



# Evidence of Enhanced K-shell Ionization in Warm, Dense Carbon

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David Bishel, on behalf of CPS Team  
NIF User Group Meeting  
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# Collaborators

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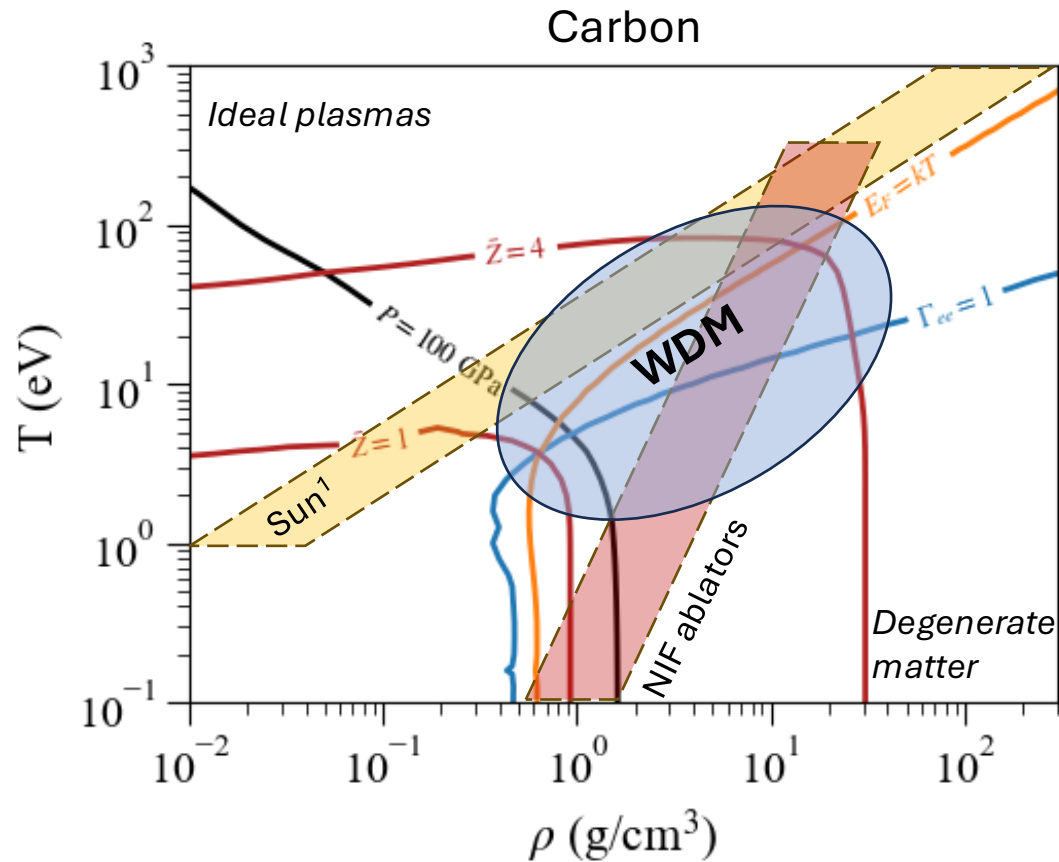


# The Colliding Planar Shocks (CPS) platform is delivering benchmark ionization measurements of C at warm-dense matter conditions

- The CPS platform assembles and characterizes a large, homogeneous volume of doubly-shocked material
  - Radiography constrains density to 15% or better
  - X-ray Thomson scattering (XRTS) constrains temperature to 20 – 30 %
- Novel analysis of XRTS, which models populations of individual atomic shells, gives evidence of **enhanced K-shell ionization**
  - Corroborated by radiograph transmission

These measurements will inform modern ionization and opacity models of warm-dense plasmas

# Warm dense matter lies at the transition between multiple limiting regimes



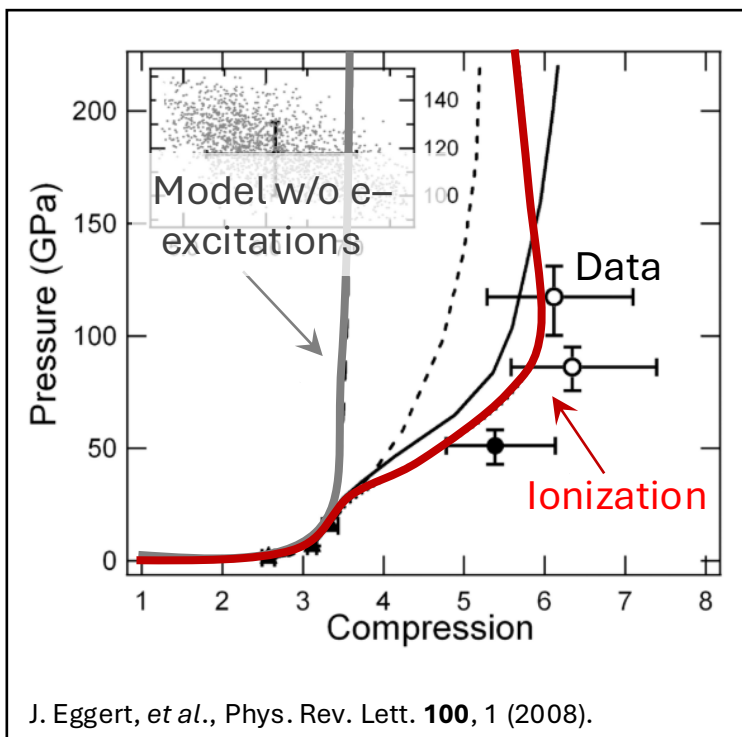
Astrophysical objects and fusion-relevant plasmas transit the WDM regime

Accurate models must include multiple effects

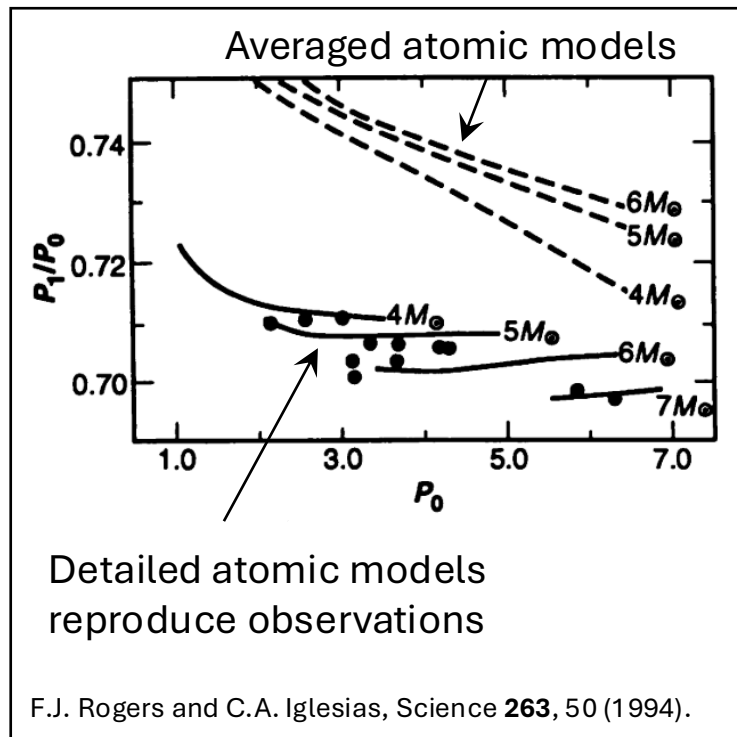
- Near degenerate → quantum effects
- Partly coupled → correlations
- Partially ionized → balance of thermal and pressure ionization

# Accurate atomic models are required to match (and predict!) HED experiments, astrophysical observations, and ICF implosions

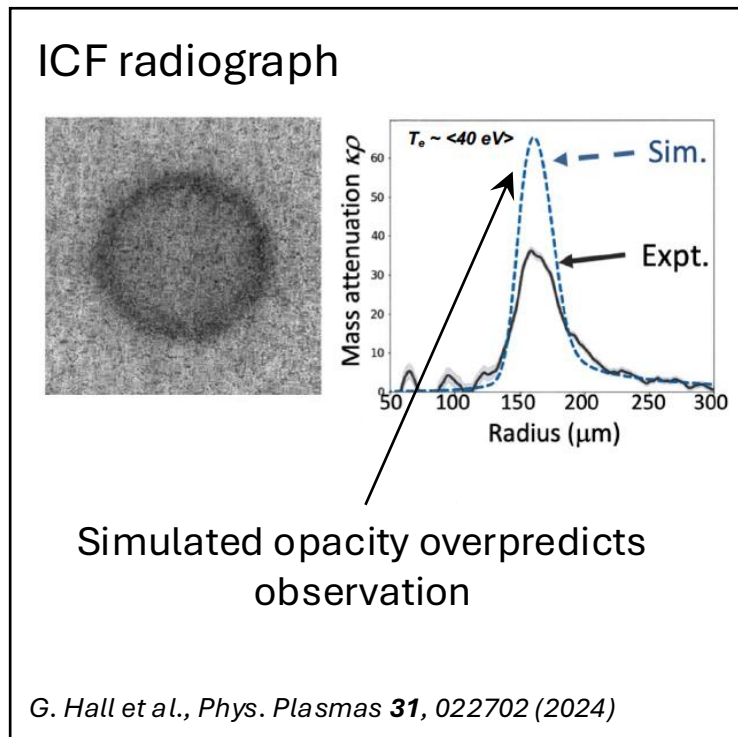
Ionization increases compressibility along Hugoniot (He)



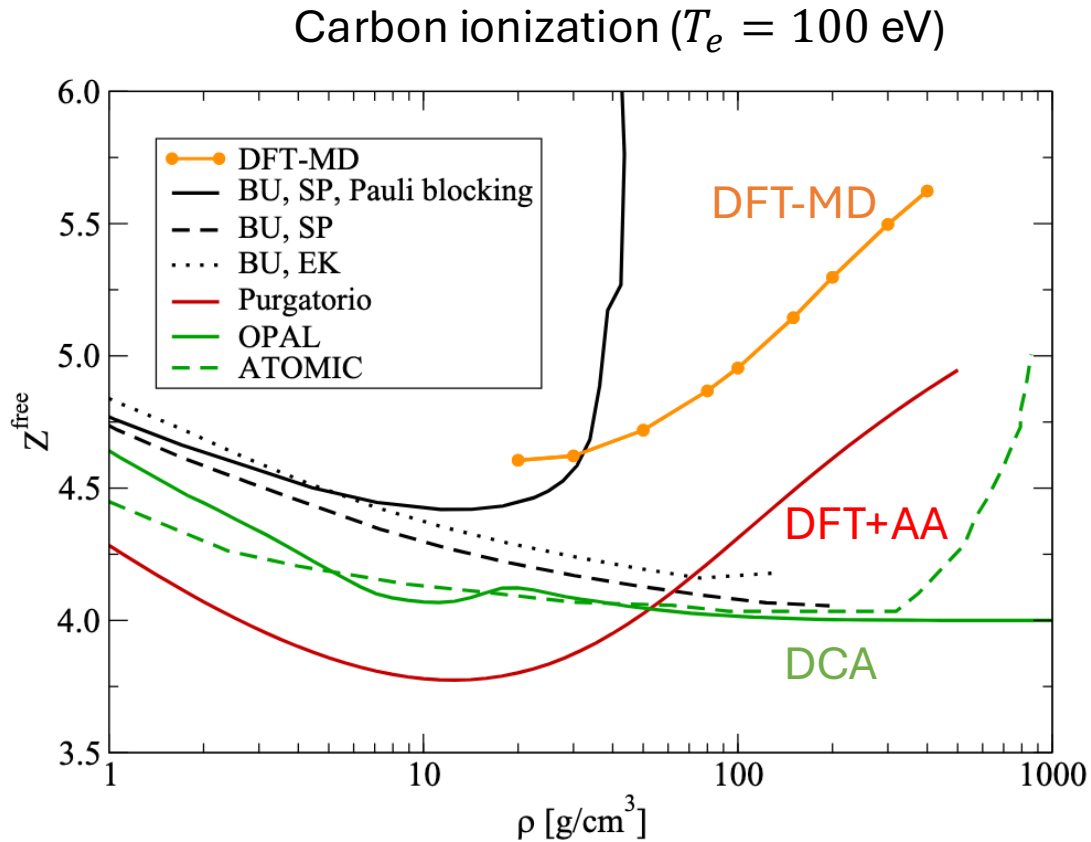
Opacity governs oscillation periods  $P_i$  of Cepheid variables



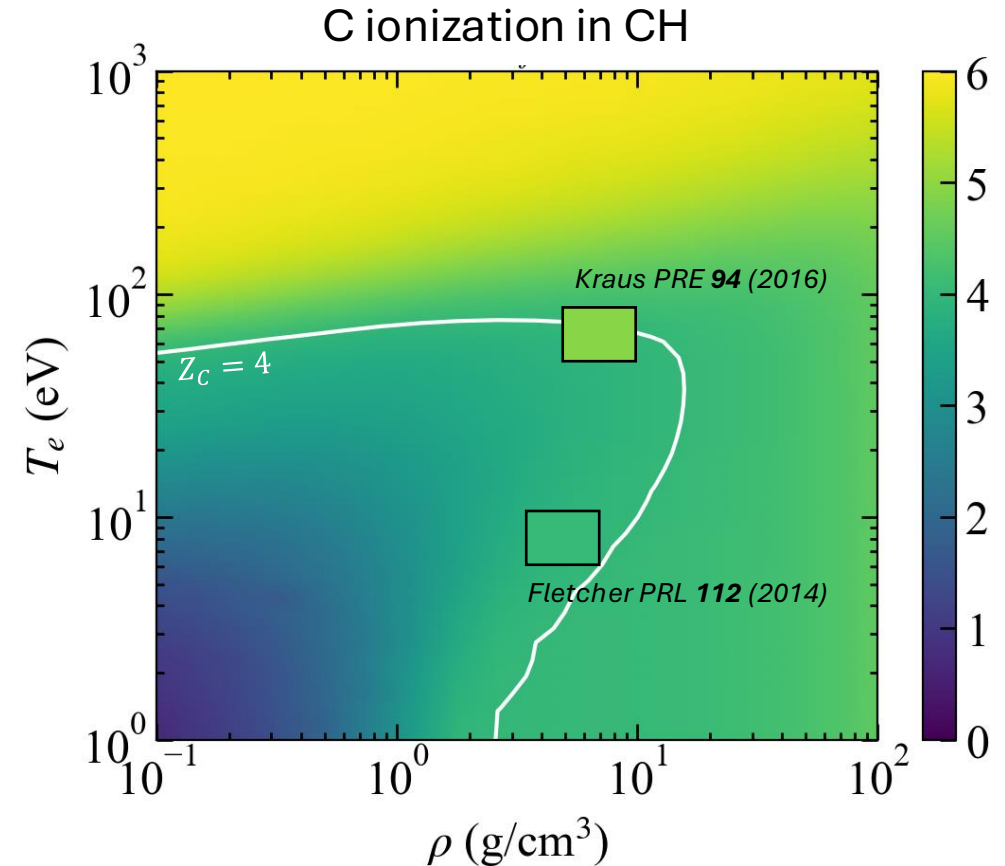
Ionization potentially explains radiography opacity problem



# Different models can vary widely in predicted ionization



M. Bethkenhagen, et al., *Phys. Rev. Res.* **2**, 023260 (2020).



There is growing theoretical and experimental evidence that traditional models underpredict ionization of WDM



# Colliding Planar Shock Platform



# The Colliding Planar Shocks (CPS) platform<sup>1</sup> simultaneously constrains density, temperature, and ionization of doubly shocked warm, dense matter

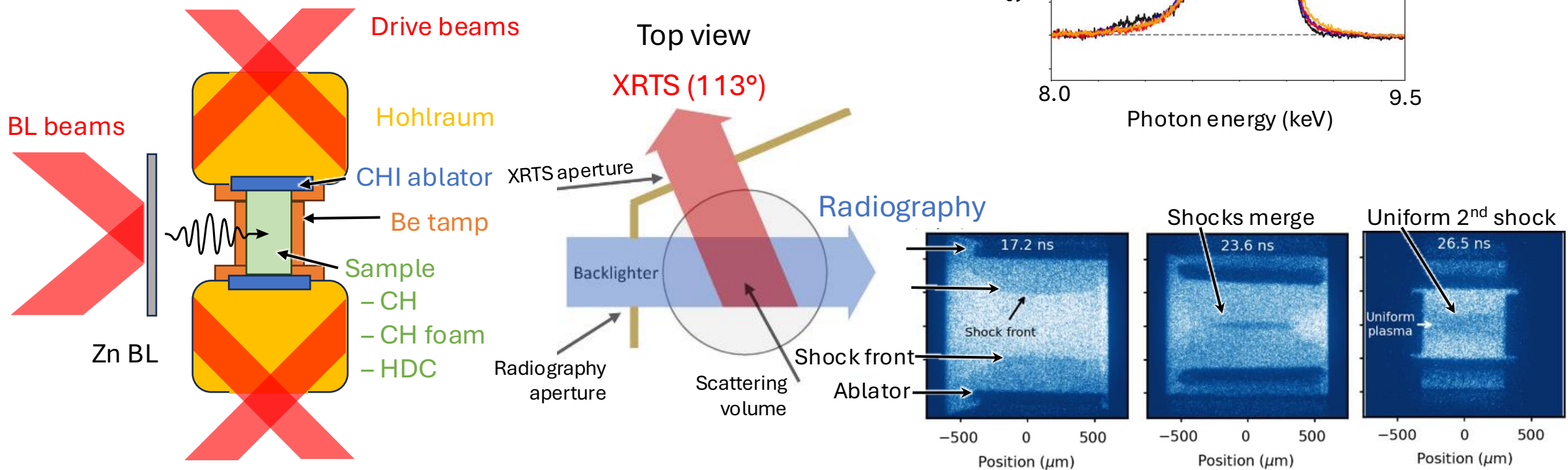
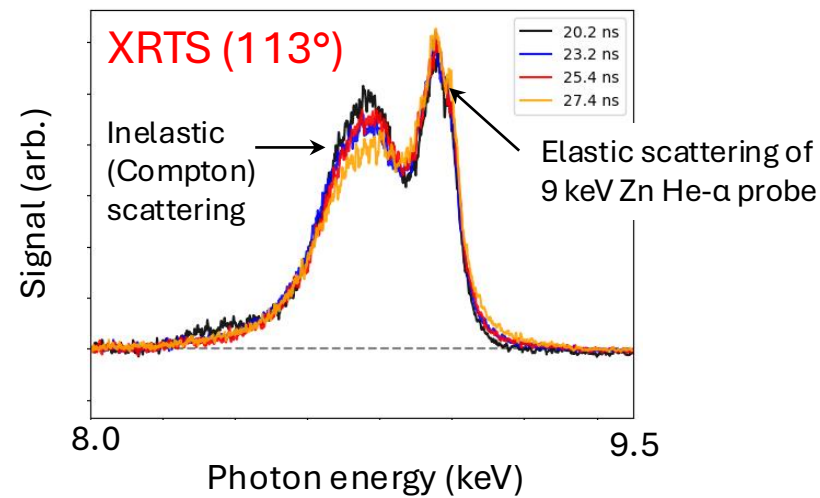
RESEARCH ARTICLE | JUNE 01 2023

