Charge Exchange Recombination Spectroscopy of W Ions for ITER Neutral H-Beam Diagnostics and more on atomic data

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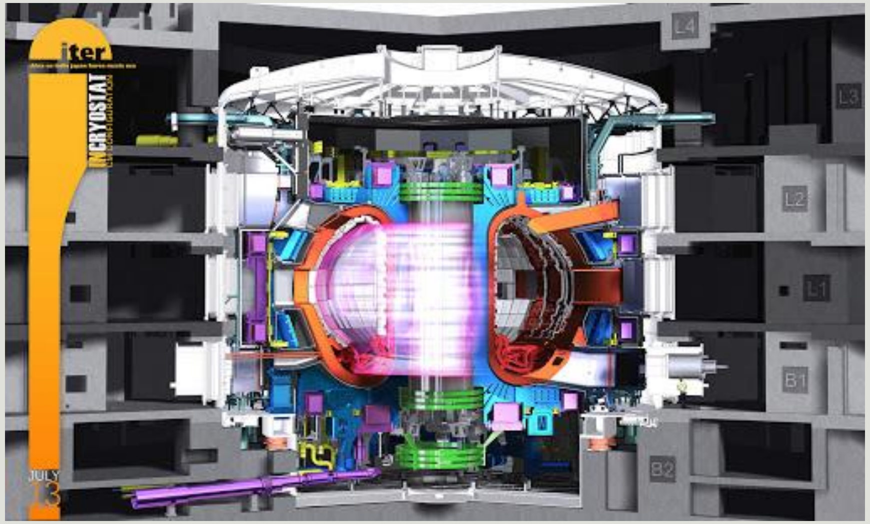


Acknowledgements

Yu. Ralchenko

C. Hill

D. Schultz

D. V. Fursa
I. Bray
H. Umar

Charge exchange recombination spectroscopy (CXRS)

$$H + A^{q+} \rightarrow H^{+} + A^{(q-1)+*}\,(nl) \rightarrow A^{(q-1)+*}\,(n'l') + h\nu$$

$n \approx q^{0.75}$, e.g., for capture into H-like Fe^{25+} ion, $n \approx 11$

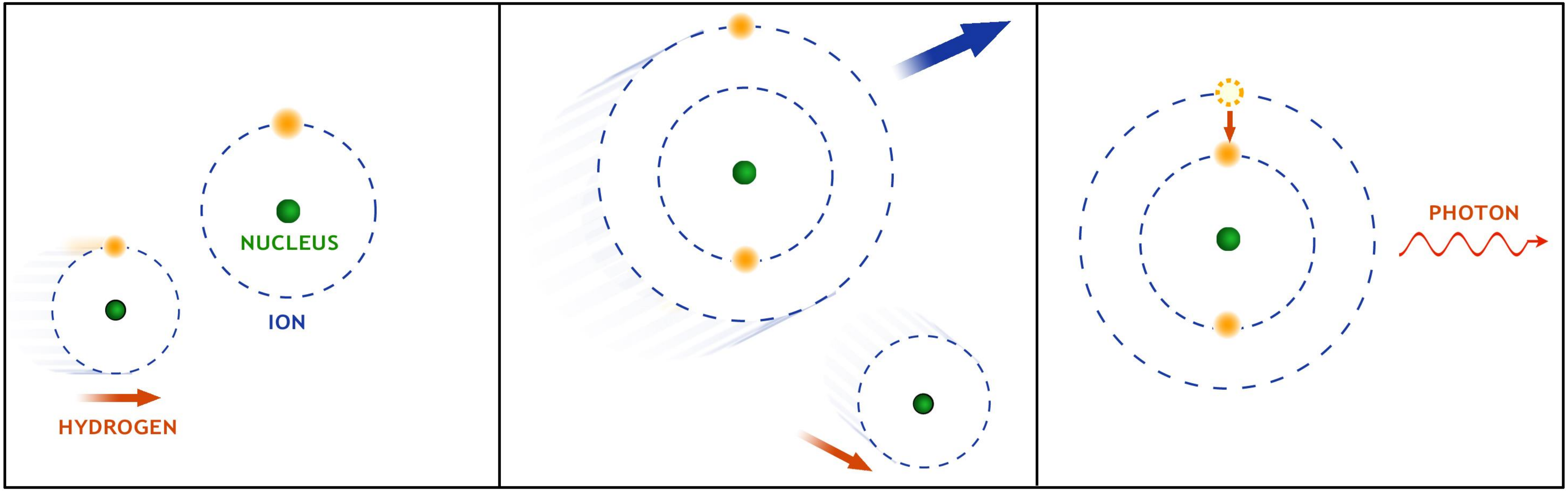
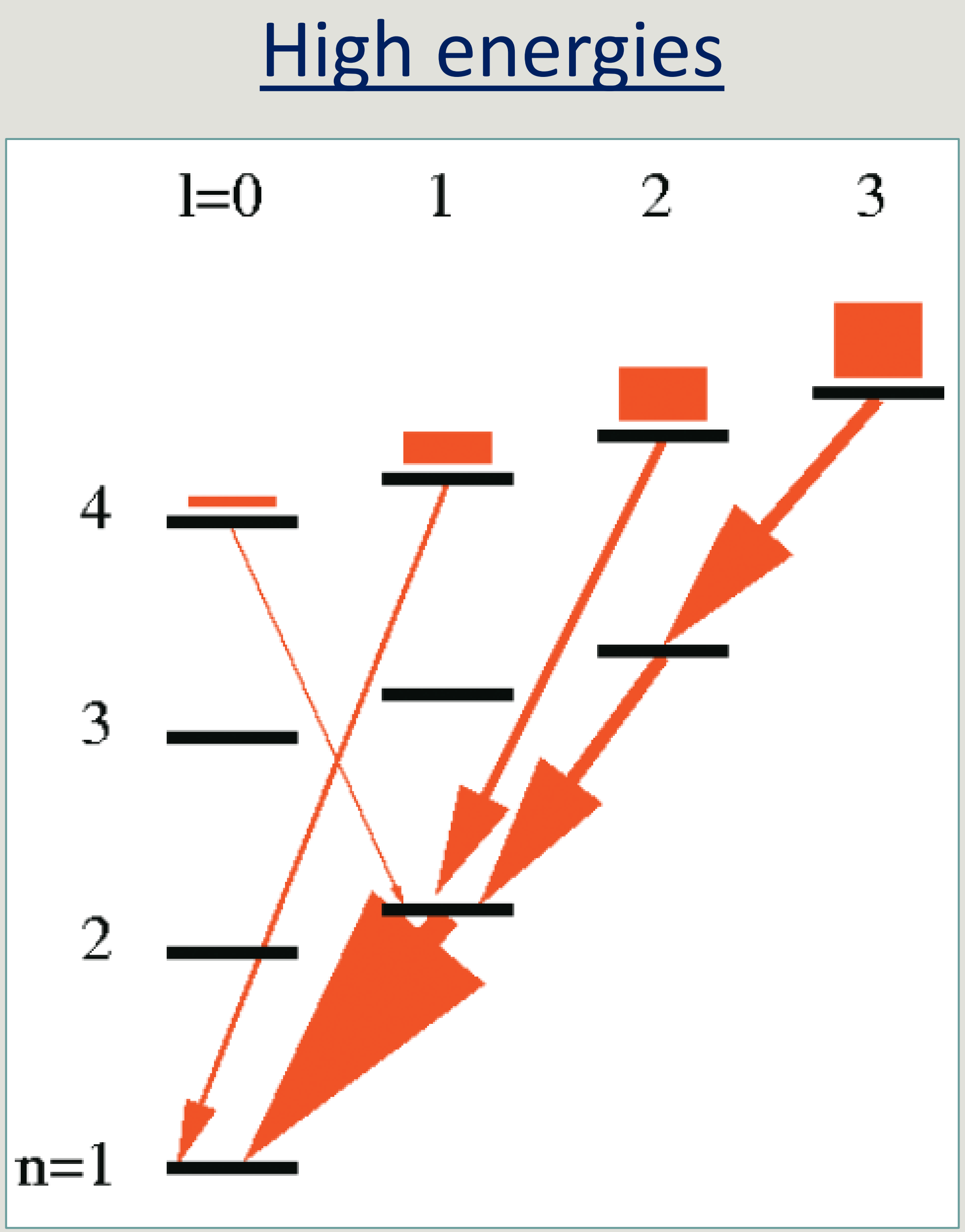
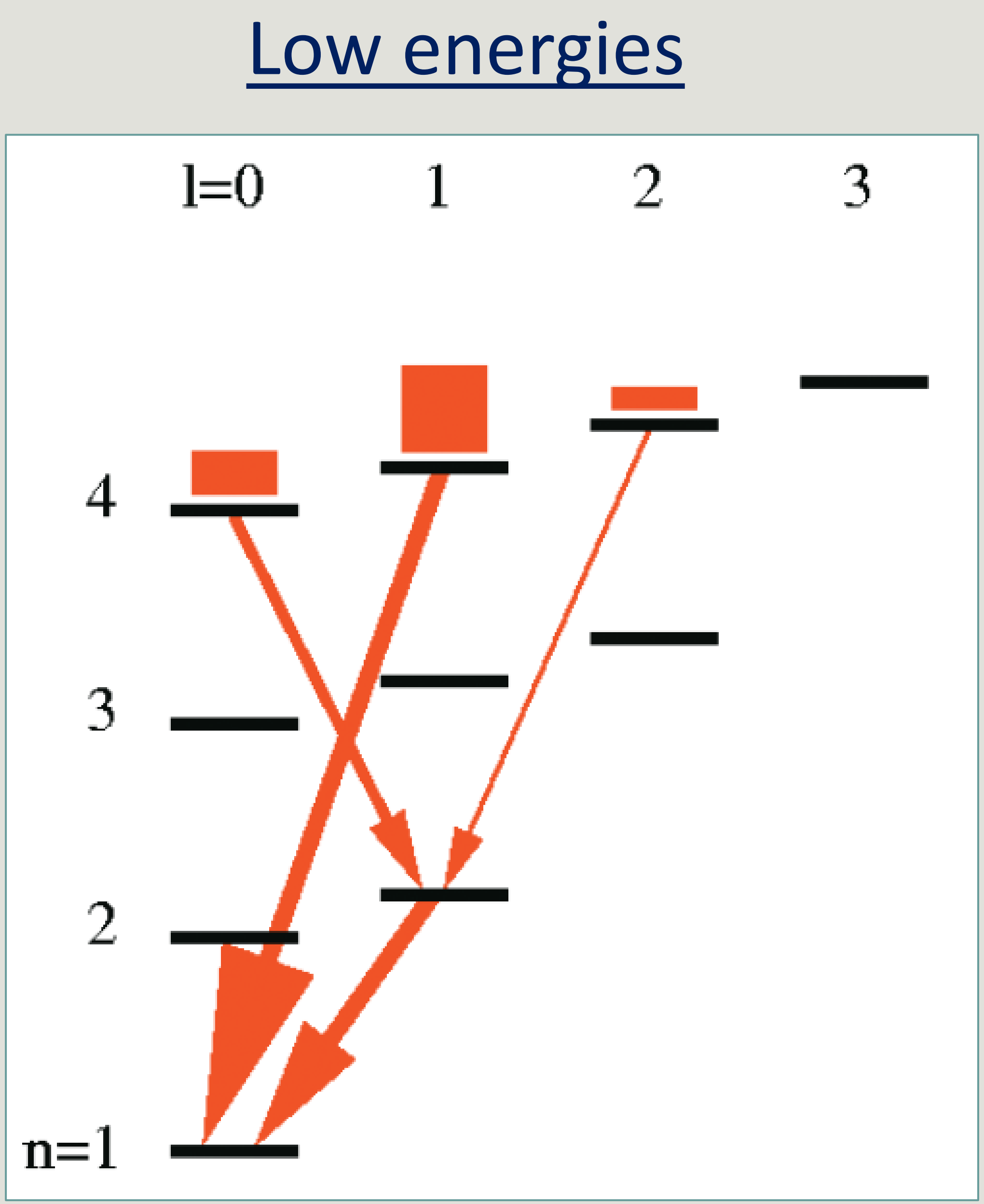


