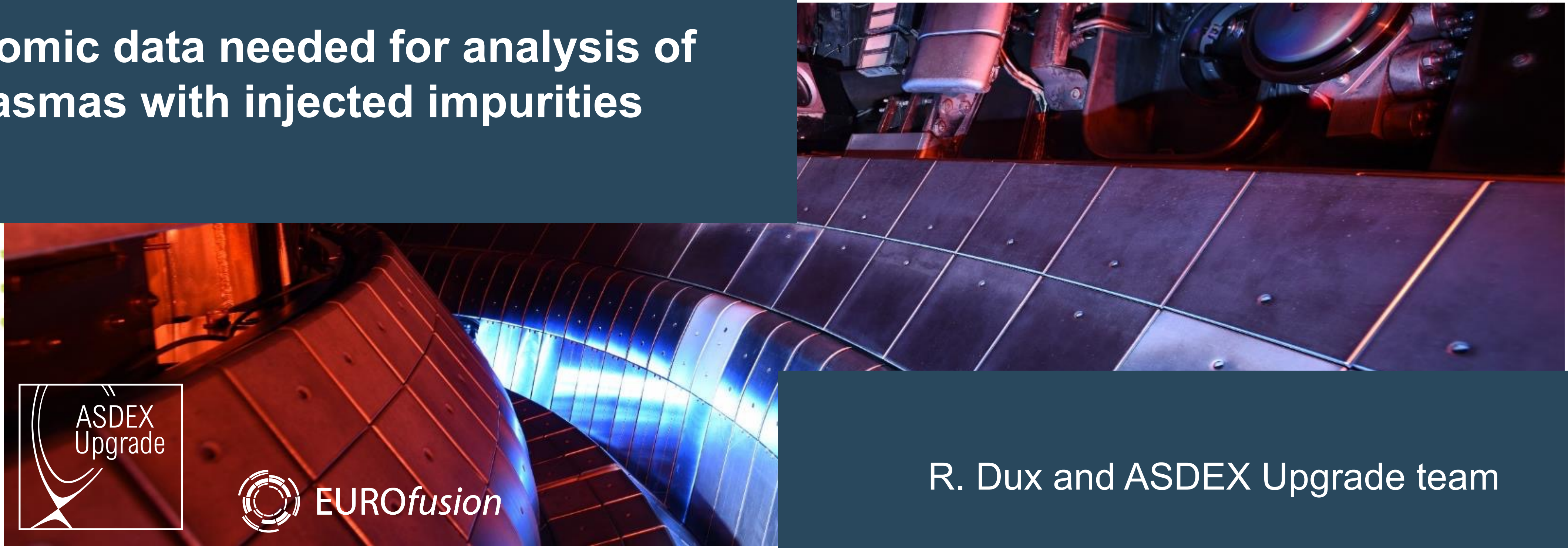
Atomic data needed for analysis of plasmas with injected impurities



R. Dux and ASDEX Upgrade team

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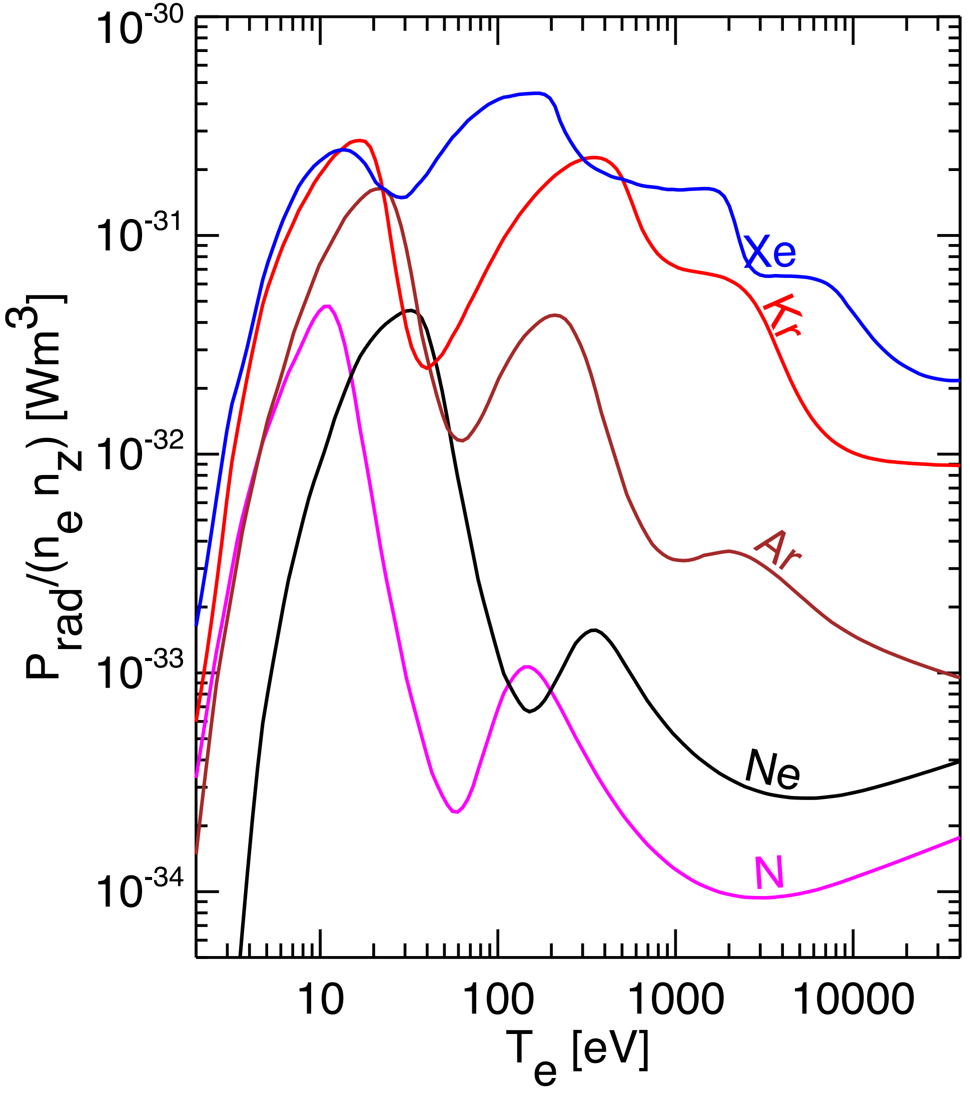
Outline

