Developing local high-Z impurity density measurements for impurity transport using high-n Rydberg transitions on DIII-D

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Motivation: Quantify tungsten transport for fusion power plants

- **Tungsten is the primary plasma facing component proposed for burning plasma experiments (ITER) and fusion pilot plants**

- **Tolerance for high-Z impurity sourcing into magnetically-confined plasmas is extremely low due to radiative losses [1]**
  - Low-z ($z \leq 10$) concentrations ~ 10^{-3}
  - High-z ($z \geq 20$) concentrations ~ 10^{-5}

- **Scenario development employing ion temperature screening may serve to create conditions for impurity pump out**
  - Experiments with impurity injection and diagnostics to measure high-Z impurity transport
  - Could benefit from a diagnostic sensitive to multiple, disparate charge states

[1] T. Pütterich, *et al.* Nuclear Fusion **59**, 056013 (2019)

Highly charged impurity ions have a proportionally large charge exchange cross section

- **Work of Janev et al.[1] showed that the charge exchange cross section increases with ion charge in a predictable way, $\sigma_{cx} \propto z$**
- **Verified by work with Argon charge exchange measurements[2]**
- **Tungsten charge exchange emission observed in tungsten pellet injection experiments on LHD[3] and as contamination lines in JET with an ITER-like wall[4] as well as other tokamaks with tungsten surfaces. More recently also on W7-X[5].**

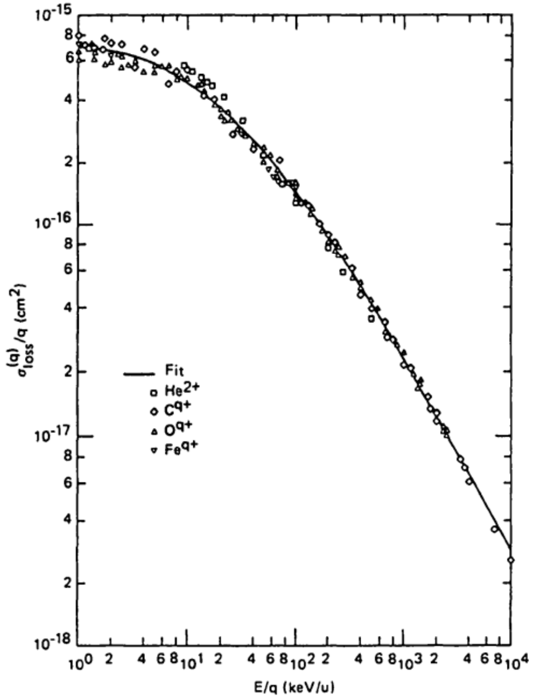
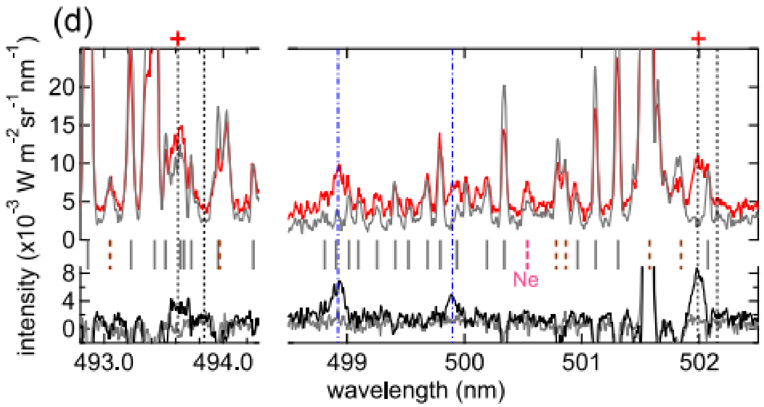
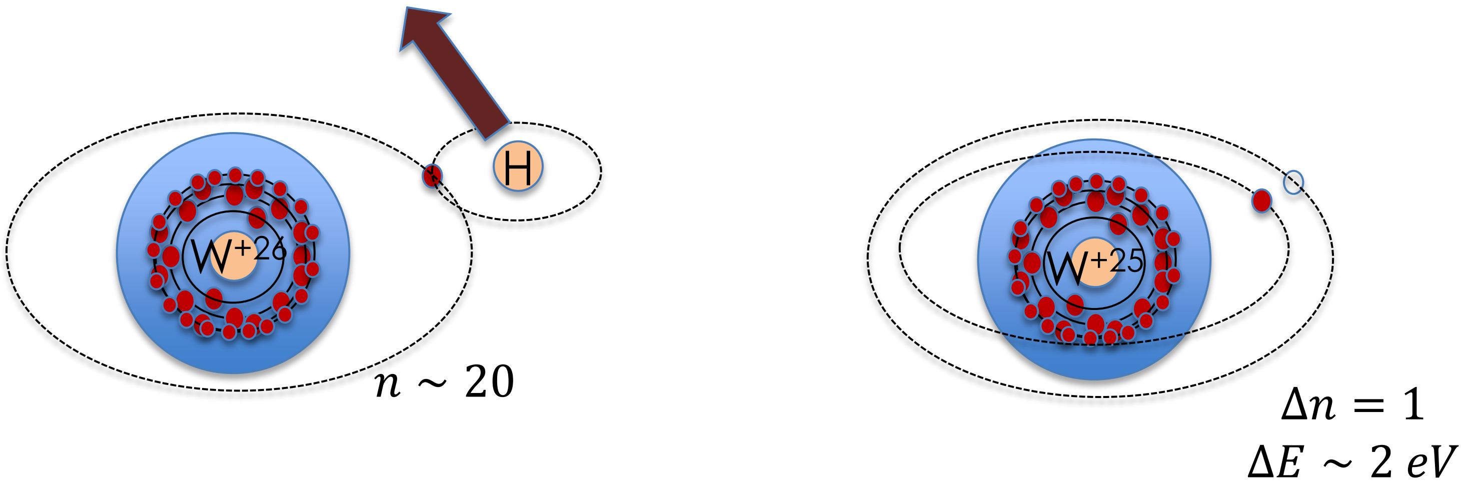


FIG. 4. q-scaled electron loss cross-section for H(1s) by impurity impact ($A^{q+} = He^{2+}, C^{q+}, O^{q+}, Fe^{q+}$).



