

# ***Sensitivity of Tokamak Transport Modeling to Atomic Physics Data: Some Examples***

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*IAEA Technical Meeting on Uncertainty  
Assessment and Benchmark Experiments for  
Atomic and Molecular Data for Fusion Applications*

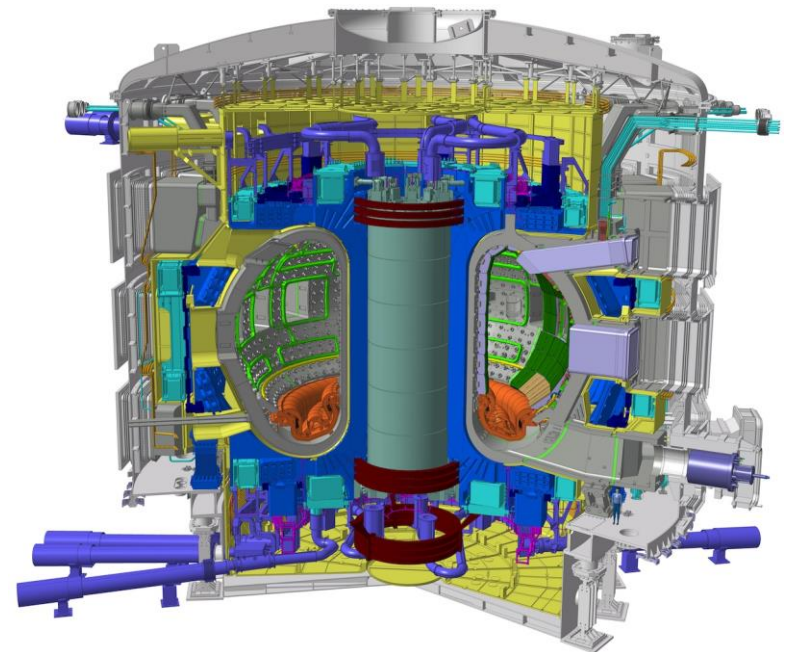
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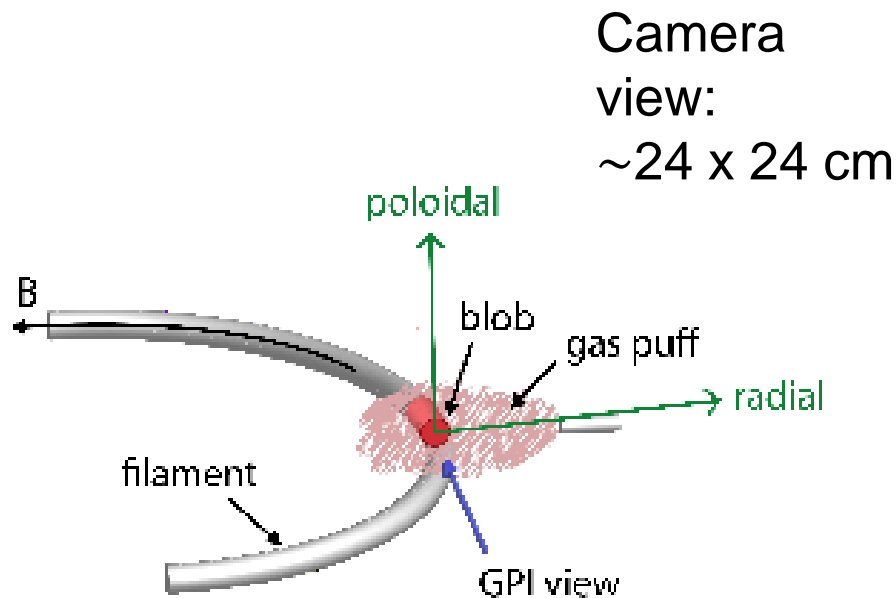