- What atomic data are needed to calculate radiation losses and to validate code calculations
- Role of recombination via charge exchange (CX) reactions
- Nitrogen vs noble gases considering NHx

Main objective of injected impurities: Increase radiation losses at the plasma edge

- Goal: little impurity radiation in the centre and much at the edge to mitigate the power load to the wall
- Edge can be the edge of the confined plasma (DEMO), the divertor (ITER) or the X-point region
- Figures of merit:
  - radiation loss at edge / radiation loss in the core
  - radiation loss at edge/ fuel dilution in the core
- TASK:
  Measure radiation and impurity densities at edge/core in present day machines (requires data for diagnostic lines) and refine code calculations using experimental data

Cooling factors



Example: code for radiation losses in confined plasma
1st step) Find radial distribution of ion stages (n_e,T_e given)

$$\frac{\partial n_z}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r} r\left(D\frac{\partial n_z}{\partial r} - v n_z \right) +$$

just radial transport

$$n_e\left(S_{z-1,z} n_{z-1} - S_{z,z+1} n_z \right) +$$

ionisation via electron collisions

$$n_e\left(\alpha_{z+1,z} n_{z+1} - \alpha_{z,z-1} n_z \right) +$$

recombination via electron collisions (radiative + di-electronic)

$$n_{D0}\left(\beta_{z+1,z} n_{z+1} - \beta_{z,z-1} n_z \right)$$

recombination via CX with D^0

- for all ion stages z of an impurity
- S, α, and β are generalized collisional-radiative (CR) rate coefficients, (e.g. including ionisation from excited states → e.g. from ADAS)

2nd step) Add up radiation losses for each ion stage

$$\mathrm{P/V} = n_e \sum_z n_z \left[l_{exc,z} + l_{rec,z} + \frac{n_{D0}}{n_e} l_{cx,z} + c_{rec,z} + c_{brems,z} \right]$$

Radiative rate coefficients
(from equilibrium solution of the CR model for each ion stage)

- $l_{exc,z}$ total line radiation due to excitation
- $l_{rec,z}$ total line radiation due to recombination
- $l_{exc,z}$ total line radiation due to charge exchange
- $c_{rec,z}$ sum of all recombination continua
- $c_{brems,z}$ bremsstrahlung

3rd step) model the diagnostic signals

Line emission as seen by passive spectroscopy

- Photon emissivity coefficients for a single multiplet due to excitation / recombination / CX

Soft X-ray

- Total radiation coefficients as above folded with the sensitivity of the soft X-ray cameras