[1] R.K. Janev et al Nucl. Fusion **29** 2125 (1989)
[2] A. Foster PhD Thesis (2008)
[3] M. Shinohara et al *Phys. Scr.* **90** 125402 (2015)
[4] A. Thorman *et al Phys. Scr.* **96** 125631 (2021)
[5] C. Swee *et al.* Nucl. Fusion **64** 086062 (2024)

These highly-excited charge-exchange ions are well-approximated as Rydberg states



- **Charge exchange populates states that differ in energy by only a few eV (visible range)**

- **Bohr’s correspondence principle suggests that a semi-classical model should give a sufficiently accurate prediction of the transition wavelengths**

Transitions between highly excited states in heavy ions require the relativistic correction of classical quantum theory

When the centripetal force is balanced against the electrostatic force the Ryberg formula is obtained: $\frac{1}{\lambda} = R\, Z^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) = \frac{\alpha^2 m_e c}{4\pi h} Z^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$

$E = \frac{hc}{\lambda} = \left(\frac{1}{2} m_e v_1^2 - \frac{1}{2} m_e v_2^2\right)$ **where** $v = \frac{Z\alpha}{n} c$ **(Sommerfeld's classical model)**

…but for highly charged ions $\frac{Z\alpha}{n}$ isn't small

we need to account for relativistic velocities

$$E = \frac{hc}{\lambda} = Z^2 \left(\frac{m_e c^2}{\sqrt{1 - \left(\frac{v_1}{c}\right)^2}} - m_e c^2 - \frac{m_e c^2}{\sqrt{1 - \left(\frac{v_2}{c}\right)^2}} + m_e c^2 \right)$$

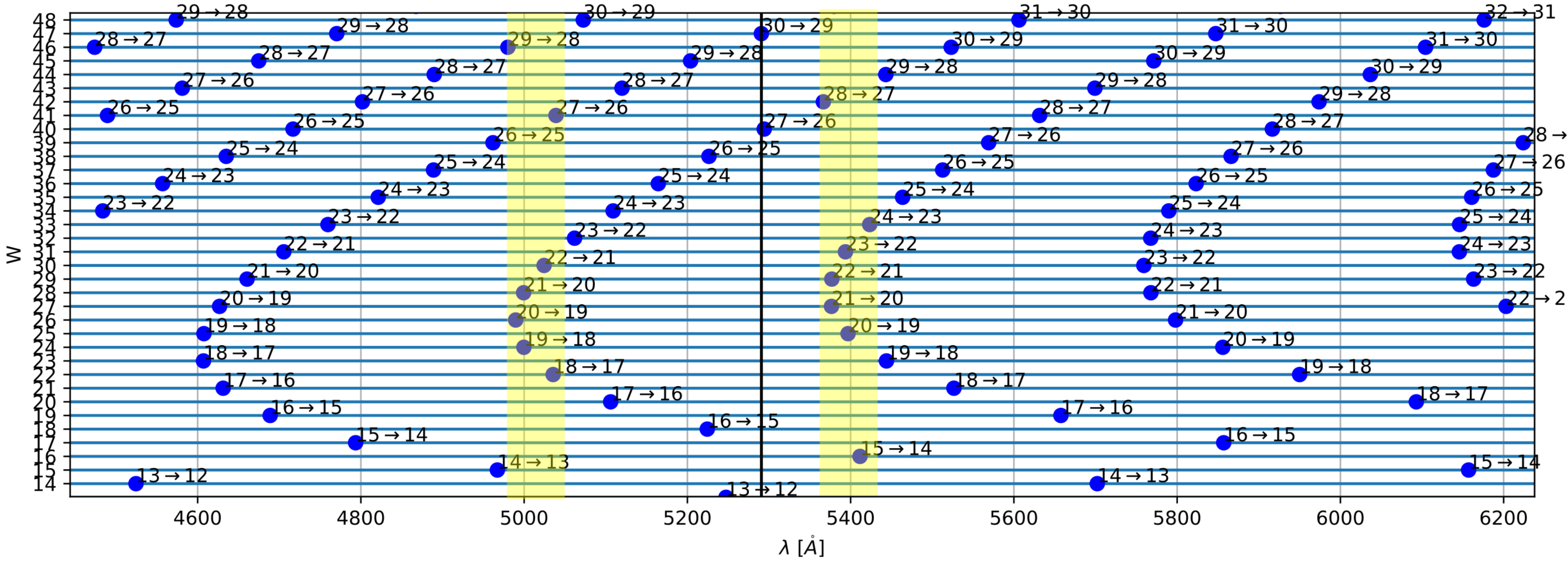
$$\lambda = \left(\frac{h}{m_e c}\right) \left(\frac{1}{\sqrt{1 - \left(\frac{Z\alpha}{n_1}\right)^2}} - \frac{1}{\sqrt{1 - \left(\frac{Z\alpha}{n_2}\right)^2}} \right)^{-1}$$

Suto, K., J. Mod. Phys., **11**, 528-534 (2020)
10.4236/jmp.2020.112018

Haug, E.G., J. Mod. Phys., **11**, 528-534 (2020)
10.4236/jmp.2020.114035

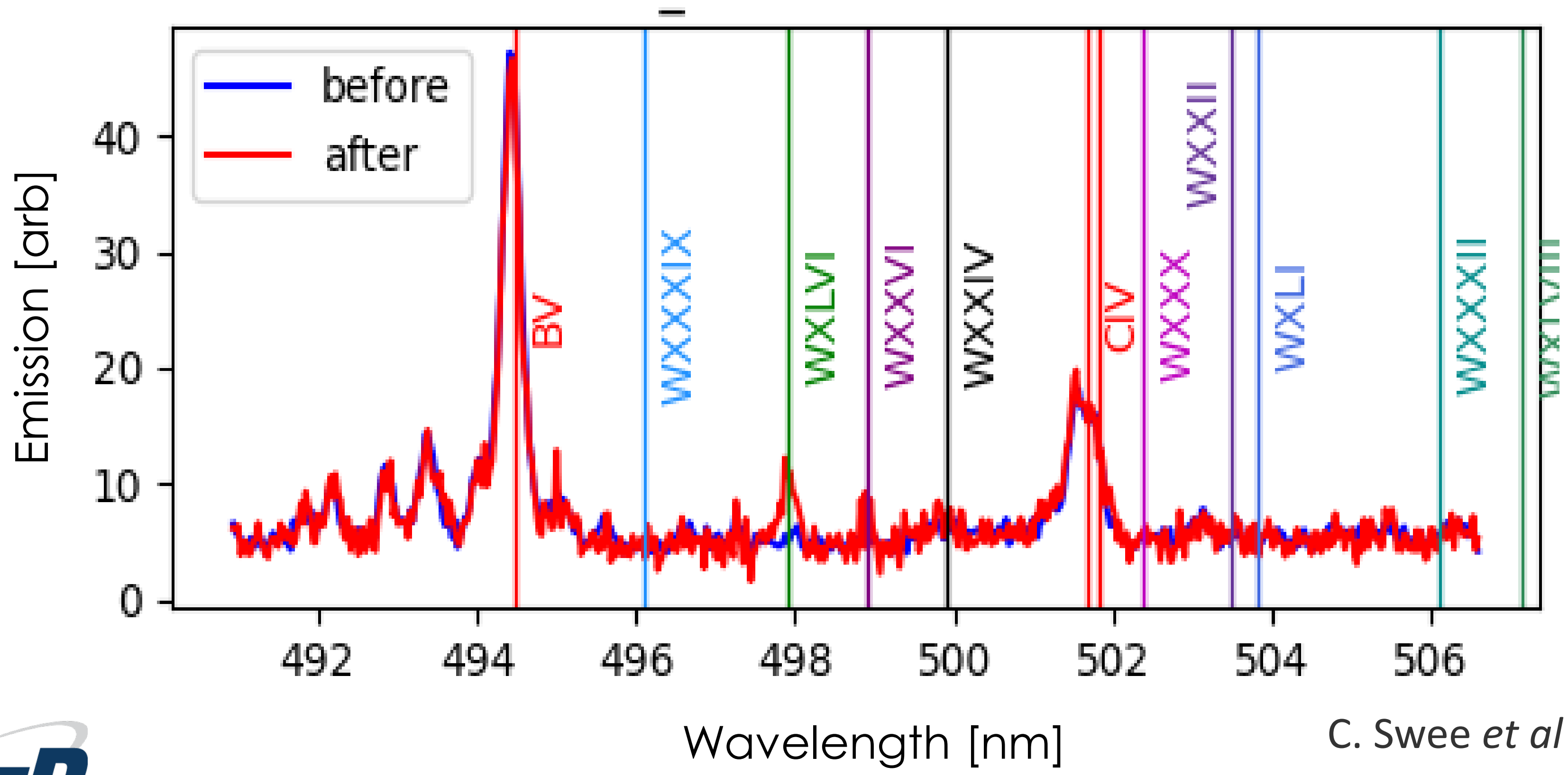
Multiple charge states are expected within narrow wavelength ranges