Illustration: NASA/CXC/M.Weiss

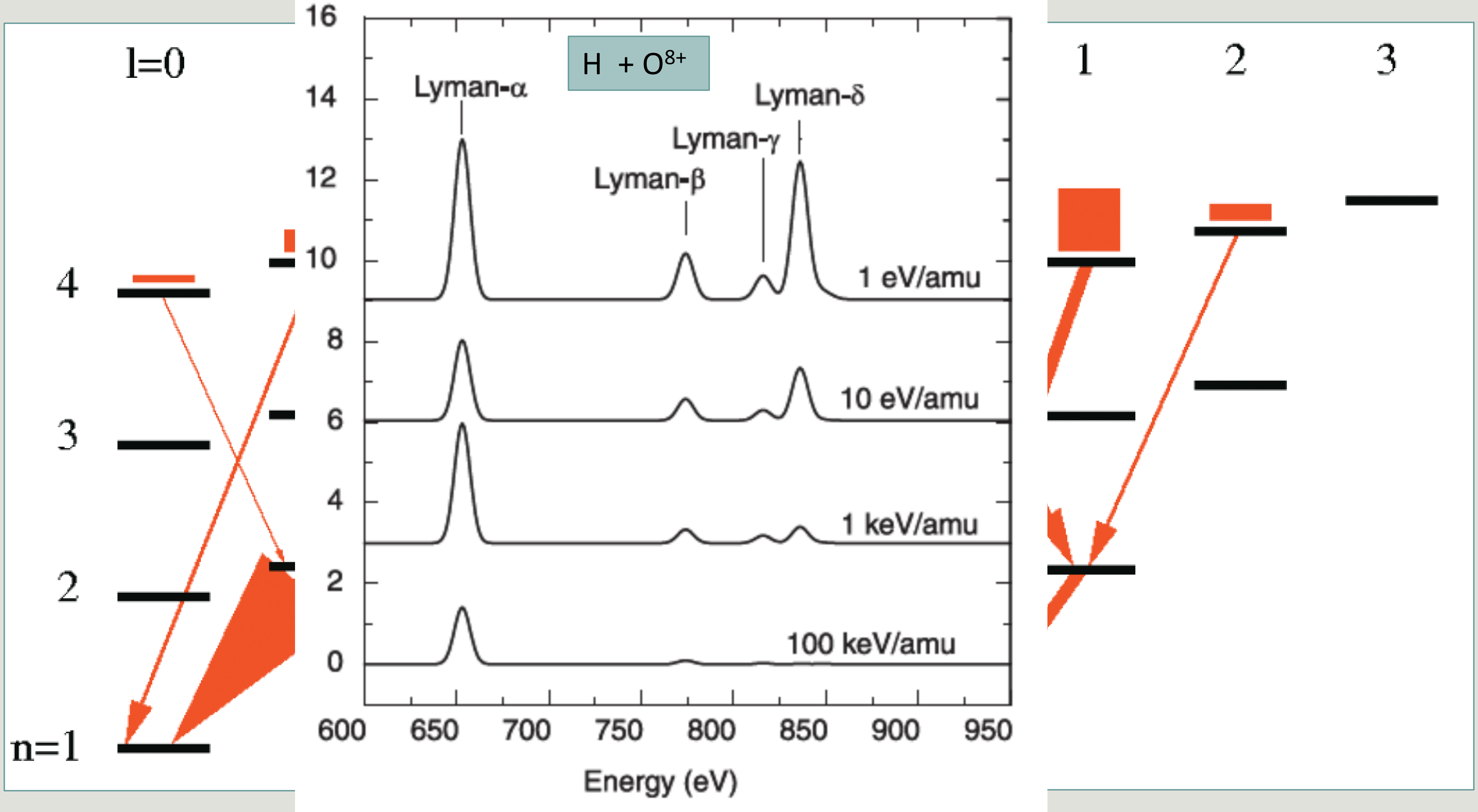




B. J. Wargelin *et al.*, Can. J. Phys. **86**, 151 (2008)

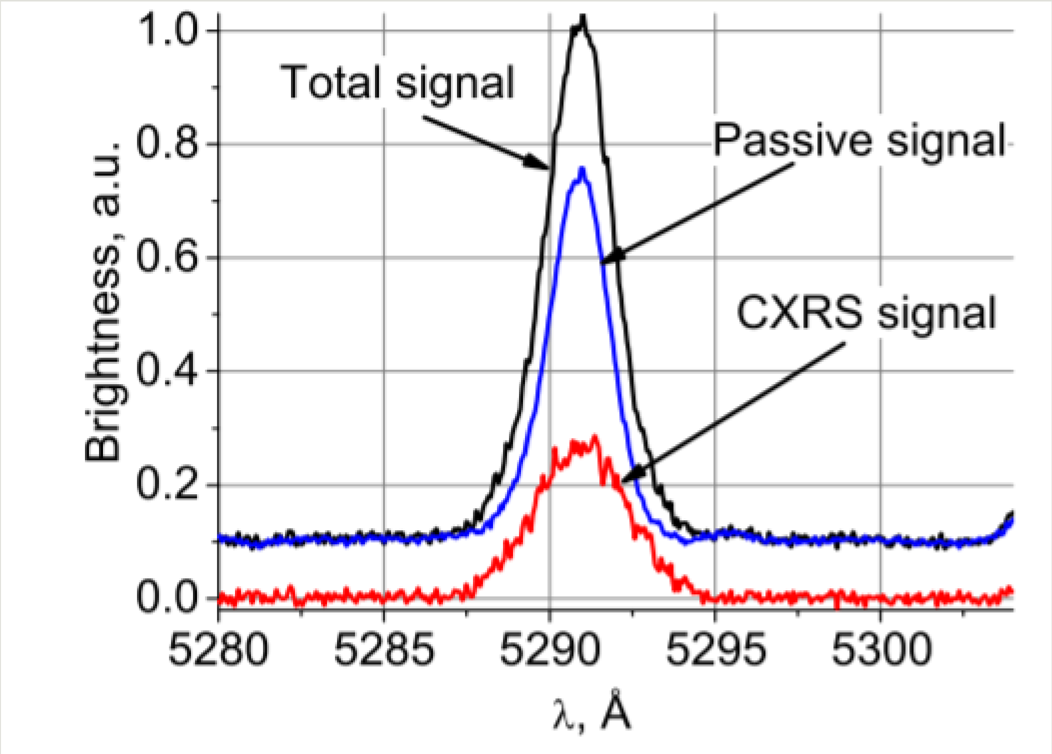
High energies

Low energies



Applications of CXRS

- Spectral diagnostics of fusion plasmas heated by neutral beam (NB)



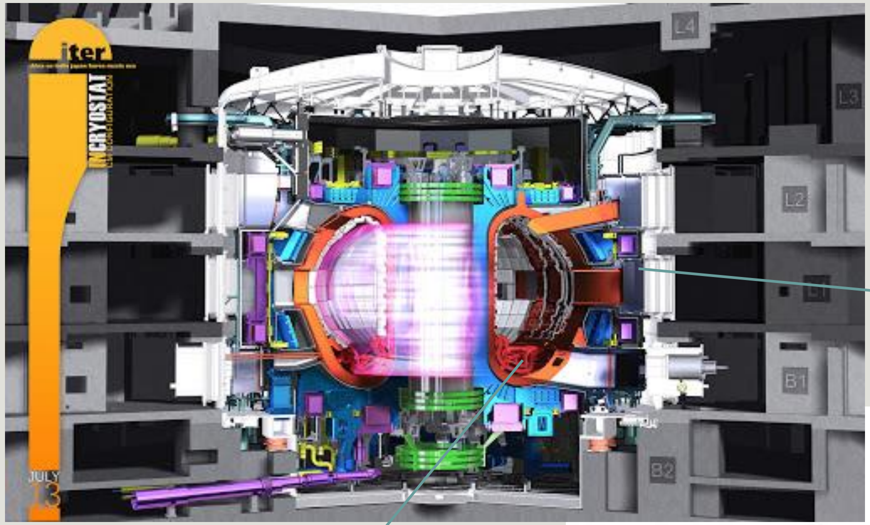
C^{5+} 7-8 transition at 5291 Å

$$T_i = 1.7 \times 10^8 M_i \left(\frac{\Delta\lambda_D}{\lambda}\right)^2$$

- Determination of ion storage times in ion traps and storage rings
- Astrophysical relevance such as solar wind charge exchange in comets and planetary atmospheres

L. A. Kluchnikov *et al.*, Rev. Sci. Instr. **87**, 053506 (2016)

ITER and the NBI

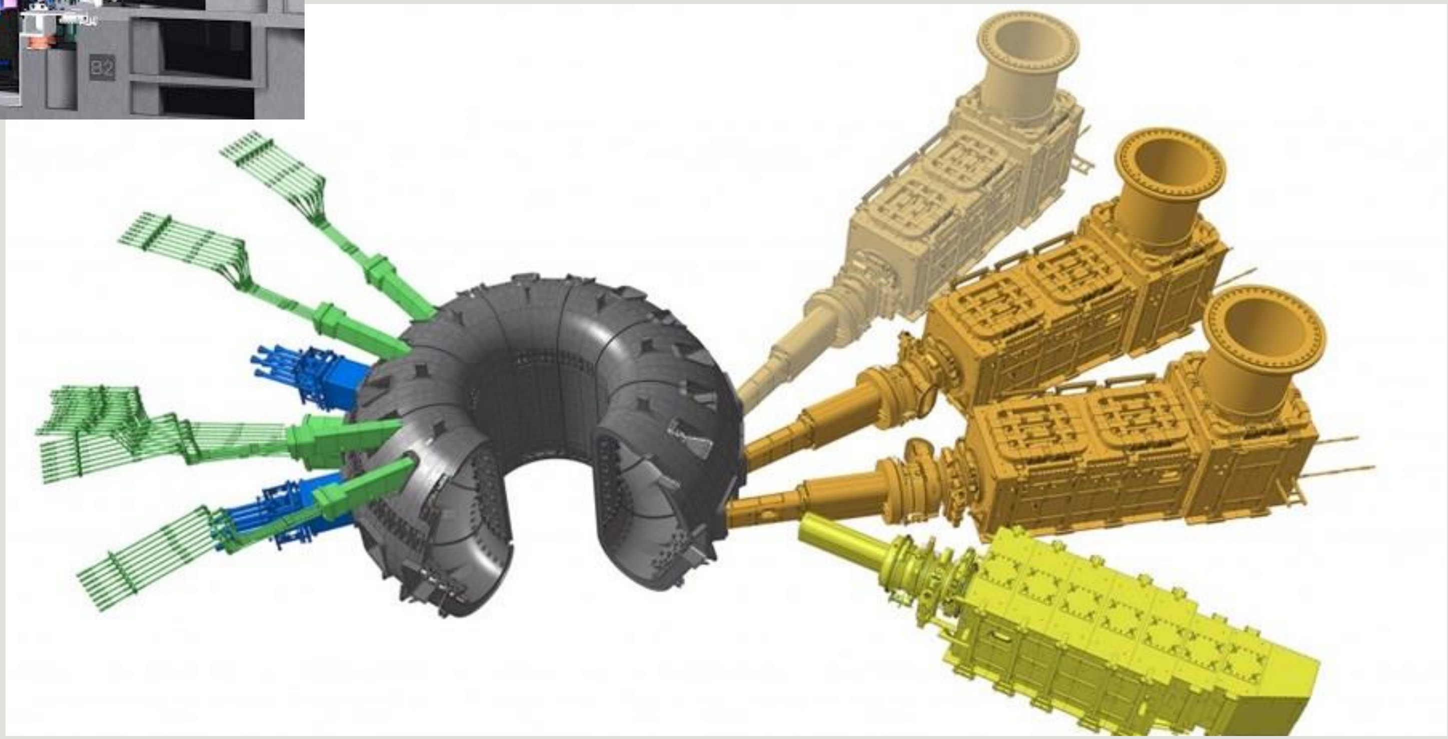


ITER is the largest international project aimed to demonstrate the scientific and technical feasibility of fusion energy as future power source.

