> 5s <sup>2</sup>	<sup>44</sup> Ru Ruthenium 101.07 [Kr]4d <sup>7</sup> 5s <sup>1</sup>	<sup>45</sup> Rh Rhodium 102.90550 [Kr]4d <sup>8</sup> 5s <sup>1</sup>	<sup>46</sup> Pd Palladium 106.42 [Kr]4d <sup>10</sup>	<sup>47</sup> Ag Silver 107.8682 [Kr]4d <sup>10</sup> 5s <sup>1</sup>	<sup>48</sup> Cd Cadmium 112.414 [Kr]4d <sup>10</sup> 5s <sup>2</sup>	<sup>49</sup> In Indium 114.818 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>1</sup>	<sup>50</sup> Sn Tin 118.710 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>2</sup>	<sup>51</sup> Sb Antimony 121.760 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>3</sup>	<sup>52</sup> Te Tellurium 127.60 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>4</sup>	<sup>53</sup> I Iodine 126.90447 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>5</sup>	<sup>54</sup> Xe Xenon 131.293 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>6</sup>	
6	<sup>55</sup> Cs Cesium 132.9054520 [Xe]6s <sup>1</sup>	<sup>56</sup> Ba Barium 137.327 [Xe]6s <sup>2</sup>		<sup>72</sup> Hf Hafnium 178.49 [Xe]4f <sup>14</sup> 5d <sup>2</sup> 6s <sup>2</sup>	<sup>73</sup> Ta Tantalum 180.94788 [Xe]4f <sup>14</sup> 5d <sup>3</sup> 6s <sup>2</sup>	<sup>74</sup> W Tungsten 183.84 [Xe]4f <sup>14</sup> 5d <sup>4</sup> 6s <sup>2</sup>	<sup>75</sup> Re Rhenium 186.207 [Xe]4f <sup>14</sup> 5d <sup>5</sup> 6s <sup>2</sup>	<sup>76</sup> Os Osmium 190.23 [Xe]4f <sup>14</sup> 5d <sup>6</sup> 6s <sup>2</sup>	<sup>77</sup> Ir Iridium 192.217 [Xe]4f <sup>14</sup> 5d <sup>7</sup> 6s <sup>2</sup>	<sup>78</sup> Pt Platinum 195.084 [Xe]4f <sup>14</sup> 5d <sup>9</sup> 6s <sup>1</sup>	<sup>79</sup> Au Gold 196.966569 [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>1</sup>	<sup>80</sup> Hg Mercury 200.592 [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup>	<sup>81</sup> Tl Thallium 204.38 [Hg]6p <sup>1</sup>	<sup>82</sup> Pb Lead 207.2 [Hg]6p <sup>2</sup>	<sup>83</sup> Bi Bismuth 208.98040 [Hg]6p <sup>3</sup>	<sup>84</sup> Po Polonium (209) [Hg]6p <sup>4</sup>	<sup>85</sup> At Astatine (210) [Hg]6p <sup>5</sup>	<sup>86</sup> Rn Radon (222) [Hg]6p <sup>6</sup>	
7	<sup>87</sup> Fr Francium (223) [Rn]7s <sup>1</sup>	<sup>88</sup> Ra Radium (226) [Rn]7s <sup>2</sup>		<sup>104</sup> Rf Rutherfordium (261) [Rn]5f <sup>14</sup> 6d <sup>2</sup> 7s <sup>2</sup>	<sup>105</sup> Db Dubnium (268) [Rn]5f <sup>14</sup> 6d <sup>3</sup> 7s <sup>2</sup>	<sup>106</sup> Sg Seaborgium (271) [Rn]5f <sup>14</sup> 6d <sup>4</sup> 7s <sup>2</sup>	<sup>107</sup> Bh Bohrium (272) [Rn]5f <sup>14</sup> 6d <sup>5</sup> 7s <sup>2</sup>	<sup>108</sup> Hs Hassium (270) [Rn]5f <sup>14</sup> 6d <sup>6</sup> 7s <sup>2</sup>	<sup>109</sup> Mt Meitnerium (276) [Rn]5f <sup>14</sup> 6d <sup>7</sup> 7s <sup>2</sup>	<sup>110</sup> Ds Darmstadtium (281) [Rn]5f <sup>14</sup> 6d <sup>8</sup> 7s <sup>2</sup>	<sup>111</sup> Rg Roentgenium (280) [Rn]5f <sup>14</sup> 6d <sup>9</sup> 7s <sup>2</sup>	<sup>112</sup> Cn Copernicium (285) [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup>	<sup>113</sup> Uut Ununtrium (284) [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>1</sup>	<sup>114</sup> Fl Flerovium (289) [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>2</sup>	<sup>115</sup> Uup Ununpentium (288) [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>3</sup>	<sup>116</sup> Lv Livermorium (293) [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>4</sup>	<sup>117</sup> Uus Ununseptium (294) [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>5</sup>	<sup>118</sup> Uuo Ununoctium (294) [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>6</sup>	
			<b>Lanthanides</b>	<sup>57</sup> La Lanthanum 138.90547 [Xe]5d <sup>1</sup> 6s <sup>2</sup>	<sup>58</sup> Ce Cerium 140.116 [Xe]4f <sup>1</sup> 5d <sup>1</sup> 6s <sup>2</sup>	<sup>59</sup> Pr Praseodymium 140.907 [Xe]4f <sup>3</sup> 6s <sup>2</sup>	<sup>60</sup> Nd Neodymium 144.242 [Xe]4f <sup>4</sup> 6s <sup>2</sup>	<sup>61</sup> Pm Promethium (145) [Xe]4f <sup>5</sup> 6s <sup>2</sup>	<sup>62</sup> Sm Samarium 150.36 [Xe]4f <sup>6</sup> 6s <sup>2</sup>	<sup>63</sup> Eu Europium 151.964 [Xe]4f <sup>7</sup> 6s <sup>2</sup>	<sup>64</sup> Gd Gadolinium 157.25 [Xe]4f <sup>7</sup> 5d <sup>1</sup> 6s <sup>2</sup>	<sup>65</sup> Tb Terbium 158.92535 [Xe]4f <sup>9</sup> 6s <sup>2</sup>	<sup>66</sup> Dy Dysprosium 162.500 [Xe]4f <sup>10</sup> 6s <sup>2</sup>	<sup>67</sup> Ho Holmium 164.93033 [Xe]4f <sup>11</sup> 6s <sup>2</sup>	<sup>68</sup> Er Erbium 167.259 [Xe]4f <sup>12</sup> 6s <sup>2</sup>	<sup>69</sup> Tm Thulium 168.93422 [Xe]4f <sup>13</sup> 6s <sup>2</sup>	<sup>70</sup> Yb Ytterbium 173.054 [Xe]4f <sup>14</sup> 6s <sup>2</sup>	<sup>71</sup> Lu Lutetium 174.9668 [Xe]4f <sup>14</sup> 5d <sup>1</sup> 6s <sup>2</sup>	
			<b>Actinides</b>	<sup>89</sup> Ac Actinium (227) [Rn]6d <sup>1</sup> 7s <sup>2</sup>	<sup>90</sup> Th Thorium 232.0377 [Rn]6s <sup>2</sup> 7s <sup>2</sup>	<sup>91</sup> Pa Protactinium 231.03588 [Rn]5f <sup>2</sup> 6d <sup>1</sup> 7s <sup>2</sup>	<sup>92</sup> U Uranium 238.02891 [Rn]5f <sup>3</sup> 6d <sup>1</sup> 7s <sup>2</sup>	<sup>93</sup> Np Neptunium (237) [Rn]5f <sup>4</sup> 6d <sup>1</sup> 7s <sup>2</sup>	<sup>94</sup> Pu Plutonium (244) [Rn]5f <sup>6</sup> 7s <sup>2</sup>	<sup>95</sup> Am Americium (243) [Rn]5f <sup>7</sup> 7s <sup>2</sup>	<sup>96</sup> Cm Curium (247) [Rn]5f <sup>8</sup> 7s <sup>2</sup>	<sup>97</sup> Bk Berkelium (247) [Rn]5f <sup>9</sup> 7s <sup>2</sup>	<sup>98</sup> Cf Californium (251) [Rn]5f <sup>10</sup> 7s <sup>2</sup>	<sup>99</sup> Es Einsteinium (252) [Rn]5f <sup>11</sup> 7s <sup>2</sup>	<sup>100</sup> Fm Fermium (257) [Rn]5f <sup>12</sup> 7s <sup>2</sup>	<sup>101</sup> Md Mendelevium (258) [Rn]5f <sup>13</sup> 7s <sup>2</sup>	<sup>102</sup> No Nobelium (259) [Rn]5f <sup>14</sup> 7s <sup>2</sup>	<sup>103</sup> Lr Lawrencium (262) [Rn]5f <sup>14</sup> 7s <sup>2</sup> 7p <sup>1</sup>	