- **There are a regions in the visible spectrum where several transitions from different charge states can be expected to be emitting**
  - (W22+),W24+, W26+, W28+, W30+, (W32+) between 4980-5070A
  - (W23+),W25+, W27+, W29+, W31+, (W33+) between 5370-5450A



High-n Rydberg transitions provide data from a wide charge state range

- **From data acquired on W7-X (S. Peiro), we can see emission lines ranging from W^{+23} to W^{+45}**
- **All resolvable within a 15 nm range!**

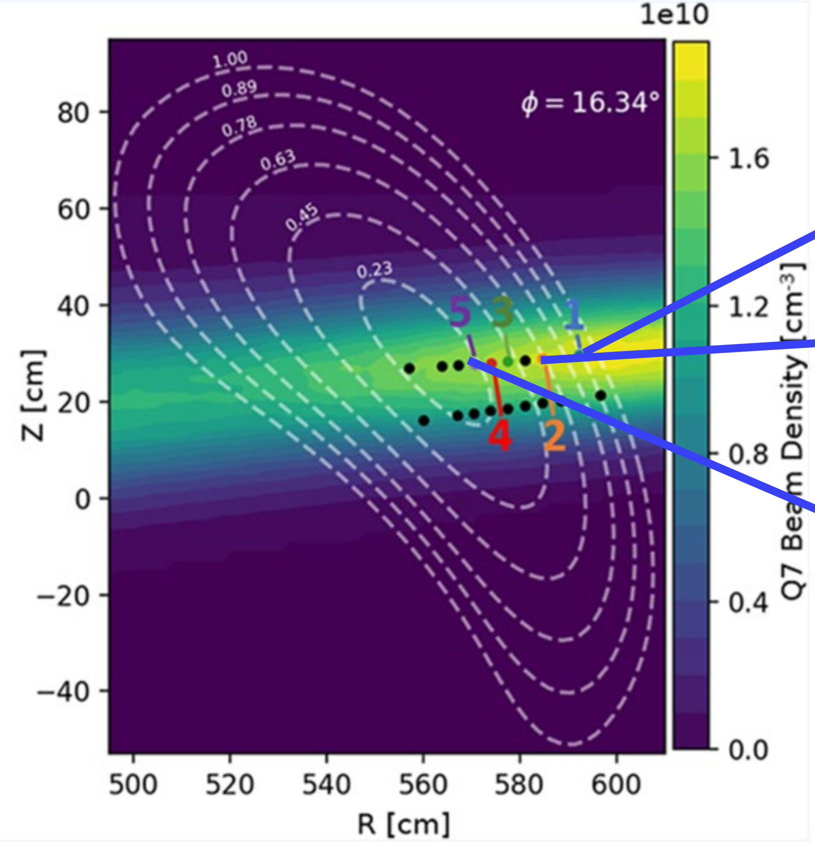


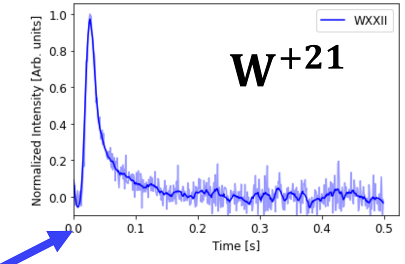
Wavelength (nm)	q	n_{upper}
496.10*	**38**	**25**
497.92*	**45**	**28**
498.91*	**25**	**19**
499.87	27	20
499.91*	**23**	**18**
502.38*	**29**	**21**
503.50*	**21**	**17**
503.82	40	26
506.11	31	22
507.15*	**47**	**29**

C. Swee *et al Nucl. Fusion* **64**, 086062 (2024)

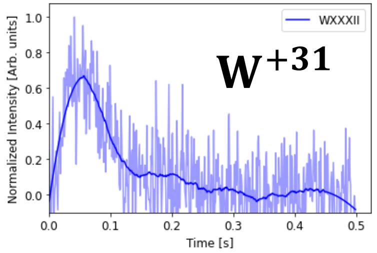
Observation of multiple charge states informs impurity dynamics

Example: Emission from different charge states following Tungsten LBO in W7-X is used for quantifying impurity transport

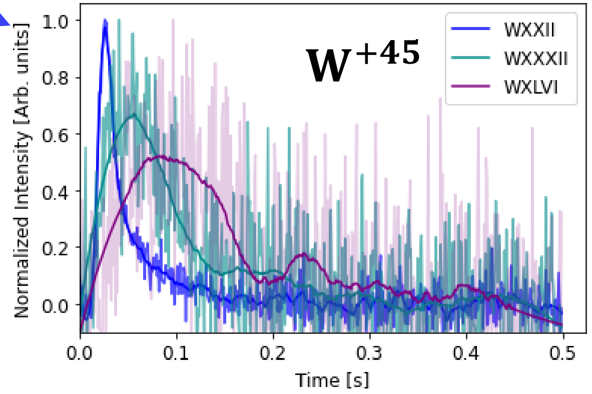




Lower charges states appear promptly near the edge



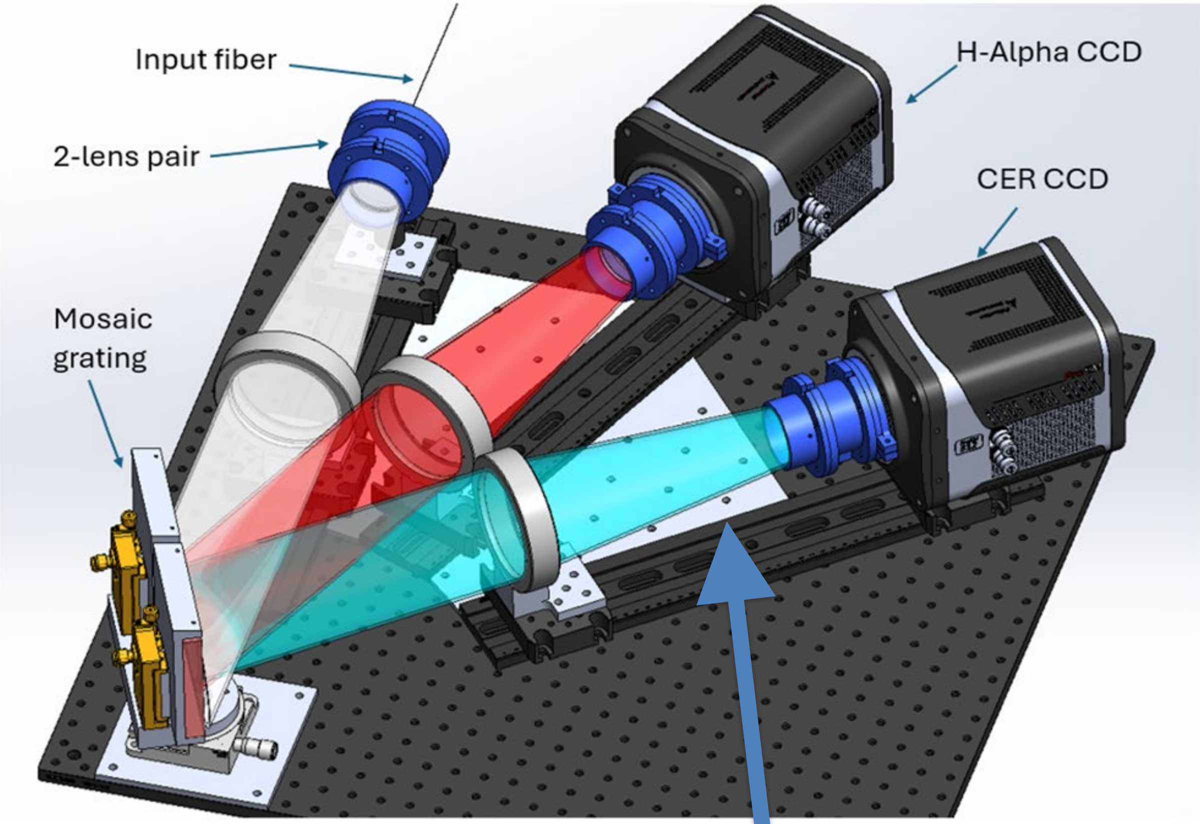
Higher charges states appear after a delay and deeper in the plasma