# Accurate Atomic Physics Data Essential for Tokamak Modeling

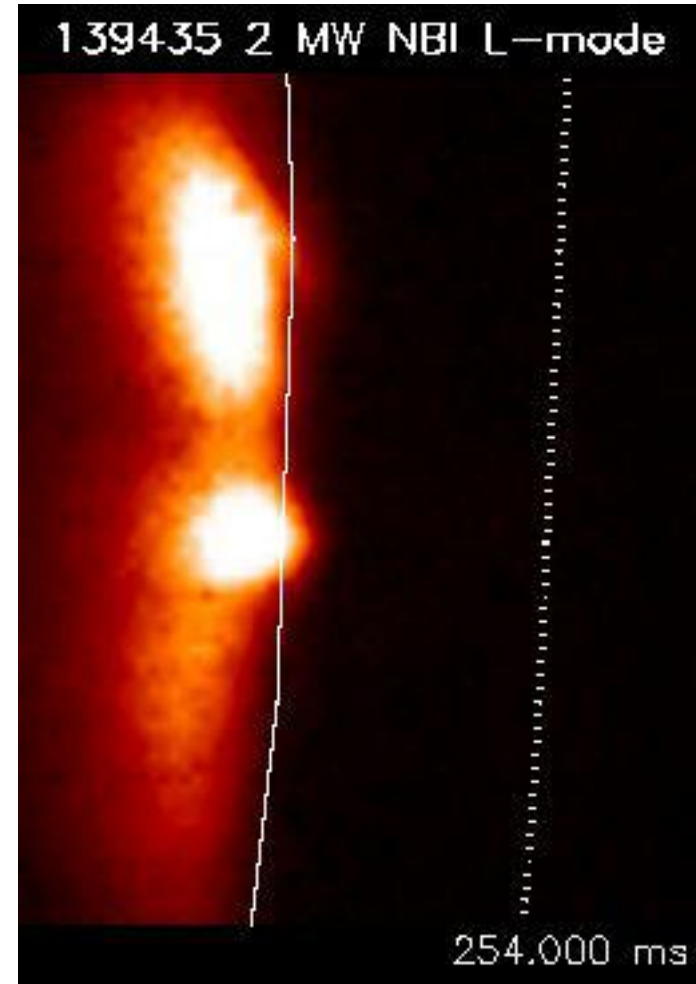
- Tokamak modeling critical for fusion energy because can't build a "small" reactor,
  - All represent extrapolation of knowledge,
  - Only approach is via 1<sup>st</sup> principles model.
  - Such models rely on atomic physics data.
  - Atomic data also needed for model validation,
    - E.g., in experimental diagnostics.
- Will show some examples:
  - Gas Puff Imaging:
    - Turbulence diagnostic,
    - Excellent opportunity for neutral transport validation.
  - High-Z impurity transport in tokamak plasmas,
    - Three examples.
  - "Closest to 1<sup>st</sup> principles" codes are kinetic,
    - Need more detailed data.