**Legend:**  
■ Solids  
■ Liquids  
■ Gases  
■ Artificially Prepared

**Example Element: Cerium (Ce)**  
 Atomic Number: 58  
 Ground-state Level: <sup>4</sup>G<sub>4</sub>  
 Symbol: Ce  
 Name: Cerium  
 Standard Atomic Weight: 140.116  
 Configuration: [Xe]4f<sup>1</sup>5d<sup>1</sup>6s<sup>2</sup>  
 Ionization Energy (eV): 5.5386

<sup>1</sup>Based upon <sup>12</sup>C. ( ) indicates the mass number of the longest-lived isotope.

\*IUPAC conventional atomic weights; standard atomic weights for these elements are expressed in intervals; see [iupac.org](http://iupac.org) for an explanation and values.

For a description of the data, visit [physics.nist.gov/data](http://physics.nist.gov/data)  
NIST SP 966 (September 2014)

Baseline

elevated

high quality



New data has:

Excitation+population model: **baseline**

Recombination data: **baseline**

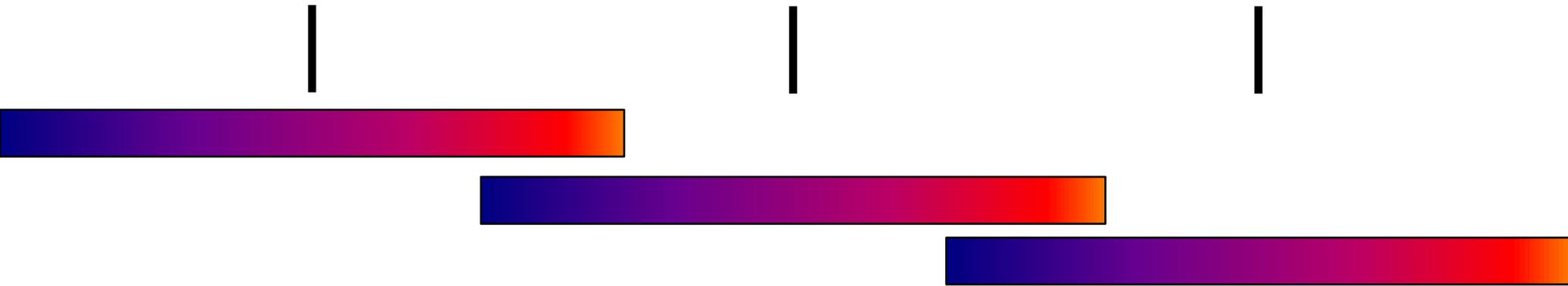
Ionisation data: **elevated**

But: **baseline** is not equal to **baseline** !

Baseline

elevated

high quality



New data has:

Excitation+population model: **baseline**

Recombination data: **baseline**

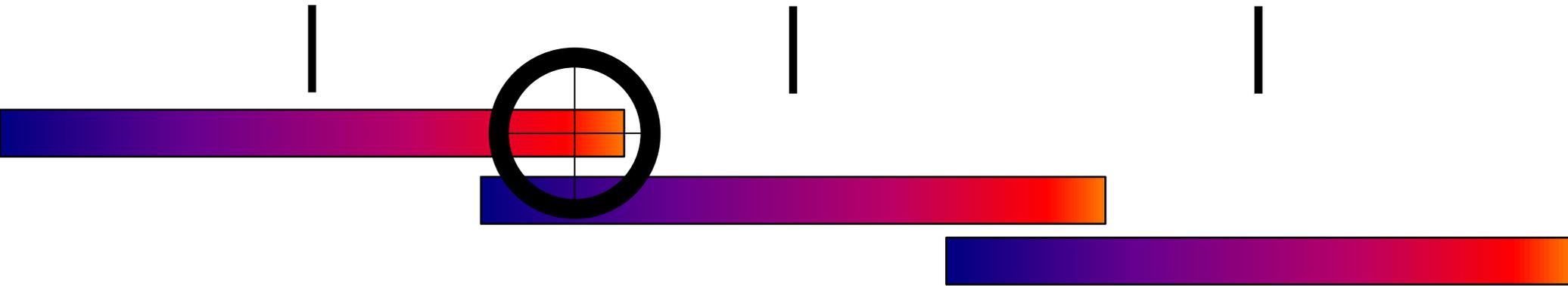
Ionisation data: **elevated**

But: **baseline** is not equal to **baseline** !

Baseline

elevated

high quality



New data has:

Excitation+population model: **baseline** (Cowan + p-w Born + basic CR)

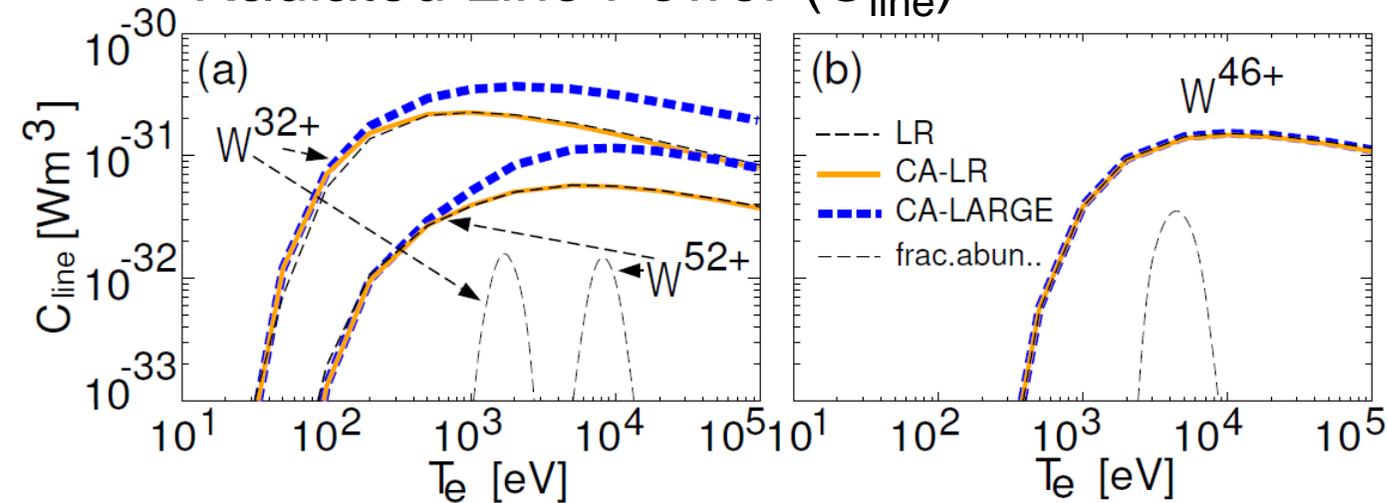
Recombination data: **baseline** (ADAS407/408 type A, parametric forms)

Ionisation data: **elevated** (CADW, but in zero-density approx.)

But: **baseline** is not equal to **baseline** !