T ~ 150 -200 million °C
Cost > $20 billion

Neutral beam injectors (NBI)

Divertor region (Plasma facing components are made of tungsten)



either 0.87 MeV H or 1 MeV D beams for heating

100 keV/u H beam for diagnostics such as ion temperature, plasma rotation, He concentration

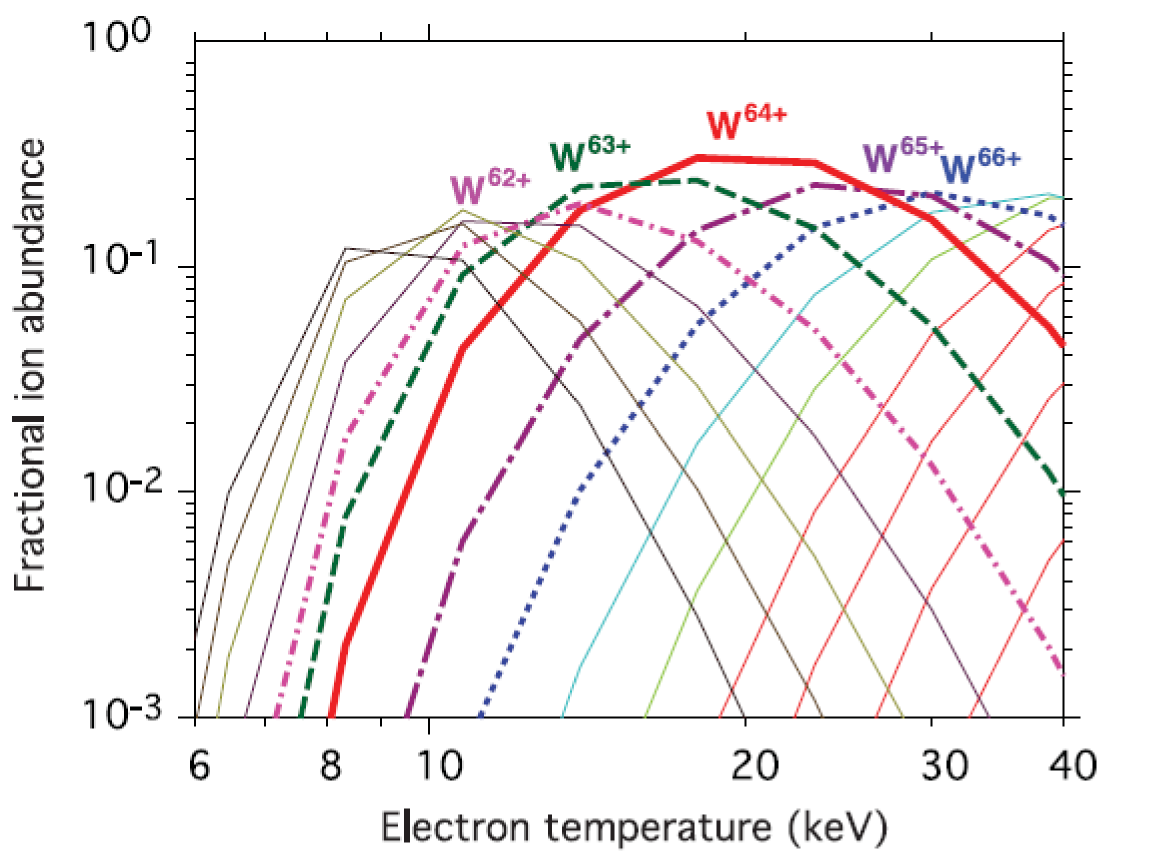
CXRS of tungsten ions for ITER NB diagnostics

- Plasma parameters:

  T = 20 keV (Ne-like W^{64+} is expected to be most abundant ion in the core of plasma)

  $n_e = 10^{14}$ cm^{-3}

- H neutral beam of energies 100 keV/u, 500 keV/u, 850 keV/u, and 1000 keV/u.

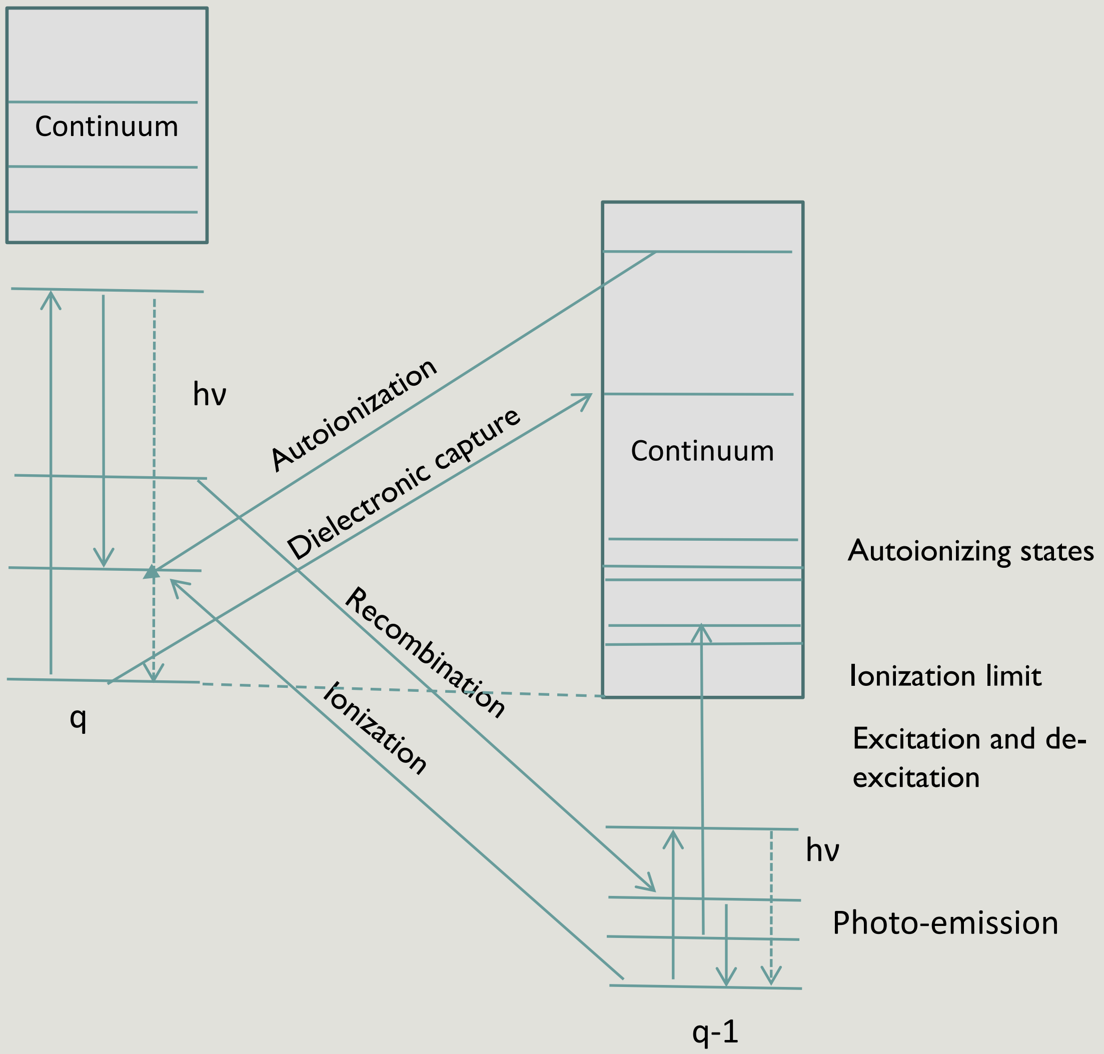


P. Beiersdorfer *et al.* JPB **43,** 144008 (2010)

Rate equations of collisional-radiative model

$$\frac{dN(t)}{dt} = R(t, N_e, T_e, \ldots)N(t) \;, \sum_{q,k} N(q,k) = 1$$

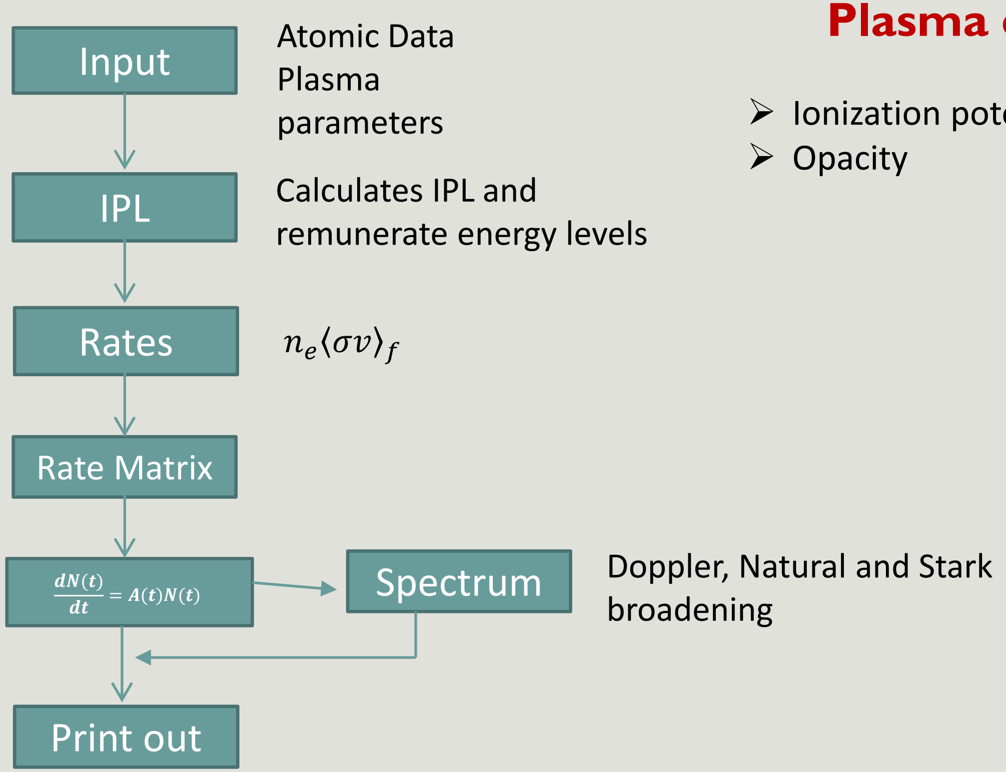
$$\frac{dN_q(k)}{dt} = -N_q(k)\sum_{j\neq k}\left(n_e X^{kj} + n_p Y^{kj}\right)$$
$$+\sum_{j\neq k} N_q(j)\left(n_e X^{jk} + n_p Y^{jk}\right)$$
$$-N_q(k)\sum_{j<k} A^{kj} + \sum_{j>k} N_q(j) A^{jk}$$
$$-N_q(k)\sum_{l} S^{kl}_{q,q+1} + \sum_{m} N_{q+1}(m)\alpha^{mk}_{q+1,q}$$
$$-N_q(k)\sum_{l} \alpha^{kl}_{q,q-1} + \sum_{m} N_{q-1}(m) S^{mk}_{q-1,q}$$



Schematic diagram of NOMAD* Code

Atomic Data (FAC#)

- Atomic structure
- Radiative decay rates (Photo excitation)
- Electron impact excitation (de-excitation)
- Electron impact ionization (three body recombination)
- Photoionization (Radiative recombination)
- Autoionization rates (Dielectronic capture)



Plasma effects

- Ionization potential lowering (IPL)
- Opacity

*Yu. Ralchenko and Y. Maron, JQSRT **71**, 609 (2001), Dipti *et al.* J. Phys. B: At. Mol. Opt. Phys. **53,** 115701 (2020).
#M. F. Gu , Can J. Phys. **86,** 675-689(2008).