# Gas Puff Imaging Allows Us to “See” & Characterize Edge Plasma Turbulence

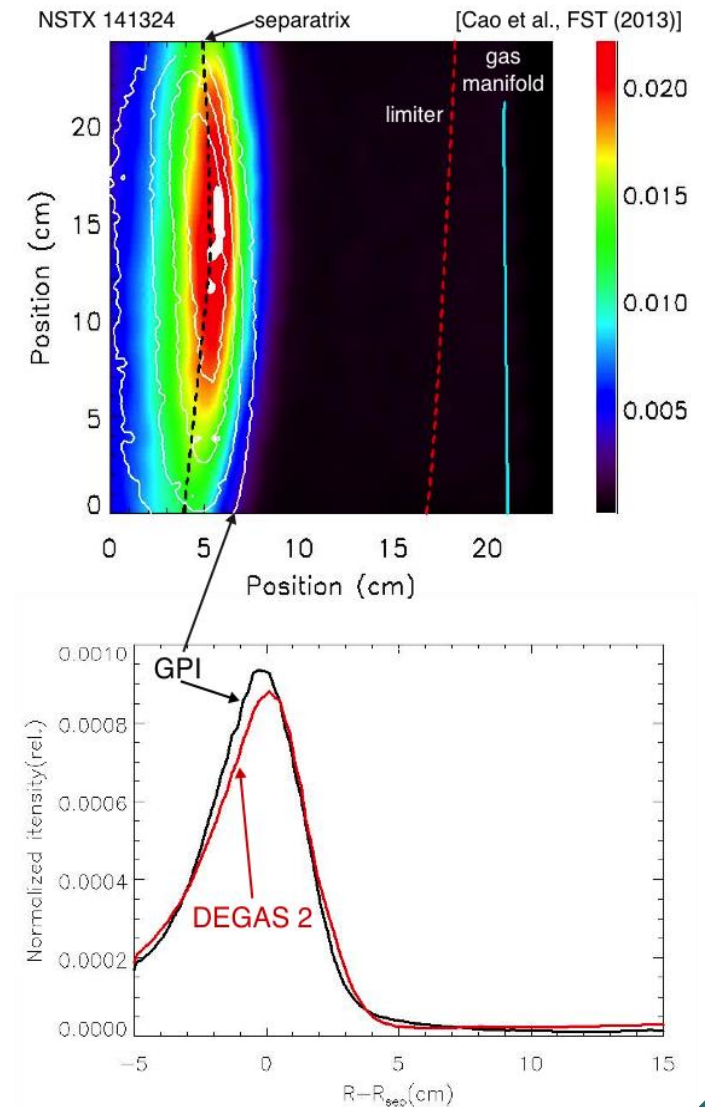


<http://w3.pppl.gov/~szweben/>  
[Zweben et al., PPCF (2016)]