Charge exchange spectroscopy

- Photon emissivity coefficients for CX into high n-levels

- all from CR models

Outline

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- **Role of recombination via charge exchange (CX) reactions**
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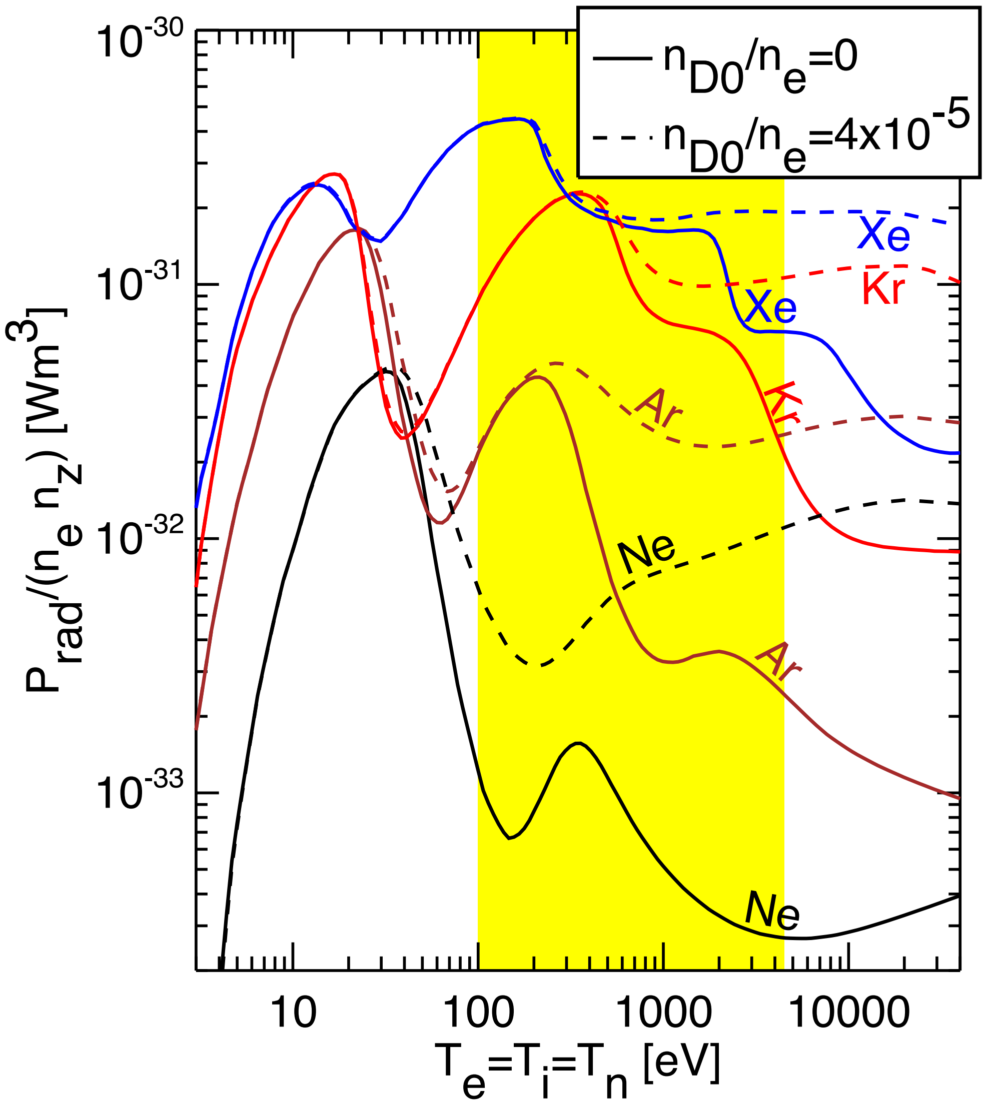
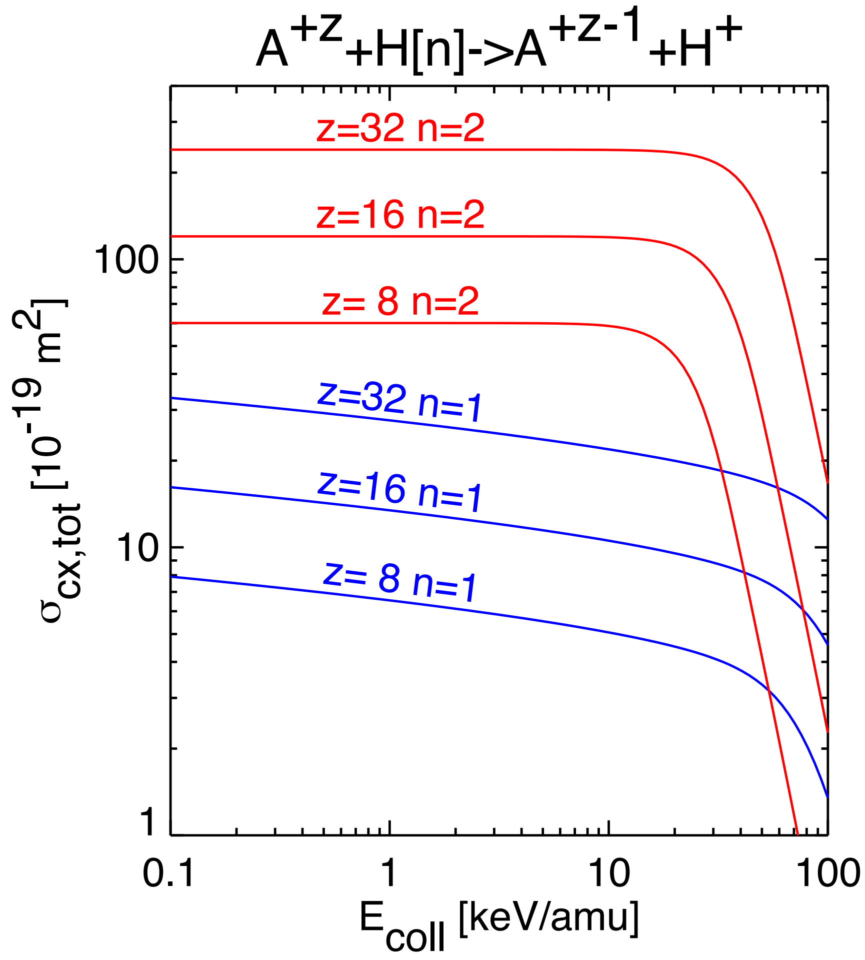
Cooling factors with/without CX

- The charge stage distribution defines how much power an impurity radiates at a certain temperature
- Even a small fraction of neutral hydrogen shifts the ionisation balance to lower ionised stages due to the additional recombination via charge exchange (CX) reactions



Cross Sections for CX between H and Impurities

- One formula for all impurities in all charge stages for H in ground state and one for H in n=2 !
- New data for total CX cross sections would be very welcome



Janev, R.K. and Smith, J.J. (1993) At. Plas. Mat. Int. Data for Fus., vol.4, p. 172-174

Fit to experimental profiles (CXRS) of Ne^{10+} and Ne^{8+} only when CX is included

- Without CX:
  density of Ne^{8+} too low
  by a factor 15-28 for $0.9<\rho_{pol}<0.98$