- Try to maximise number of configs
- Include the ,important‘ configs
- Strategy:
  - ⇒ Use configurations as identified for W  
(PhD Pütterich, PPCF 2008, NF 2010)
  - ⇒ Level resolved calculations for
    - ⇒ Predicting spectra
    - ⇒ Running adas407/408
  - ⇒ Configuration averaged calculations for cooling factors

## Radiated Line Power ( $C_{\text{line}}$ )

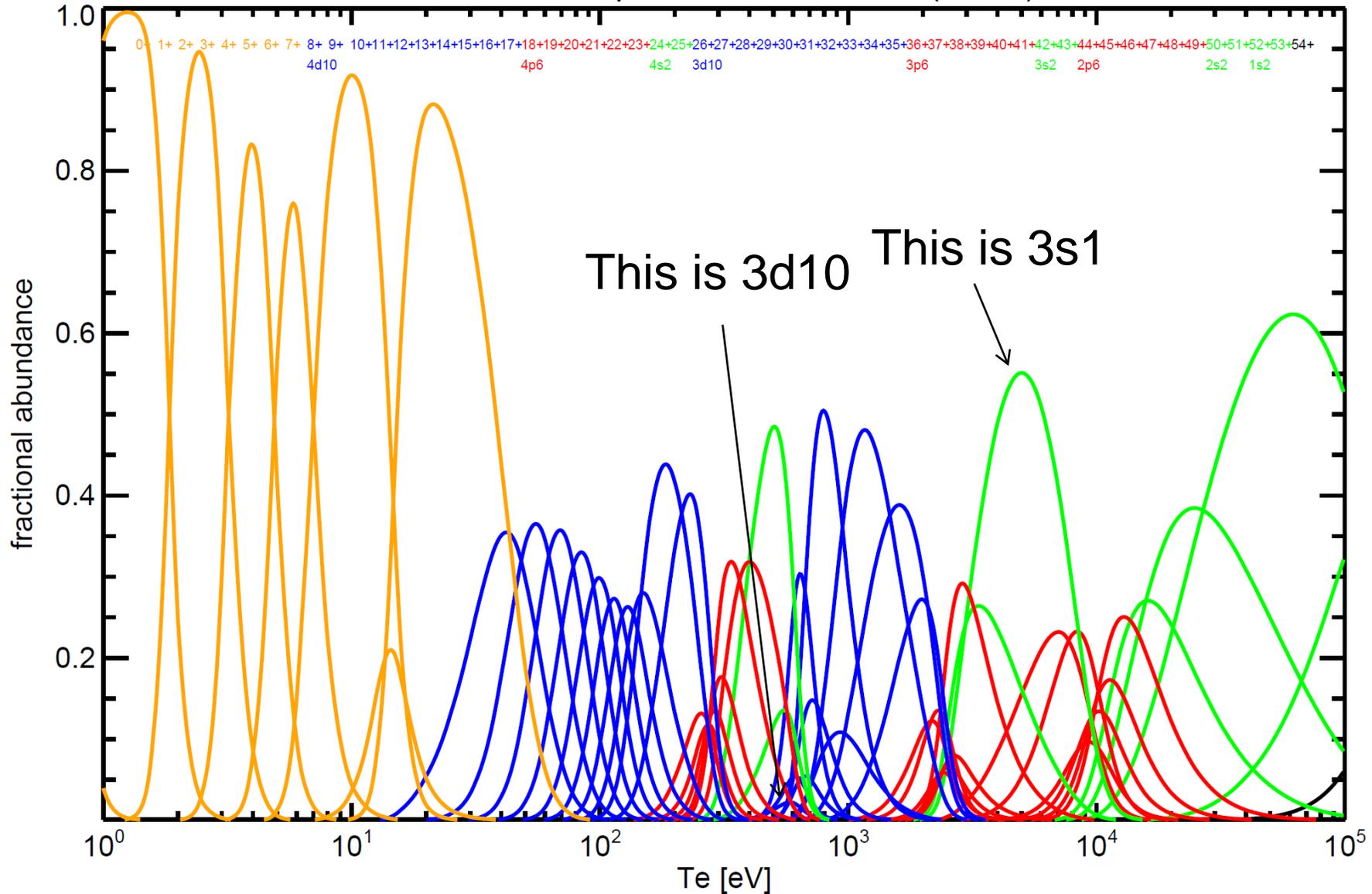


- Level-resolved LR
- Config.-average CA
  - ⇒ LR set of configs
  - ⇒ Large set of configs ~#30

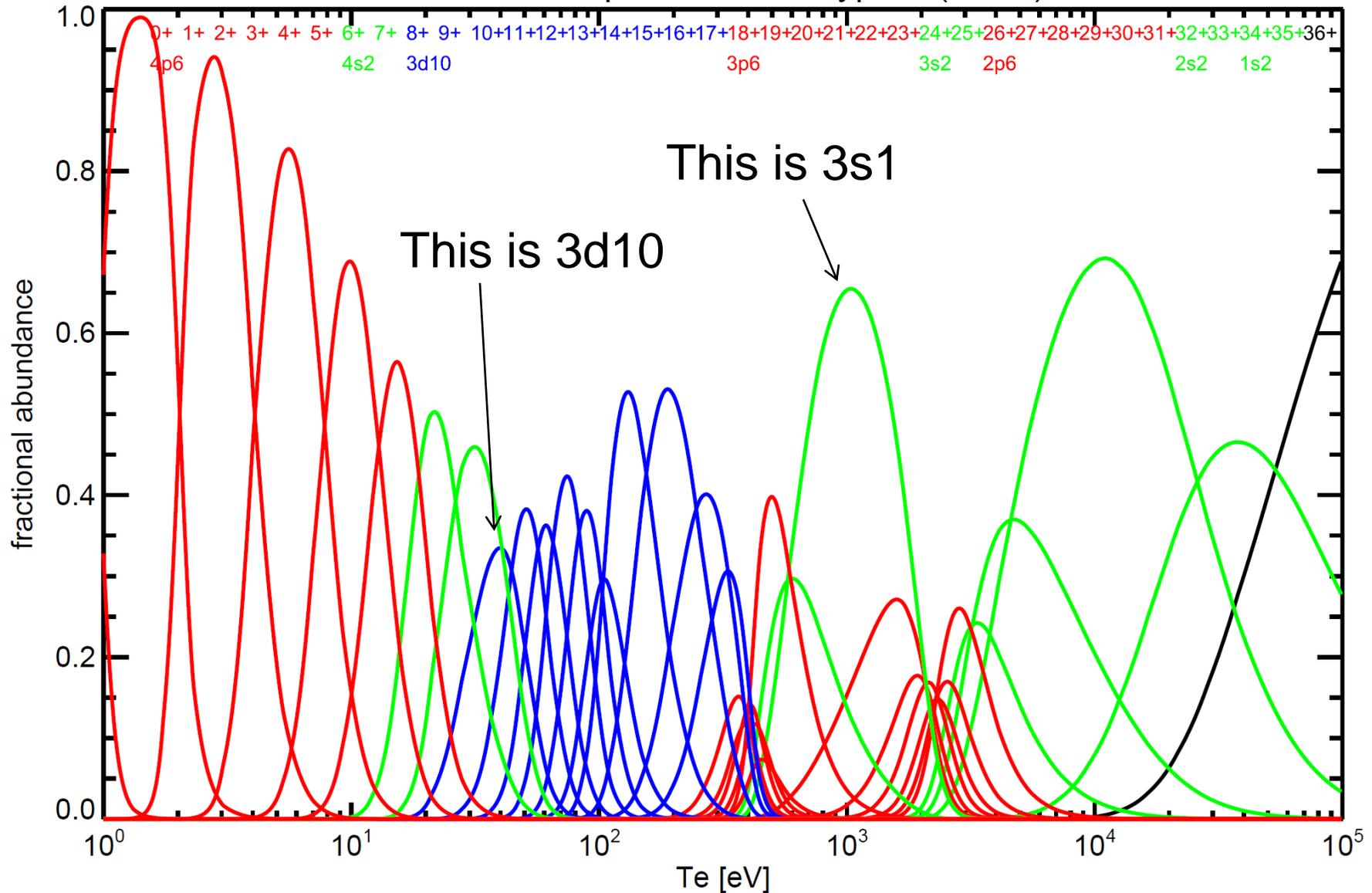
Pütterich NF 2010

	LR/CA-LR	CA-LARGE
Mo-like $W^{32+}$	$4d^6, 4d^5 4f \rightarrow 4d^5 5f,$ $4p^5 4d^7,$ $\Sigma = 7$	$4d^6, 4d^5 4f \rightarrow 4d^5 5g,$ $4p^5 4d^7 \rightarrow 4p^5 4d^6 5g,$ $4s 4p^6 4d^7 \rightarrow 4s 4p^6 4d^6 5g,$ $3d^9 4s^2 4p^6 4d^7 \rightarrow 3d^9 4s^2 4p^6 4d^6 5g; \Sigma = 28$