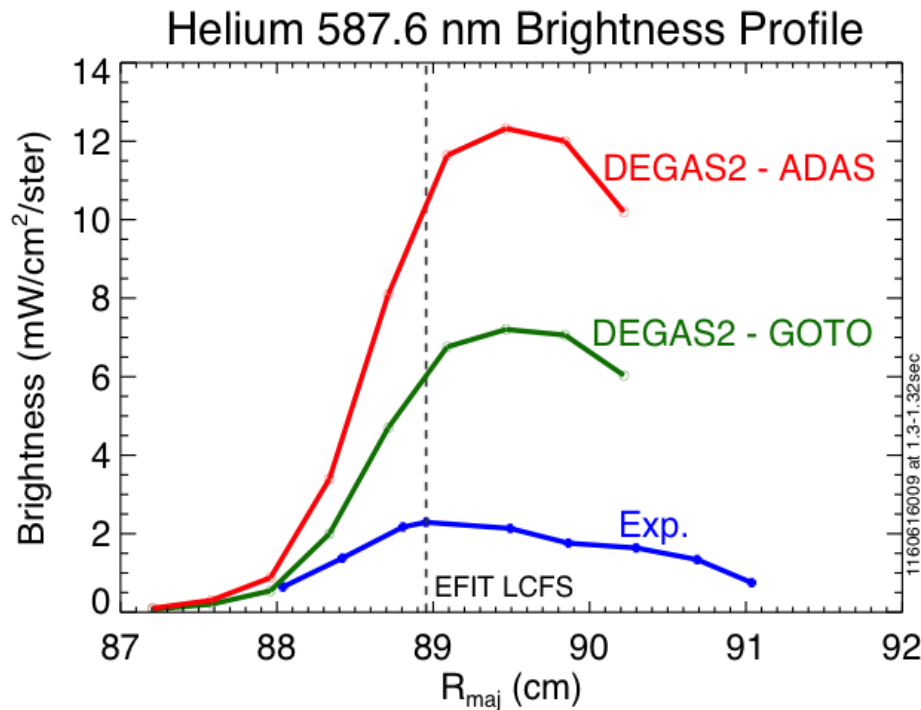


# GPI Provides Nearly Ideal Opportunity for Validating Neutral Transport Codes

- And atomic physics data!
  - $\Rightarrow$  Identify sensitivities & minimize uncertainties.
- Is “ideal” because:
  - Source & plasma well characterized,
  - Plasma-material interaction effects minimal,
  - Results can be directly compared with experiment.
- But, not completely:
  - Complex geometry,
  - Light emission nonlinear function  $\Rightarrow \langle S(n) \rangle \neq S(\langle n \rangle)$ .
  - Turbulence complicates  $n_e$ ,  $T_e$  measurement.
- NSTX D<sub>2</sub> validation:
  - Observed: 1/89 D <sub>$\alpha$</sub>  photons / atom  $\pm$  34%,
  - Simulated: 1/75  $\pm$  18%.
- Doesn't include atomic physics uncertainty!
  - Subsequent update to  $n = 1 \rightarrow 3, 4, 5 \Rightarrow \sim 10\%$  change in emission.
    - How uncertain are these data?
  - D<sub>2</sub> dissociation contributes  $\sim 30\%$  of D <sub>$\alpha$</sub>  at peak & is more uncertain.



# Simulated He GPI Emission in Alcator C- Mod Way Too Large!

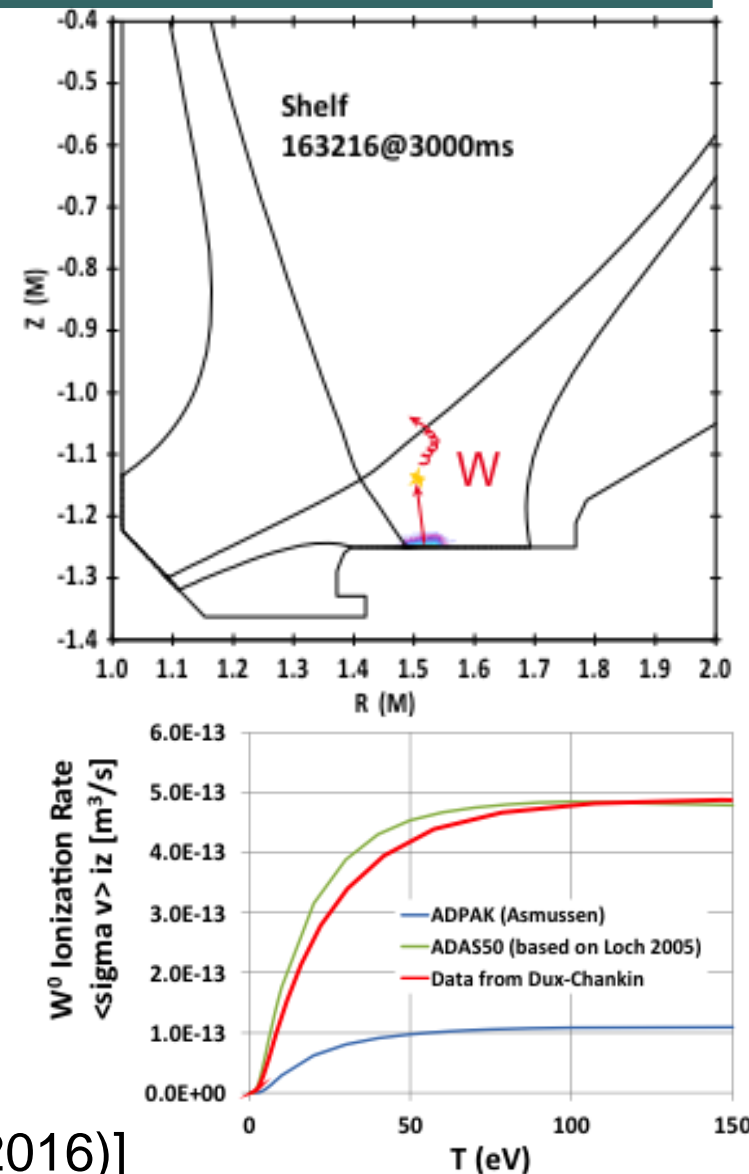


[S. Baek et al., APS-DPP (2016)]

- $D_2$  comparison similar to NSTX.
- Two He CR models:
  - M. Goto, JQSRT 76, 331 (2003),
  - S. Loch et al., PPCF 51, 105006 (2009).
- How accurate are these data?
- Alternative explanations dismissed:
  - Boundary conditions,
  - 4.1 T singlet-triplet mixing (Goto).
- Still to check:
  - Radiation trapping,
  - Turbulence effects.