**The colliding planar shocks platform to study warm dense matter at the National Ignition Facility**  

M. J. MacDonald ; C. A. Di Stefano ; T. Döppner ; L. B. Fletcher ; K. A. Flippo ; D. Kalantar ; E. C. Merritt ; S. J. Ali ; P. M. Celliers ; R. Heredia ; S. Vonhof ; G. W. Collins ; J. A. Gaffney ; D. O. Gericke ; S. H. Glenzer ; D. Kraus ; A. M. Saunders ; D. W. Schmidt ; C. T. Wilson; R. Zacharias ; R. W. Falcone 

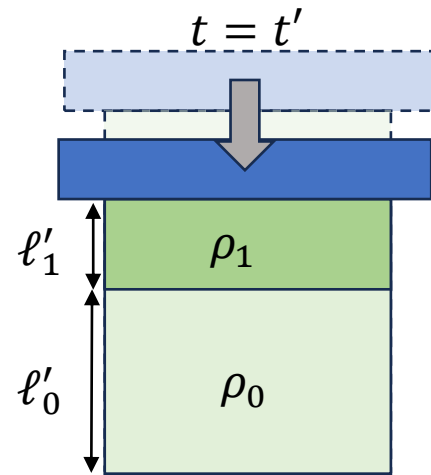
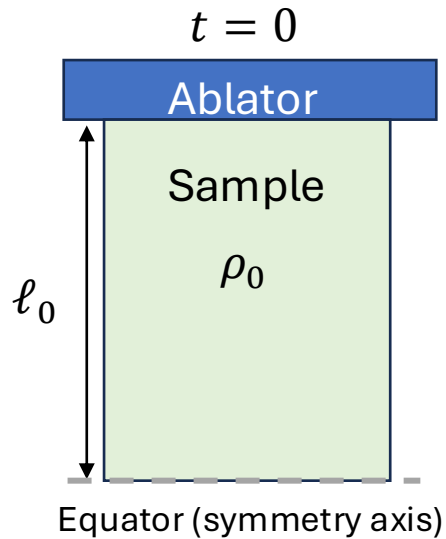


*Physics of Plasmas* 30, 062701 (2023)  
<https://doi.org/10.1063/5.0146624>



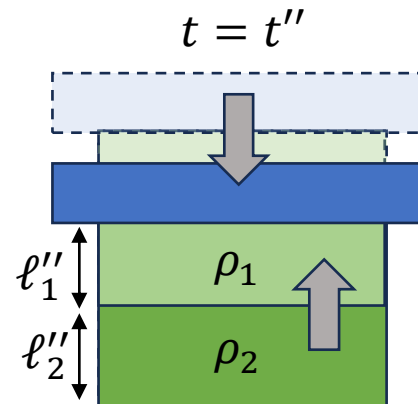
<sup>1</sup> MacDonald, M. J. et al. *Physics of Plasmas* 30, (2023).

# Radiography from the side-mounted Zn foil constrains the shocked densities

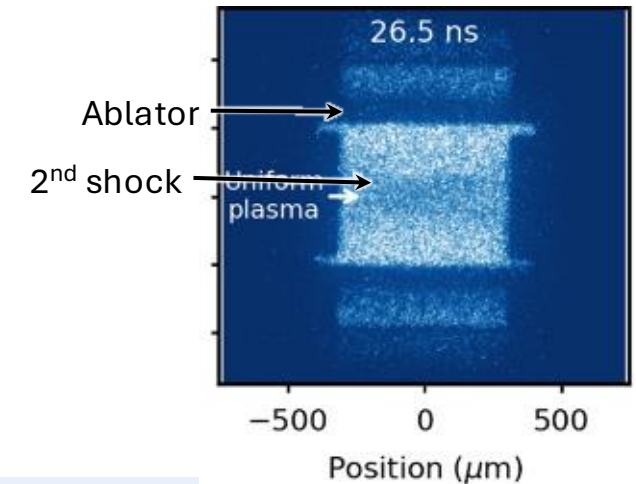
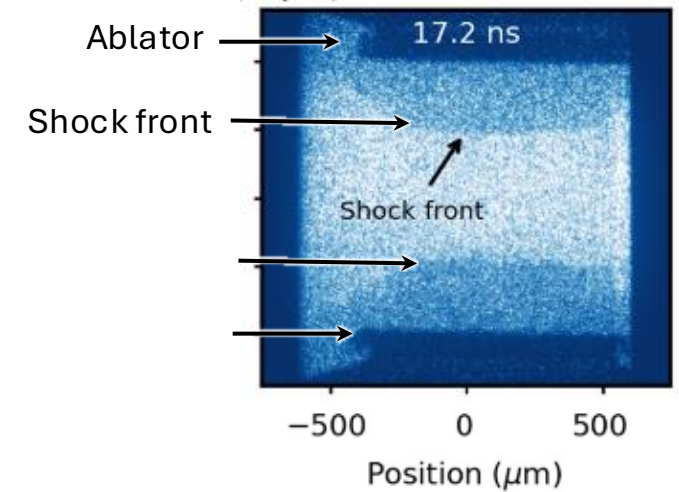


Density inferred from conservation of mass

$$\frac{\rho_1}{\rho_0} = \frac{l_0 - l'_0}{l'_1}$$



$$\frac{\rho_2}{\rho_0} = \frac{l_0}{l''_2} \left[ 1 - \frac{\rho_1}{\rho_0} \frac{l'_1}{l_0} \right]$$

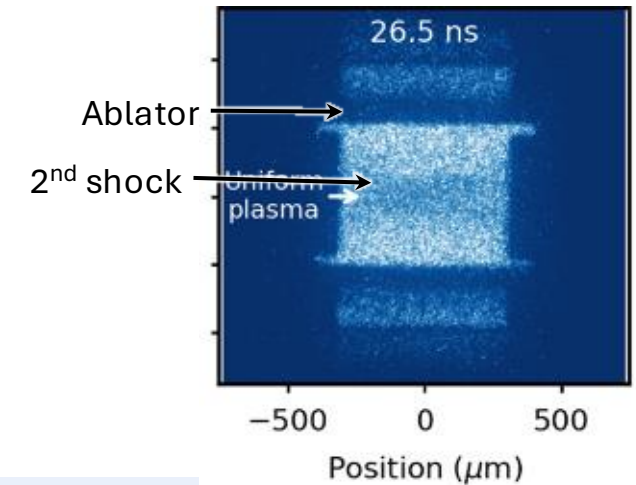
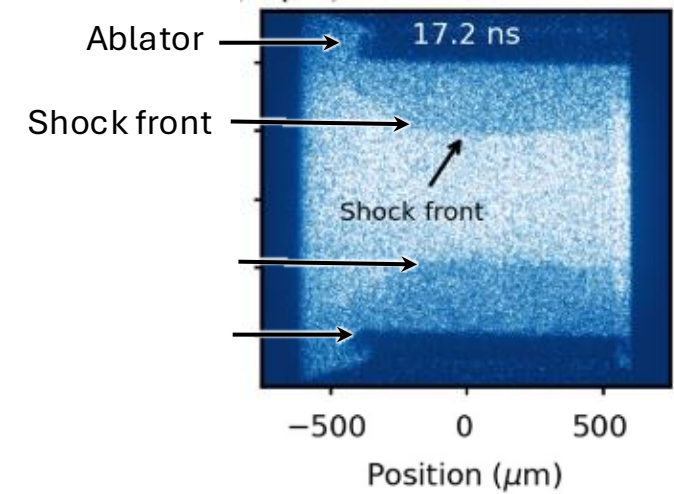
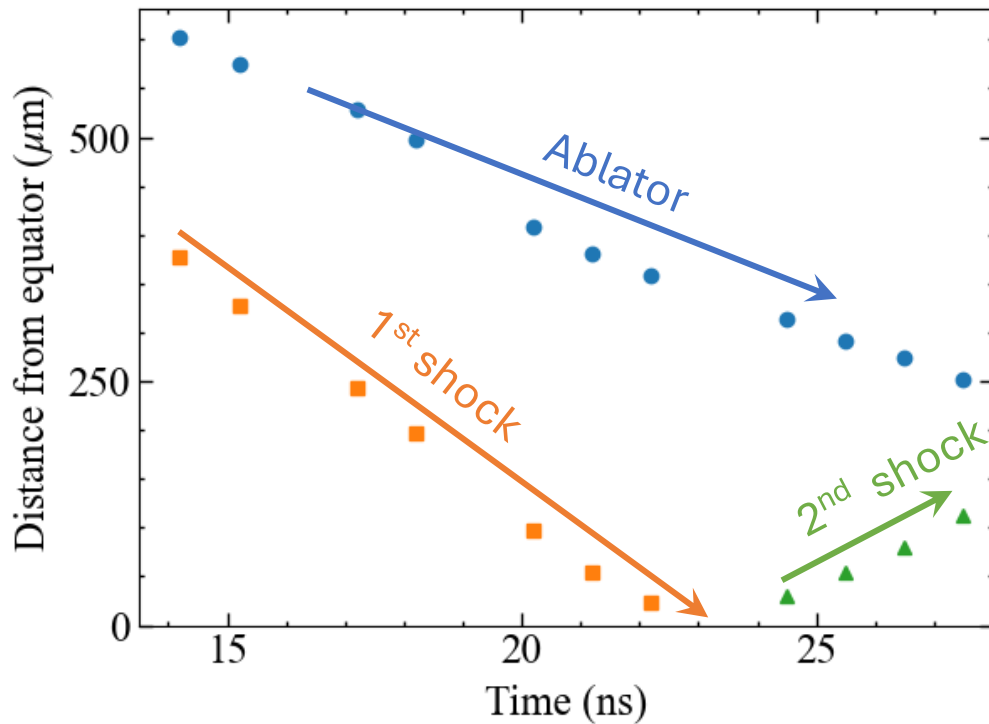


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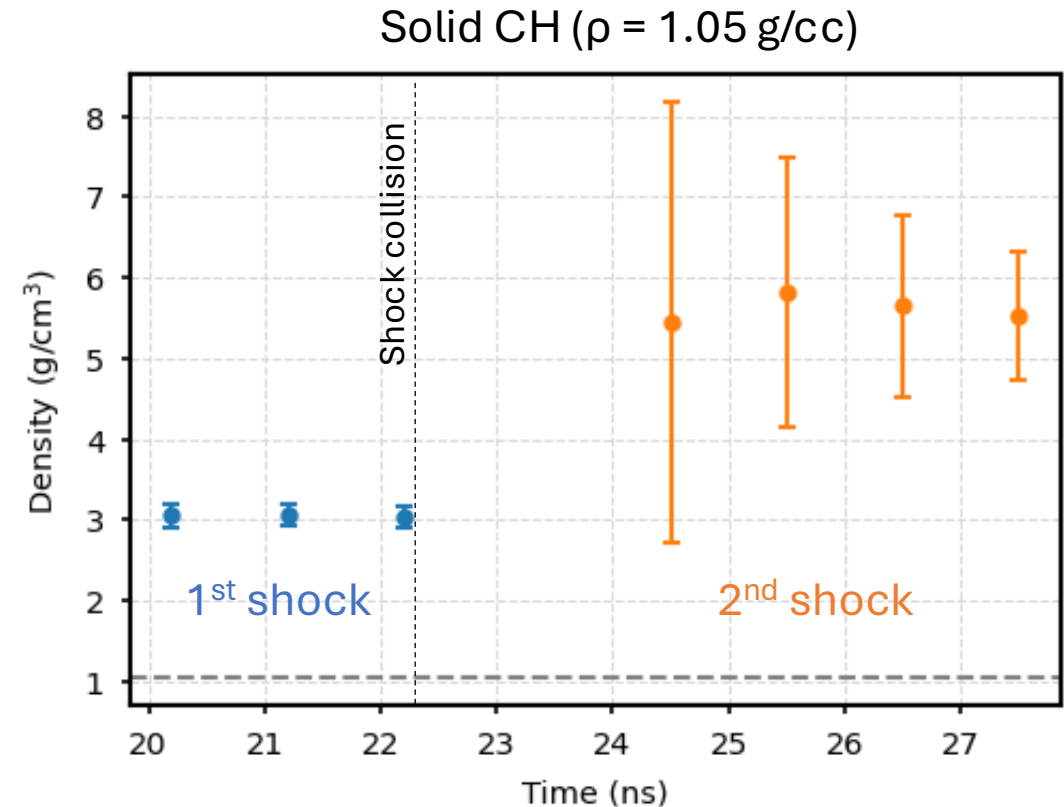
Monte Carlo error propagation of measured values

$$\frac{\rho_1}{\rho_0} = \frac{\ell_0 - \ell'_0}{\ell'_1} \qquad \frac{\rho_2}{\rho_0} = \frac{\ell_0}{\ell''_2} \left[ 1 - \frac{\rho_1}{\rho_0} \frac{\ell''_1}{\ell_0} \right]$$

Uncertainty is minimized as shocked volume increases

$$\frac{\sigma_{\rho_1}}{\rho_1} \geq \frac{\sigma_{\ell}}{\ell'_1} \qquad \text{First shock}$$

$$\frac{\sigma_{\rho_2}}{\rho_2} \geq \frac{\sigma_{\ell}}{\ell''_2} \sqrt{1 + \left( \frac{\rho_1}{\rho_2} \right)^2} \qquad \text{Second shock}$$

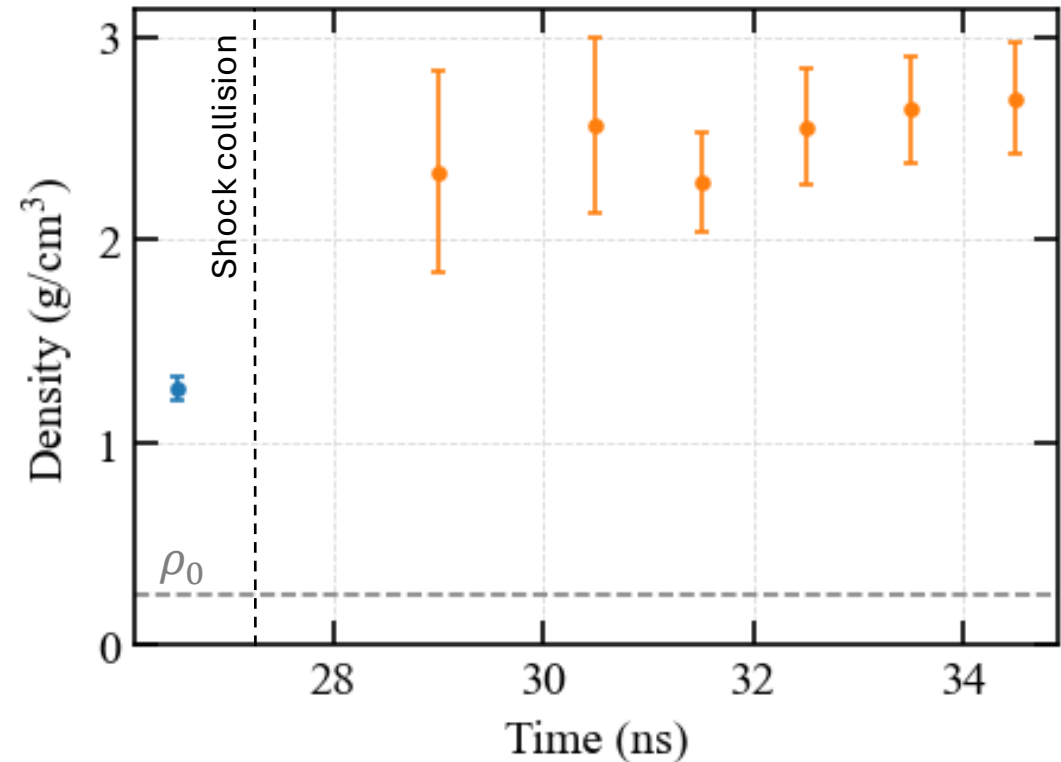
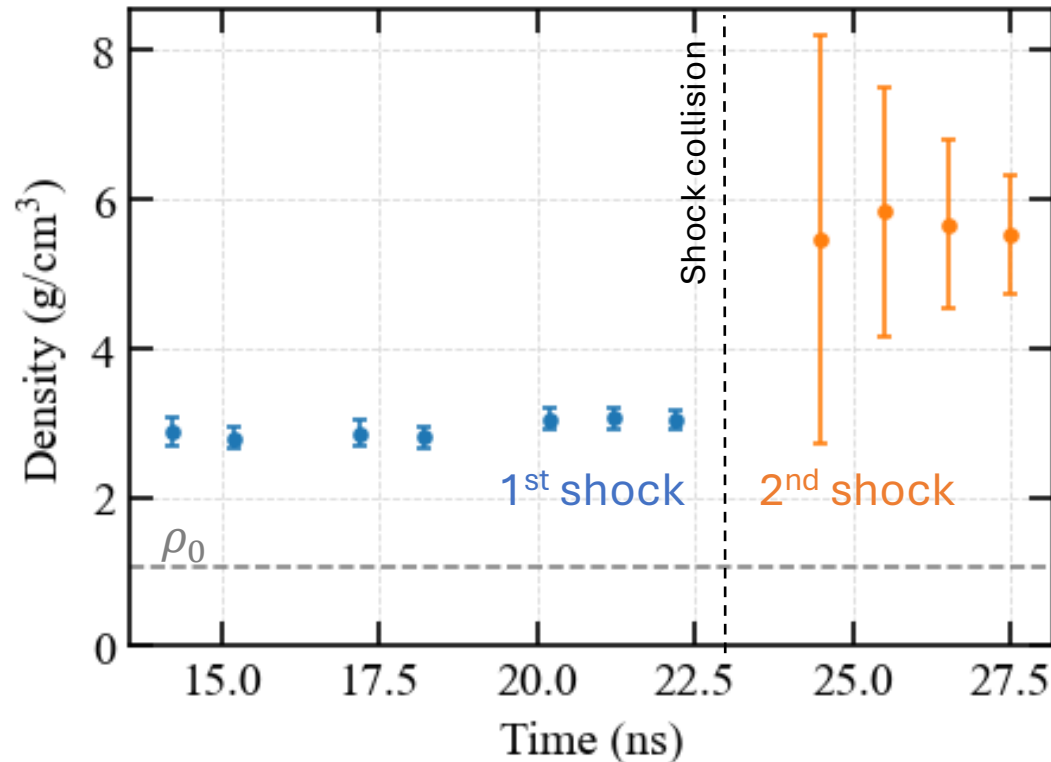