Peiro, *et al.*, Hidden Symmetries and Fusion Energy Retreat (2025)

DIII-D NATIONAL FUSION FACILITY

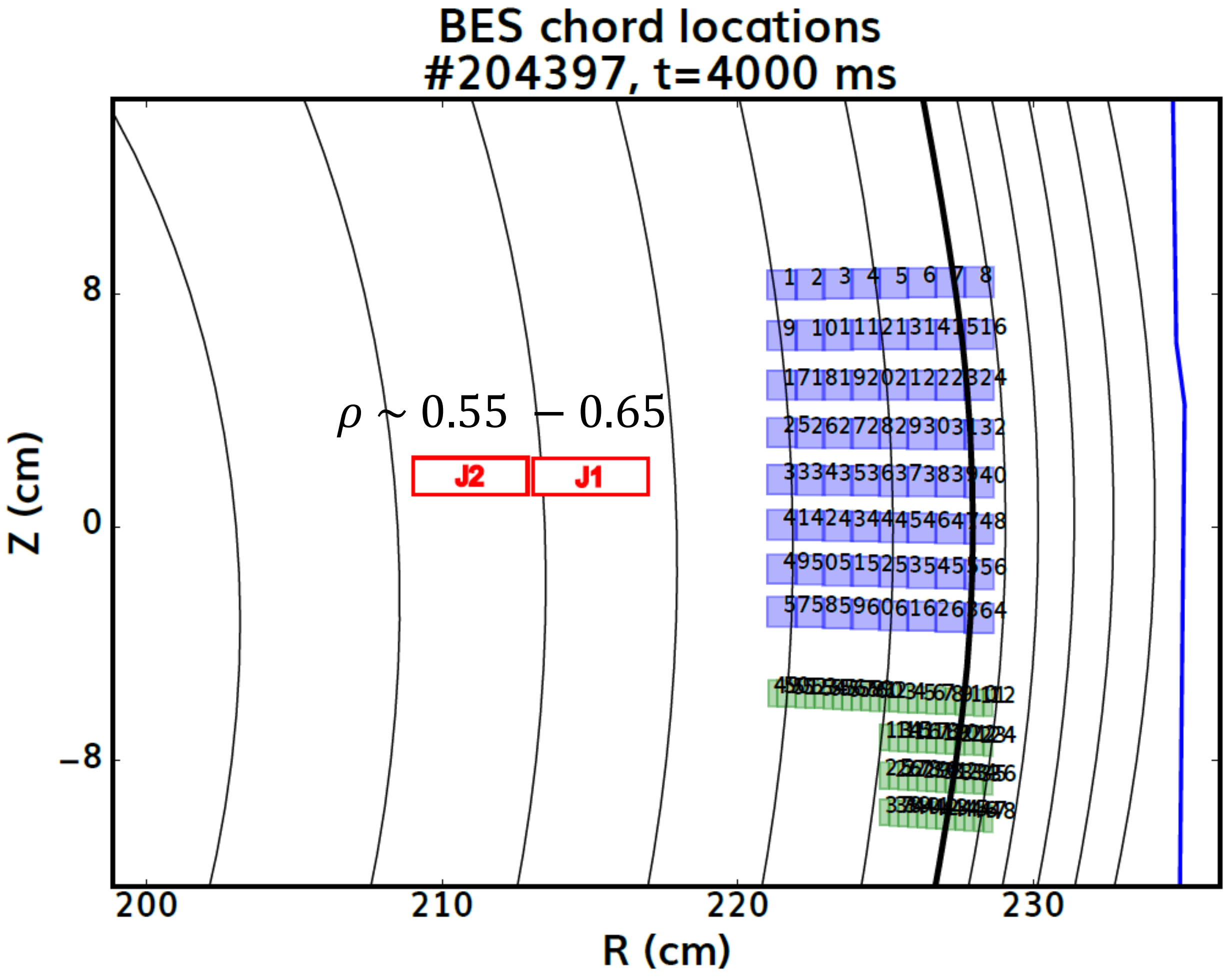
We modified the Edge J_R and CXR spectrometer to look for these transitions in DIII-D plasmas



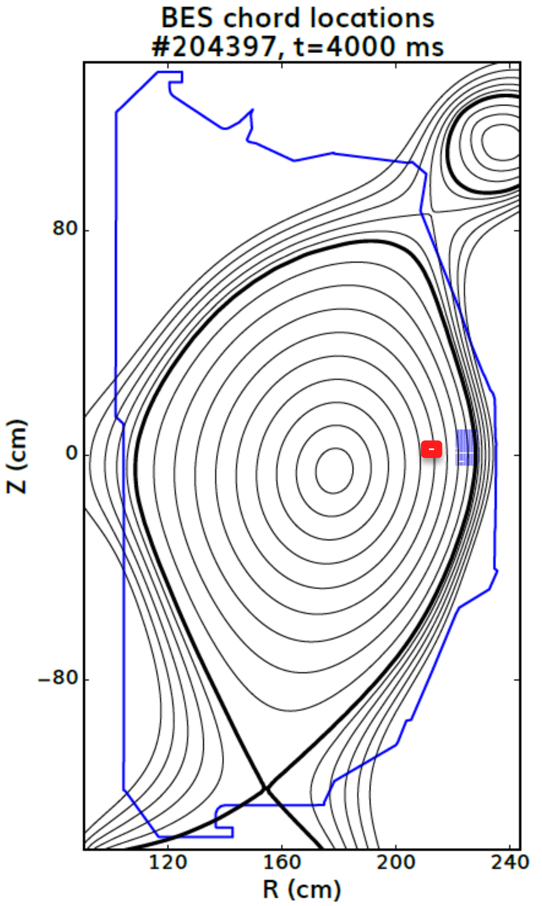
Configuration	Angle	Wavelength Range [nm]
Original Carbon CER	43.7°	519 to 532
New high-n CER	47.7°	495 to 508