- Prad of Ne in confined plasma increases by factor 5 when CX is included

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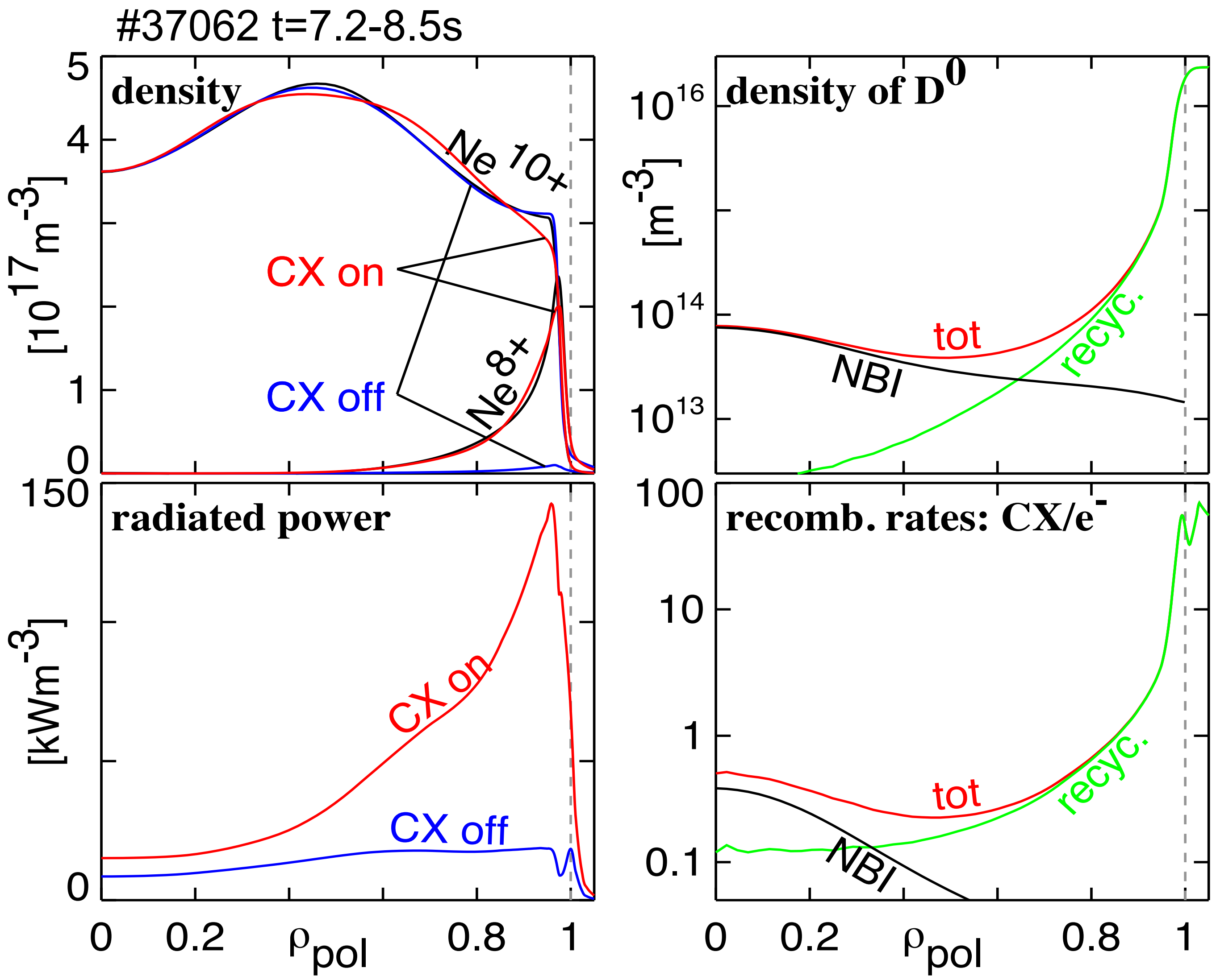
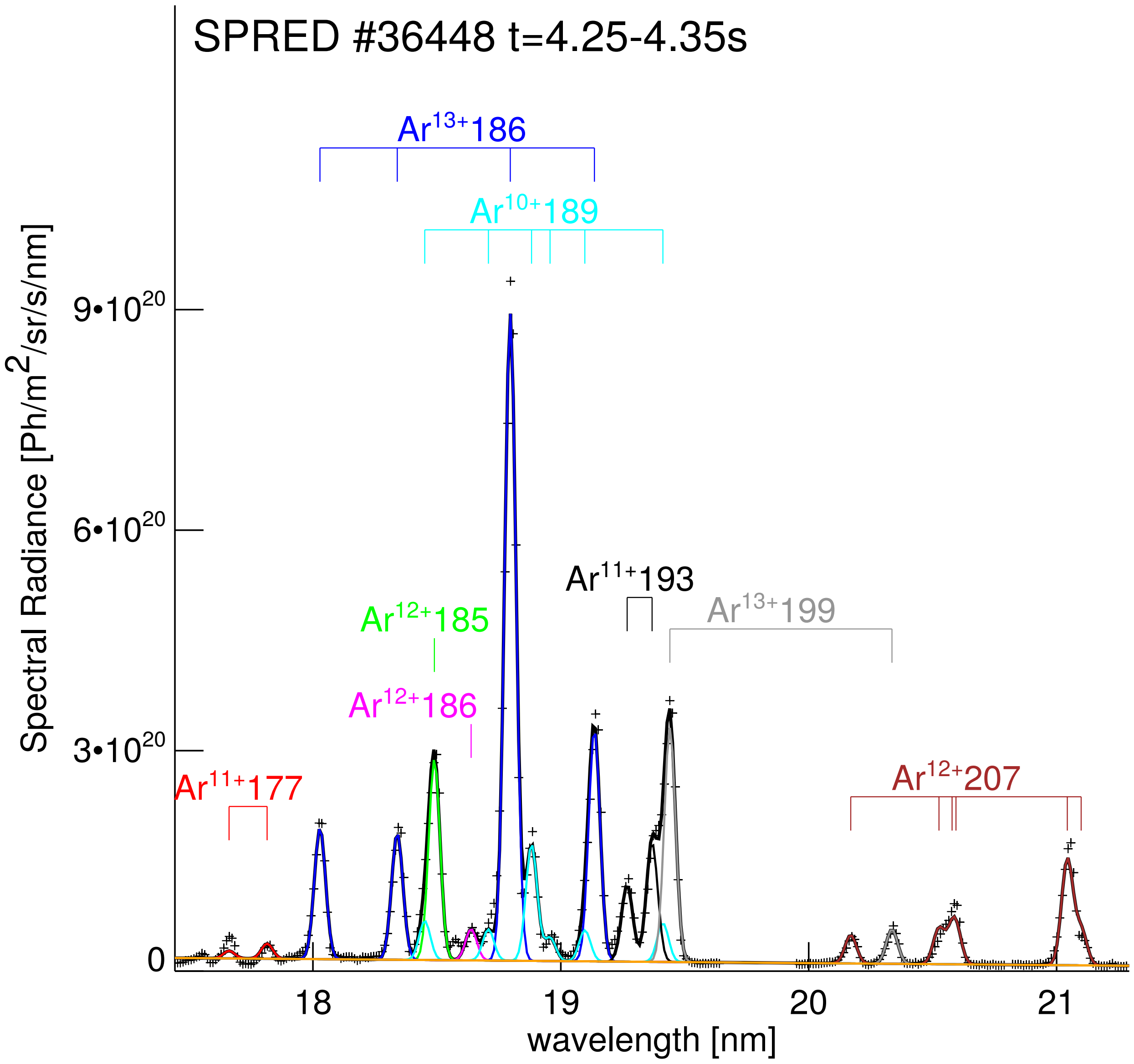