Density of doubly-shocked CH is constrained to within 15%

# Lower initial density of CH foam allows tuning of doubly-shocked state

Solid CH ( $\rho_0 = 1.05 \text{ g/cc}$ )

CH foam ( $\rho_0 = 0.25 \text{ g/cc}$ )



Recent shots on HDC access higher densities



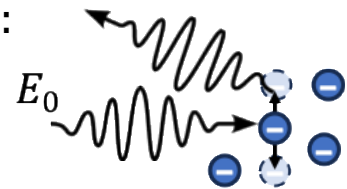
# Temperature, ionization from X-ray Thomson Scattering



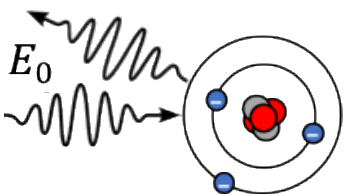
# X-ray Thomson scattering (XRTS) is a powerful diagnostic for warm-dense matter, encoding temperature, density, and ionization

Measured signal  $\propto$  dynamic structure factor<sup>2</sup>  $S(k, \omega)$ :

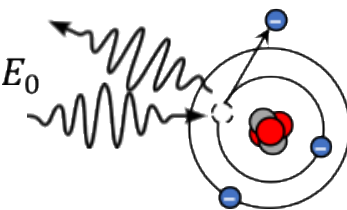
$$S(k, \omega) = Z_f S_{ee}^0(k, \omega) \quad \text{[Free electrons]}$$



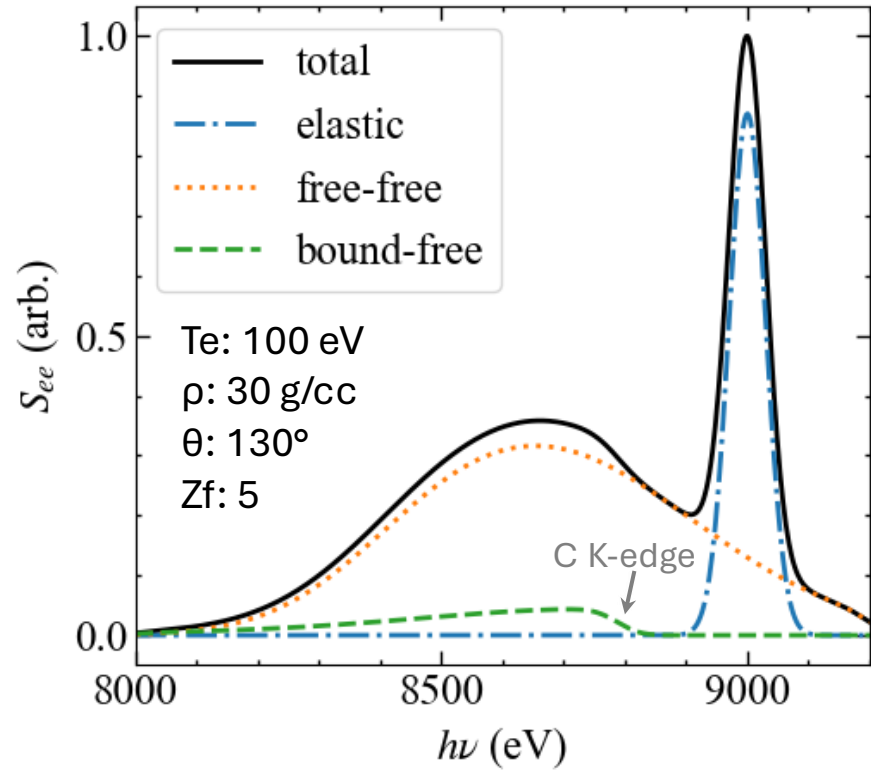
$$+ |f_I(k) + q(k)|^2 S_{ii}(k) \delta(\omega) \quad \text{[Elastic]}$$



$$+ Z_b \int S_{ce}(k, \omega - \omega') S_s(k, \omega') d\omega' \quad \text{[Bound-free]}$$



Simulated XRTS<sup>1</sup> from C in CH



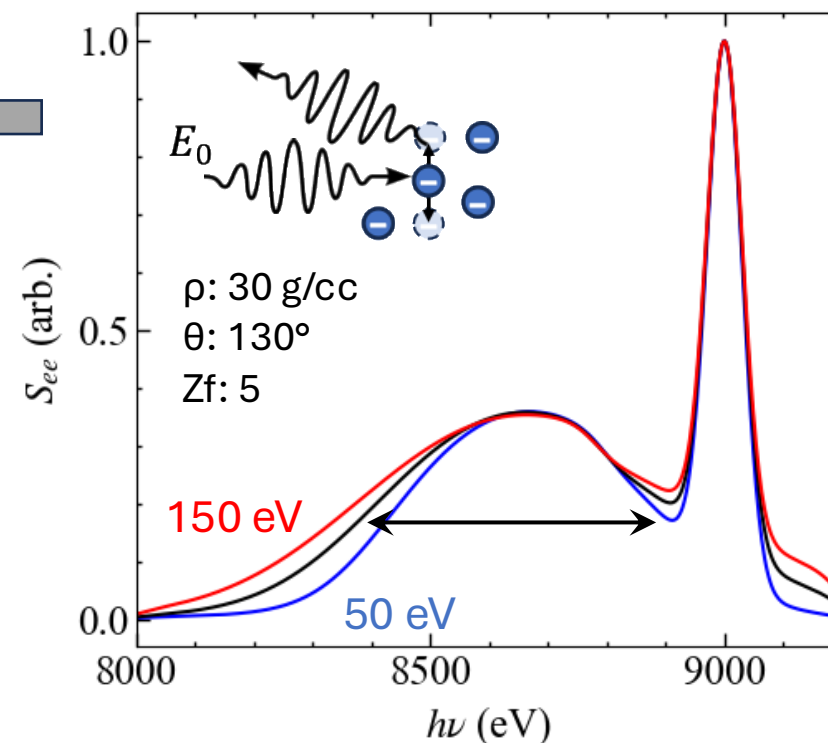
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 & + Z_b \int S_{ce}(k, \omega - \omega') S_s(k, \omega') d\omega' && \text{[Bound-free]}
 \end{aligned}$$



Scattering from **free electrons** encodes the **thermodynamic state**



Temperature is encoded in the width of the inelastic Compton feature

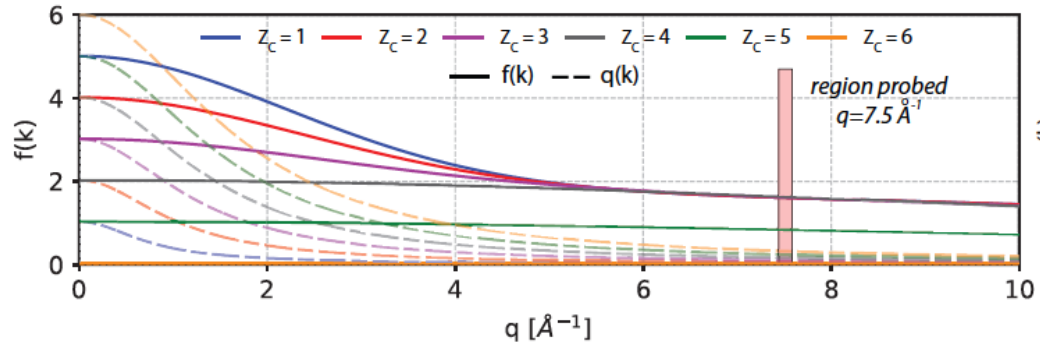
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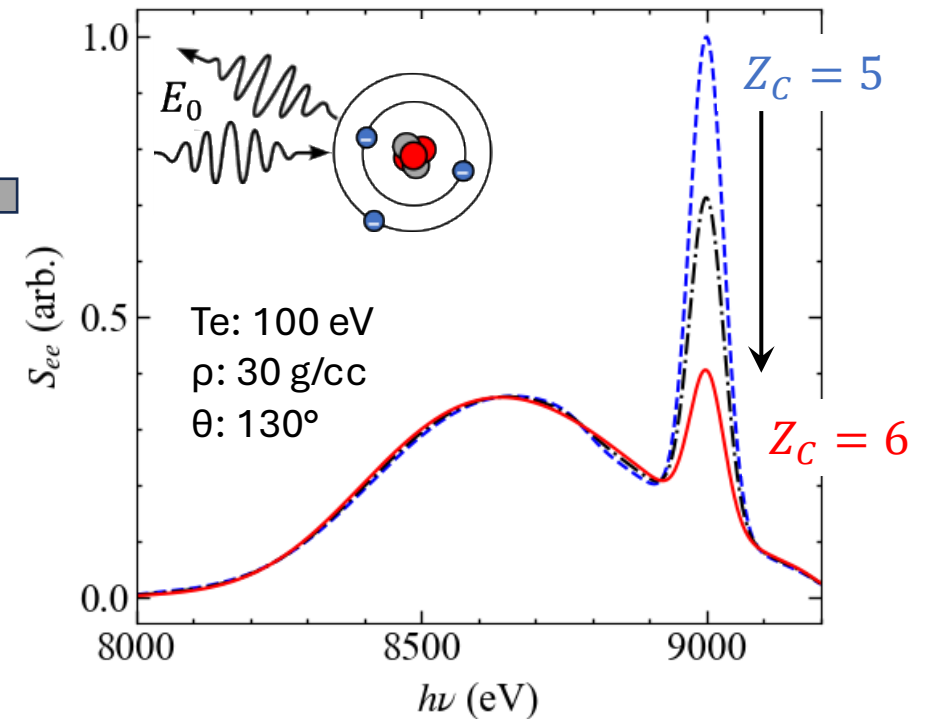
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$$+ |f_I(k) + q(k)|^2 S_{ii}(k) \delta(\omega) \quad \text{[Elastic]}$$

Atomic form factor ( $f_I$ ) and screening ( $q$ ) for various C ionization

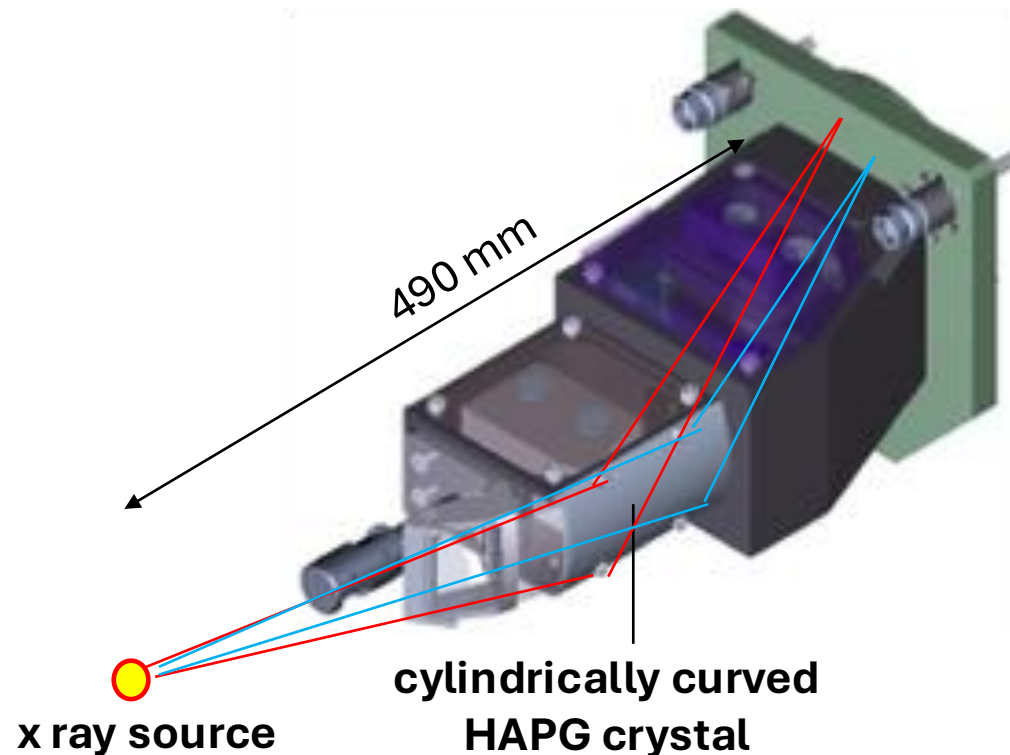


Scattering from tightly **bound electrons** encodes **ionization**



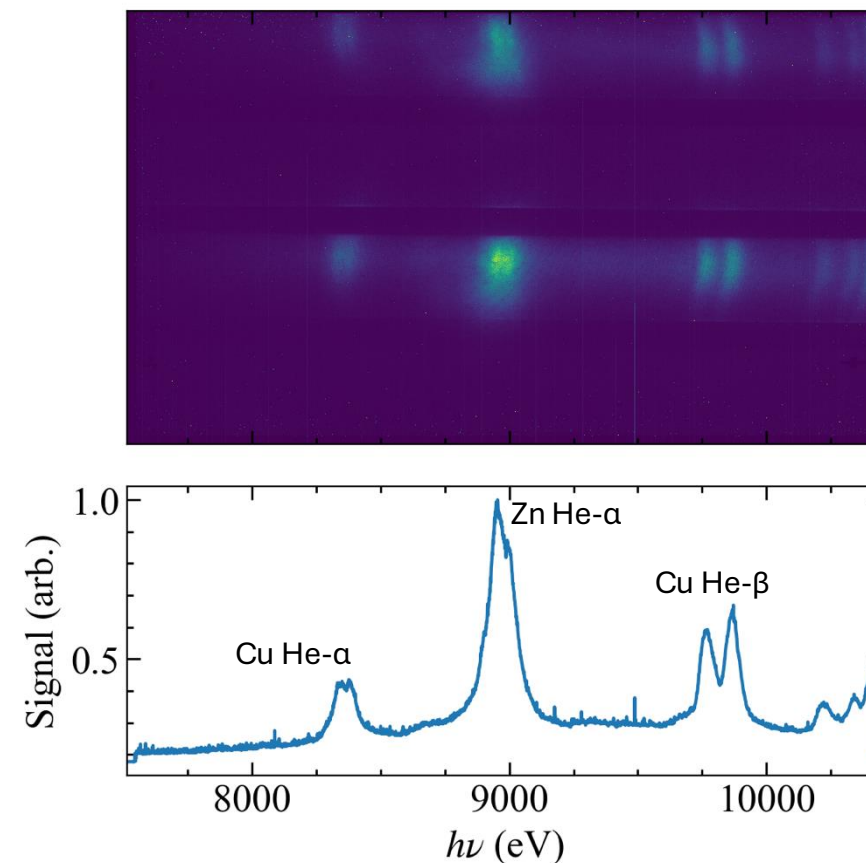
Ionization is encoded in the ratio of elastic-to-inelastic scattering