Collisional-radiative Model

- includes Si-like W^{60+} through the O-like W^{66+} ions and the ground state of N-like W^{67+} ion.

- Atomic structure has been calculated using relativistic configuration

For an L-shell ion

$1s^2 2s^2 2p^k$ (ground state configuration)
$1s^2 2s^2 2p^{k-1} nl$ (**$n \leq 50$**)
$1s^2 2s 2p^k nl$ ($n \leq 15$)
$1s^2 2s^2 2p^{k-2} 3l nl'$ ($n \leq 5$)

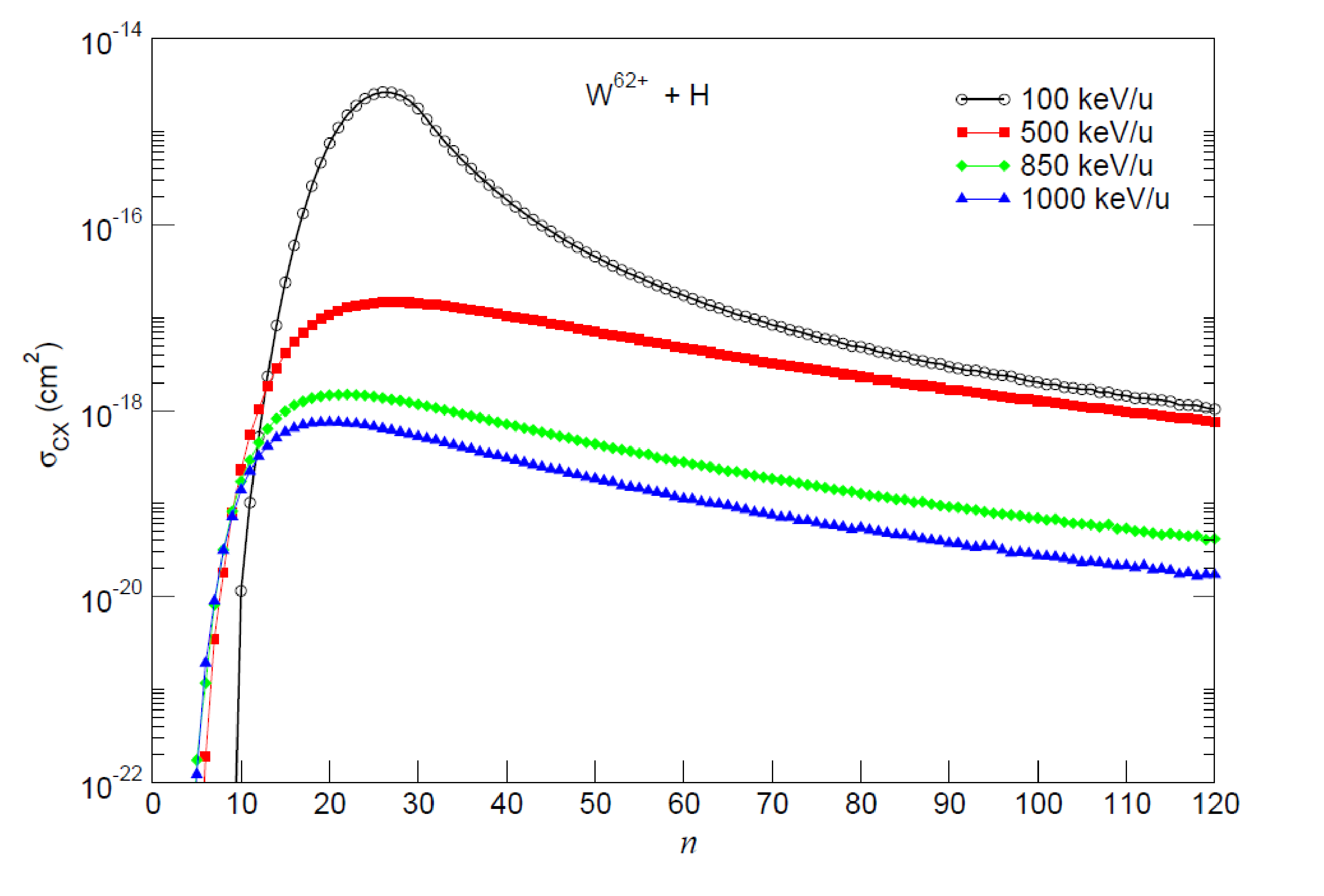
$n \approx q^{0.75} \approx 22$

Total number of levels included in the model are about **48 000**.

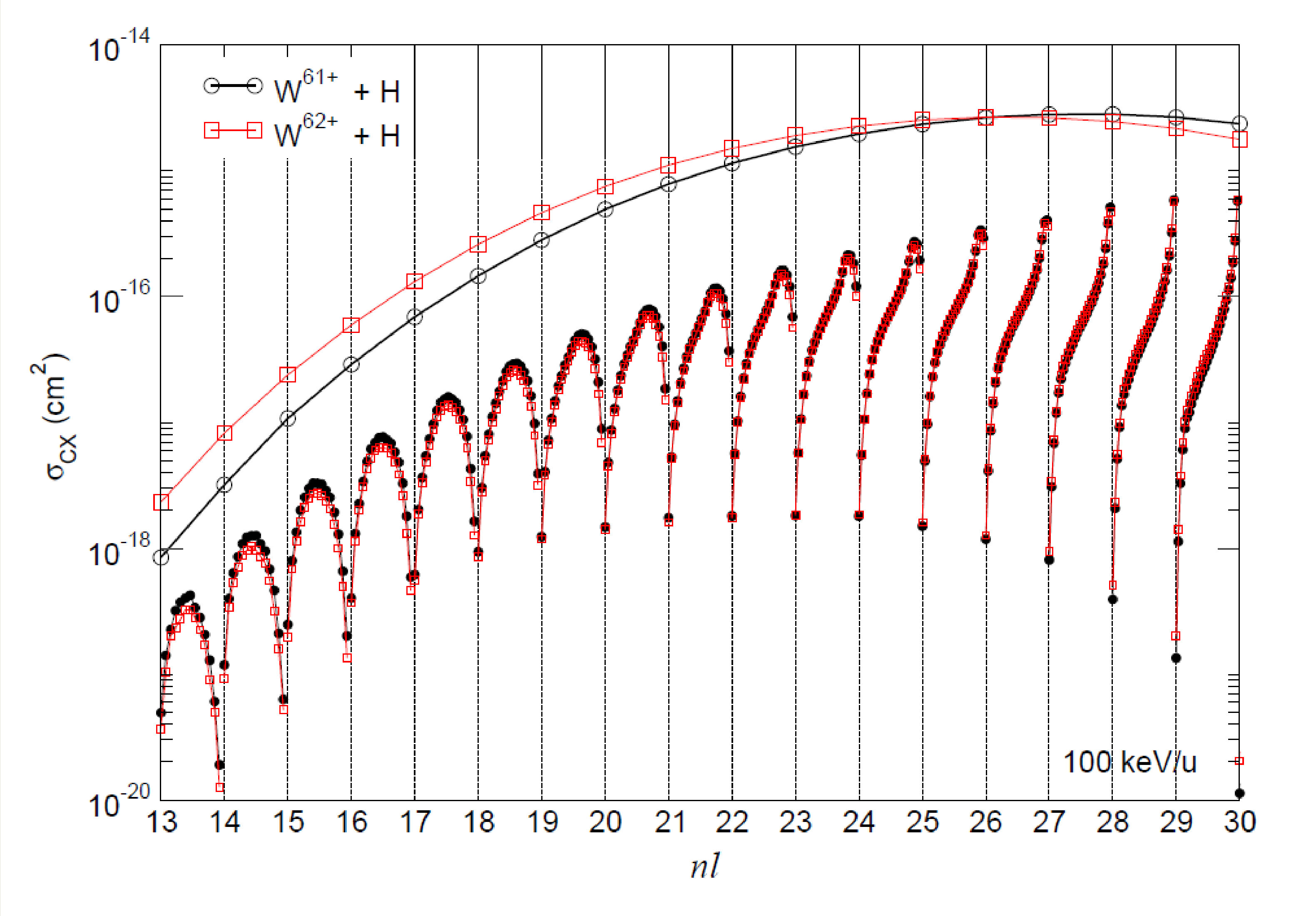
- nl-resolved CX cross sections were calculated using the classical trajectory Monte Carlo simulations by D. R. Schultz

$$\text{Rate (CX)} = n_o v_r \sigma_{CX} \quad (n_o v_r = 10^{15}\ cm^{-2}s^{-1} - 10^{17}\ cm^{-2}s^{-1})$$