VUV Line Emission Ar^{6+} - Ar^{15+}

SPRED

(Survey Poor Resolution Extended Domain)

- **1 radial line-of-sight at mid-plane**
- **12-90 nm**
- **lines from Ar^{6+} - Ar^{15+}**
- **here just a small region of the spectrum**

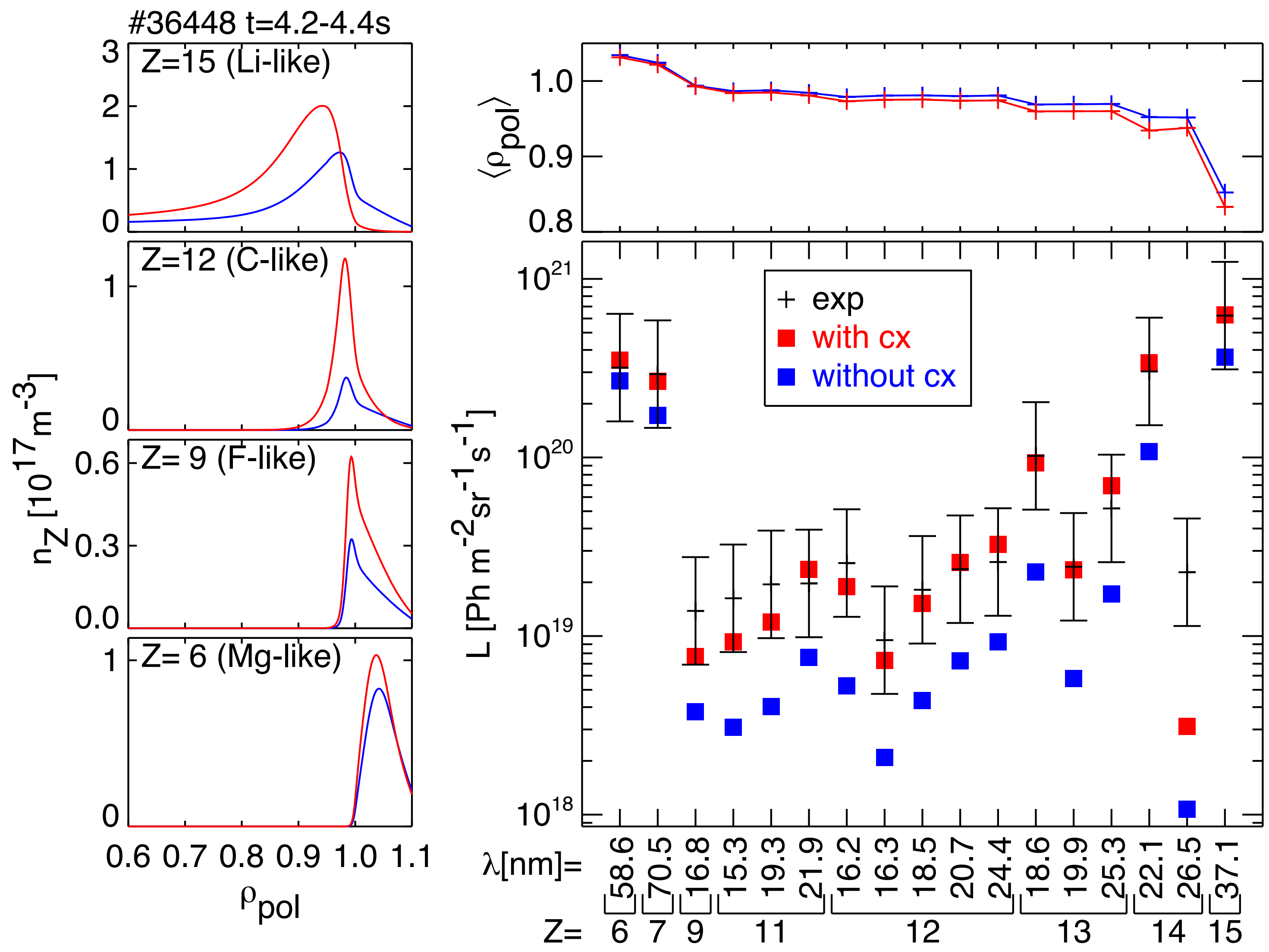


VUV Line Emission Ar^{6+} - Ar^{15+}

photon emissivity coefficients from new atomic data* for all Ar ions

CX on

- **the radiance of almost all lines from ions Ar^{6+} - Ar^{15+} fit the measurement**
- **mean deviation = 24%**
- **max deviation = - 44%**
- **outlier: ArXV at 26.5nm: off by a factor of 7.4**