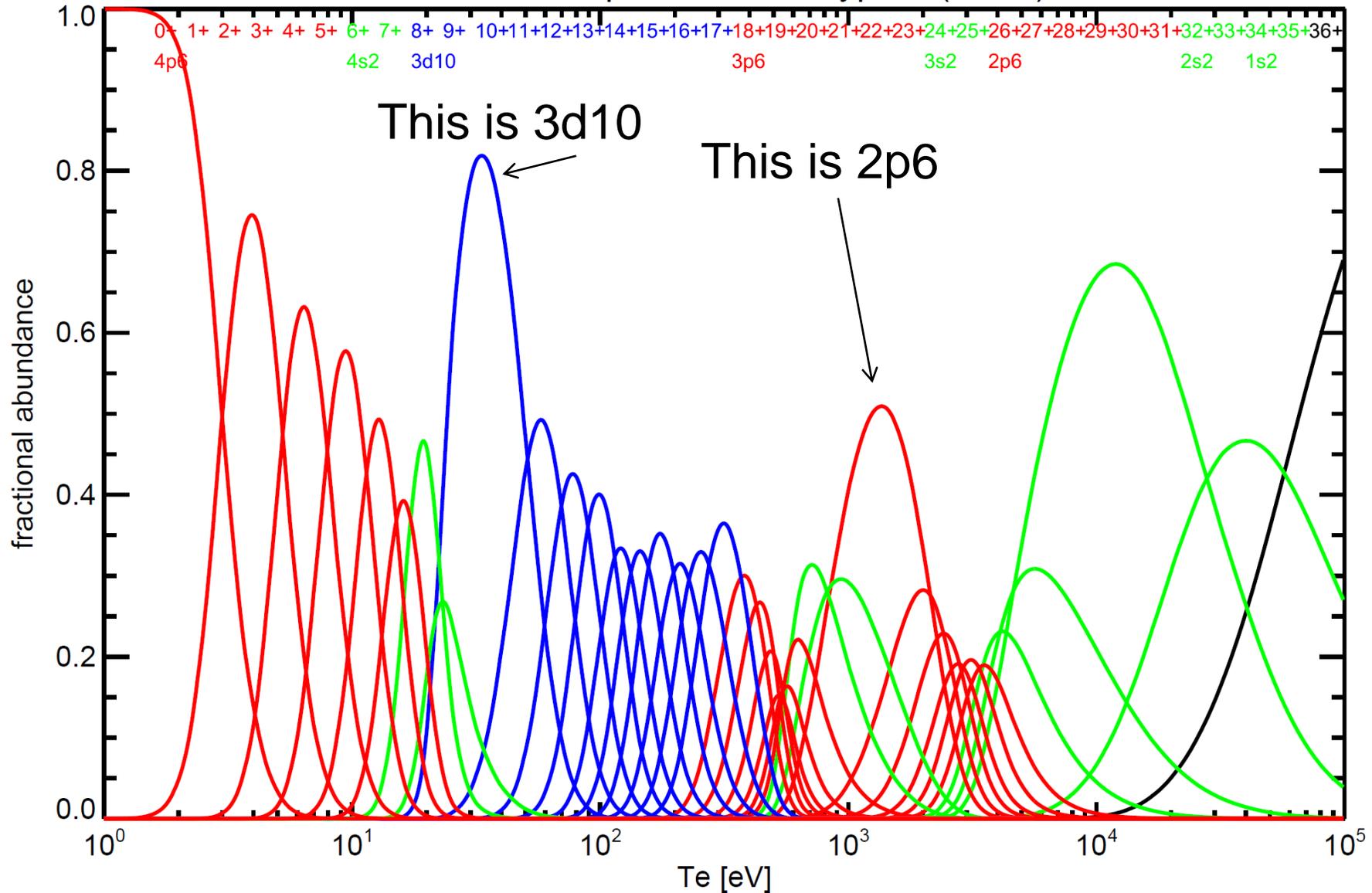
## Ionization Equilibrium of Xenon (Z=54)



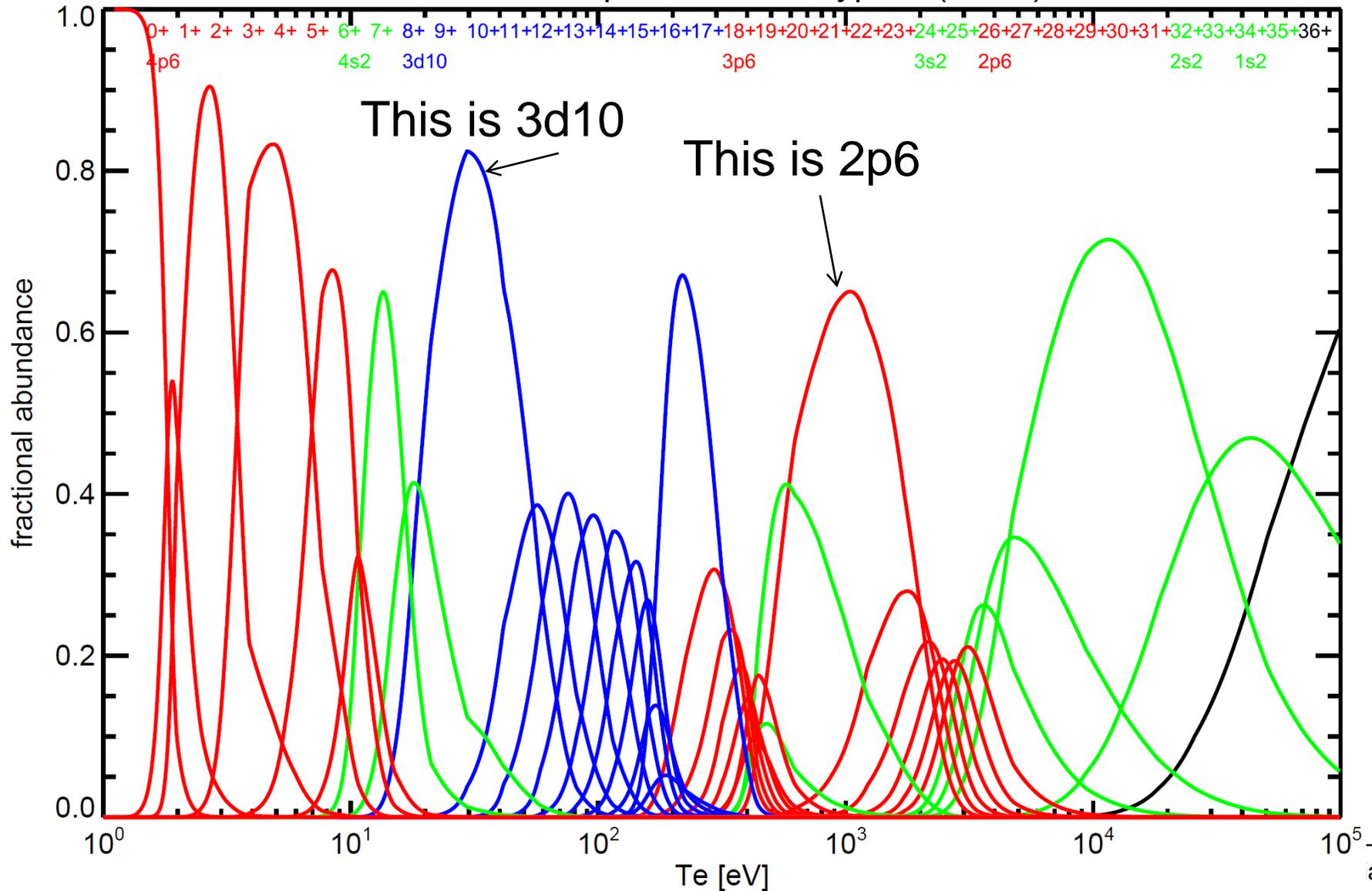
## Ionization Equilibrium of Krypton (Z=36)