n-resolved CX cross sections

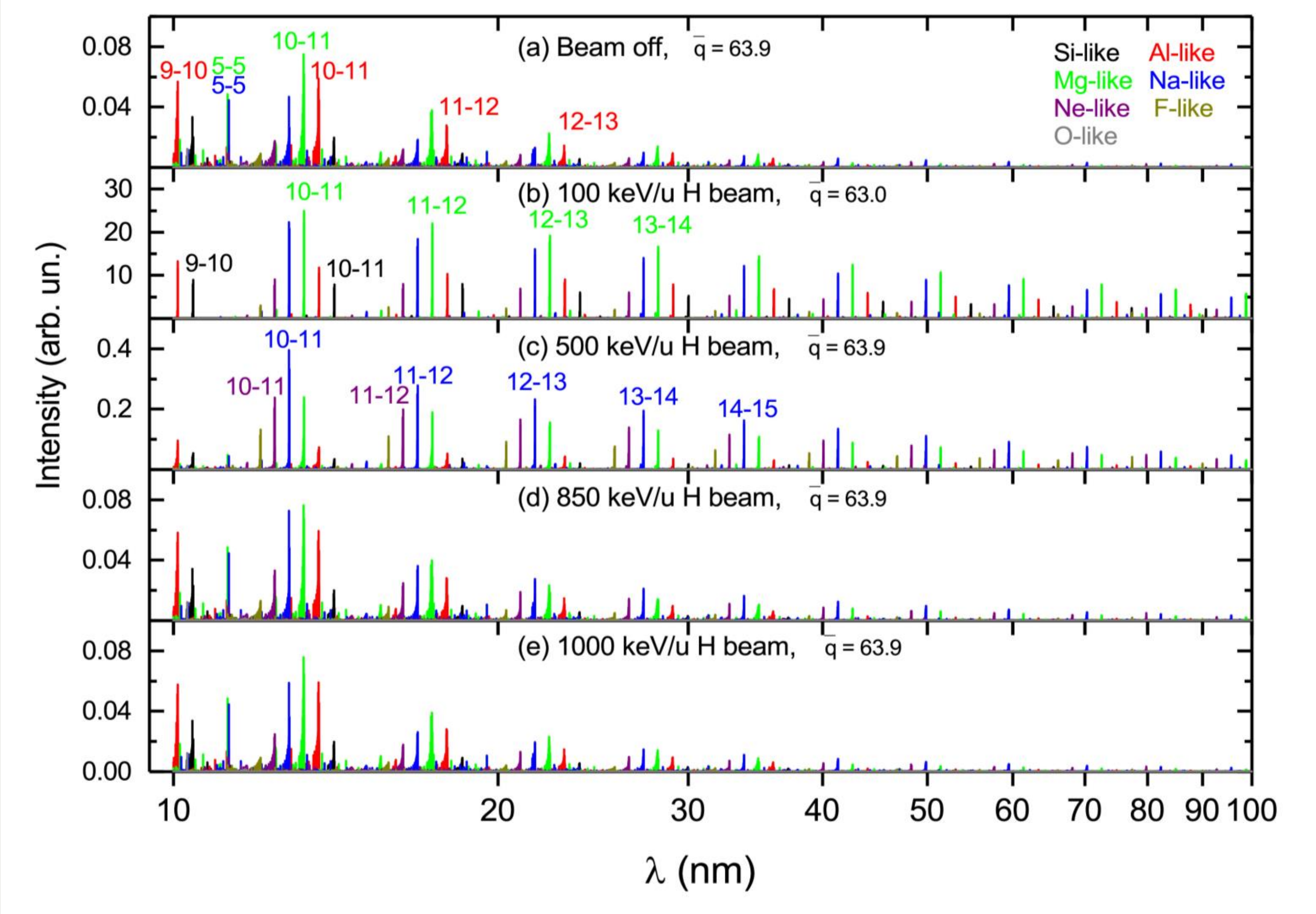


nl-resolved CX cross sections



Simulated spectra in 0.1 nm to 1000 nm

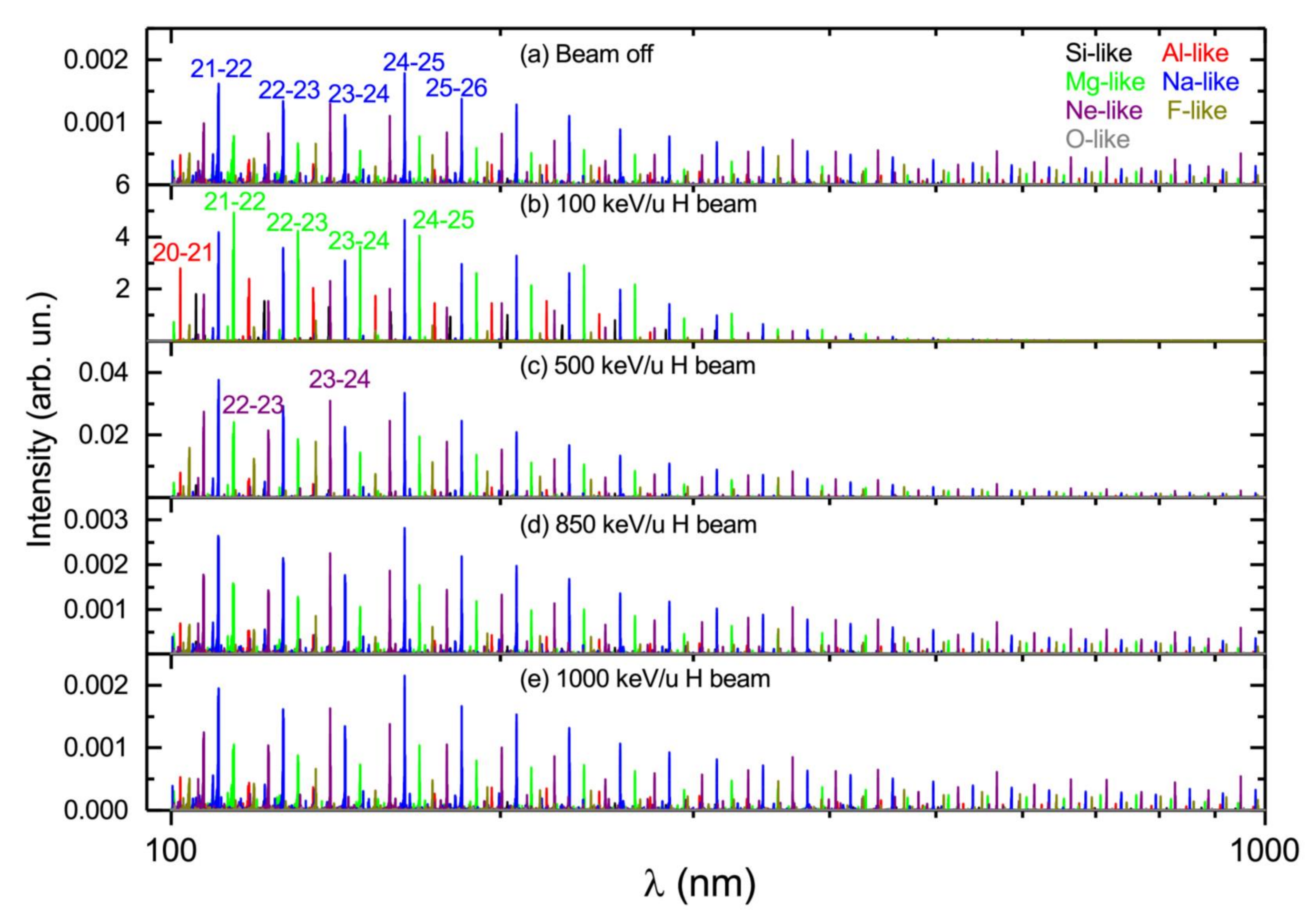
T_e = 20 keV, n_e= 10^{14} cm^{-3}, $n_o v_r$ = 10^{16} cm^{-2}s^{-1}



Spectra in lower wavelength 0.1 nm to 10 nm are not affected by CX.

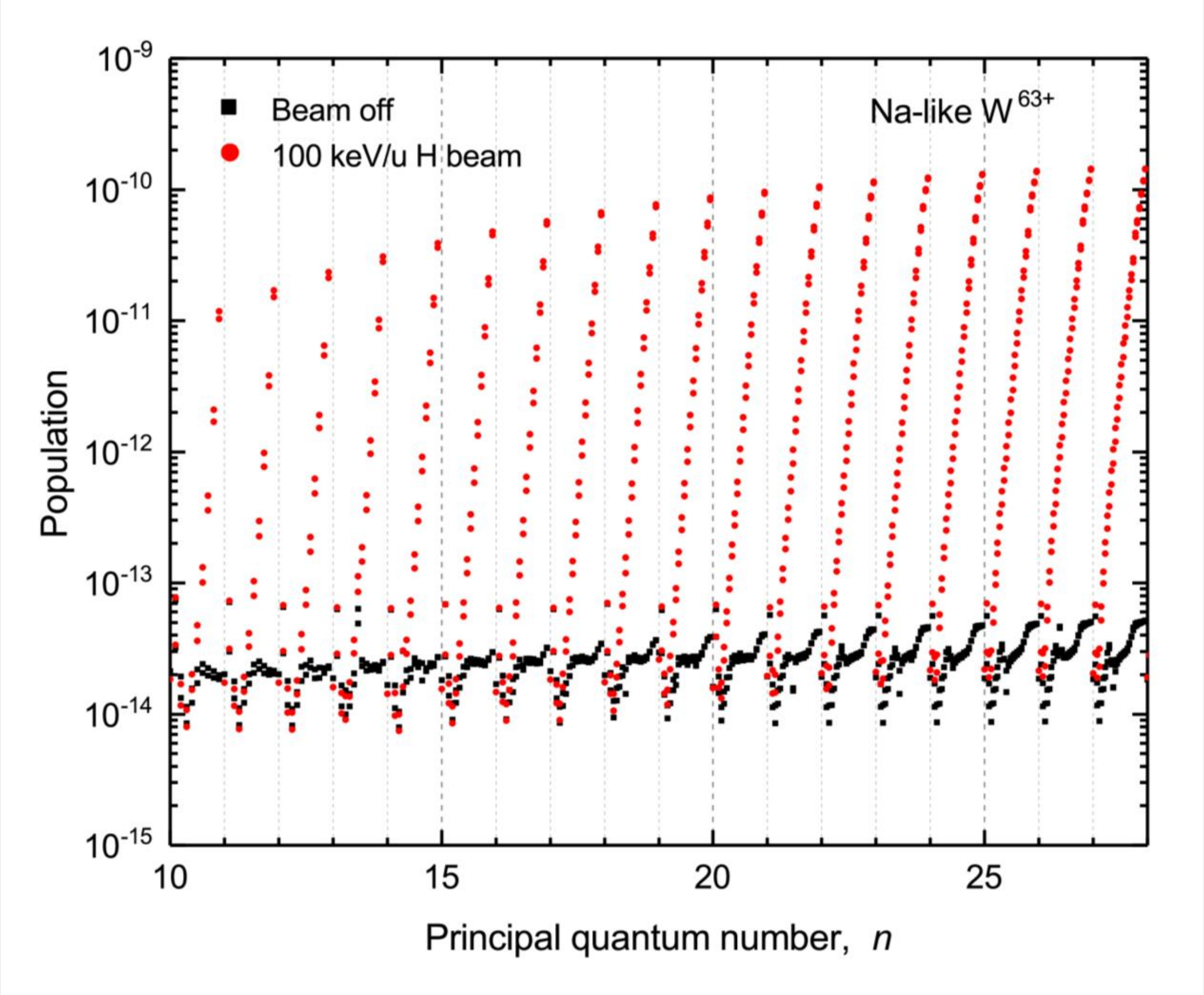
Transitions 2-3, 3-3, 3-4, 3-5

Simulated spectra.....



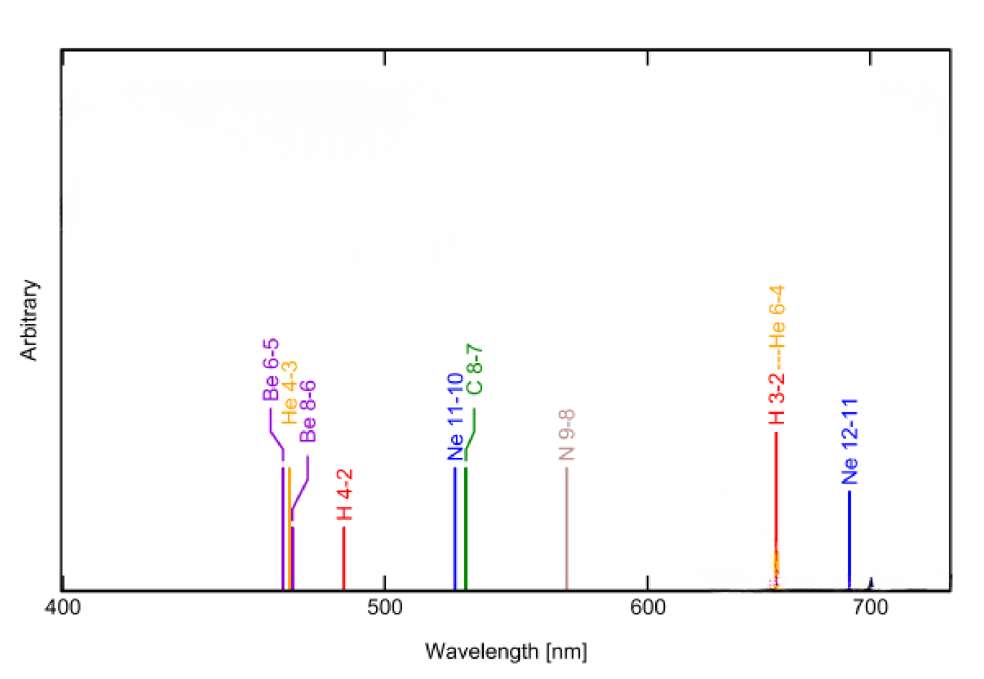
Population distribution with and without CX for DNB