* M.M. Bluteau (2019) PhD thesis, Univ. Strathclyde

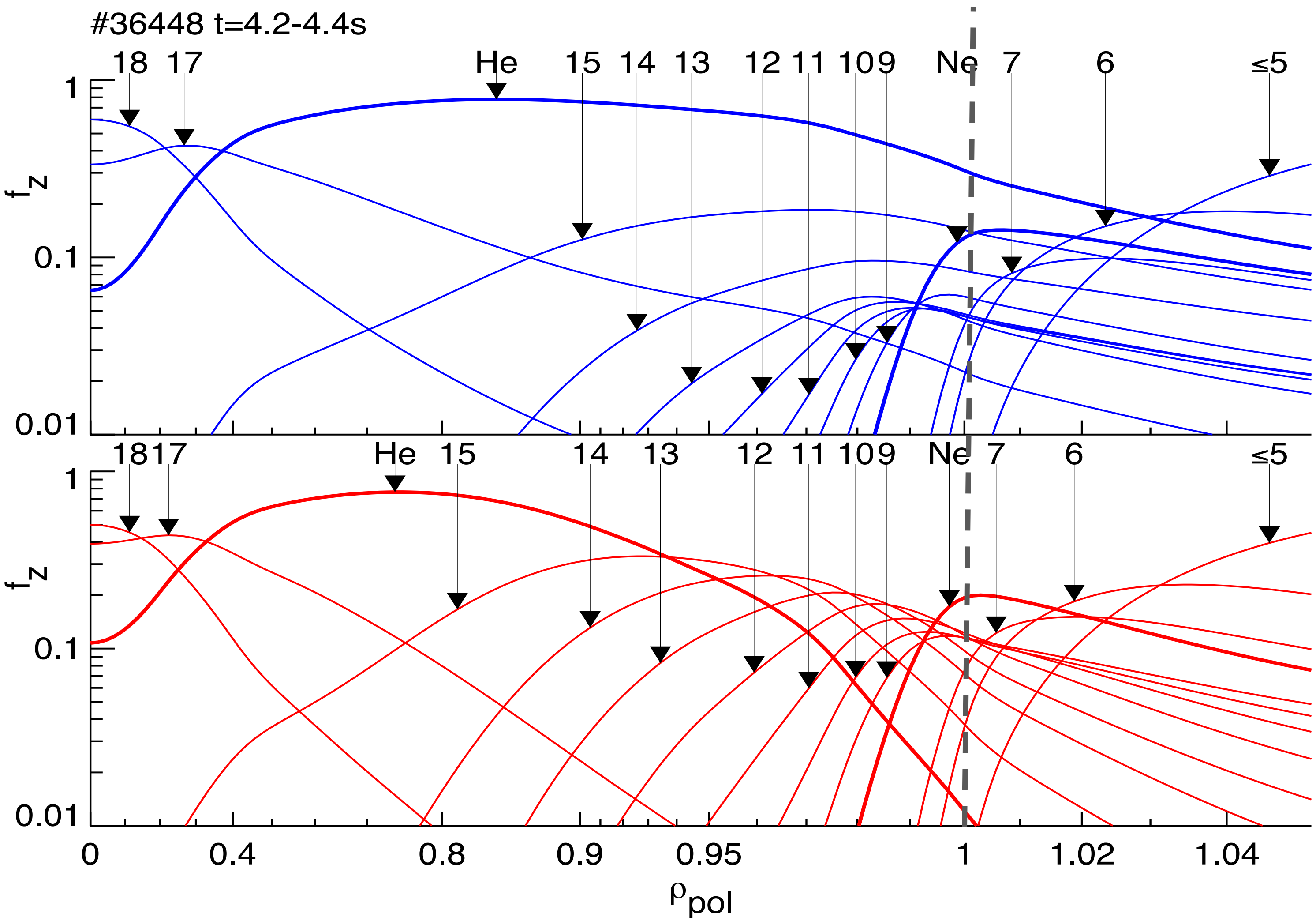
Effect of CX on Ar near separatrix
Ion stages below He-like have much higher abundances

CX off:

- **He-like Ar has the highest fractional abundance in most of the plasma even at the separatrix**

CX on:

- **Li-, Be-, B-, …stages become the dominant charge stages in the pedestal region**