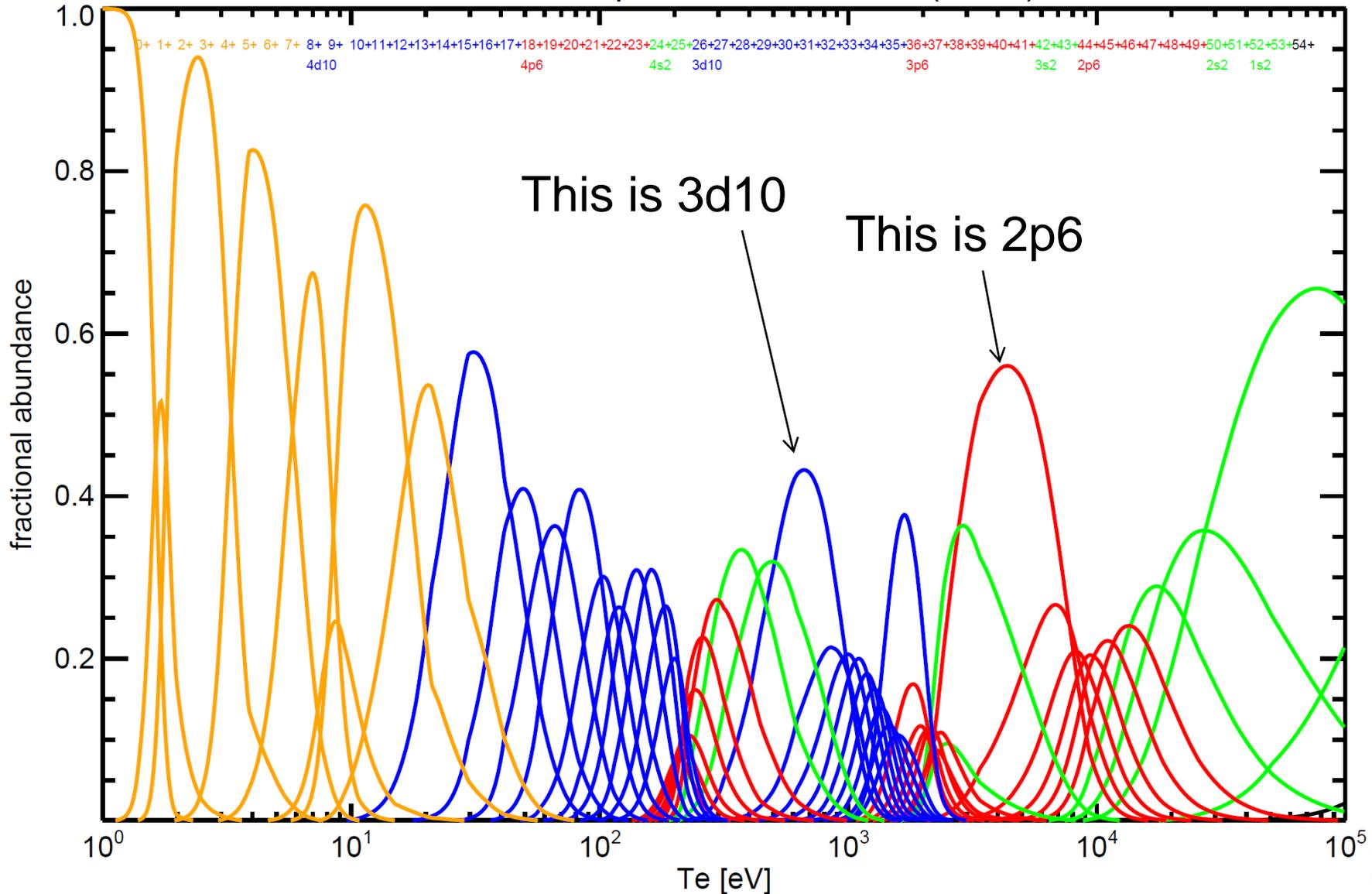
Ionization Equilibrium of Krypton (Z=36)