T_e = 20 keV, n_e= 10^{14} cm^{-3}, $n_o v$ = 10^{16} $cm^{-2}s^{-1}$

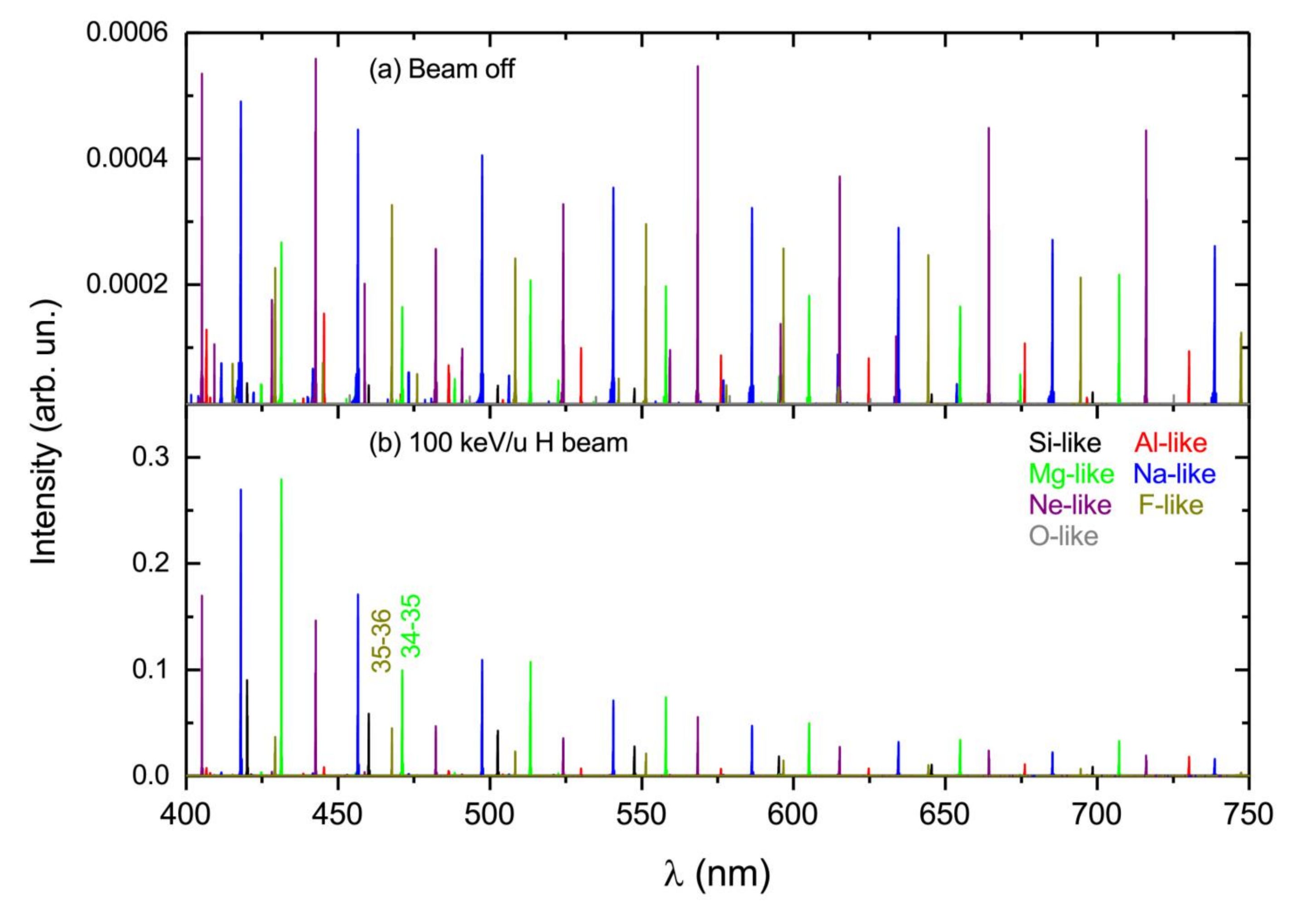


Visible CXRS diagnostic for ITER and other tokamaks

He^{+}: n=3-4 transitions at 468.8 nm
Be^{3+}: n= 5-6 and n=6-8 transitions at 465.9 nm and 468.6 nm



Lines of interest for CXRS for JET*

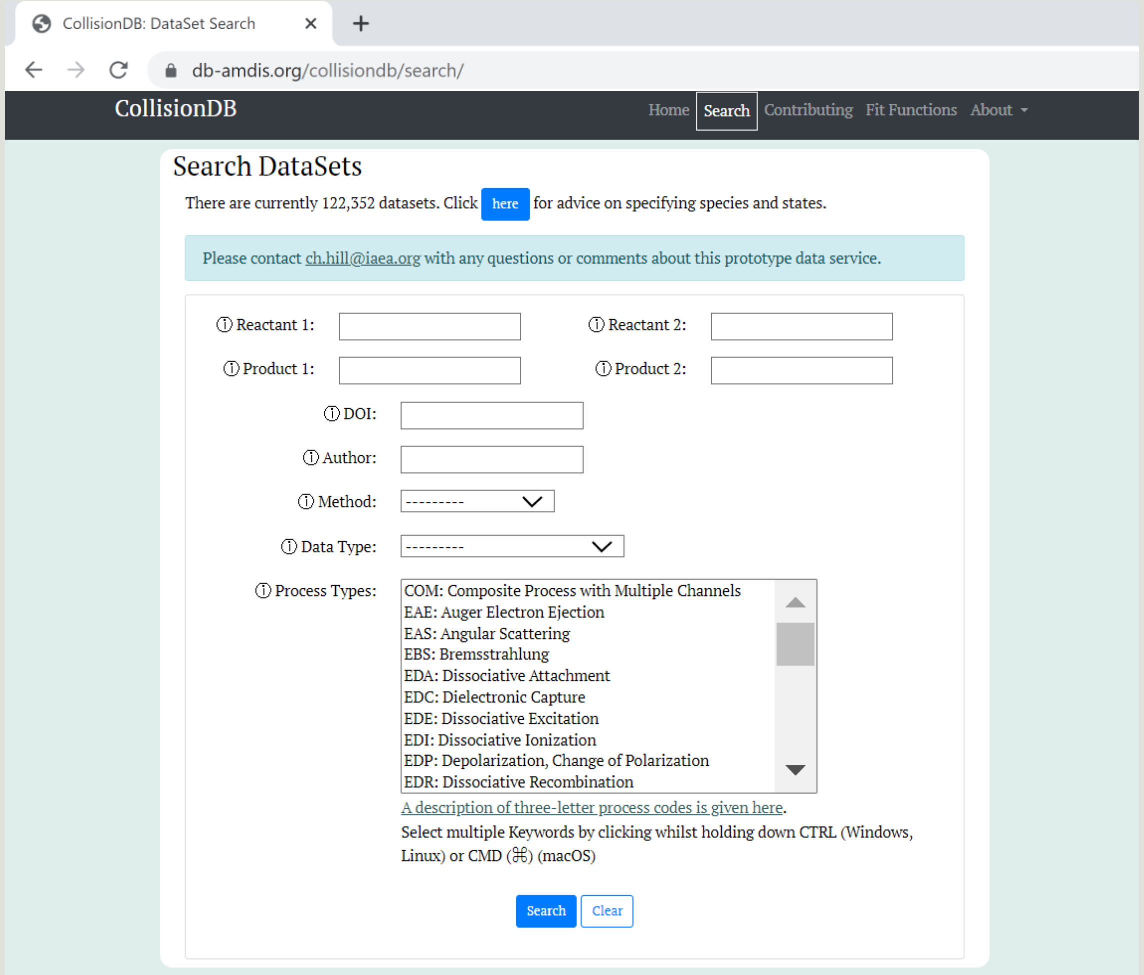


CX cross sections are available in IAEA's database: CollisionDB.

*N. C. Hawkes *et al.*, Rev. Sci. Instrum. **89**, 10D113 (2018)
Dipti, D. R. Schultz, and Yu. Ralchenko, Plasma Phys. Control. Fusion **63**, 115010 (2021)

CollisionDB : Database of Plasma collisional processes

- Cross sections and rate coefficients for atomic and molecular collisional processes to support fusion and other areas of plasma research
- Evaluated data from IAEA’s old database ALADDIN.
- Data is described with rich metadata and provided in standardized format
- Data retrievable by search and identifier from a browser and through an API



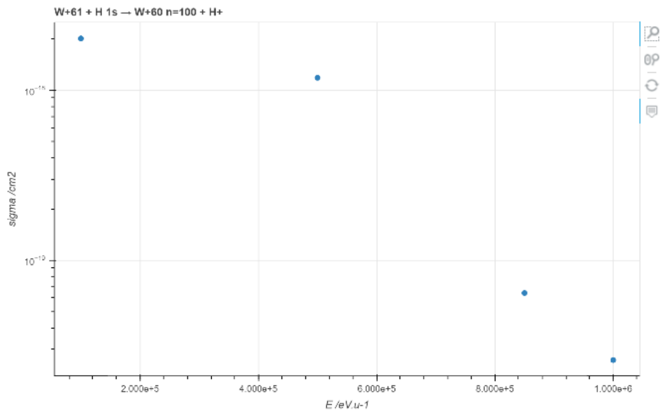
CollisionDB

Home Search Contributing Fit Functions About

DataSet D76390

$$\mathrm{W}^{61+} + \mathrm{H}\ 1s \rightarrow \mathrm{W}^{60+}\ n = 100 + \mathrm{H}^{+}$$

Process	HCX: Charge Transfer
Data type	cross section | uploaded on 2022-05-26
comment	Total and state-selective charge exchange cross sections for recombination of O-like to Al-like W ions with atomic hydrogen at collision energies relevant to the ITER neutral beams. The n- or nl-resolved cross sections not listed in the database for a given value in (n ≤ 120, l ≤ n-1) are 0 at all considered energies.
Method	CTMC: Classical trajectory Monte Carlo
Frame	Target
Columns	1. E /eV u^{-1} 2. sigma /cm^2
Ref	B22: Dipti, D. R Schultz, Y. Ralchenko, "Charge exchange recombination spectroscopy of W (q+) (q = 61-66) for application to ITER neutral hydrogen beam diagnostics ", *Plasma Physics and Controlled Fusion* **63**, 115010 (2021). [10.1088/1361-6587/ac206c]
Data	Download




```
{
  "qid": "D76390",
  "reaction": "W+61 + H 1s \u2192 W+60 n=100 + H+",
  "process_types": { "HCX": "Charge Transfer" },
  "data_type": "cross section",
  "refs": { "B22": { "doi": "10.1088/1361-6587/ac206c" } },
  "json_comment": { "comment": "Total and state-selective CX cross sections for recombination of O-like to Al-like W ions" },
  "json_data": {
    "method": "CTMC",
    "columns": [
      {
        "name": "E",
        "units": "eV.u-1"
      },
      {
        "name": "sigma",
        "units": "cm2"
      }
    ]
  }
}
------------------------------------------------------------------------
1.000e+05 2.015e-18
5.000e+05 1.184e-18
8.500e+05 6.41e-20
1.000e+06 2.585e-20
```

PyCollisionDB: API Library

- Python package for interacting with the CollisionDB API ; data exploration, data transformation, plotting, etc.