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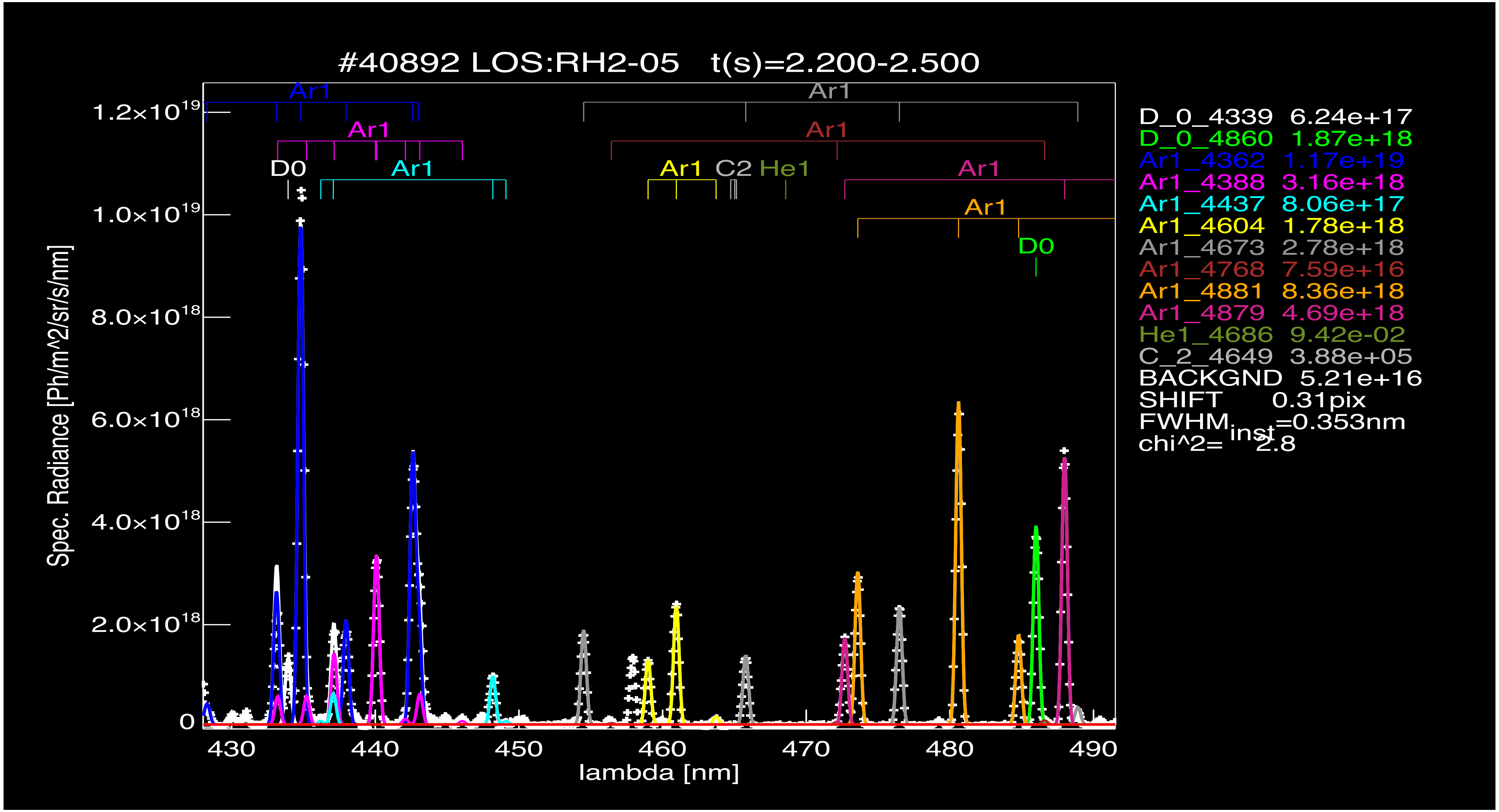
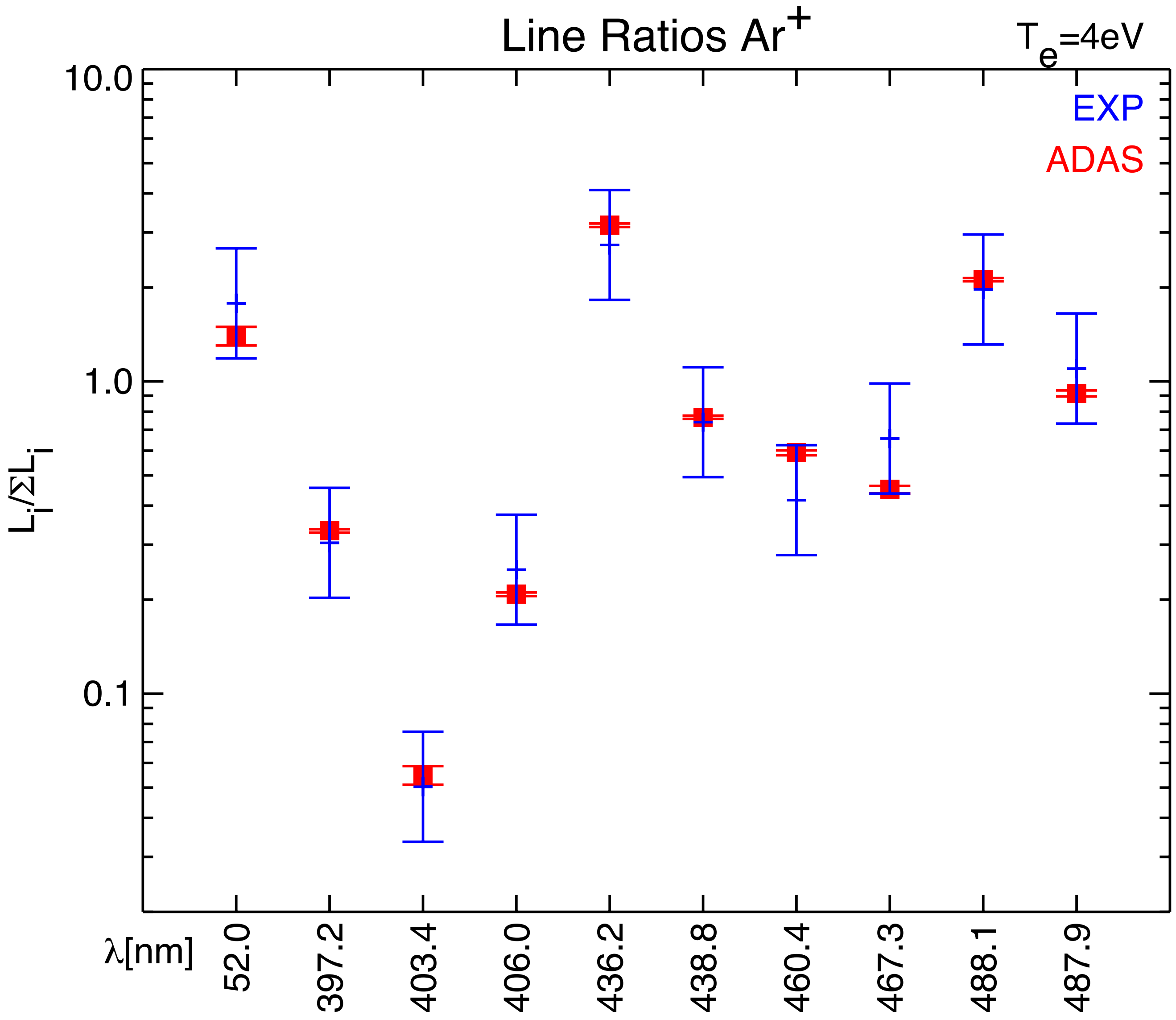
Ar1+ spectrum around 460nm



Line Ratios of Ar^+

Experiment vs ADAS*:

- **$n_e \approx 5x10^{19} m^{-3}$ $T_e \approx 4eV$**
- **within a factor of 1.5 in agreement**