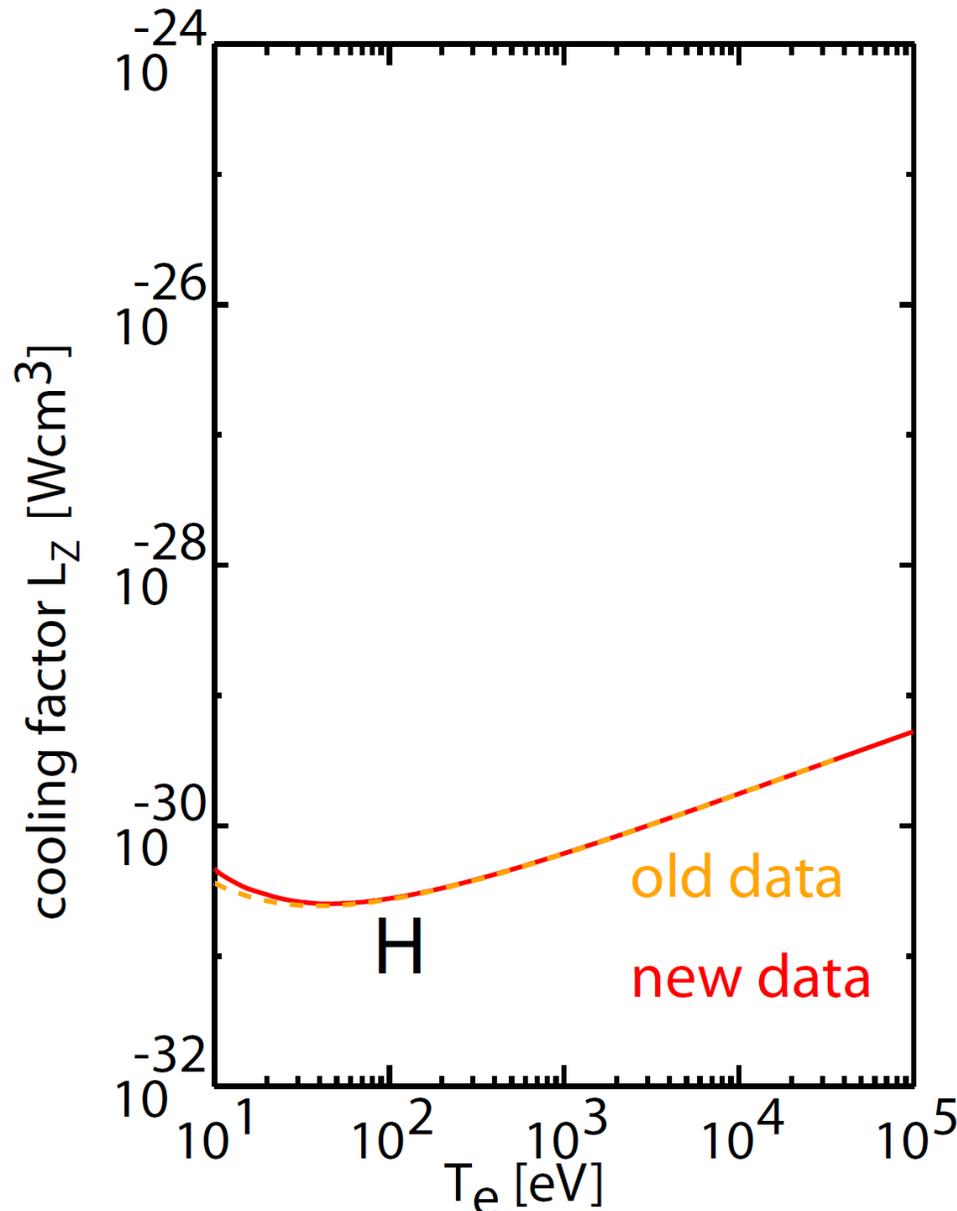


## Ionization Equilibrium of Krypton (Z=36)

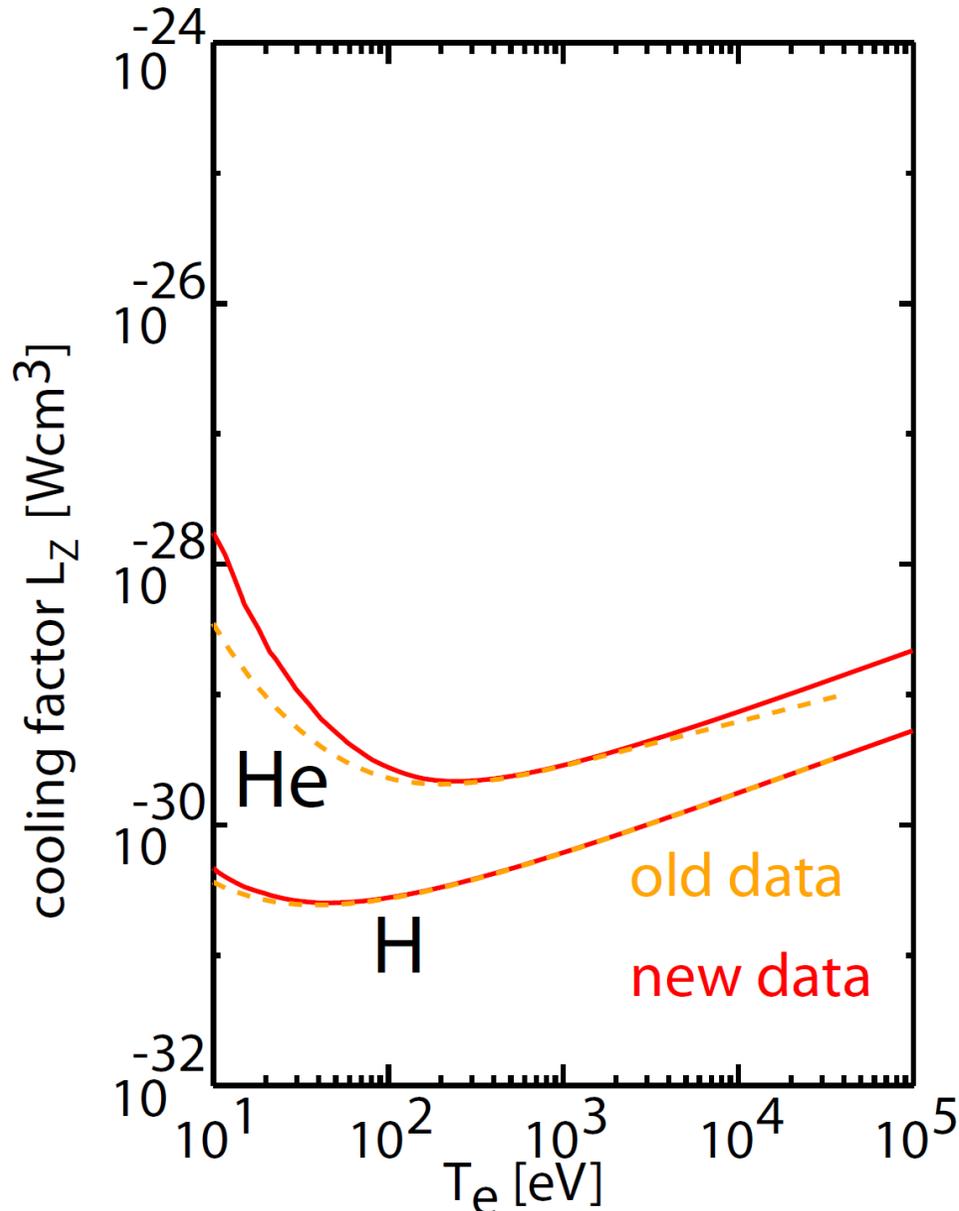


## Ionization Equilibrium of Xenon (Z=54)

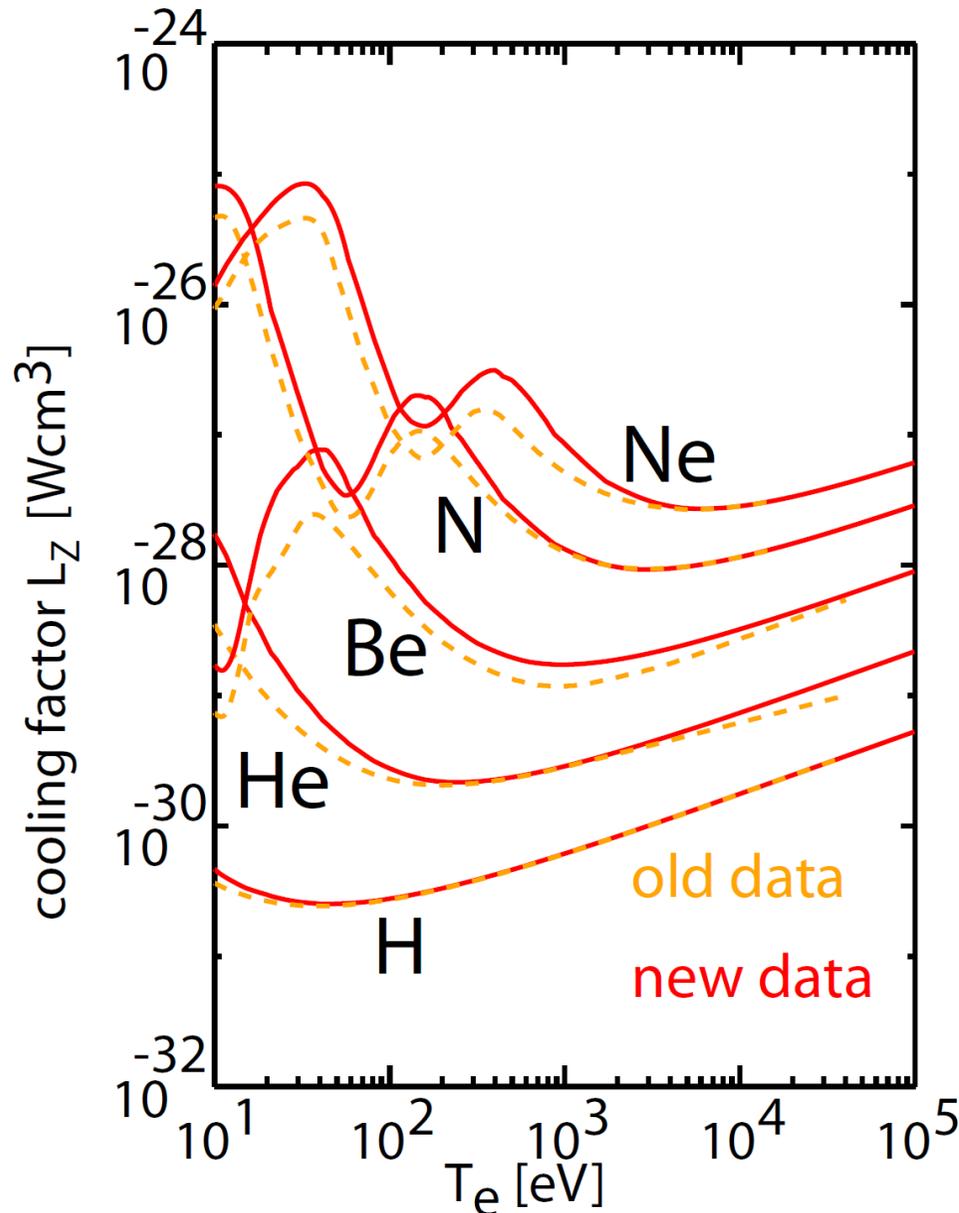




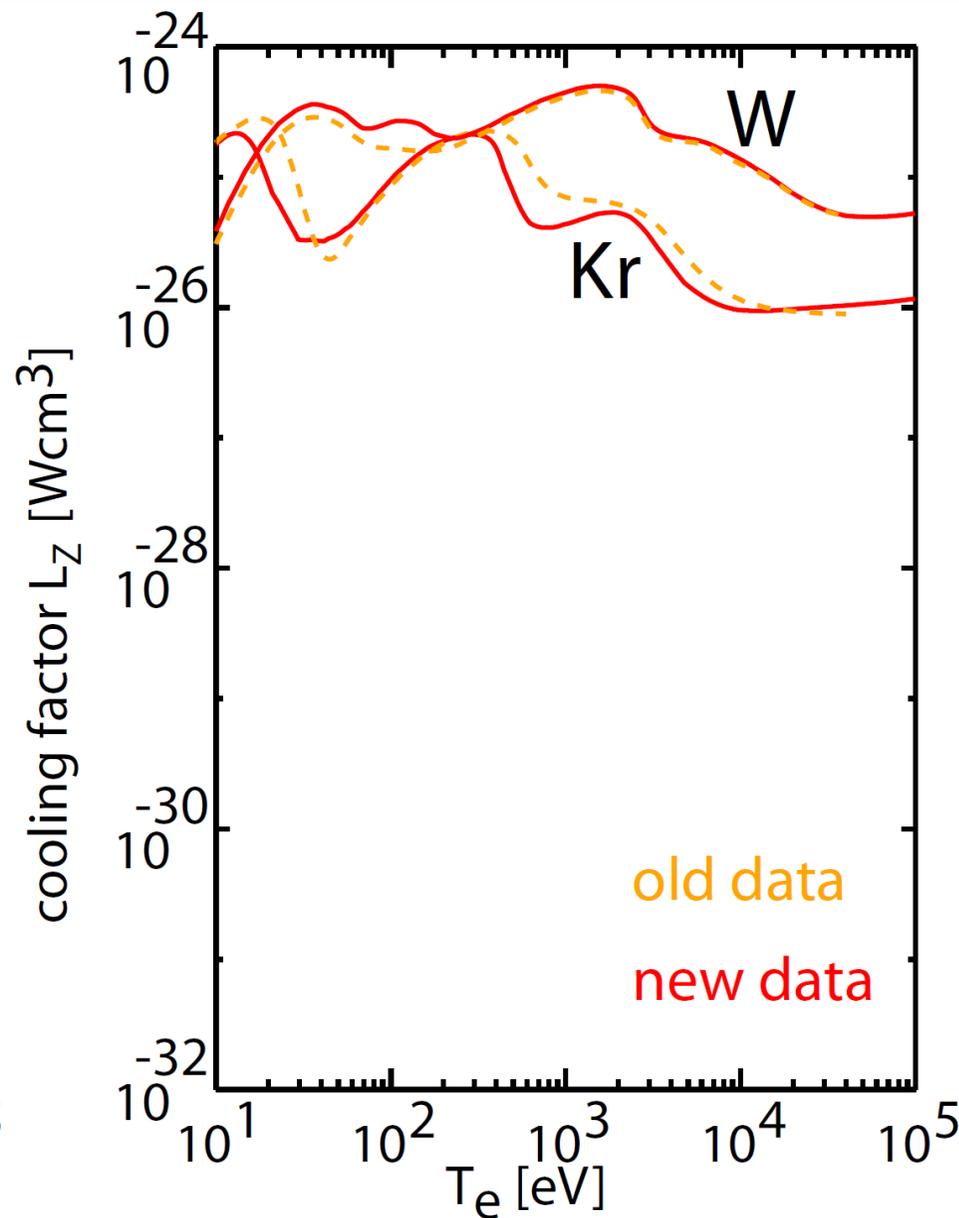