Example:

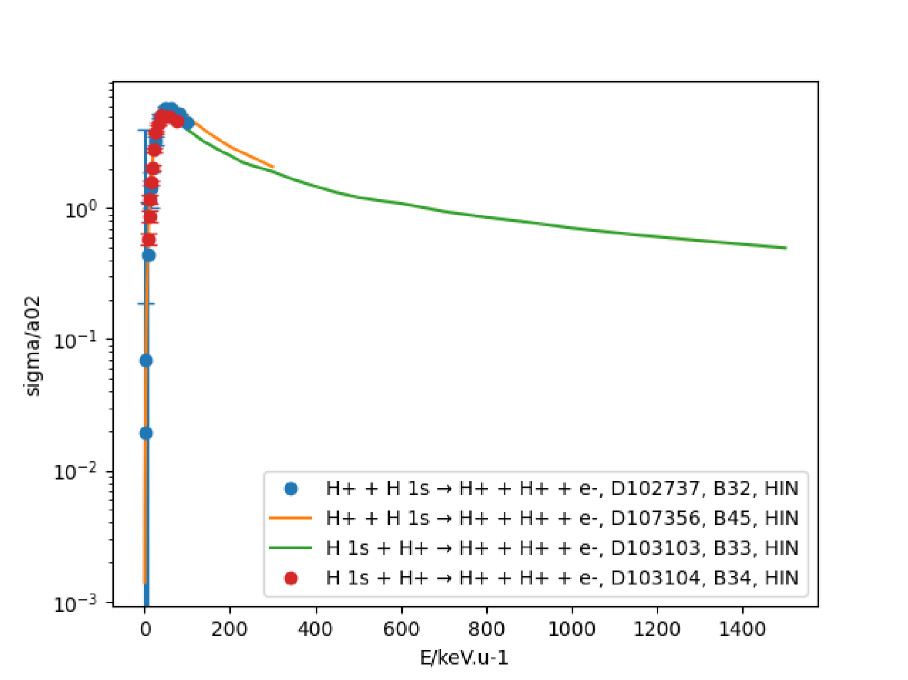
```
>>> from pycollisiondb.pycollisiondb import PyCollision
```

```
>>> # Proton-impact ionization of H.
>>> query = {'reactants': ['H+', 'H 1s'],
                    'process_types': ['HIN'],
                   'data_type': 'cross section'}
>>> pycoll = PyCollision.get_datasets(query=query)
```

```
>>> # Datasets retrieved from the server as a dict keyed by pk ID.
>>> pycoll.datasets
{102737: D102737: H+ + H 1s → H+ + H+ + e-,
 107356: D107356: H+ + H 1s → H+ + H+ + e-,
 103103: D103103: H 1s + H+ → H+ + H+ + e-,
 103104: D103104: H 1s + H+ → H+ + H+ + e-}
```

```
>>> # Energy is changed from eV.u-1 (default) to keV.u-1 and sigma from
cm2 (default) to a02.
>>> # This accesses the pyqn library.
>>> pycoll.convert_units({'E': 'keV.u-1', 'sigma': 'a02'})
```

```
>>> import matplotlib.pyplot as plt
>>> %matplotlib notebook
>>> fig, ax = plt.subplots()
>>> pycoll.plot_all_datasets(ax, label=('reaction', 'qid', 'refs', 'process_types'))
>>> plt.legend()
```



Data evaluation: recommended collisional data for Be I

Atomic Data and Nuclear Data Tables 127–128 (2019) 1–21

Contents lists available at ScienceDirect

Atomic Data and Nuclear Data Tables

journal homepage: www.elsevier.com/locate/adt

Recommended electron-impact excitation and ionization cross sections for Be I

Dipti [a,*], T. Das [b,1], K. Bartschat [c], I. Bray [d], D.V. Fursa [d], O. Zatsarinny [c], C. Ballance [e], H.-K. Chung [b,2], Yu. Ralchenko [a,*]

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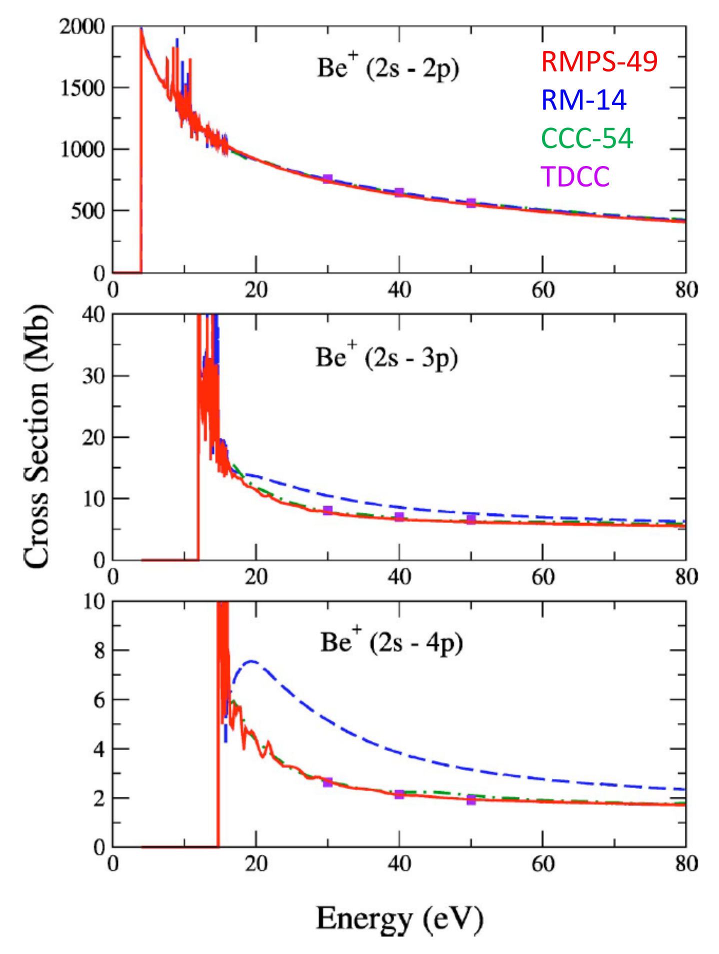
[b] *International Atomic Energy Agency, A-1400 Vienna, Austria*
[c] *Department of Physics and Astronomy, Drake University, Des Moines, IA 50311, USA*
[d] *Curtin Institute for Computation and Department of Physics, Astronomy and Medical Radiation Science,Curtin University, GPO Box U1987, Perth, WA 6845, Australia*
[e] *School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, United Kingdom*

Recommended collisional data for Be II: Overview of data

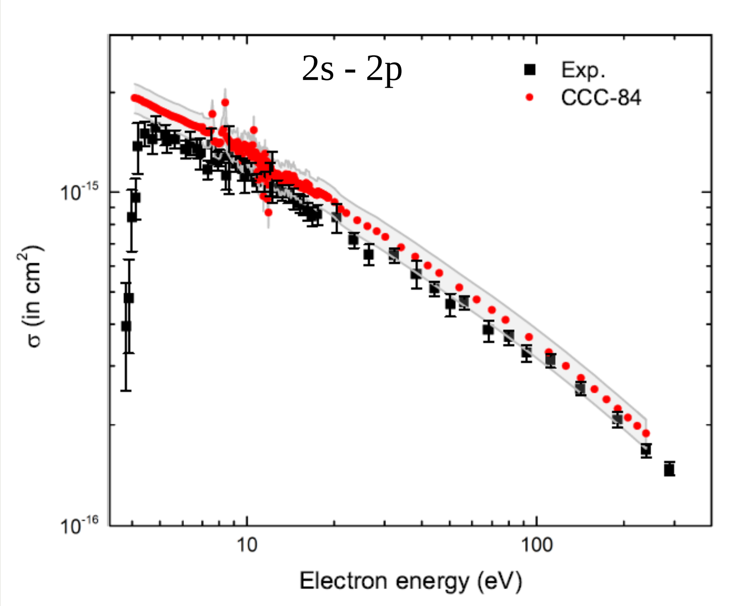
- Ground state: $1s^2 2s\ ^2S$
- $1s^2 nl\ ^2L$ ($n \leq 4$; $l \leq n-1$)



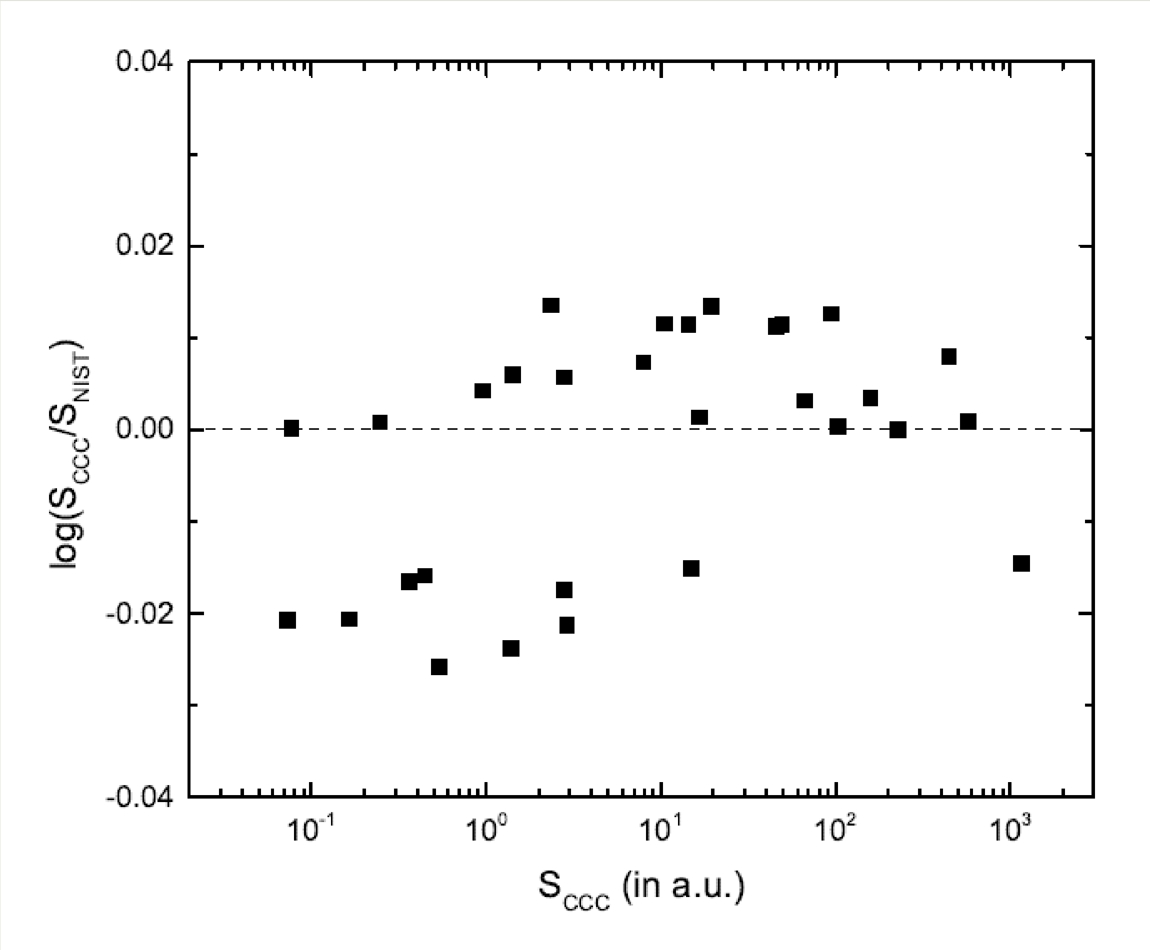
C. P. Balance et al. PRA 68, 062705 (2003)

- R-matrix (RM-14)
- R-matrix with pseudo states (RMPS-26, RMPS-49)
- Convergent-close-coupling (CCC-54, CCC-64)
- K-matrix (KM-20)
- Time-dependent close-coupling
- Distorted-wave method
- .....