R. Albosta *et al.*
Rev. Sci. Instrum. **95**, 093519 (2024)
Rev. Sci. Instrum. **93**, 113546 (2022)

Moved spectrometer channels to hotter region of plasma where desired charge states of W are predicted from collisional-radiative modelling



$\rho \sim 0.55 - 0.65$

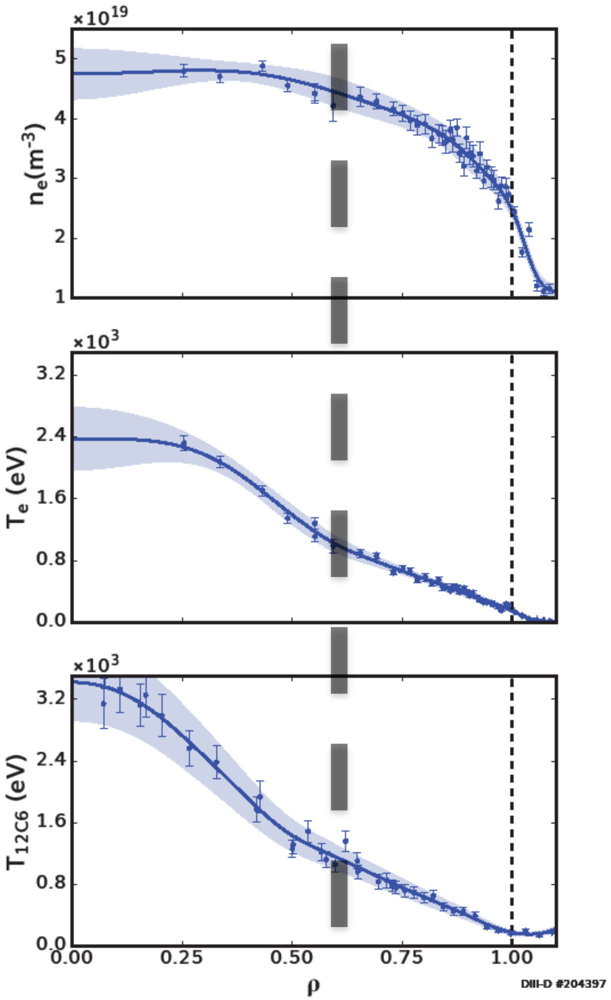


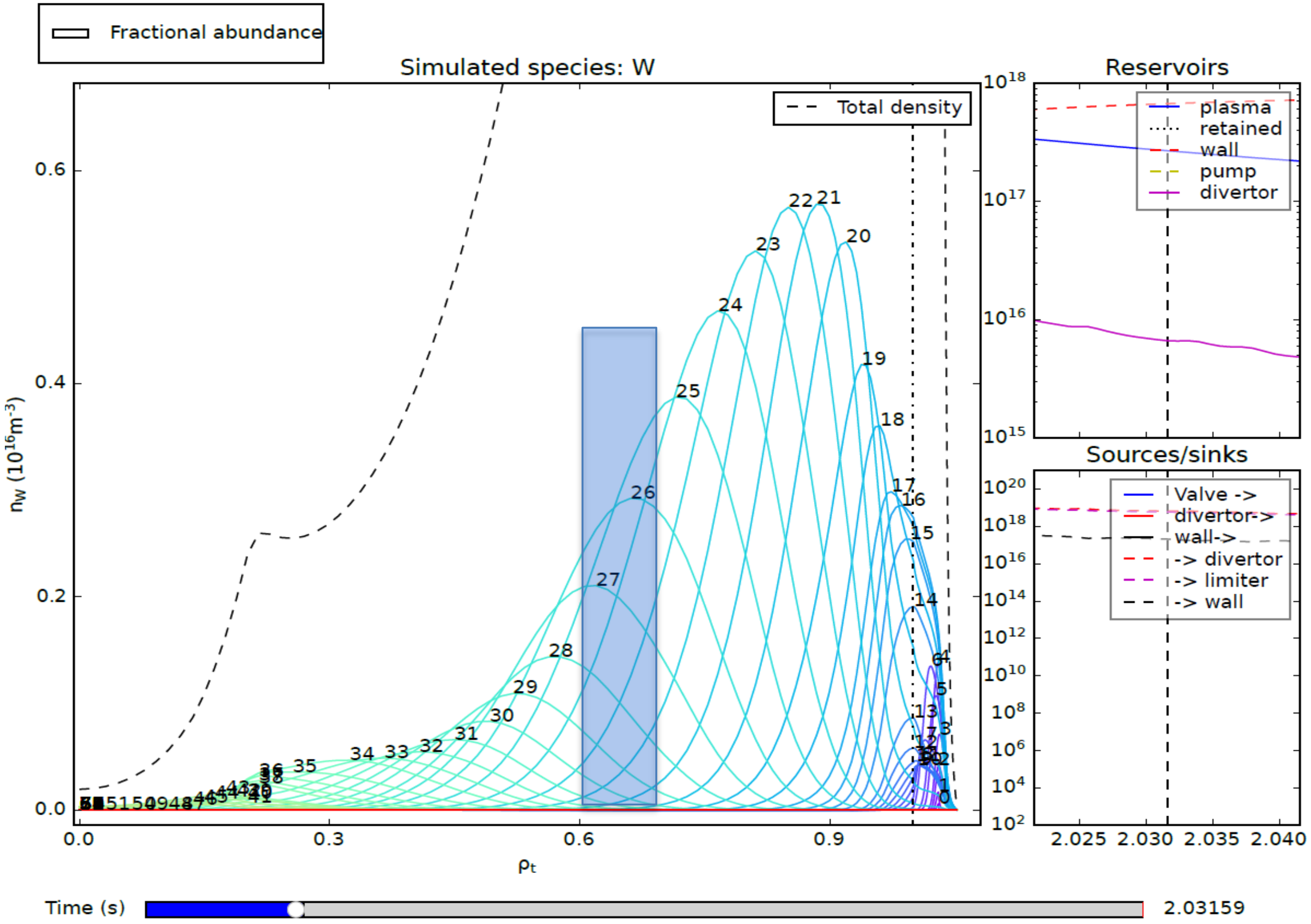
Impurity transport modelling with Aurora using SXR emission shows $W^{+24,+26,+28}$ present at measurement locations

Electron density & temperature profiles measured with Thomson Scattering and C^{+6} temperature measured through CXR at time of LBO

Tungsten charge state balance determined using Aurora collisional-radiative transport code