# XRTS is collected throughout the experiment with the high-throughput, two-crystal MACS spectrometer

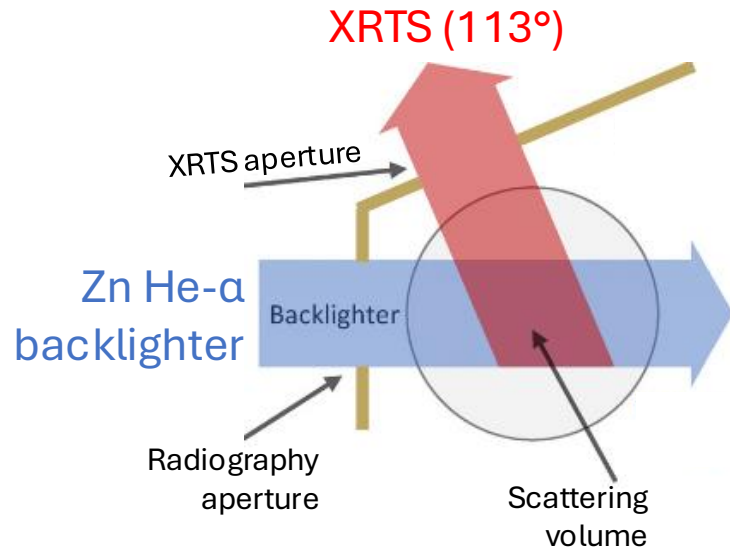


- Focusing geometry
- Mosaic crystal: high reflectivity
- Moderate resolution:  $E/dE \sim 600$

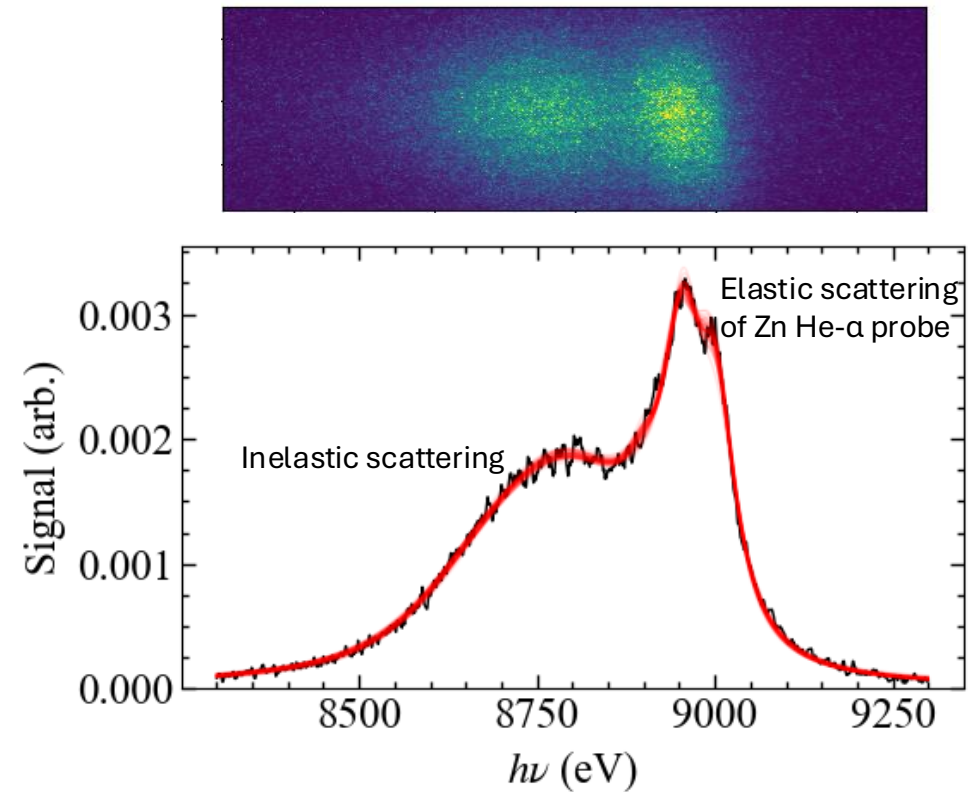
Brass (Cu/Zn) source spectrum



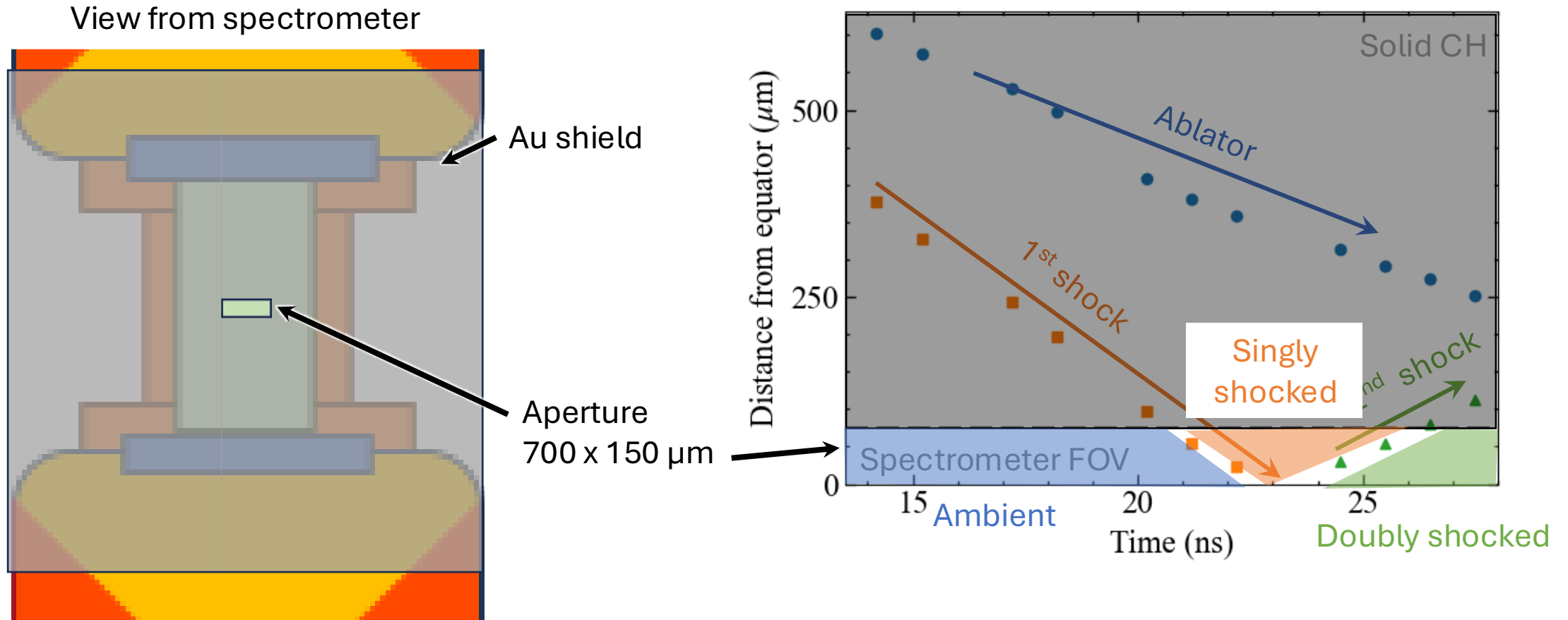
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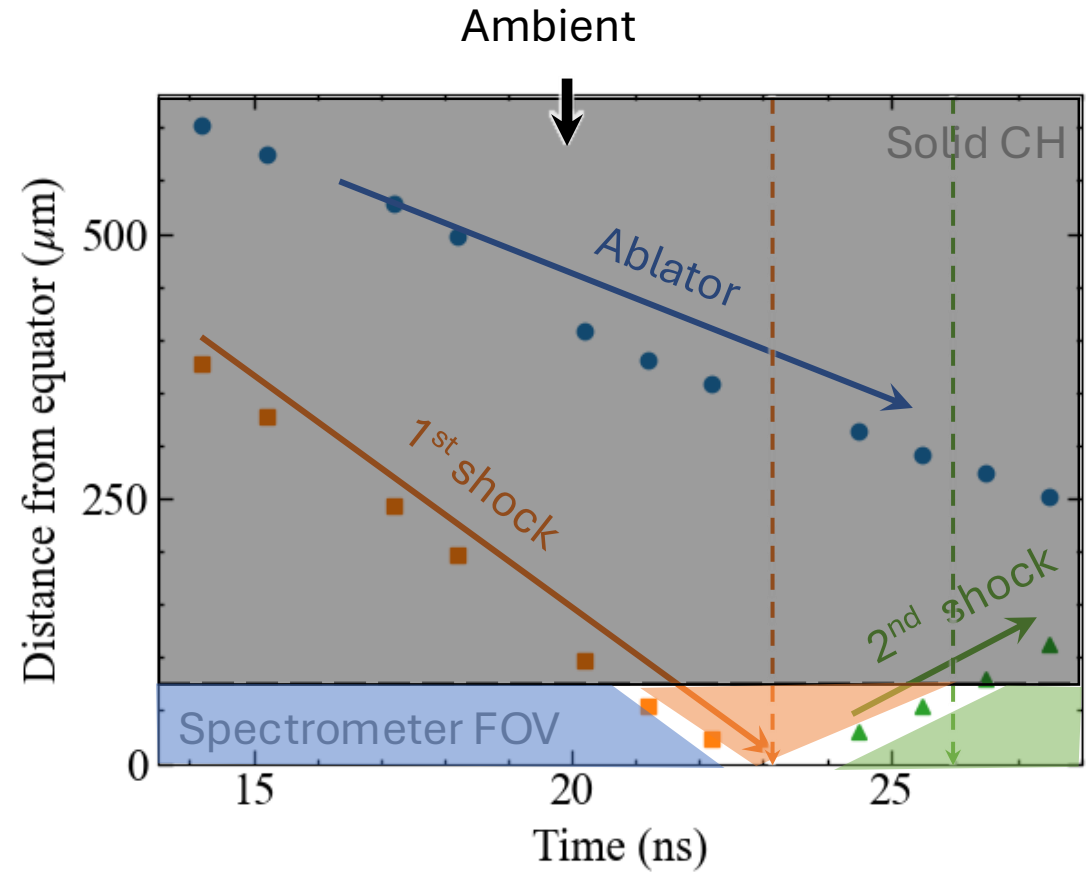
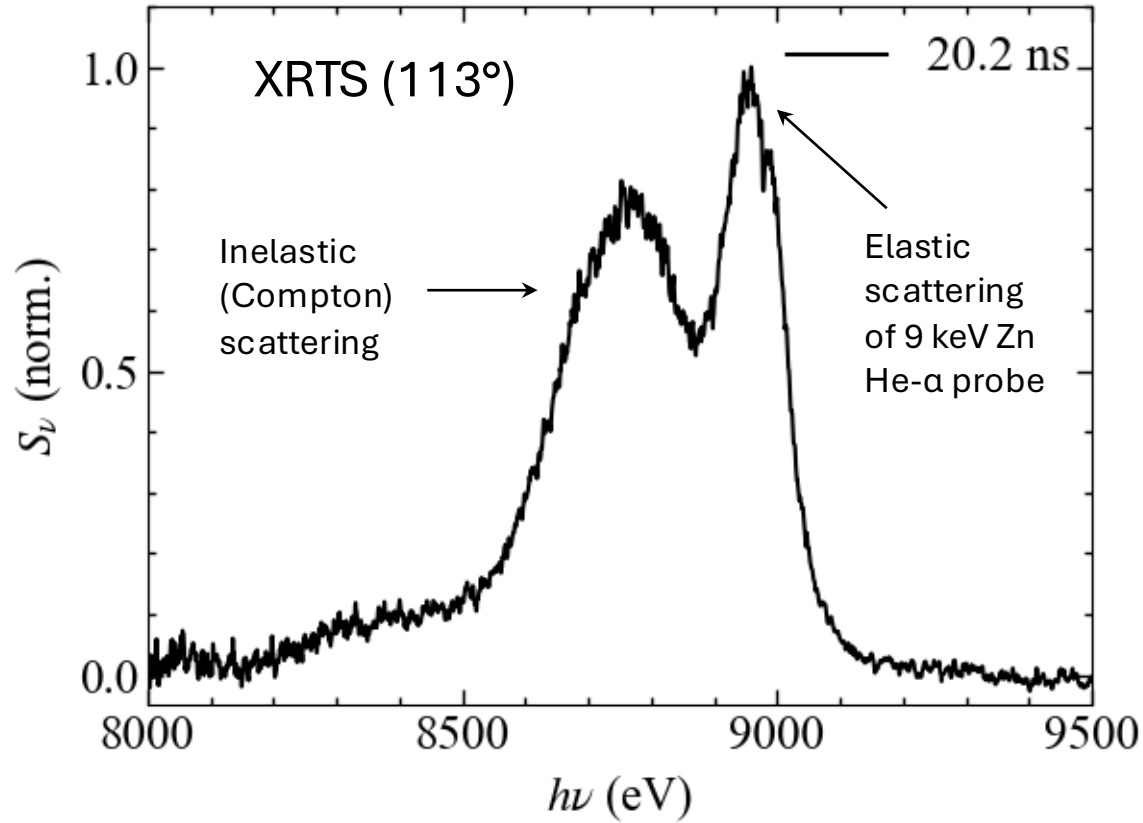
Scattering from doubly-shocked CH



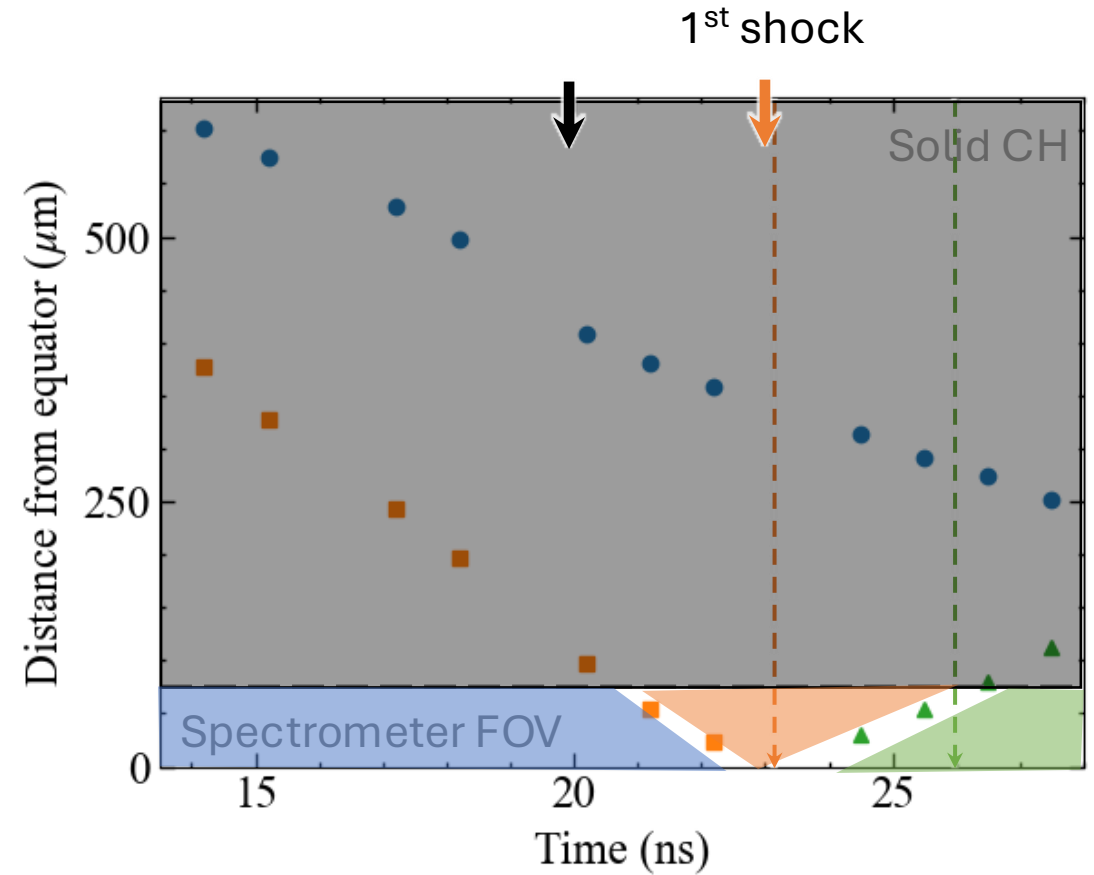
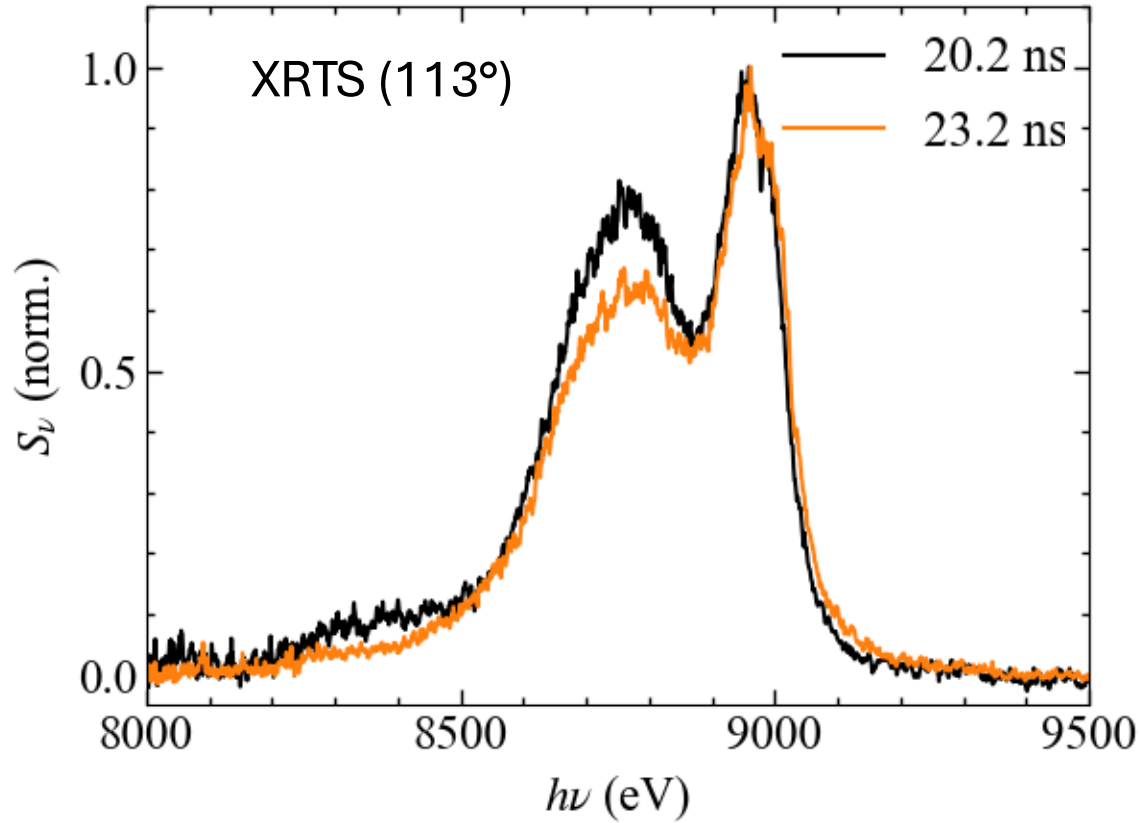
# An aperture on the XRTS line-of-sight restricts the measurement to single-density states near the shock collision plane