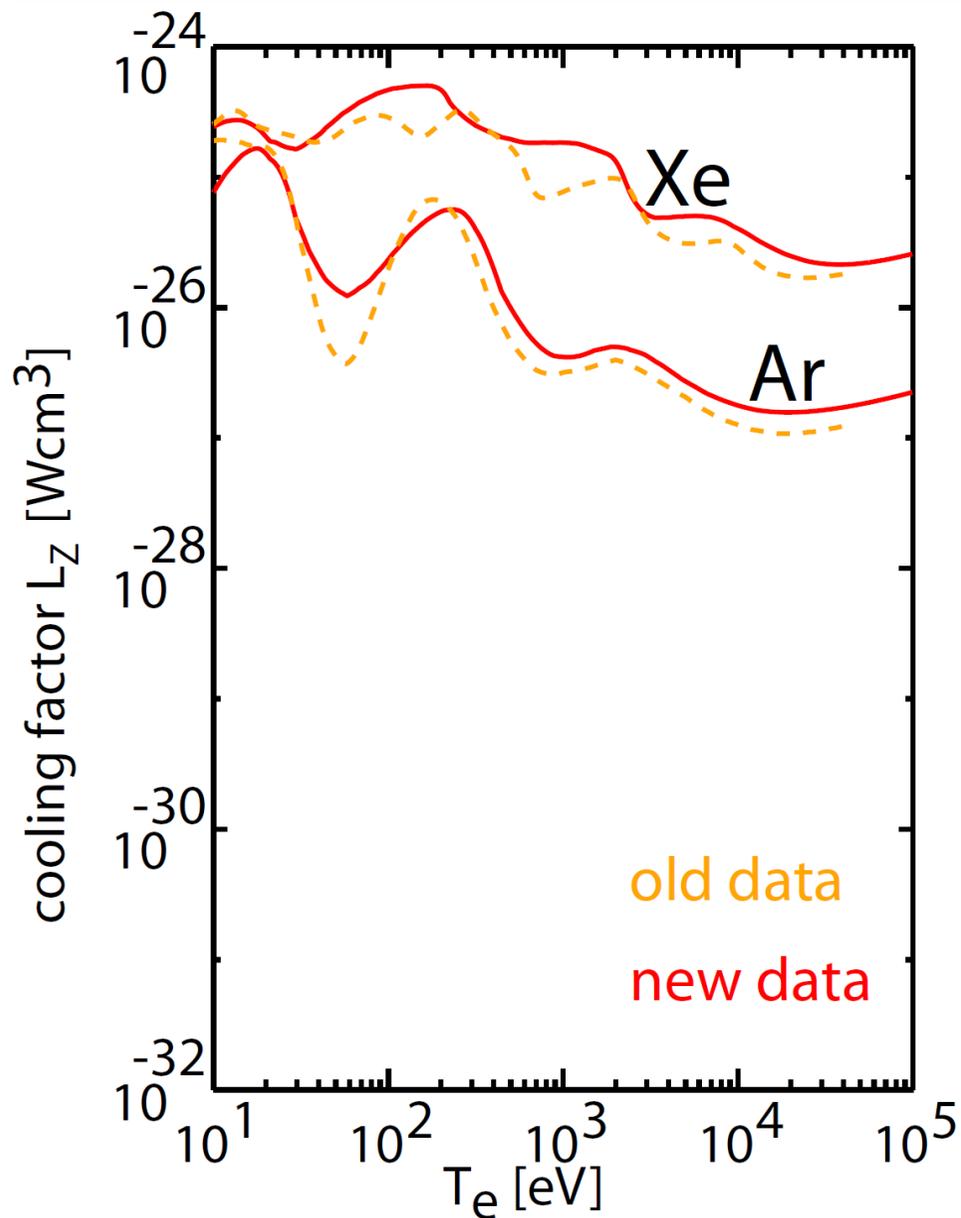
- Old data up to  $\sim 40\text{keV}$  available
- Continuum Radiation in agreement slight deviations for line radiation
- For low-Z, old data may be better for line rad. (or not?)