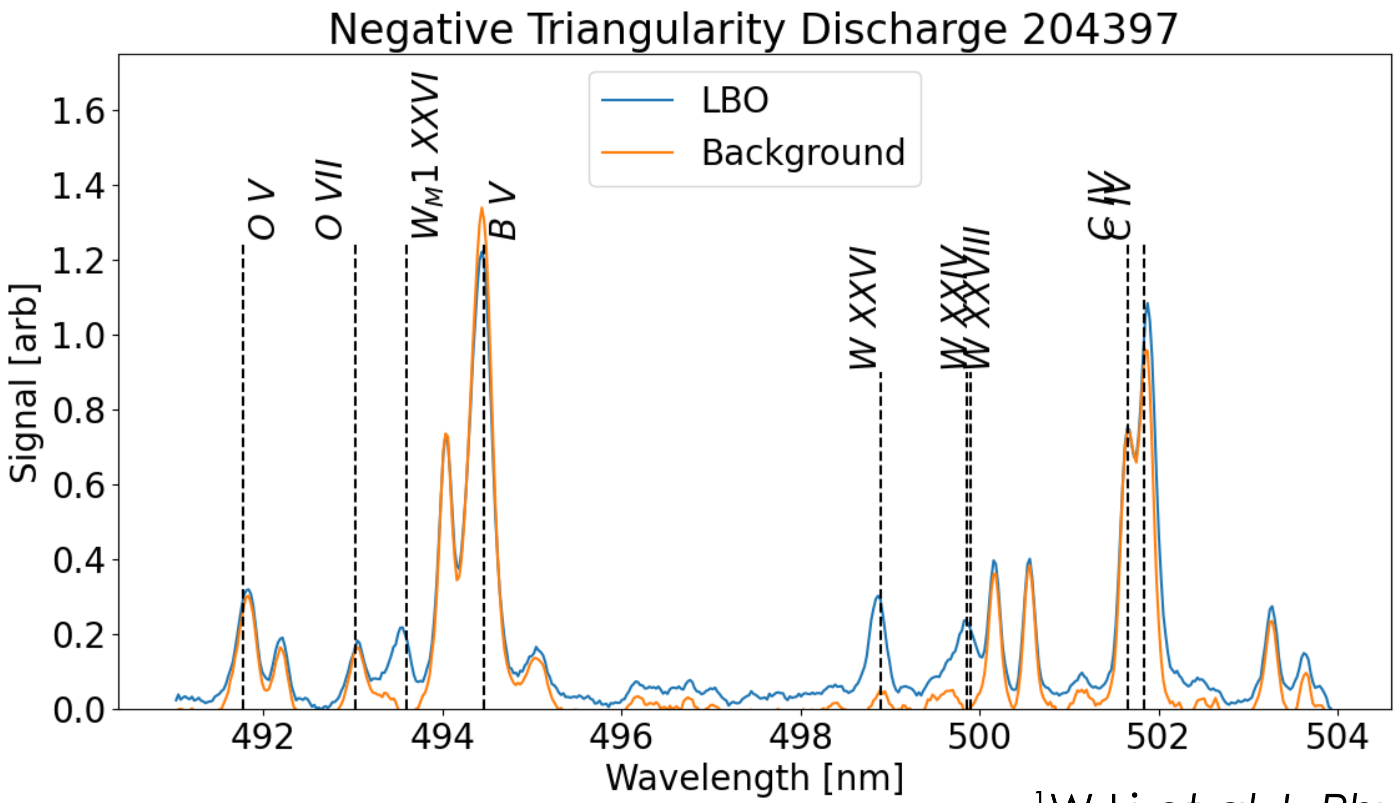
Recall: Ion charge states will recombine through charge exchange with a neutral beam hydrogen atom to form W^{+23}, W^{+25}, and W^{+27}





Emission from both Rydberg transitions in $W^{+23,+25,+27}$ and an W^{+25} M1 transition observed from LBO events

2025/07/09	Particle and impurity transport in negative triangularity discharges	Tomas Odstrcil, A. Biwole, *et al.*	MP 2025-15-01



- Wavelength calibrations corrected using surrounding known emission lines of carbon and oxygen

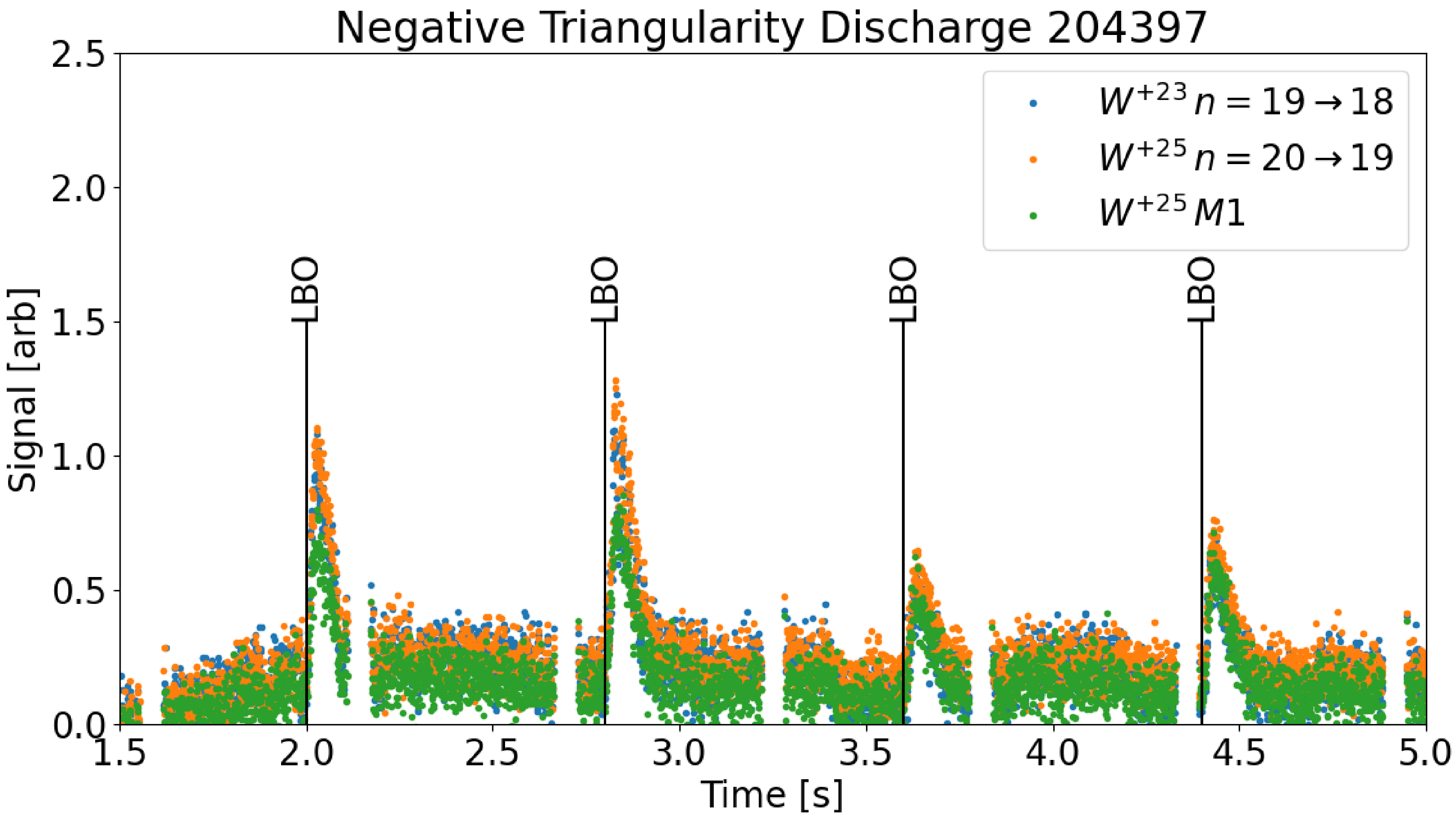
- Rydberg transitions observed:
  $W^{+25}\ n = 20 \rightarrow 19$
  $W^{+23}\ n = 19 \rightarrow 18$
  $W^{+27}\ n = 21 \rightarrow 20$