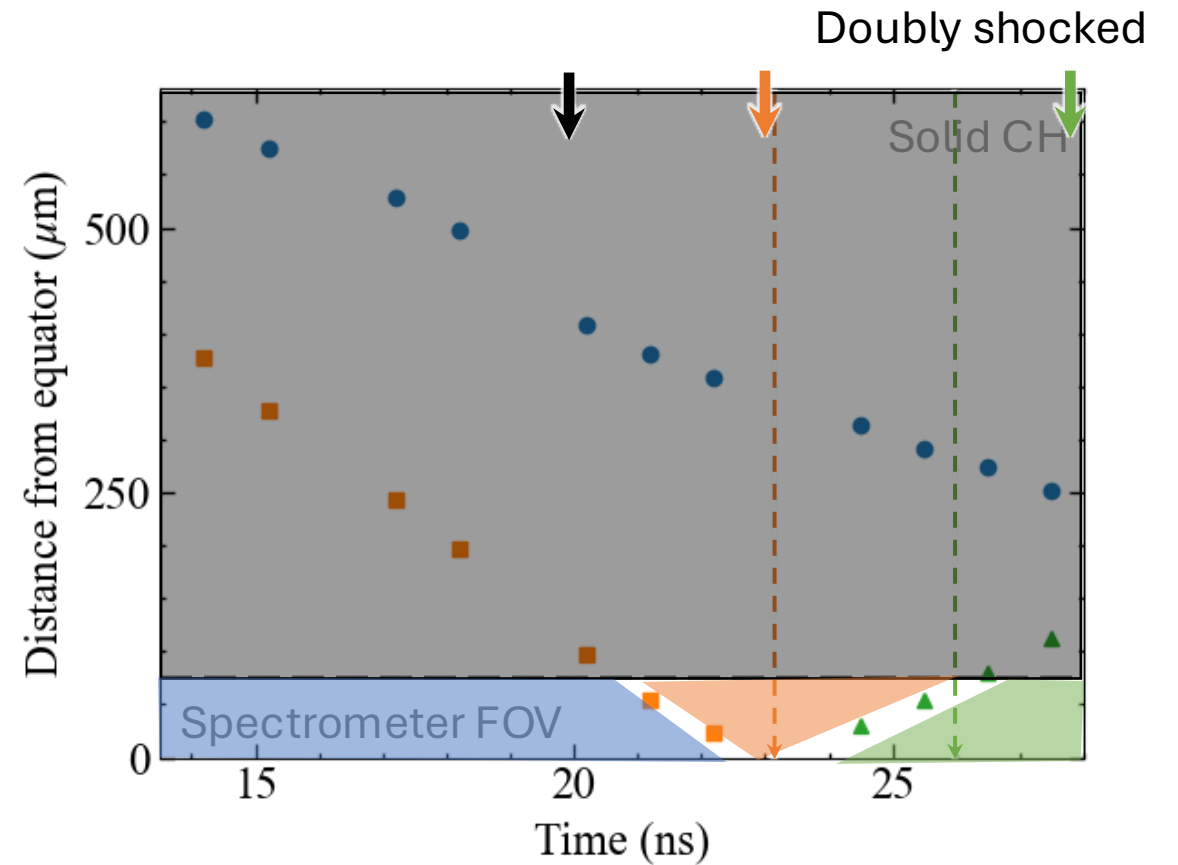
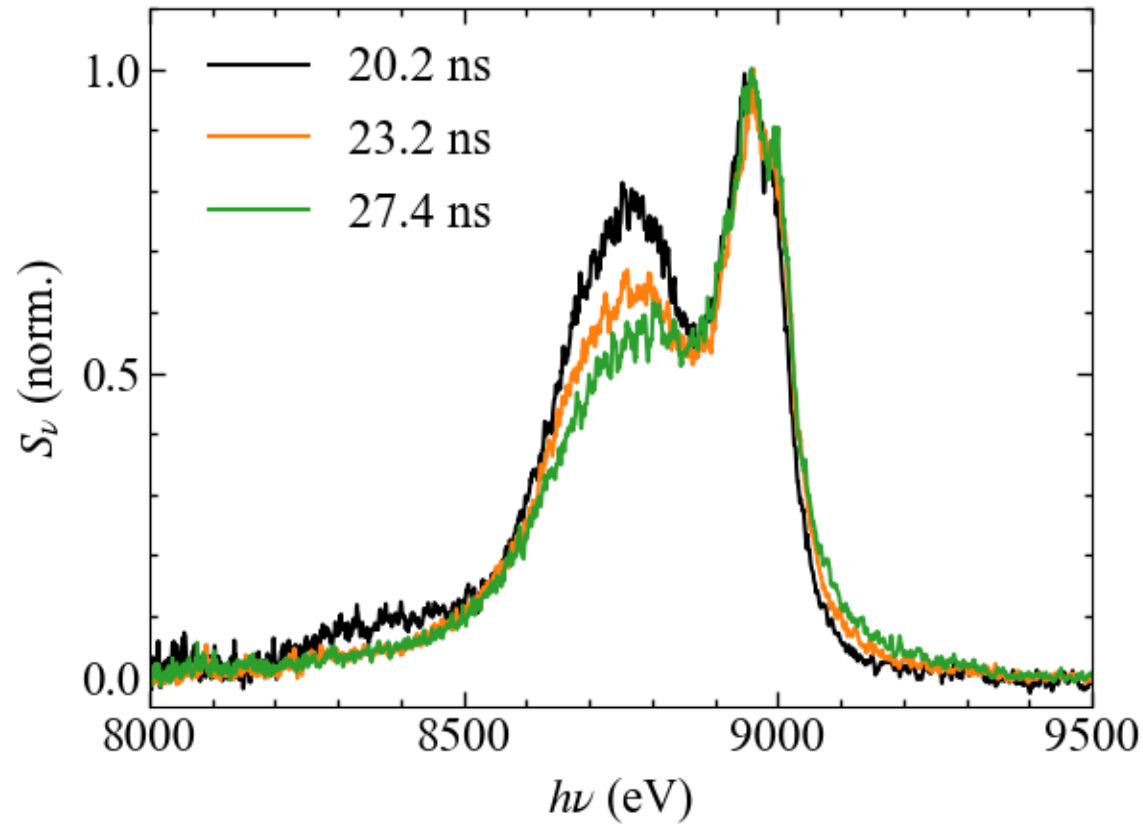
# XRTS spectra are collected throughout the shock sequence on multiple shots



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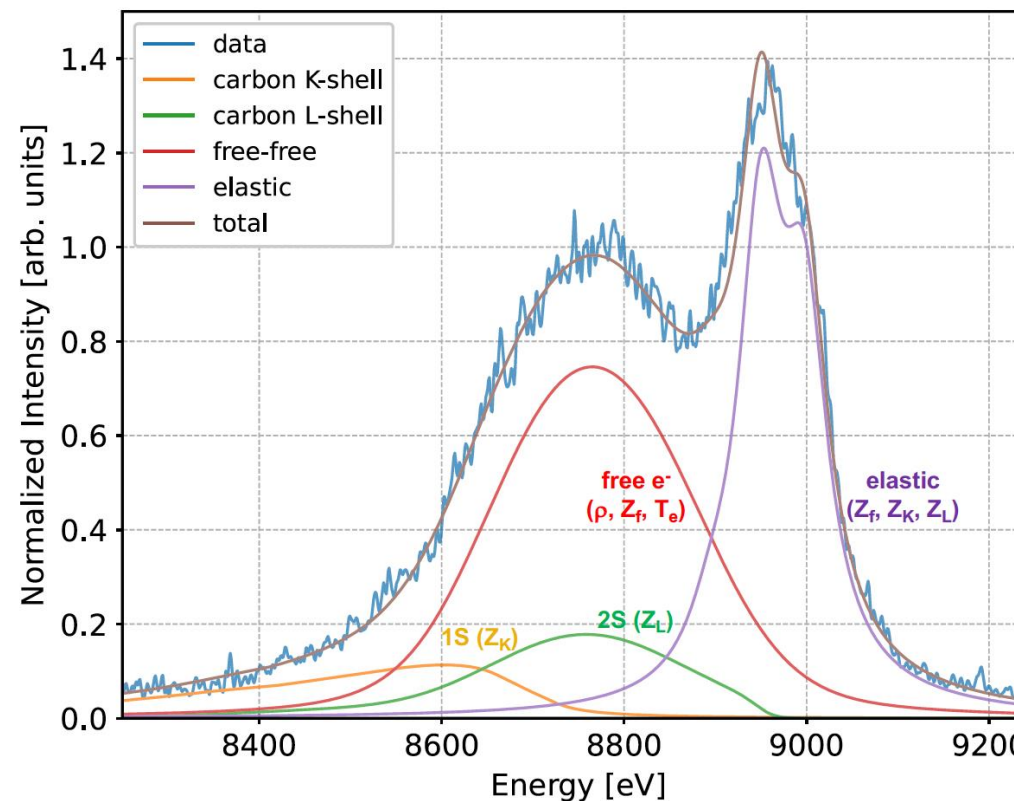
# XRTS is modeled with K-, L-shell populations as free parameters, allowing direct inference of ionization

$$S(k, \omega) = Z_f S_{ee}^0(k, \omega) \quad \text{[Free electrons]}$$

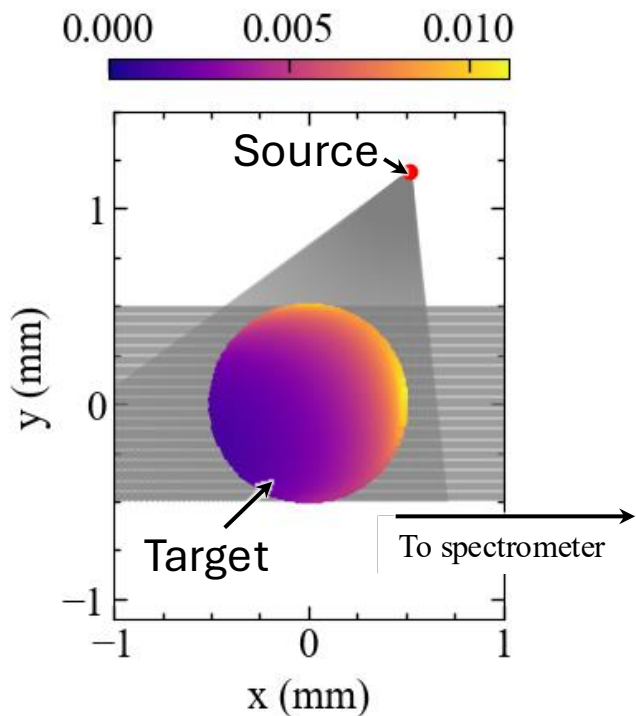
$$+ \left| \sum_{n\ell} f_{n\ell}(k) + q(k) \right|^2 S_{ii}(k) \delta(\omega) \quad \text{[Elastic]}$$

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**XRTS model with separate L-shell and K-shell ionization states**