New calculations with CCC-84 for $1s^2 nl\ ^2L$ ($n \leq 5$; $l \leq n-1$) by D. V. Fursa and his group



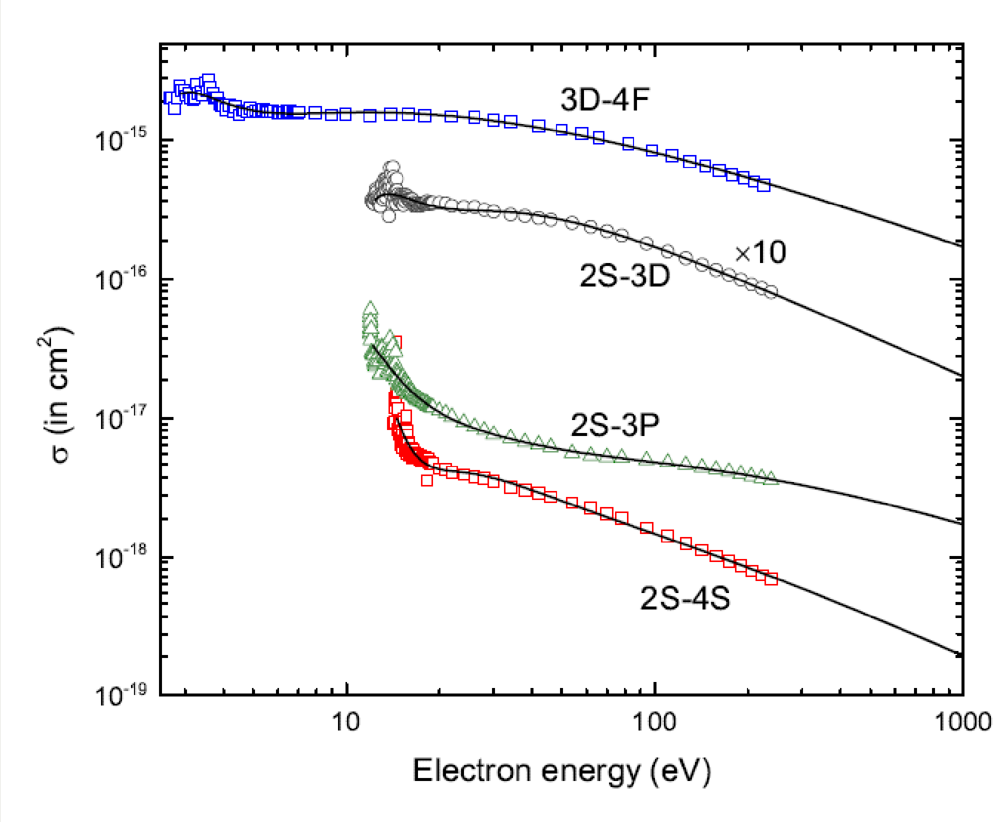
Atomic Structure calculations for Be II: line strengths (S)

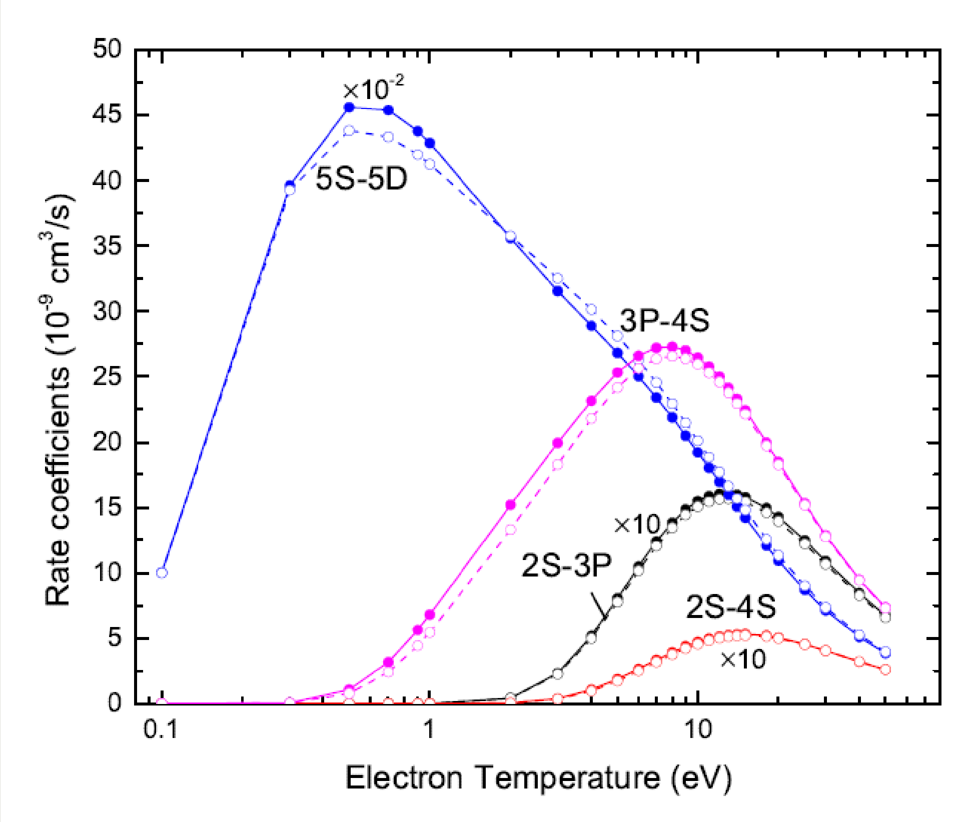


Uncertainty ≈ 5 %

Analytic fits for excitation

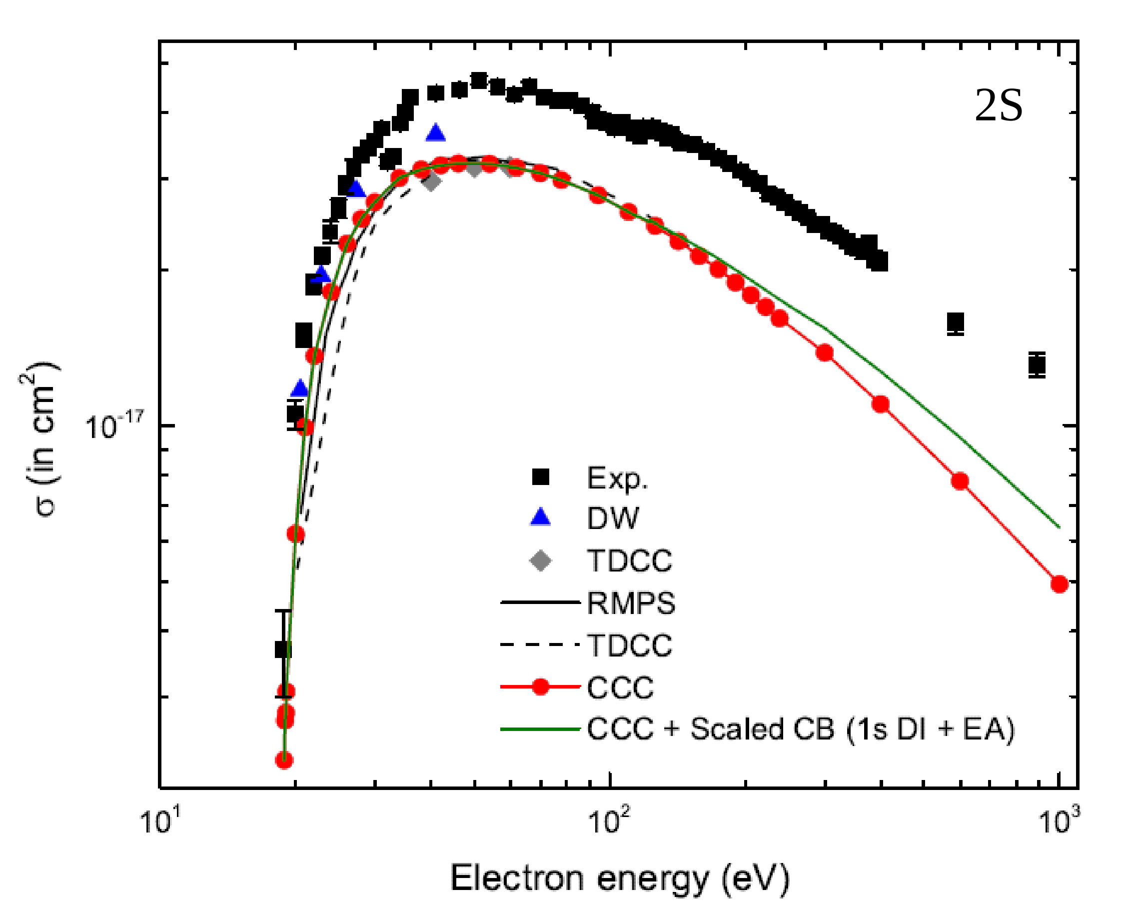
- Dipole-allowed (ΔL = ±1) : $\Omega(x) = A_0^2 \ln(x) + A_1 + \frac{A_2}{x} + \frac{A_3}{x^2} + \frac{A_4}{x^3} + \frac{A_5}{x^4}$
- Dipole-forbidden (ΔL ≠ ±1) : $\Omega(x) = A_0^2 + \frac{A_1}{x} + \frac{A_2}{x^2} + \frac{A_3}{x^3} + \frac{A_4}{x^4}$

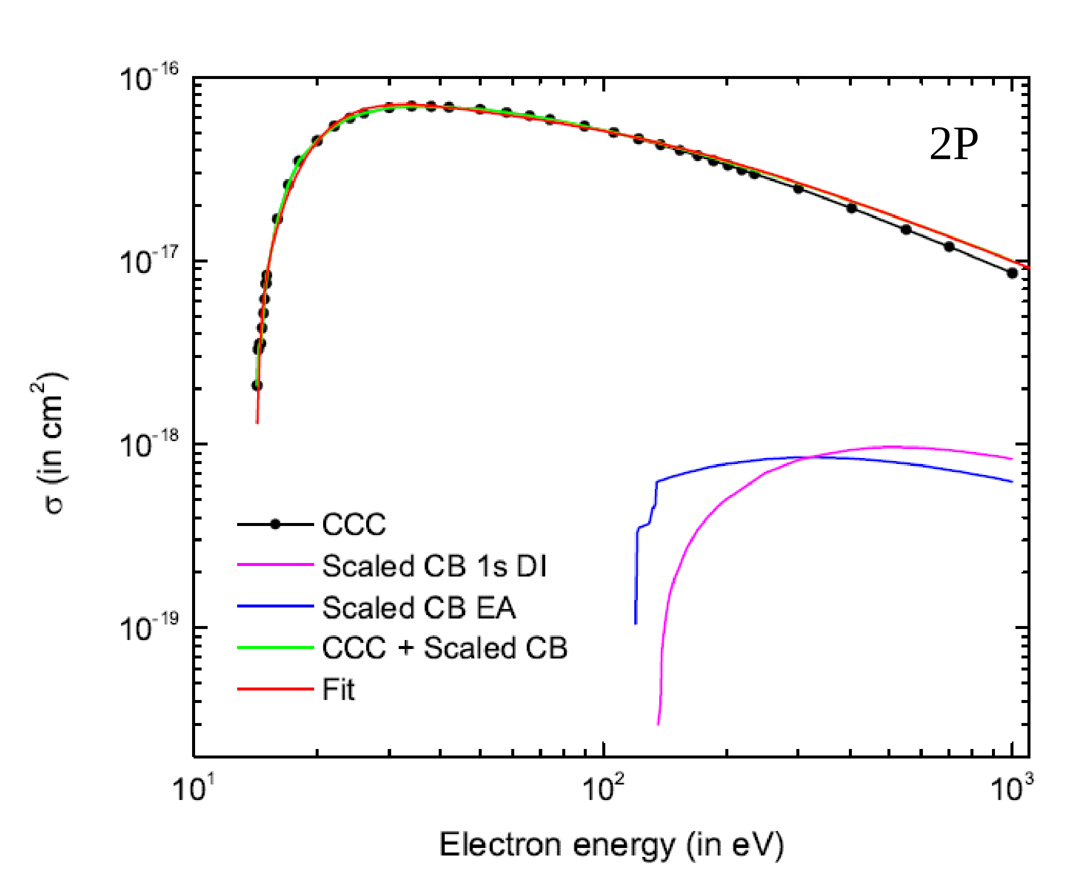




correct asymptotic behaviors

Ionization





Thank you for your attention !!!