- W^{+25} M1 forbidden transition[1,2] was also observed

[1] W Li *et al J. Phys. B: At. Mol. Opt. Phys.* **49** 105002 (2016)

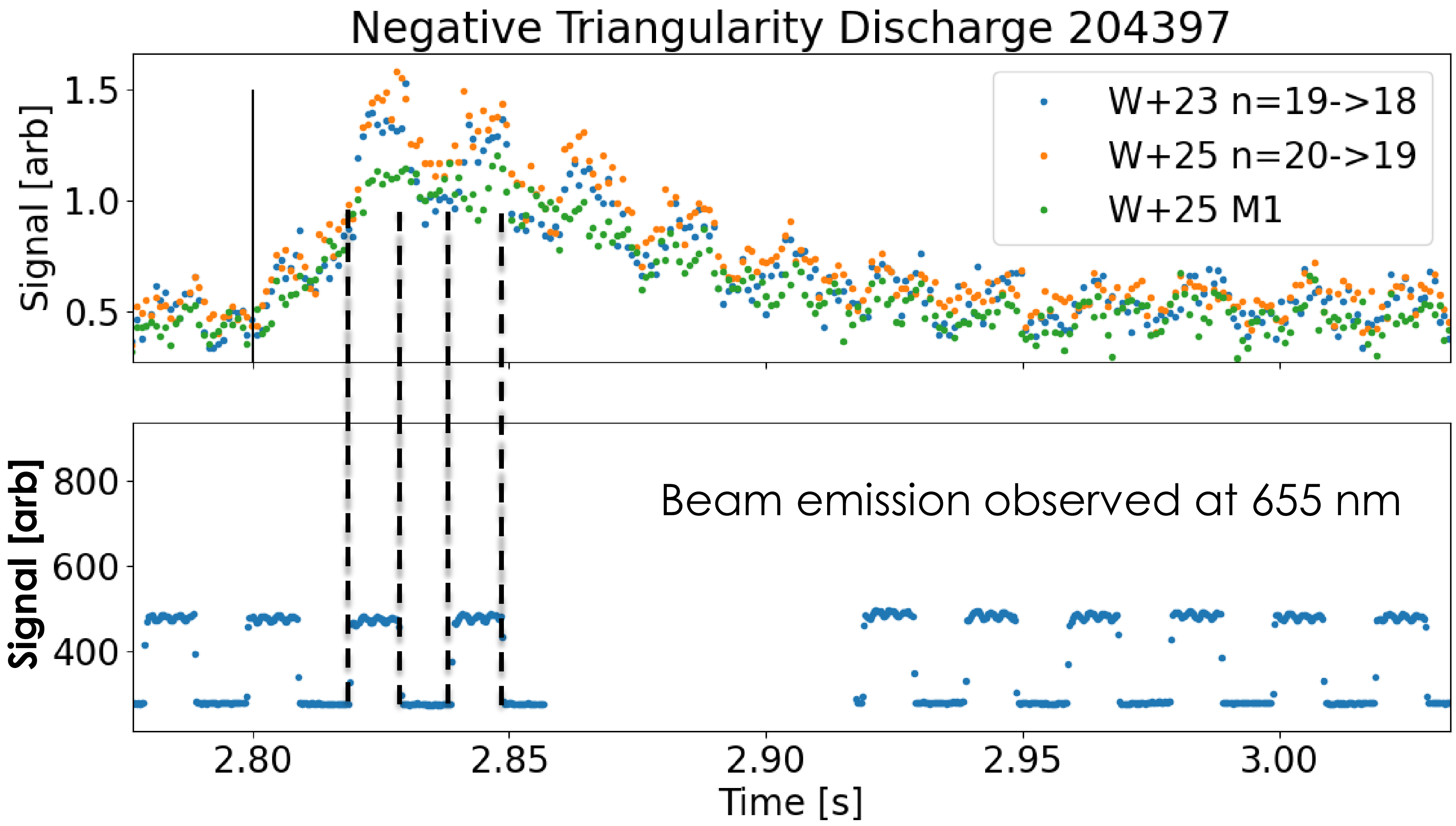
[2] A. Thorman *et al* 2021 *Phys. Scr.* **96** 125631

Evidence of W^{+23} and W^{+25} in DIII-D LBO discharges



- Charge states ranging from +23 and +25 show similar time dynamics
- Decay time after peak emission is ~ 50 ms, of order the impurity particle transport time

Beam modulation shows that the active charge exchange emission is comparable to the passive background emission



Strategy for determining photon emissivity coefficients for W charge exchange emission

- **The population of these highly-excited states is governed by a rate equation**

$$\frac{dn_k^z}{dt} = \underbrace{-n_k^z \sum_{i<k} A_{k,i}}_{\text{Spontaneous emission}} + \underbrace{\sum_{n>k} (n_n^z A_{n,k}}_{\text{Cascade from higher levels}} + \underbrace{n_0^{z+1} \sigma_n^{z+1} n^0 \, v_{\mathrm{beam}} \,)}_{\text{NBI charge exchange}} \underbrace{= 0}_{\text{Quasi-static equilibrium}}$$

$$\overleftrightarrow{A} \cdot \overrightarrow{\left(\frac{n^z}{n_0^z} \right)} = \left(\frac{n_0^{z+1}}{n_0^z} \right) \sigma_n^{z+1} n_{\mathrm{beam}}^0 v_{\mathrm{beam}}$$

- **To accurately model the population of the upper state of our desired transition we need to account for the cascade from charge exchange into higher levels $n > k$**
  - Spontaneous decay has a scaling $A_{n,k} \sim n^{-\frac{9}{2}}$
  - Level-resolved charge exchange cross section scales as $\sigma_n^{z+1} \sim n^{-3}$
  - We should have accuracy to about 1% if we evaluate the next 5 higher levels

Janev, J. Phys. Chern. Ref. Data, Vol. 12, No.4, 1983

To determine the impurity density from CX emission measurements requires solving a collisional radiative model for the newly formed ions

- **To determine the amount of light produced from the quasi-static excited state population we will need to calculate**

$$\varepsilon = \int n_k^z(\ell)\, A_{k,k-1}\, d\ell = \sum_E \int n_0^{z+1}\, n_{\mathrm{beam},E}^0\, q_{\mathrm{eff},E}\, d\ell$$

$$\text{where} \quad q_{eff,\mathrm{E}} = \frac{n_k^z\, A_{k,k-1}}{n_0^{z+1}\, n_{\mathrm{beam,E}}^0}$$

- **Solving for the quasi-static n_k^z population involves a matrix inversion for which we will need to know the n-resolved cross sections and the Einstein A coefficients**

$$\begin{bmatrix} -\sum_{i=1}^{1} A_{2\to i} & A_{3\to 2} & A_{4\to 2} & \cdots & A_{k_{\mathrm{max}}\to 2} \\ 0 & -\sum_{i=1}^{2} A_{3\to i} & A_{4\to 3} & \cdots & A_{k_{\mathrm{max}}\to 3} \\ 0 & 0 & -\sum_{i=1}^{3} A_{4\to i} & \cdots & A_{k_{\mathrm{max}}\to 4} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -\sum_{i=1}^{k_{\mathrm{max}}-1} A_{k_{\mathrm{max}}\to i} \end{bmatrix} \begin{bmatrix} N_{z,2} \\ N_{z,3} \\ N_{z,4} \\ \vdots \\ N_{z,k_{\mathrm{max}}} \end{bmatrix} = -N_0\, v_{\mathrm{beam}} \begin{bmatrix} \sigma_{z+1,2} \\ \sigma_{z+1,3} \\ \sigma_{z+1,4} \\ \vdots \\ \sigma_{z+1,k_{\mathrm{max}}} \end{bmatrix}$$