# Core Penetration Fraction Sensitive to $W$ Ionization Rate

- Predictive OEDGE simulations of DIII-D  $W$  ring experiments.
- For “shelf” geometry:
  - ADAS50: 0.3%  $W$  reach core,
  - ADPAK: 16%!
  - Factor of 5 difference in ionization rate  $\Rightarrow$  factor of 50 difference in core penetration.
  - Similar results for “floor” geometry.
- Sensitivity enters via prompt redeposition model.
- Actual experiments will have  $WI$  data  $\Rightarrow$  can quantify source,
  - & core bolometry will give data on core concentration.
  - $\Rightarrow$  may be able to reduce uncertainties.



[J. D. Elder et al., PSI (2016)]



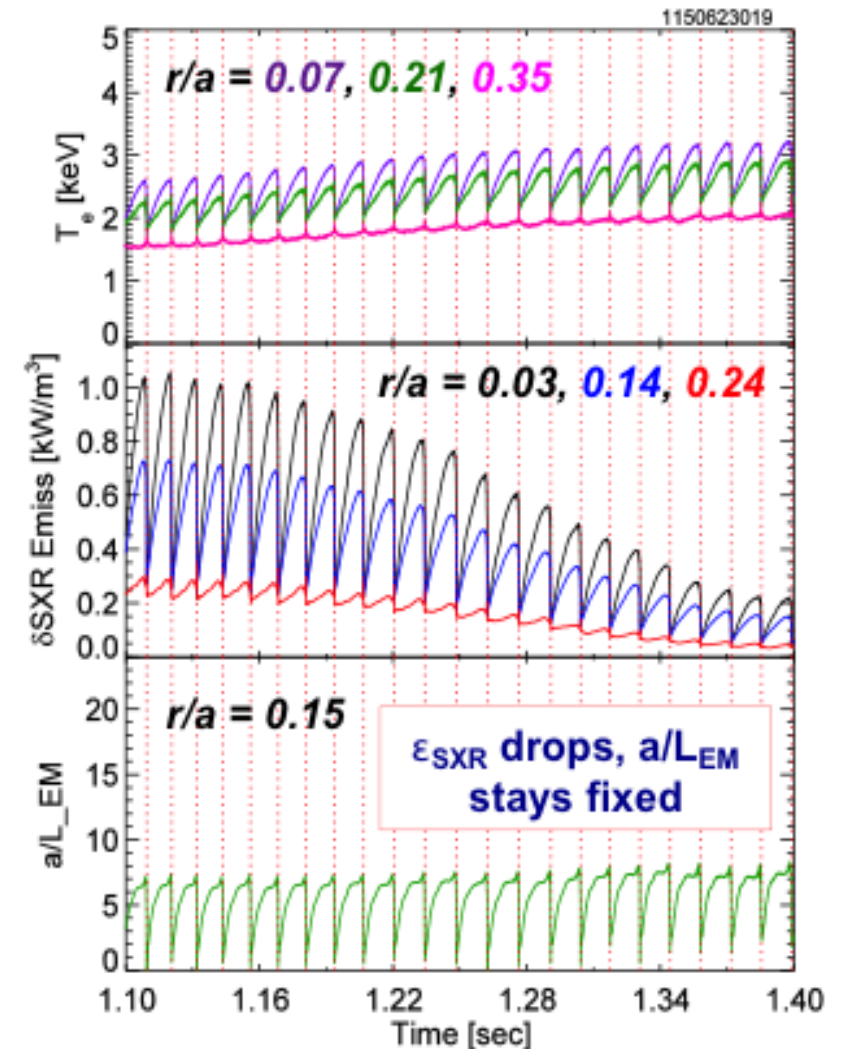
# Optimization of Fusion Operating Scenarios