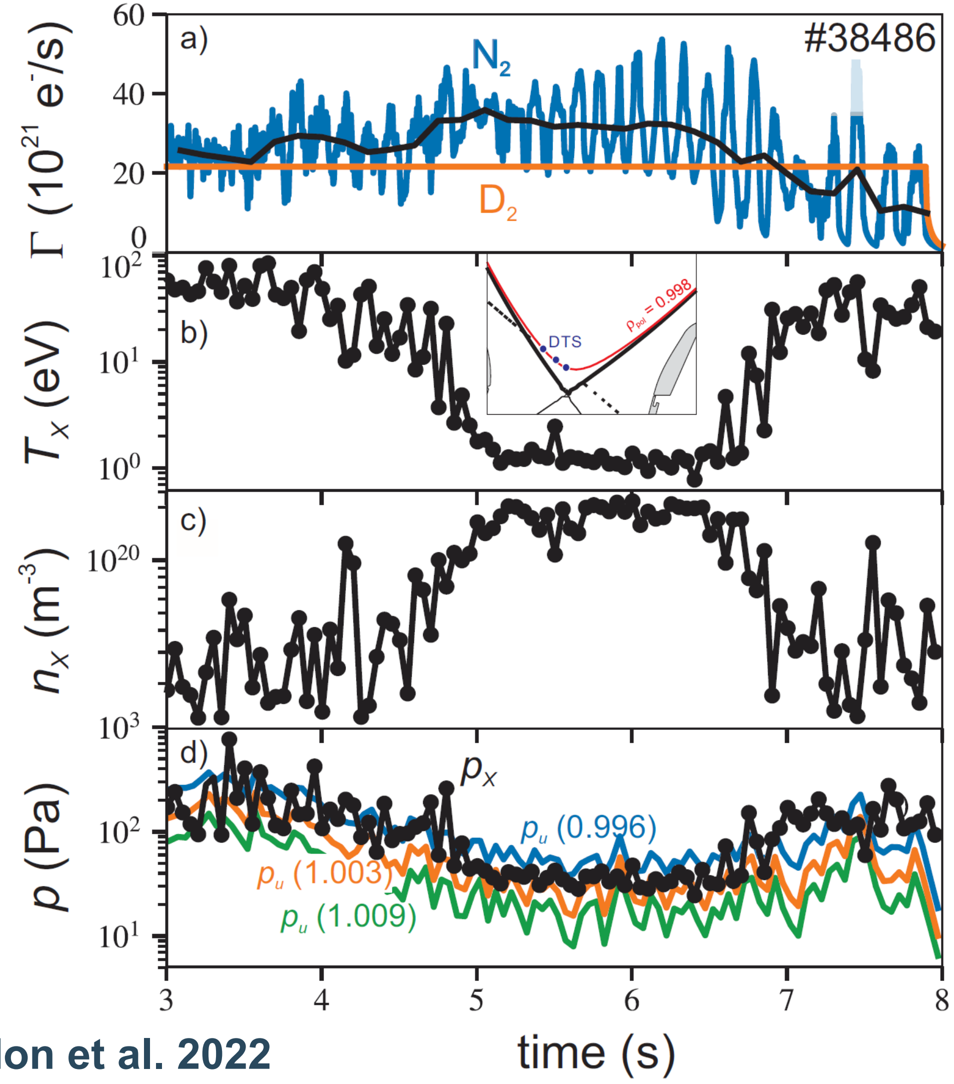


*** M.M. Bluteau (2019)
PhD thesis, Univ. Strathclyde**

Nitrogen vs noble gases considering NHx

- much better radiator than Ne in small machines
- highly questionable radiator for ITER due the strong hydrogen chemistry
- SOLPS ITER modelling predicts difference between N and Ne to disappear in large devices (needs further validation)
- what counts is the radiated power per fuel dilution
- if N does not outperform Ne or Ar in this parameter, N should be avoided
- I would invest the manpower in atomic data and CR modelling to allow for a good comparison of N, Ne, Ar, (and Kr) radiators

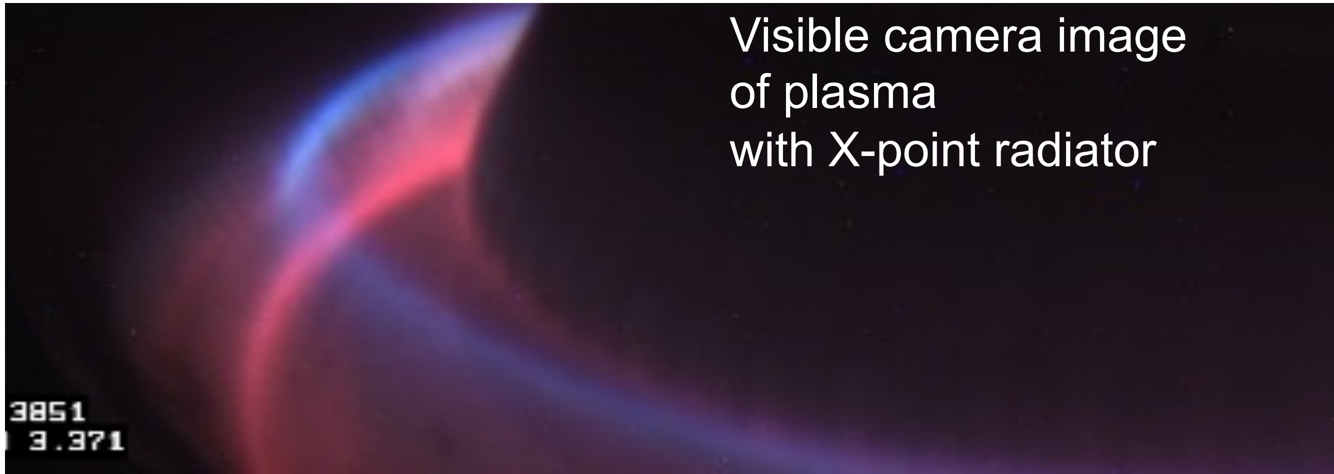
Temperature range for atomic data has to be wide: 1eV–10 keV



Cavedon et al. 2022
NF (62) 066027

Divertor TS measurements during a transition into the X-point radiator regime in AUG

- *T* drops to about 1eV and *n* increases at constant pressure on flux surface



Visible camera image
of plasma
with X-point radiator