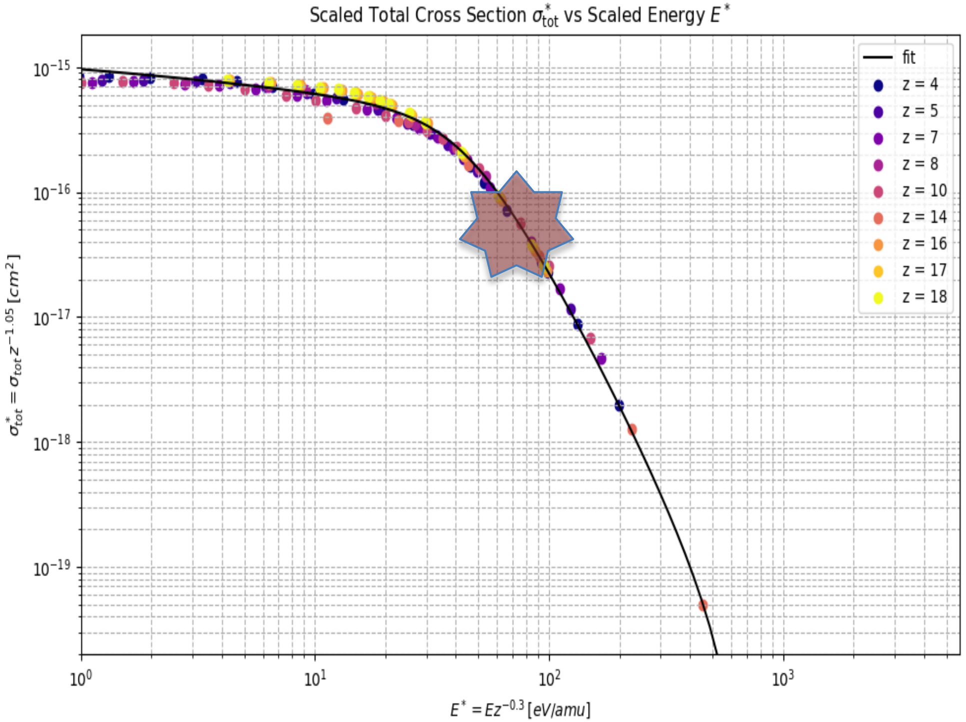
- **We can use the calculated $q_{eff,\mathrm{E}}$ to calculate the expected emission and compare with measurements to validate the approximation techniques**

Charge exchange cross sections show very similar energy scaling with ion charge and quantum level *n*

- **Universal scaling law observed for ion charge exchange based on ion charge z**

$$\sigma^*_{tot} = \frac{A log_{10}\left(\frac{B}{E^*}\right)}{1 + CE^* + DE^{*^2} + FE^{*^3} + GE^{*^4}}$$

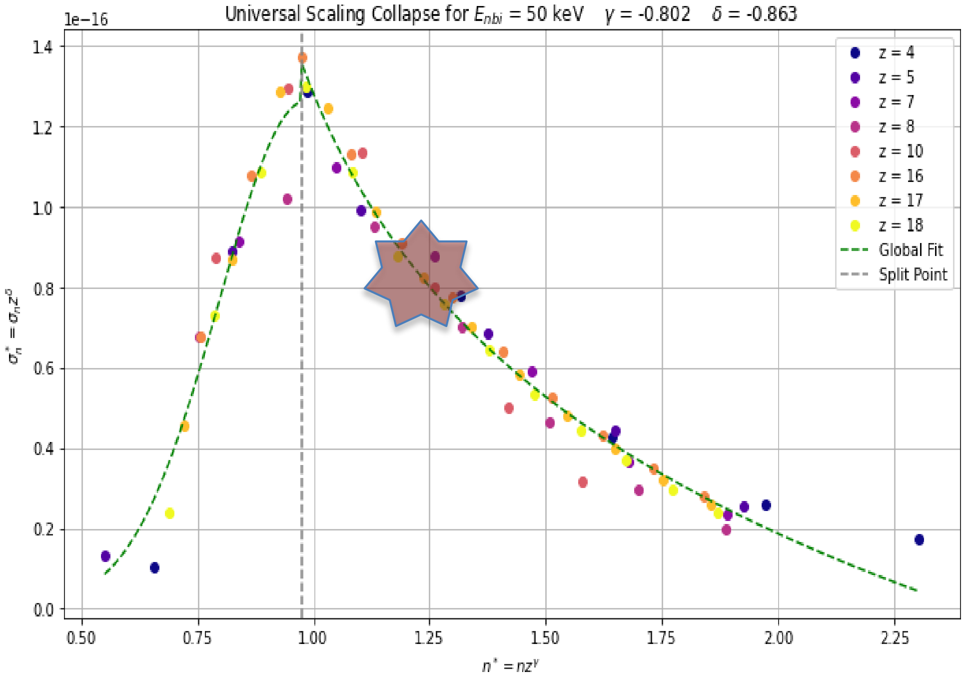
$$E^* = E \times z^{\beta} \qquad \sigma^*_{tot} = \sigma_{tot} \times z^{\alpha}$$



- **Since highly excited states tend to look hydrogen-like, the n-resolved charge exchange cross section also shows a scaling with quantum level n**

$$\sigma^*_n = \sigma_n \times z^{\delta}$$

$$n^* = n \times z^{\gamma}$$



Ongoing work and challenges

- **While the electronic configuration for Cu-like W^{+45} is fairly simple $(3d^{10}\ 4s^{1})$ the other charge states have much more complicated configurations requiring a much larger atomic structure calculation**
  - We are looking into using hydrogenic approximations for the Einstein *A* coefficients to see if they are adequate
  - For those excited states for which we have AUTOSTRUCTURE calculations we will check whether we may use the hydrogenic scaling to extrapolate to higher *n* to limit the needed cascade calculations
  - Even with these rates, past cross section approximations have reproduced the correct relative energy scaling, but not the absolute value. We can provide a dataset to help resolve these discrepancies

- **Radiance calibrations will be performed to complete the empirical determination of the photon emissivity coefficients**

Summary

- **Highly charged Tungsten ions generate sufficient charge exchange emission to serve as an impurity diagnostic**
  - The relativistic Rydberg formula provides accurate wavelength predictions
  - Impurity transport can be determined from emission measurements of many different charge states within a narrow visible spectral range
  - Background emission is comparable to the beam-induced charge exchange emission (this is different from experience in W7-X)

- **Charge exchange cross sections and emission rate coefficients of highly-charged ions are otherwise unavailable**
  - Reviewing accuracy of approximation techniques for determining scaling of charge exchange cross section (an *n*-resolved cross section) with ion charge
  - Reviewing accuracy of hydrogenic *n*-scaling of Einstein *A* coefficients for highly excited states