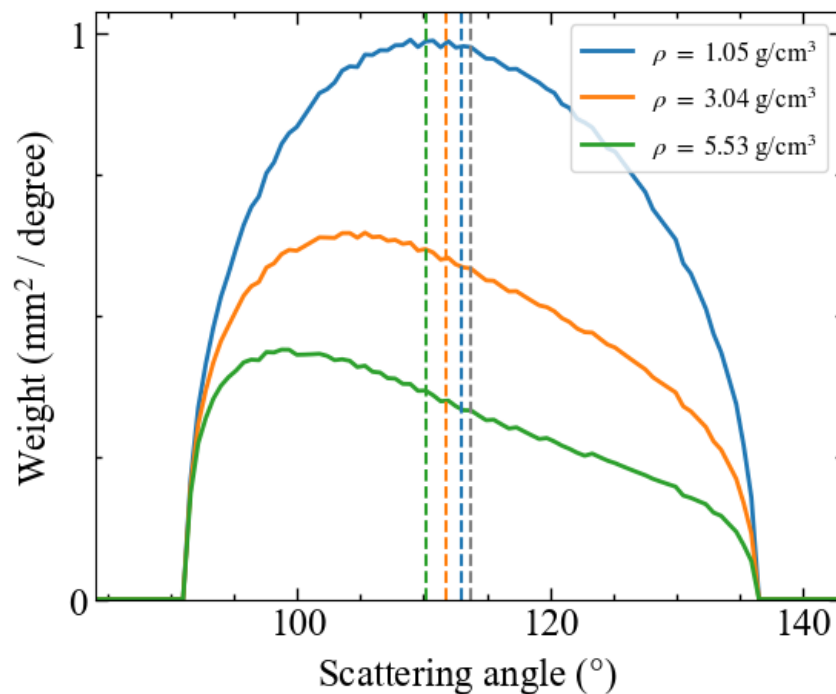


# XRTS from multiple scattering angles must be summed together due to the proximity of the target to the backlighter



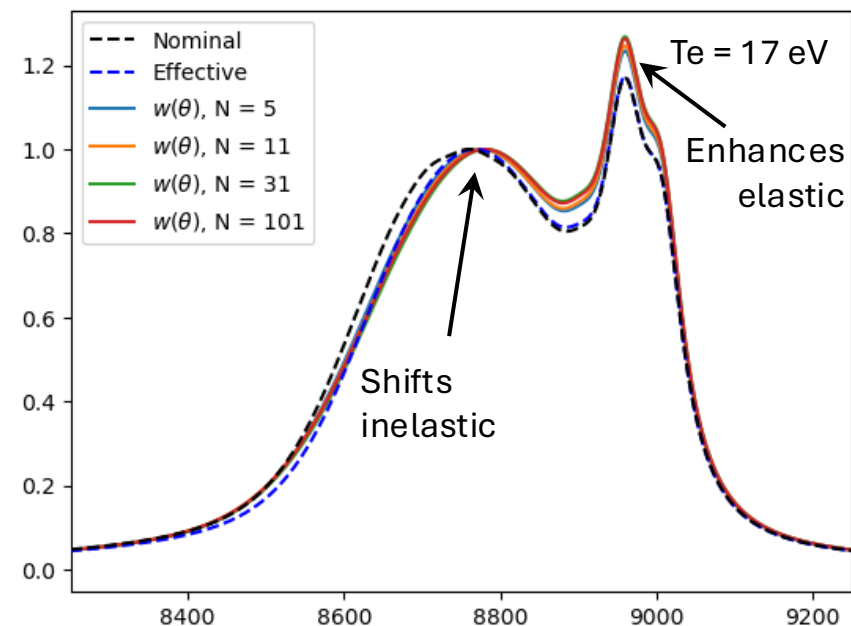
- Weights due to plasma attenuation

Angle-resolved weights



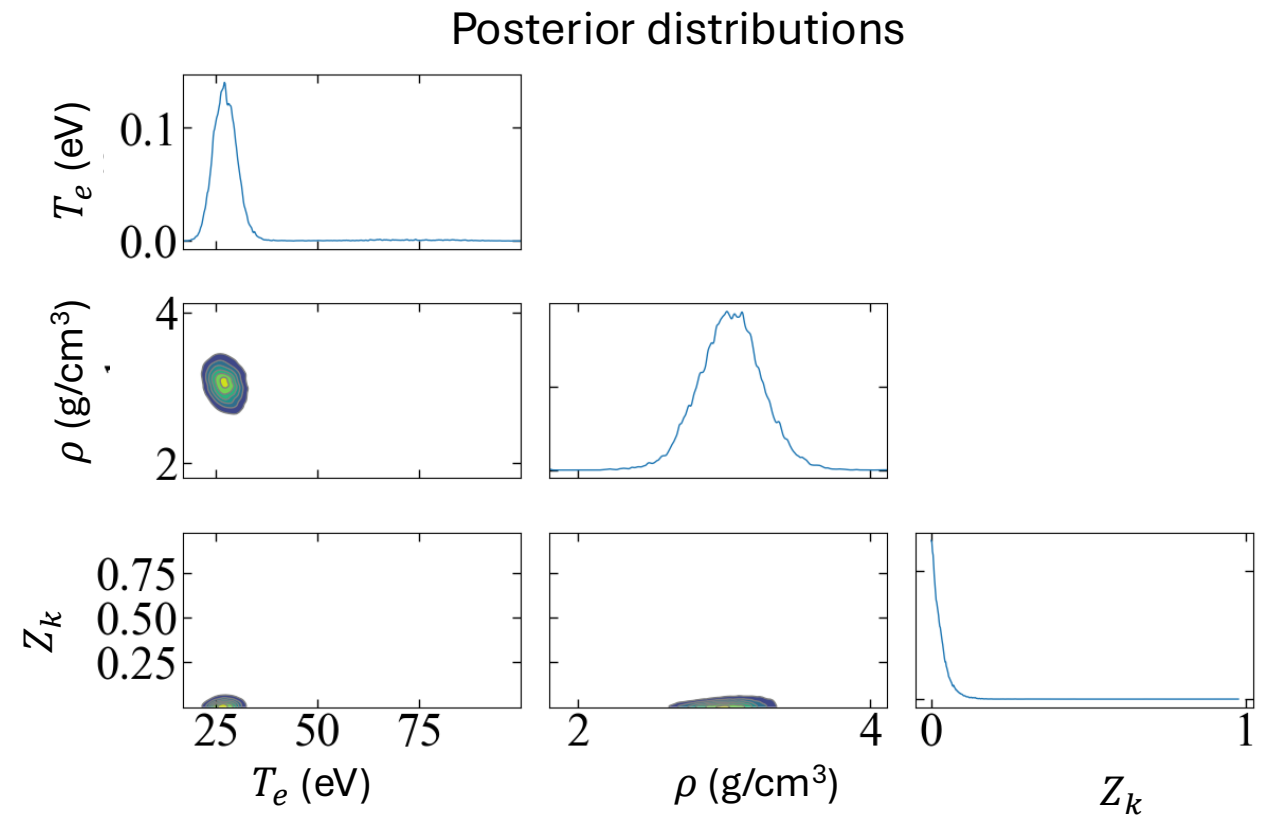
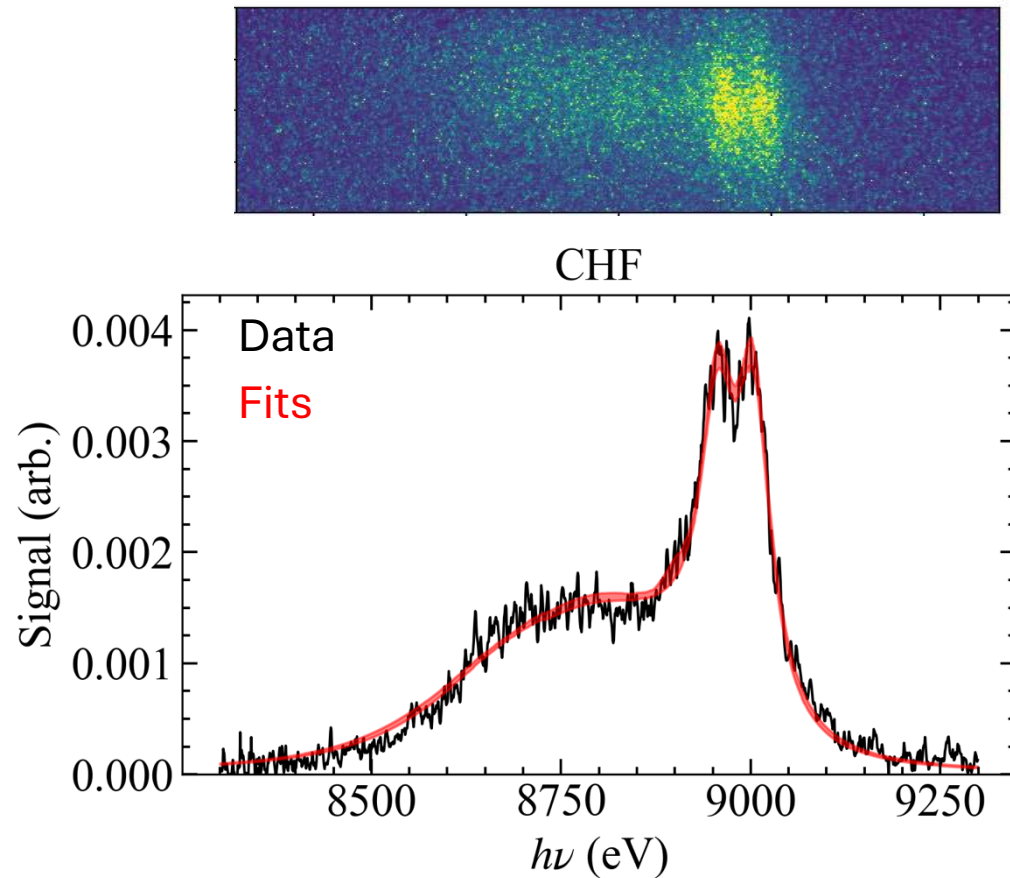
- Skew towards smaller angle

CHF, 2<sup>nd</sup> shock

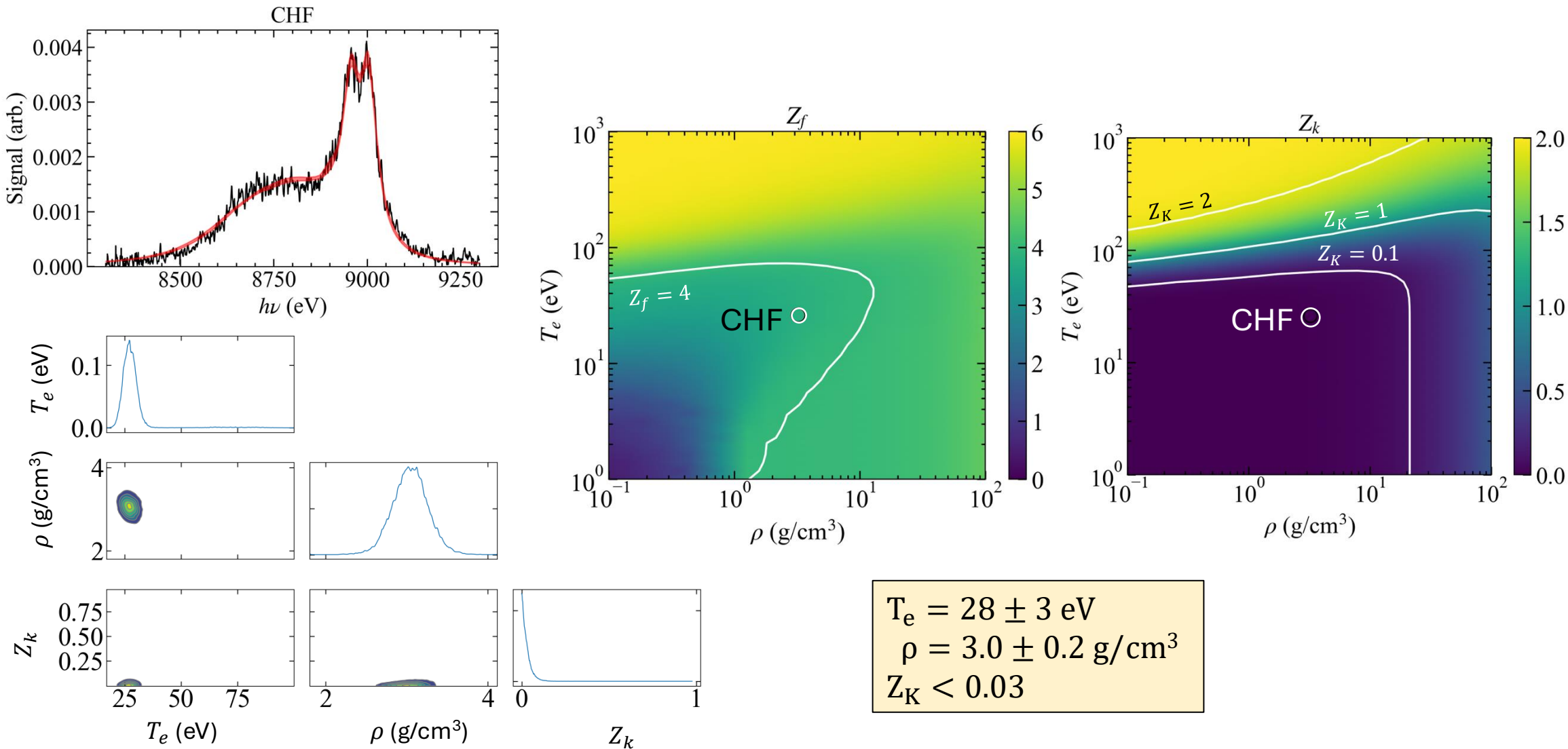


XRTS at average  $\langle \theta \rangle$  only shifts inelastic peak

# The XRTS forward model is wrapped in a Markov Chain Monte Carlo sampler, giving access to parameter uncertainties and correlations

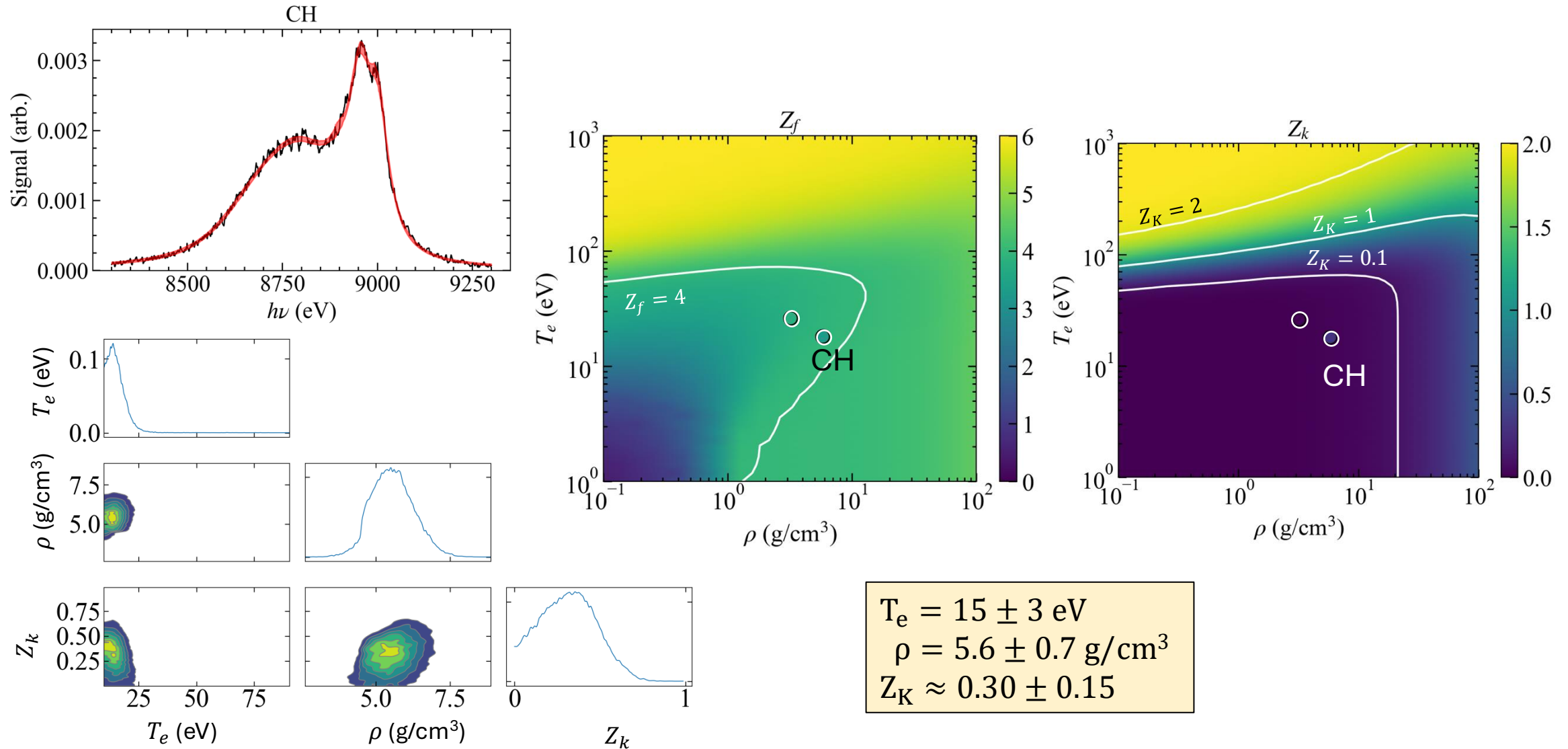


# CH foam ( $\rho_0 = 0.25 \text{ g/cm}^3$ ) data are consistent with no K-shell ionization



$T_e = 28 \pm 3 \text{ eV}$   
 $\rho = 3.0 \pm 0.2 \text{ g/cm}^3$   
 $Z_K < 0.03$

# CH ( $\rho_0 = 1.05 \text{ g/cm}^3$ ) data are consistent with enhanced K-shell ionization $Z_K = 0.3$



# Enhanced K-shell ionization is corroborated by transmission measurements

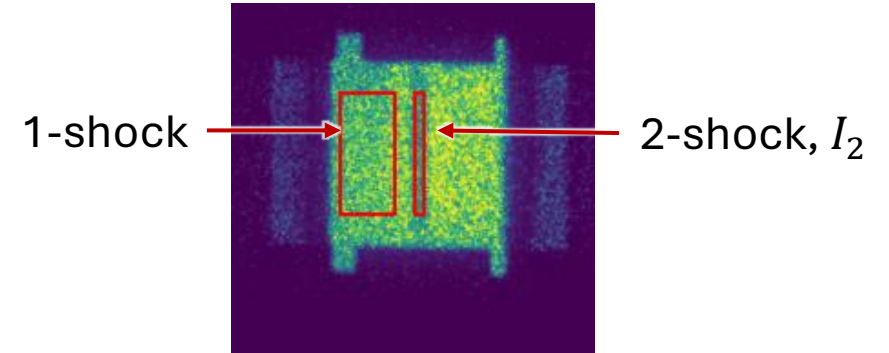
- Ratio of measured signals constrains  $\kappa\rho$ :

$$T_i = \frac{I_i}{I} = e^{-\rho\kappa\ell}$$

$I_i$  : transmitted signals  
 $i = 0$  : ambient  
 $i = 1$  : 1-shock  
 $i = 2$  : 2-shock

$$\rho_2\kappa_2 = \frac{1}{\kappa_2\ell} \ln\left(\frac{I_1}{I_2}\right) + \rho_1\kappa_1$$

- $\rho_1, \rho_2$  known from radiography  
 $\rightarrow \kappa_2 = 0.75 \kappa_0$
- Reduced inferred opacity can be interpreted as enhanced K-shell ionization
- Note: if  $\kappa_1$  also decreases,  $\kappa_2$  must be *further* reduced



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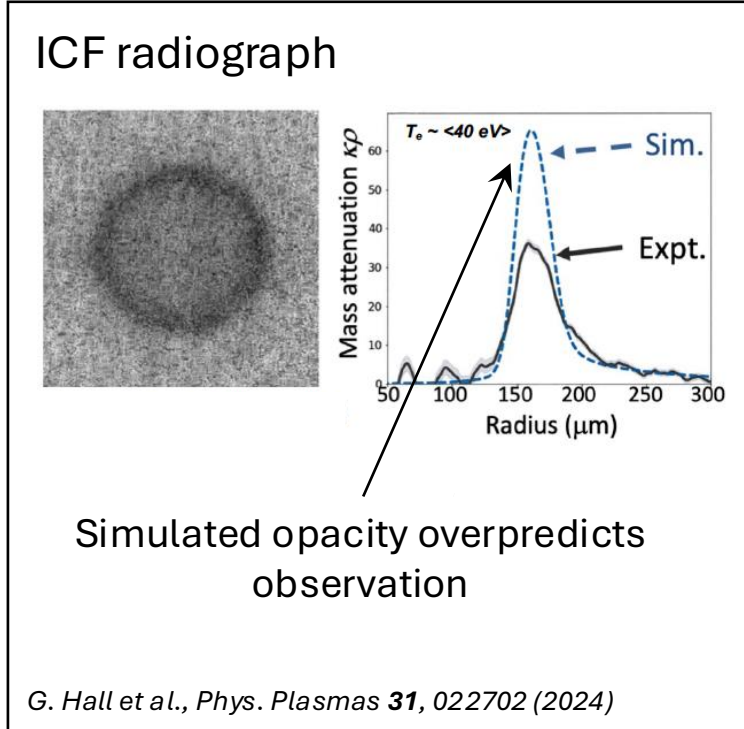
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Ionization potentially explains radiography opacity problem



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  - X-ray Thomson scattering (XRTS) constrains temperature to 20 – 30 %
- Novel analysis of XRTS, which models populations of individual atomic shells, gives evidence of **enhanced K-shell ionization**
  - Corroborated by radiograph transmission
- Future developments will further constrain ionization models
  - HDC samples to benchmark ionization at higher densities / coupling parameters
  - Use of a new streaked x-ray spectrometer to measure full evolution of XRTS
  - Comparison to novel DFT simulations (A. Bergermann)