## Benefits from Accurate $L(T_e)$

- Optimize  $n_i$  &  $T_i$  profiles to maximize pressure ( $\rightarrow P_{fus}$ ) & high  $J_{boot}$  ( $\downarrow$  recirculating power),
  - High-Z content must be controlled to do this.
- C-Mod experiments targeted at validation those control mechanisms:
  - Neoclassical transport,
  - Radio-frequency heating effects.
- Assess  $W$  transport via sawteeth!
  - How much peaking due to  $n_W$ ?
  - How much to  $T_e$ ?
  - Peaking  $\leftrightarrow$   $\square$  gradients  $\Rightarrow$  need  $dL/dT_e$ !

$$n_W = \frac{\epsilon_{SXR}(r)}{n_e L_Z(T_e)}$$

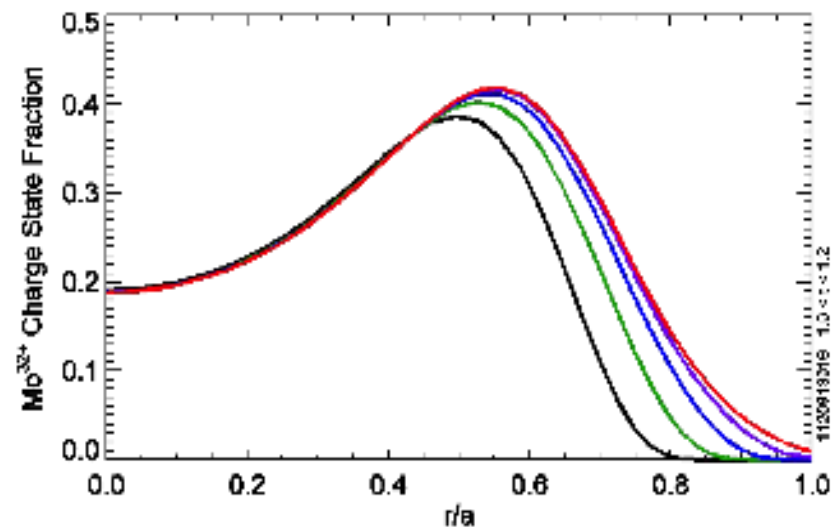
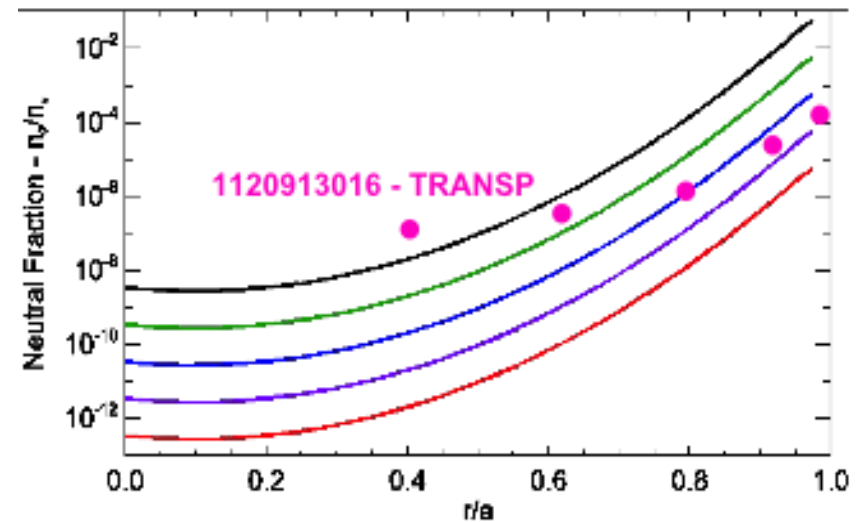
$$\frac{\nabla n_W}{n_W} = \frac{\nabla \epsilon_{SXR}}{\epsilon_{SXR}} - \frac{T_e}{L_Z} \left( \frac{\partial L_Z}{\partial T_e} \right) \frac{\nabla T_e}{T_e} - \frac{\nabla n_e}{n_e}$$



[Reinke et al., IAEA FEC (2016),  
Loarte et al., PoP (2015)]