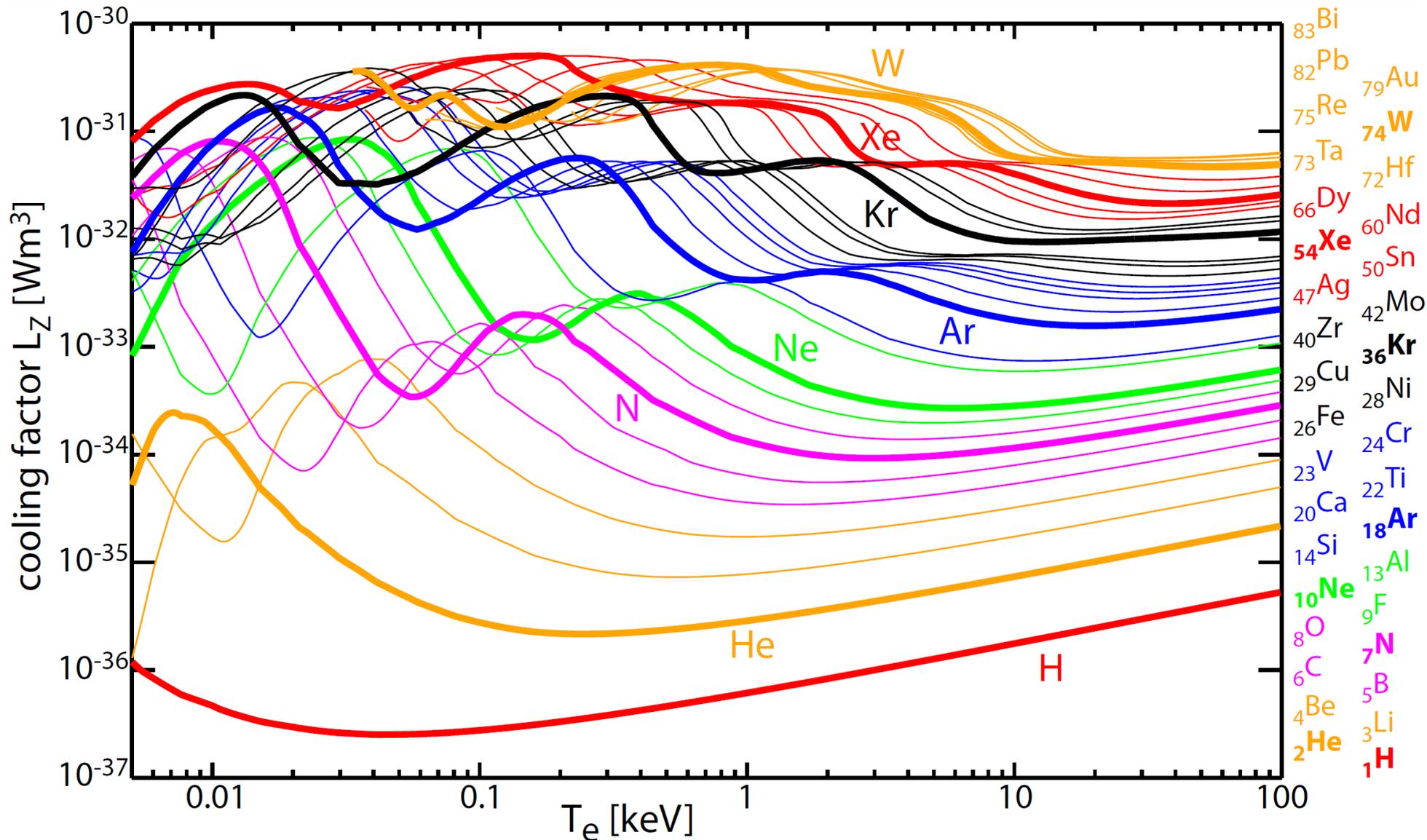
- Old data up to  $\sim 40\text{keV}$  available
- Continuum Radiation in agreement slight deviations for line radiation
- For low-Z, old data may be better for line rad. (or not?)
- Helium: Continuum rad. In old data has wrong T-dependence - extrapolation?



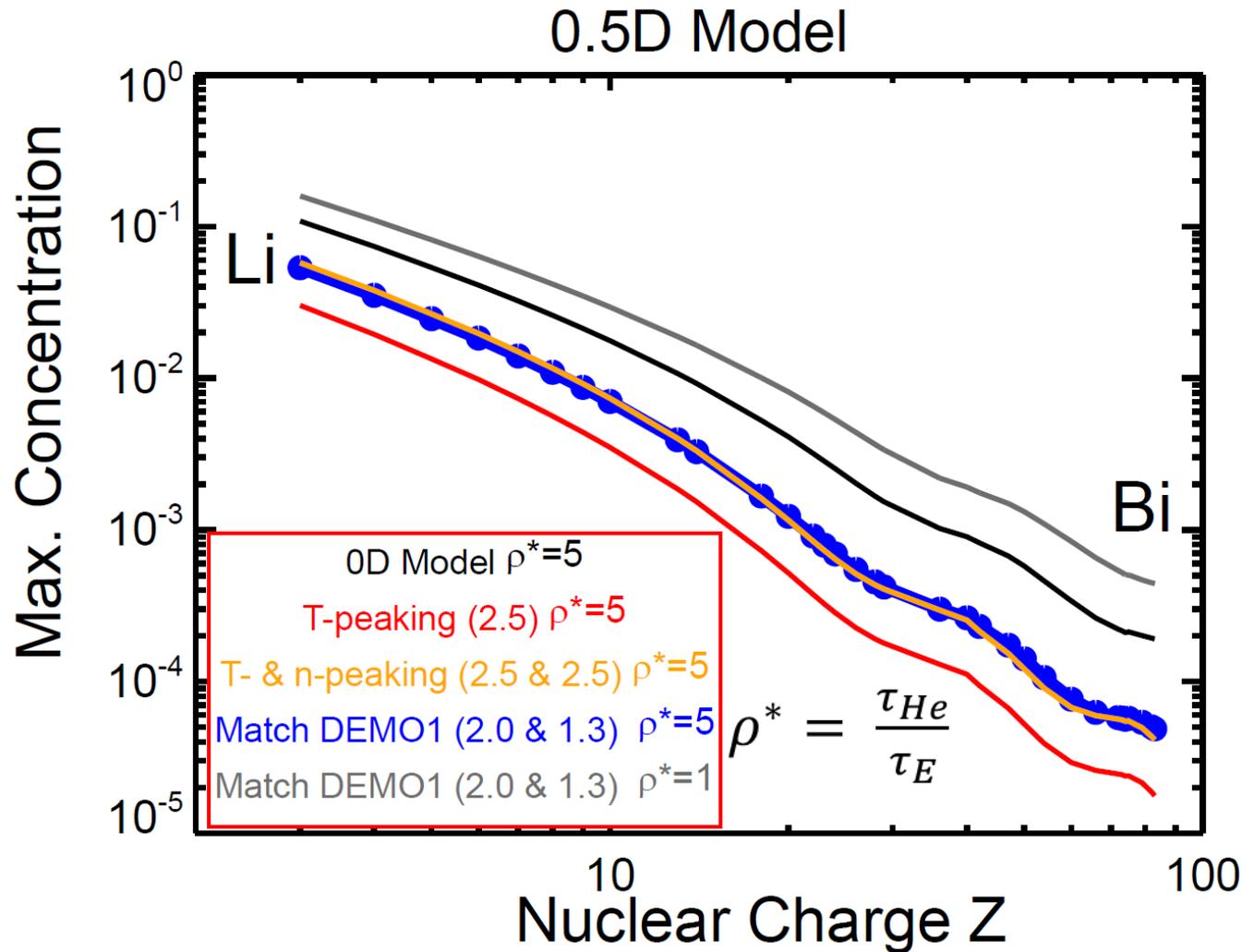
- Old data up to  $\sim 40\text{keV}$  available
- Continuum Radiation in agreement slight deviations for line radiation
- For low-Z, old data may be better for line rad. (or not?)
- Helium: Continuum rad. In old data has wrong T-dependence - extrapolation?



# New Data Behaves Straight Forward



- Motivation
  - ⇒ Impurities in Fusion Plasmas
  - ⇒ Issues with existing data
  
- New Calculations using ADAS codes
  - ⇒ What quality has the new data?
  - ⇒ First tests with the new data
  
- First Applications of the new data
- Course of Action?



- All reactor models require cooling factors to model impurity radiation
- Here, very simple 0.5D model is used to evaluate impurity limit for each element

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- Data for plasma emissions have been calculated for all ions of 35 elements
- The same procedure has been used for all elements, thus systematical trends in the data can be better observed
- The quality is good for baseline calculations
- For elements with  $Z$  higher than  $\sim 18$  the new data is probably an improvement
- Include all data in ADAS? Dedicated benchmarking?