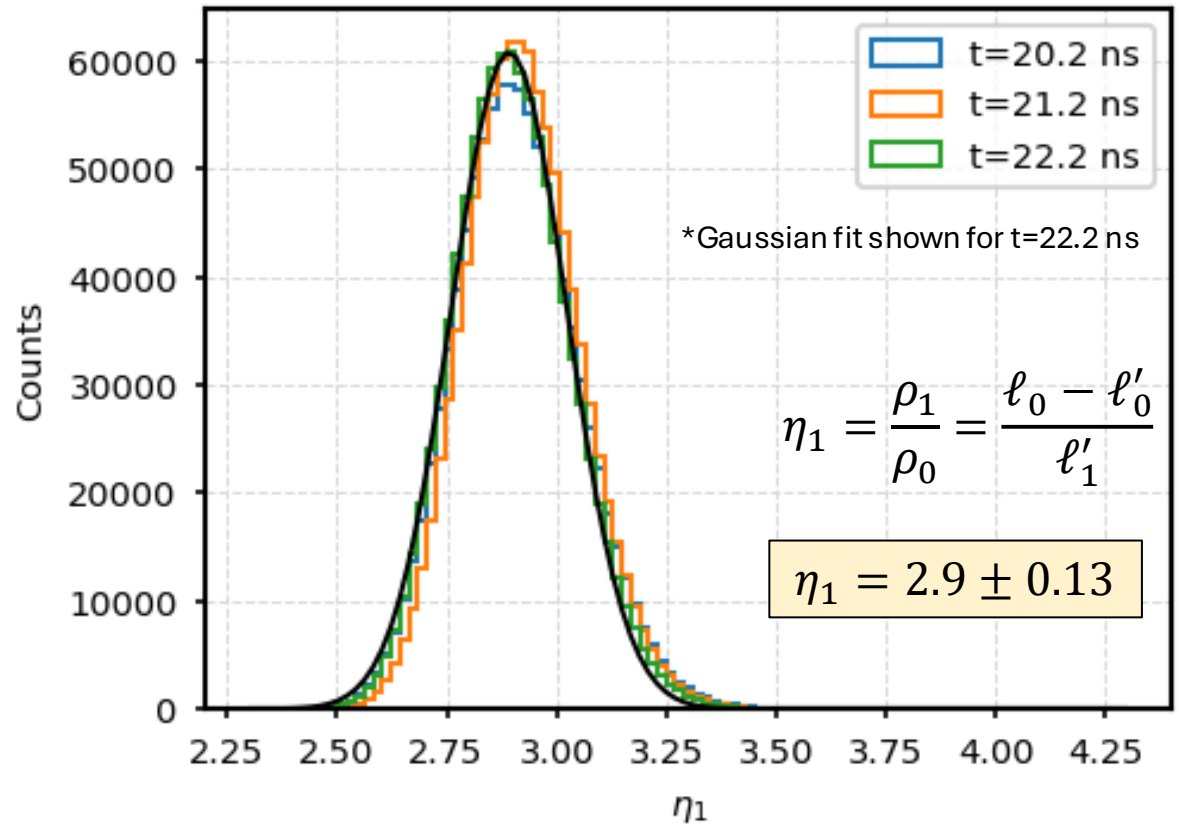
These measurements will inform modern ionization and opacity models of warm-dense plasmas



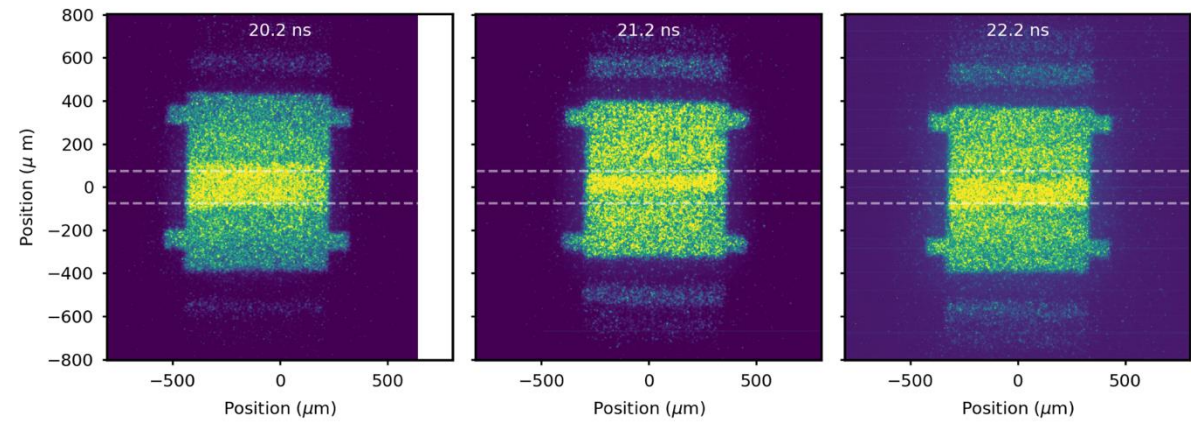


# Backups

# Compression uncertainties by MC 1<sup>st</sup> shock – 5% relative uncertainty



$\ell'_0, \ell'_1 \sim G(\mu = \text{measured}, \sigma = 20 \mu\text{m})$

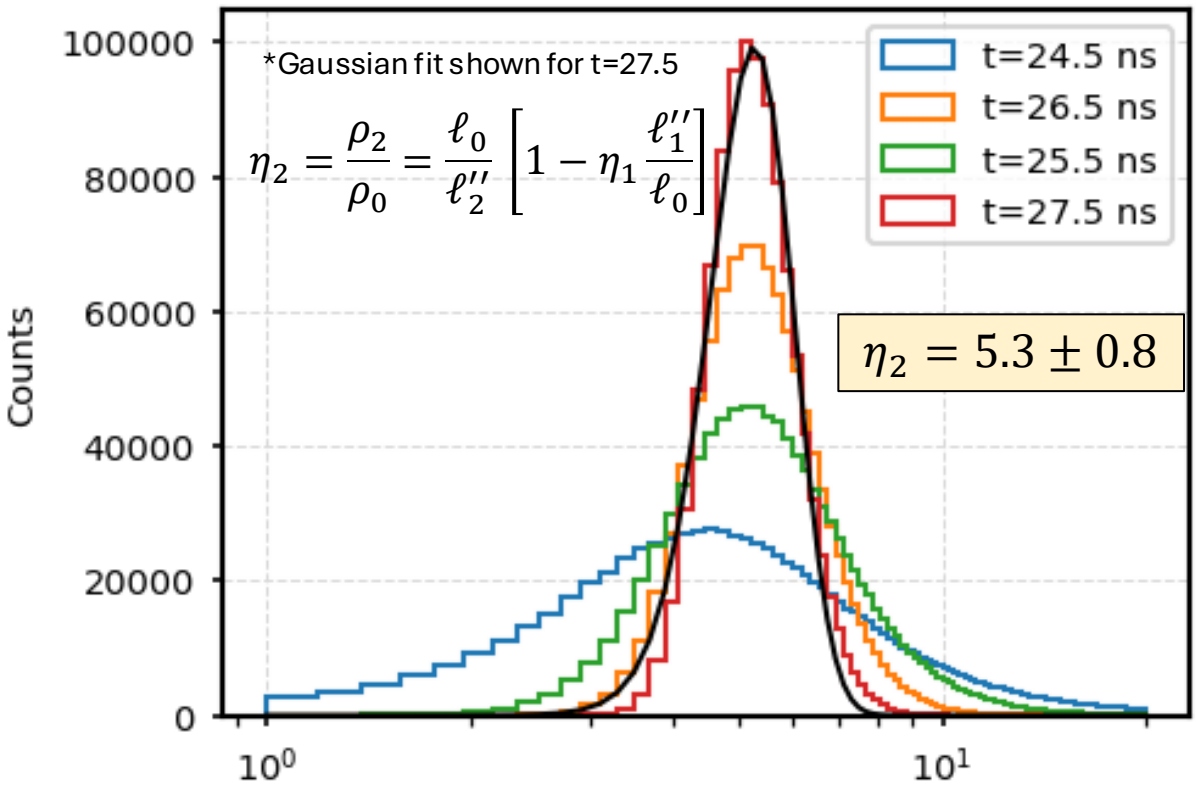


- MC distribution slightly asymmetric
- Taylor approximation representative of MC distributions
- $\sigma_\eta \propto 1/\ell'_1$ 
  - small because volume is close to 100% 1-shock
  - All images have similar  $\ell'_1$ , hence similar  $\sigma_\eta$

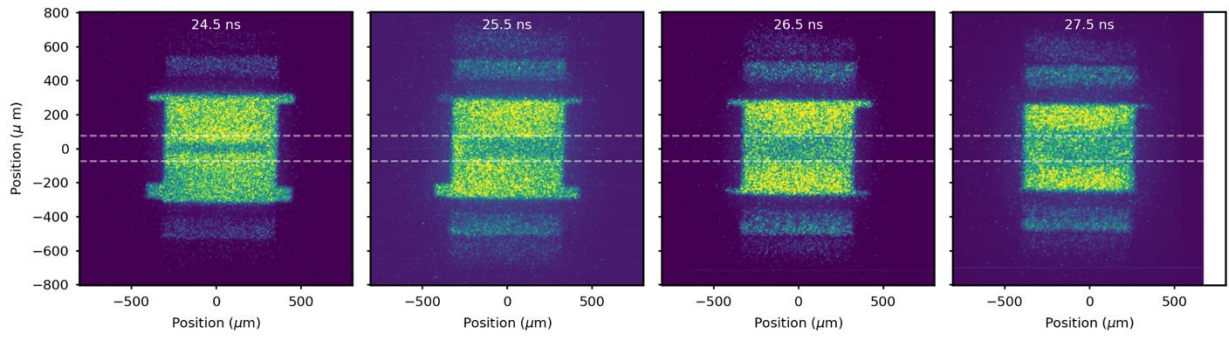
Mag = 5.6x

# Compression uncertainties by MC

## 2<sup>nd</sup> shock – 15% relative uncertainty



$\ell_1'', \ell_2'' \sim G(\mu = \text{measured}, \sigma = 20 \mu\text{m})$   
 $\eta_1 \sim 1^{\text{st}} \text{ shock analysis (note: different shot)}$   
 Could enforce  $\eta_1$  as a minimum

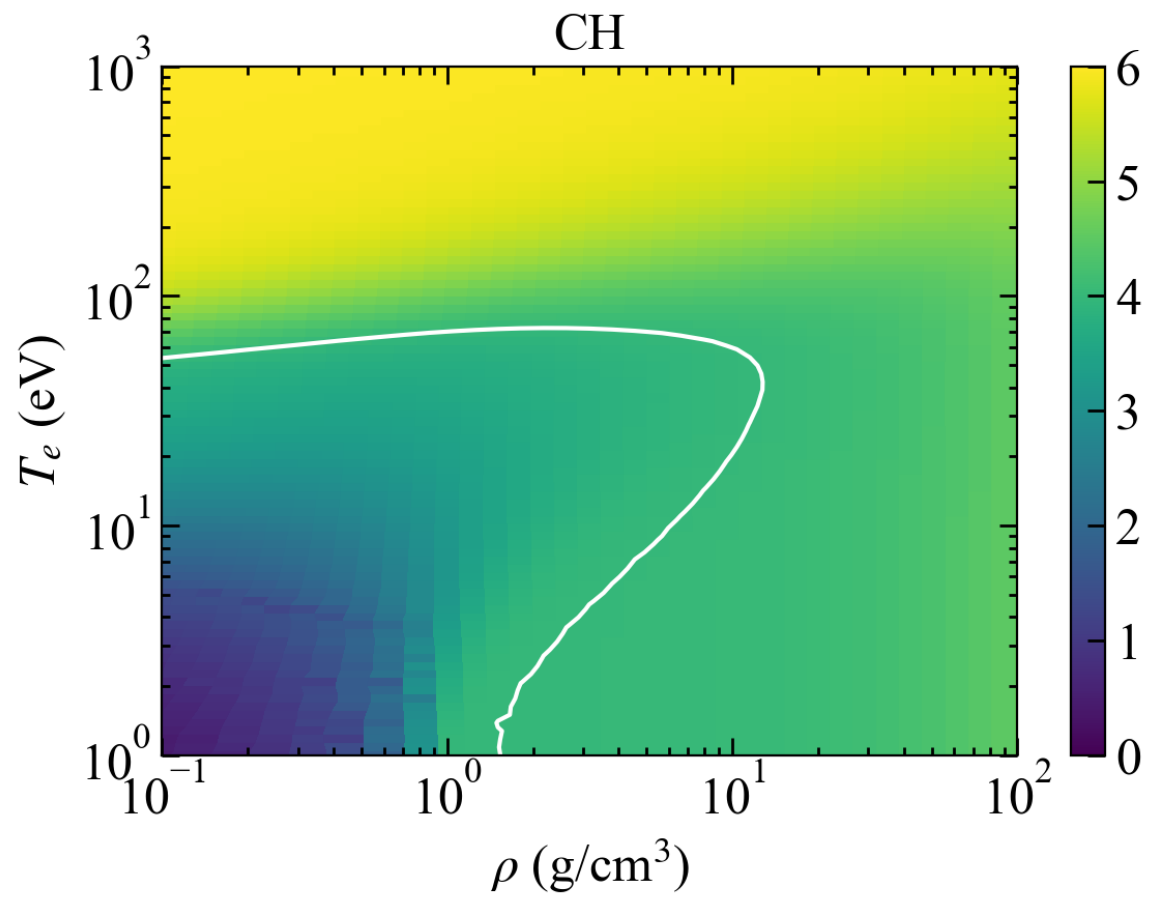
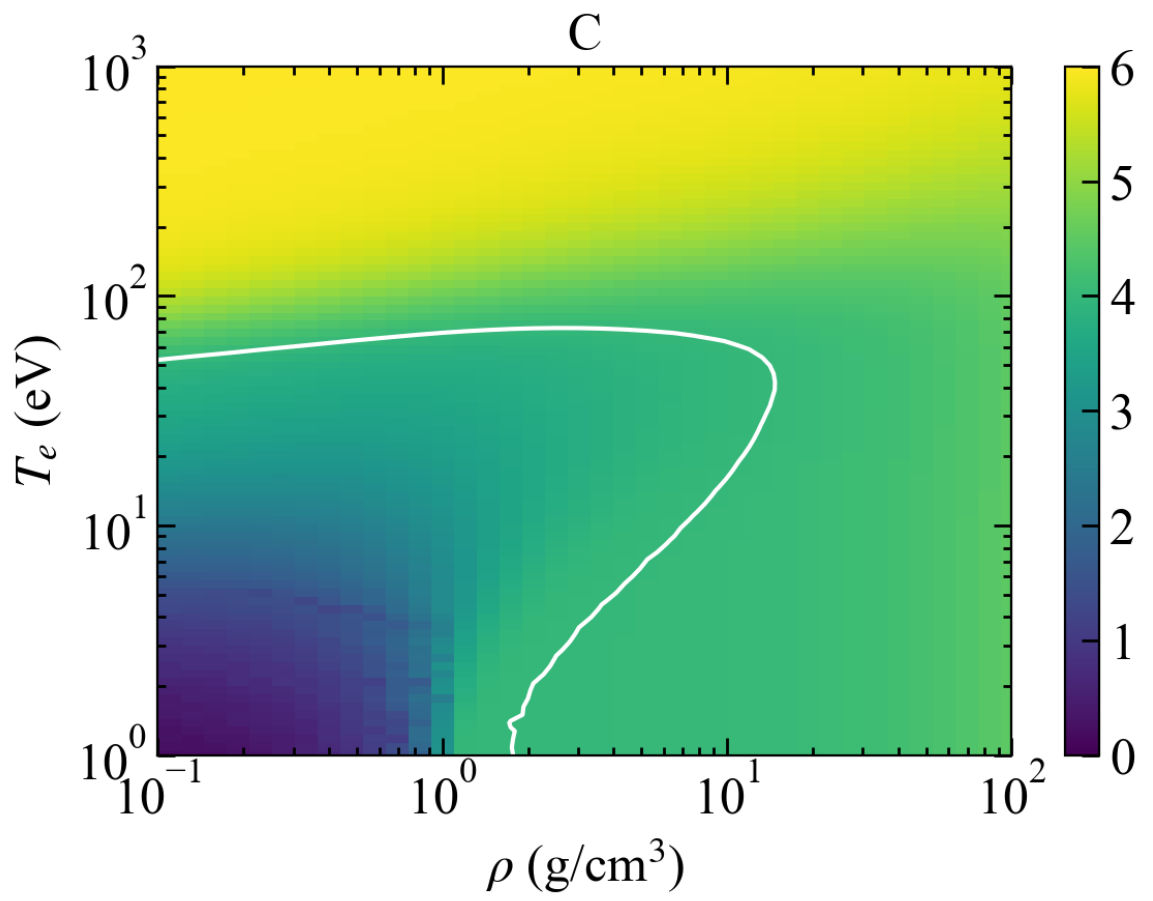


- MC distributions asymmetric
- Possibly log-normal
- $\sigma_{\eta_2} \propto 1/\ell_2''$
- Later time radiographs exhibit reduced  $\sigma$ , due to larger 2-shock volume
- Even still, mean is surprisingly robust