# CX Recombination Affects Ionization Balance & Diagnostic Interpretation

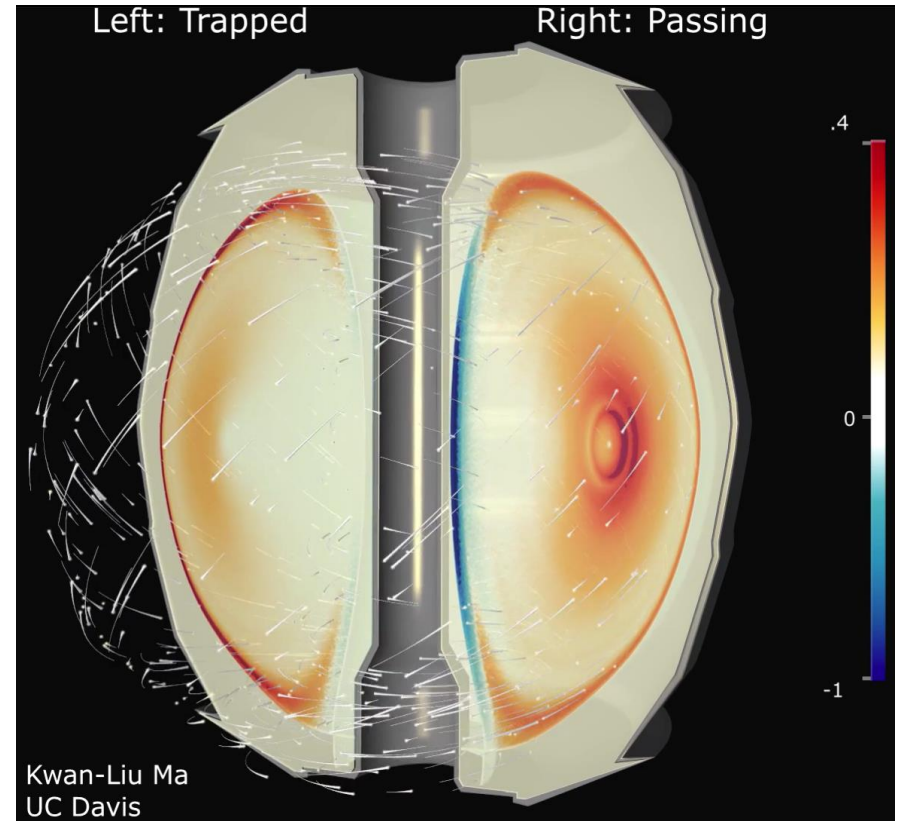
- Assume  $n_0/n_e$  profiles & calculate  $\text{Mo}^{32+}$  distributions:
  - Net effect of CX recombination equivalent to  $\Delta r \sim 0.1 a$ !
- Impacts transport model based on  $\text{Mo}^{32+}$  diagnostic,
  - E.g., ignoring CX would require pinch to match observed  $\text{Mo}^{32+}$ .
- Relevant for diagnostic analysis, e.g., C-Mod XICS [Reinke, RSI (2012)].
- More important in devices with NBI!
- But, CX recombination data hard to find for W, Ca, ...
  - Can rough estimates be made without much effort?





# Kinetic Codes Will Need More Detailed Data

- 6-D codes track velocities of all reactants & products.
- E.g., [Tskhakaya CPP (2016):
  - $H^+ + e$  radiative recombination from photoionization,
  - 3-body recombination from ionization.
- Large scale gyrokinetic / drift kinetic codes are 5-D.
  - Focus is on ion distribution.
  - & electrons in atomic processes treated heuristically.
  - But, want correct electron energetics.



Bootstrap current calculation with XGCa  
[Hager PoP (2016)]

# Conclusions

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- From Gas Puff Imaging:
  - D collisional radiative model in good shape,
    - Molecular contributions more uncertain.
  - Are there problems with He model?
- High- Z Impurity Transport:
  - W first ionization critical,
  - Knowing  $dL/dT_e$  accurately would be useful,
  - Data for CX recombination of closed shell ions needed for diagnostic interpretation.
- 1<sup>st</sup> principles kinetic codes need velocity data for all reactants & products.