Mag = 5.6x

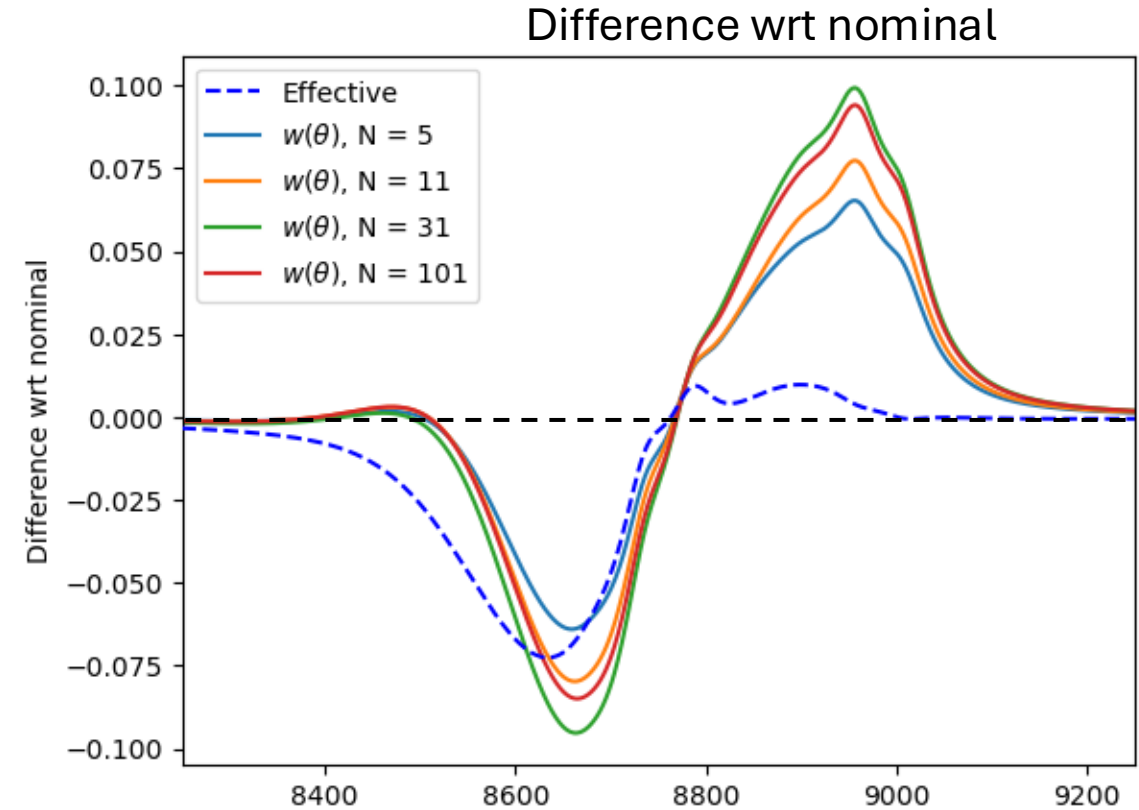
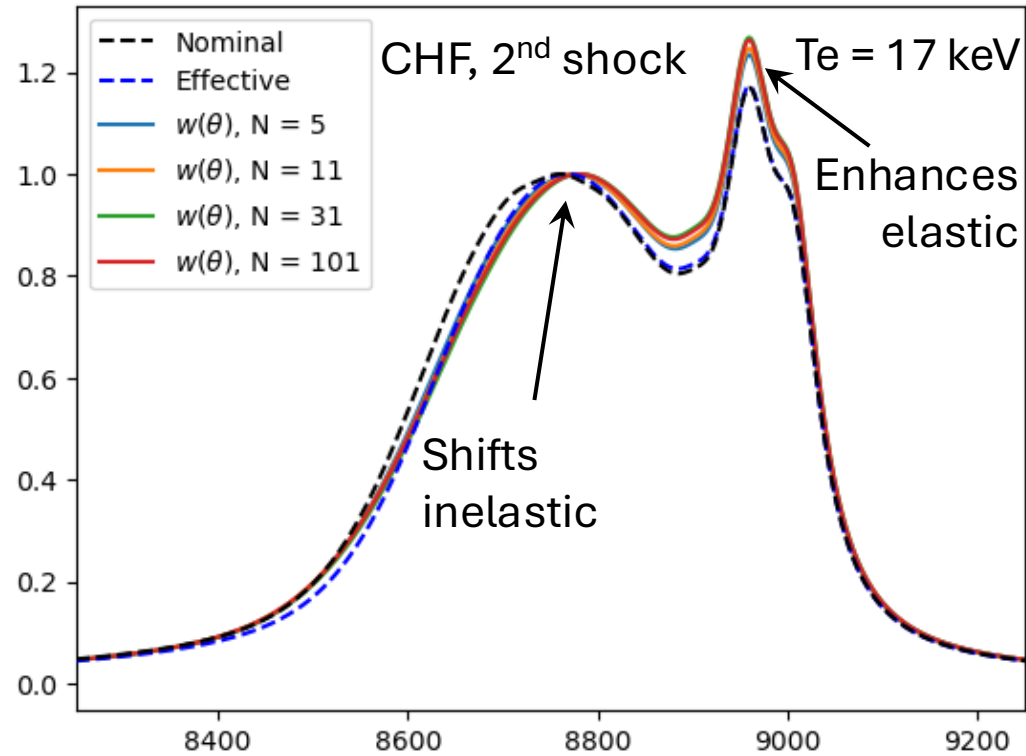


# C vs CH ionization



CH ionizes at ~0.9 the density of pure C

# XRTS summed over angle distribution $w(\theta)$ increases elastic peak and shifts inelastic peak to higher photon energy

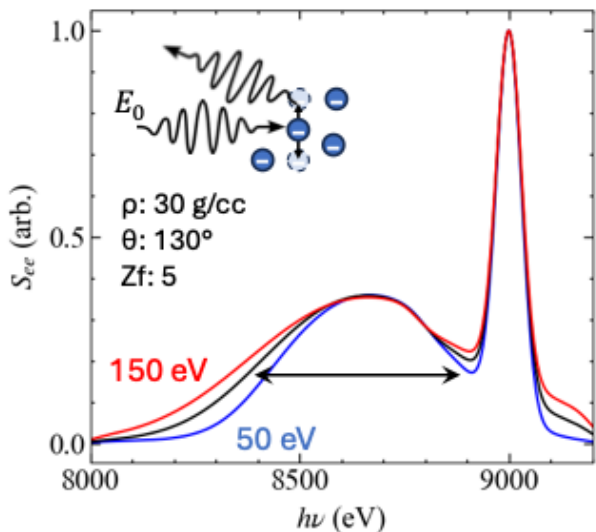


XRTS at average  $\langle \theta \rangle$  only shifts inelastic peak

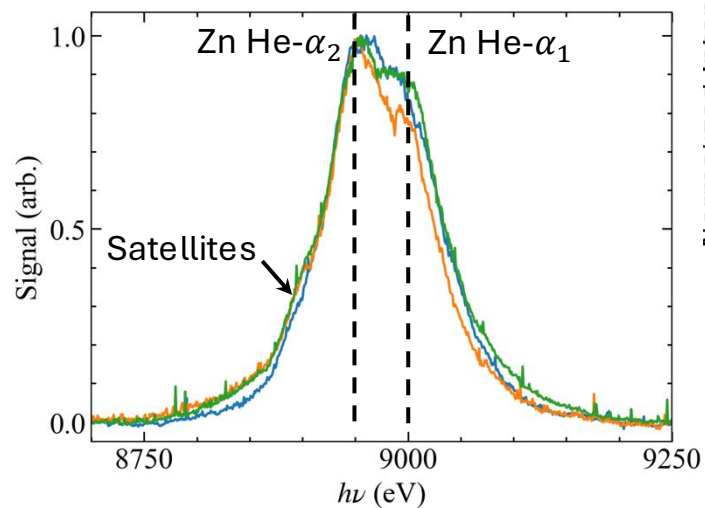
# We include source variations in uncertainty analysis

Observed spectrum  $\propto S(k, \omega) * I(\omega)$

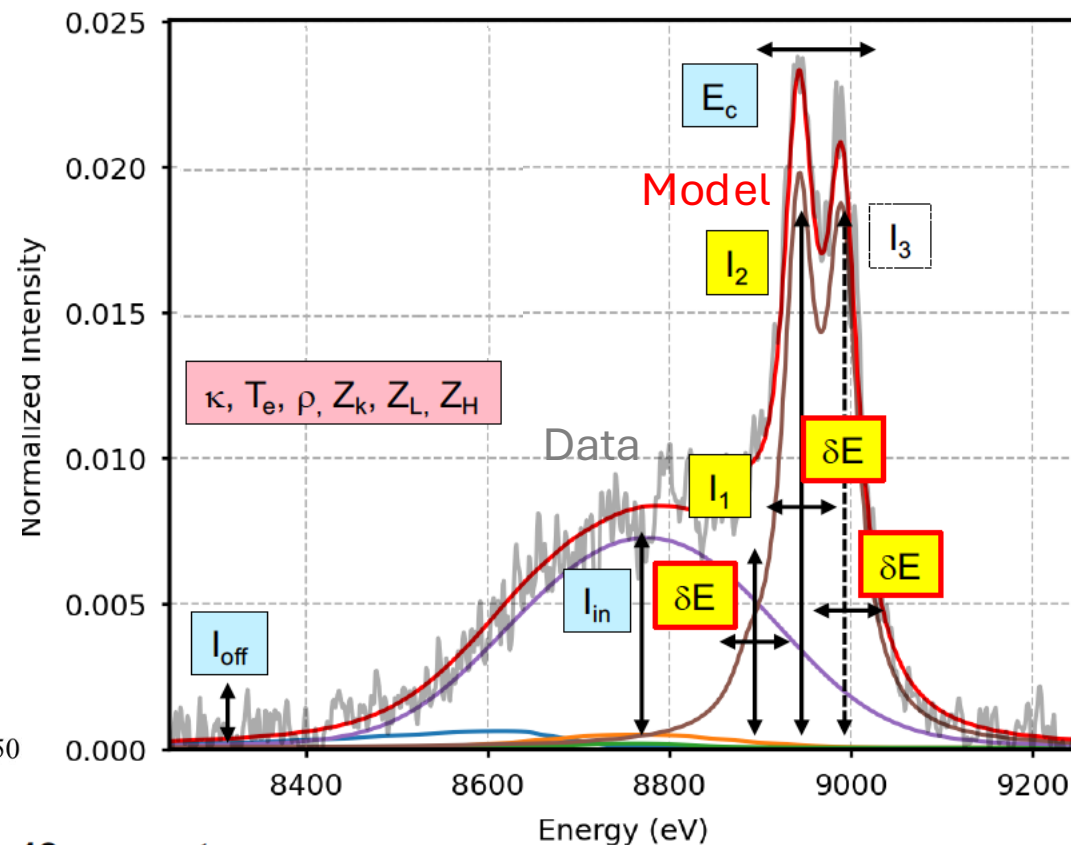
$f(T, \rho, Z)$



Source-instrument function



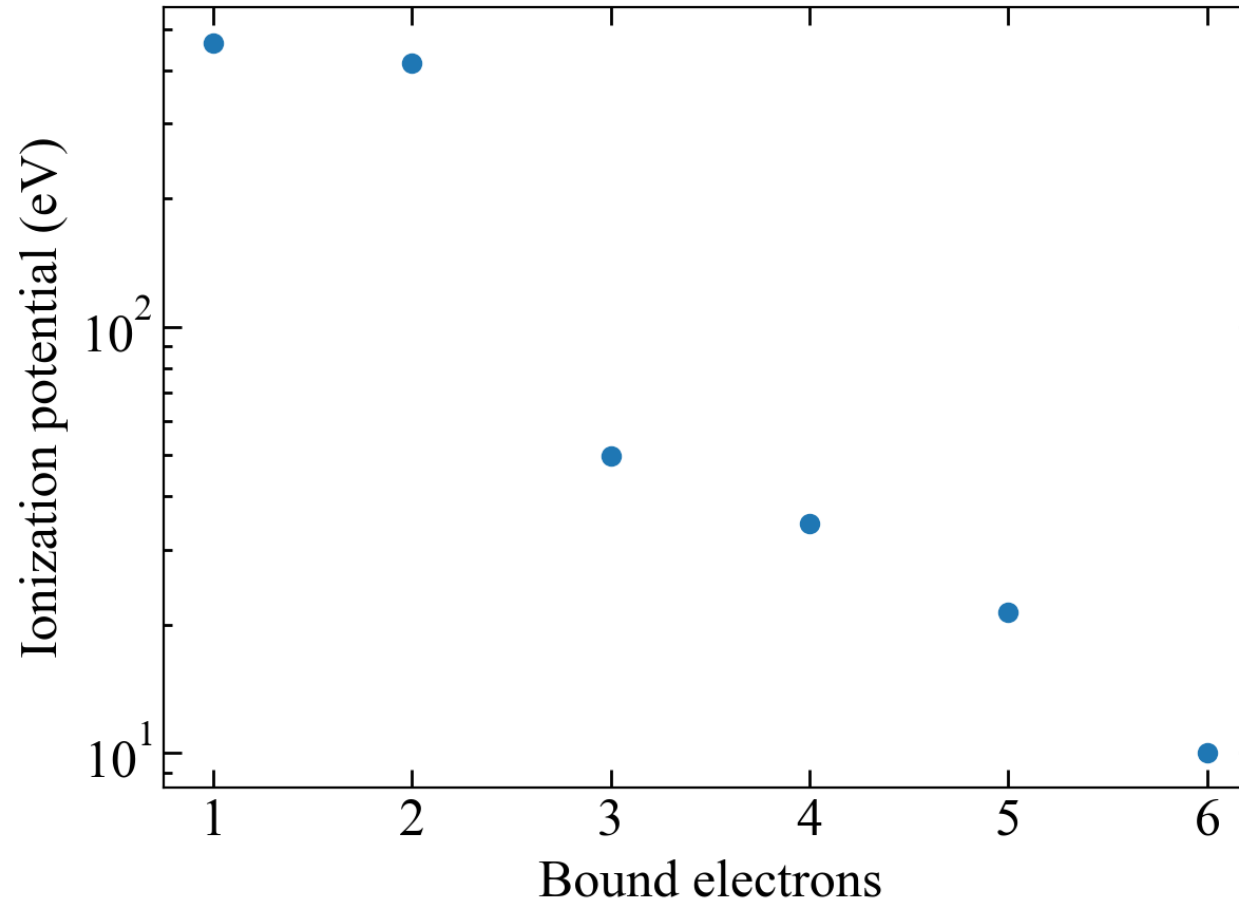
Zn He- $\alpha$  spectra from three experiments



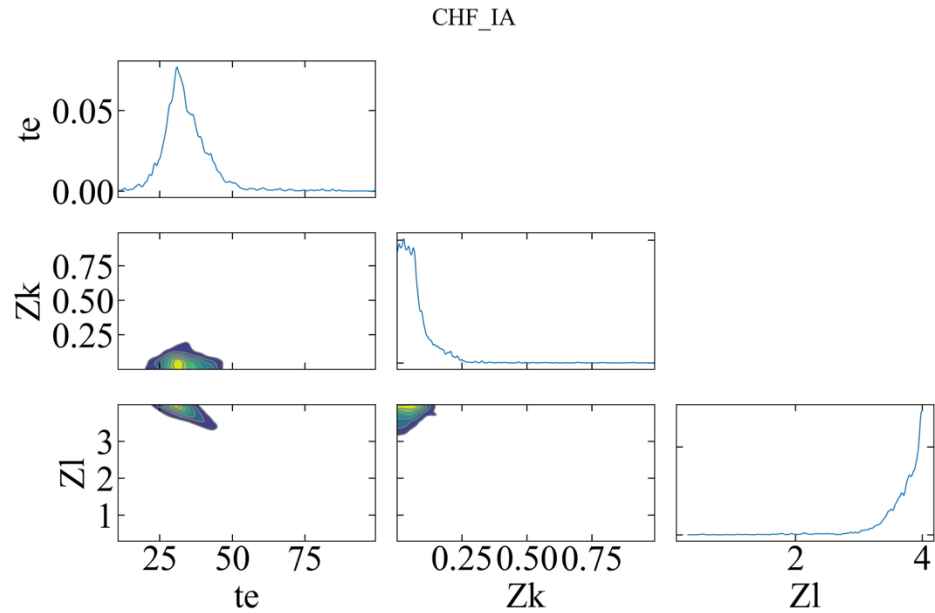
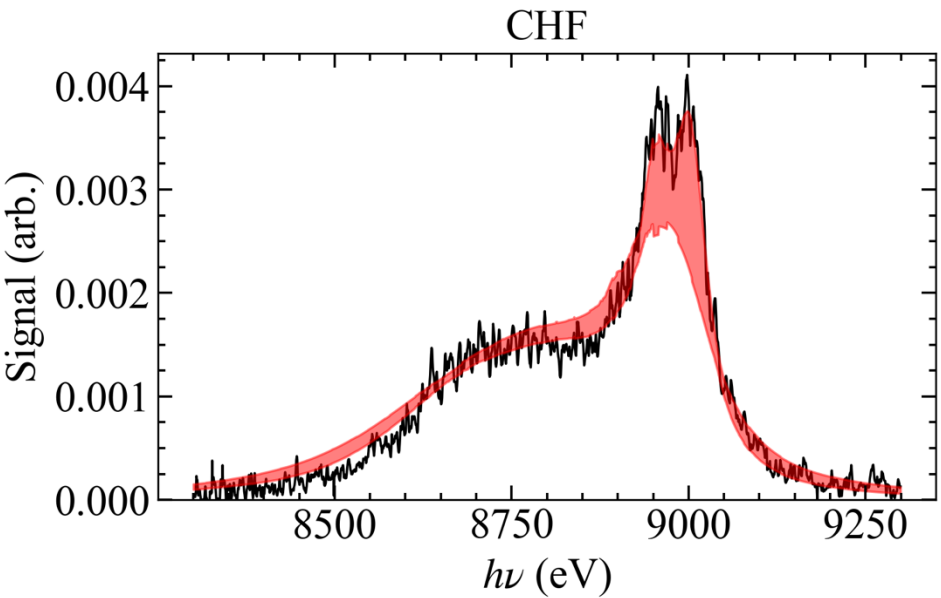
**12 parameters:**

- XRTS variables
- Source func. variables
- "Processing" variables

# C ionization potential



# Fit to CHF XRTS with constant density yields higher $T_e \approx 34$ eV, but still no K-shell ionization



Shape of fit is similar  
 Note: fewer samples