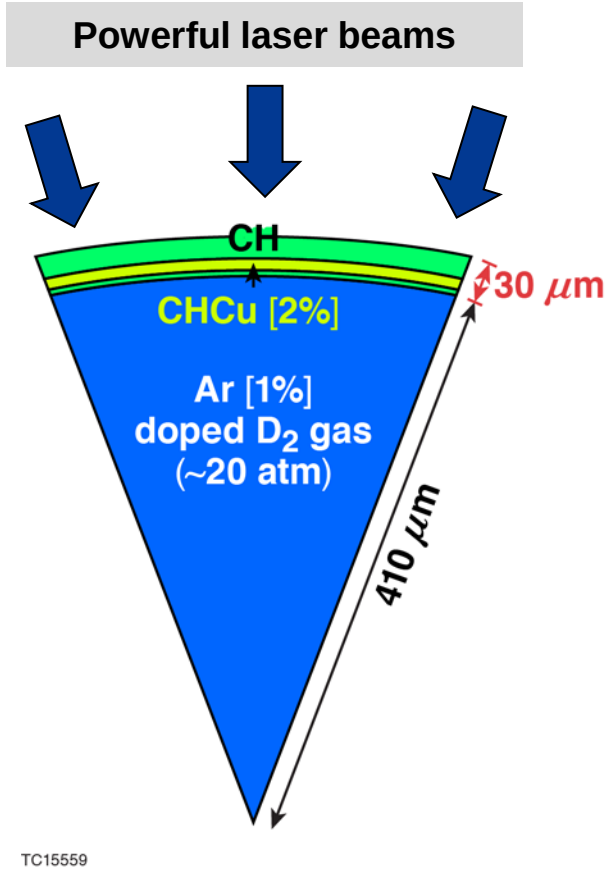
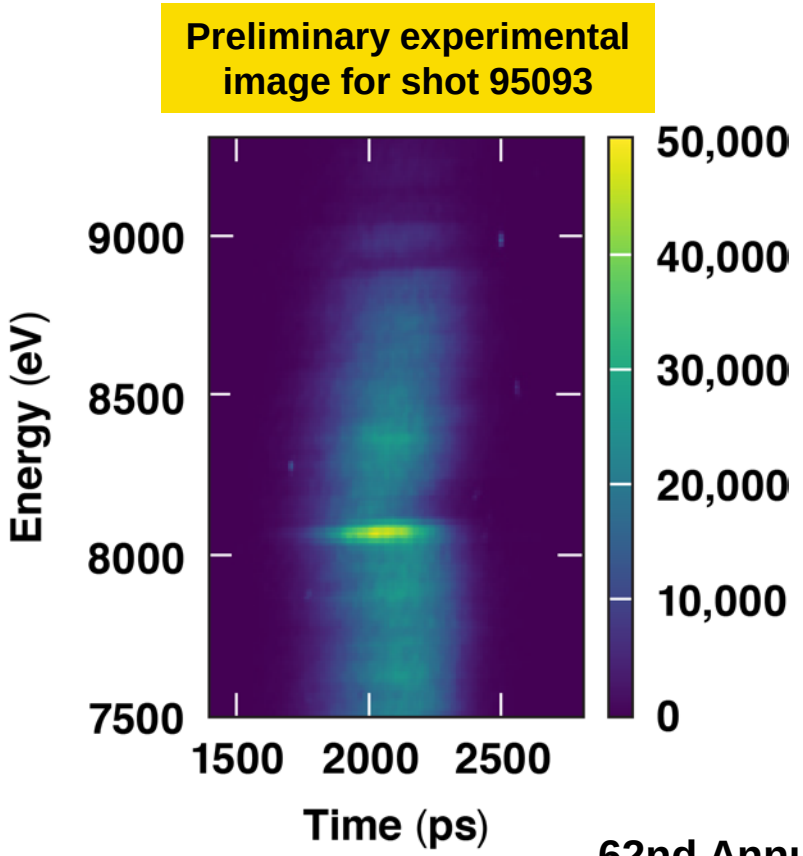
Extreme Atomic Physics at 5- to 100-Gbar Pressures





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Summary

In collaboration with SNL and Prism, we have established an experiment–theory-combined program to understand extreme atomic physics under HED conditions

- Using a high-resolution time-resolved spectroscopy technique, we have conducted spherical implosion campaigns on OMEGA to measure K_{α} and K_{β} emission/absorption of Cu at 5- to 100-Gbar pressures
- Post-processing hydro simulations of these experiments, we could not find a single atomic-physics model giving a full count of the spectroscopic features observed in experiments
- A DFT-based NLTE-modeling code (*VERITAS*) is under development, in which the *ab-initio* calculations provide the essential shifts and transitions of K_{α} from emission to absorption during heat-wave propagation

DFT-based NLTE modeling would offer a self-consistent understanding of exotic atomic physics at extreme HED conditions.

SNL: Sandia National Laboratories
HED: high energy density
DFT: density-functional theory
NLTE: non local thermodynamic equilibrium

Collaborators

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Sandia National Laboratories

T. Walton and I. E. Golovkin

Prism Computational Sciences

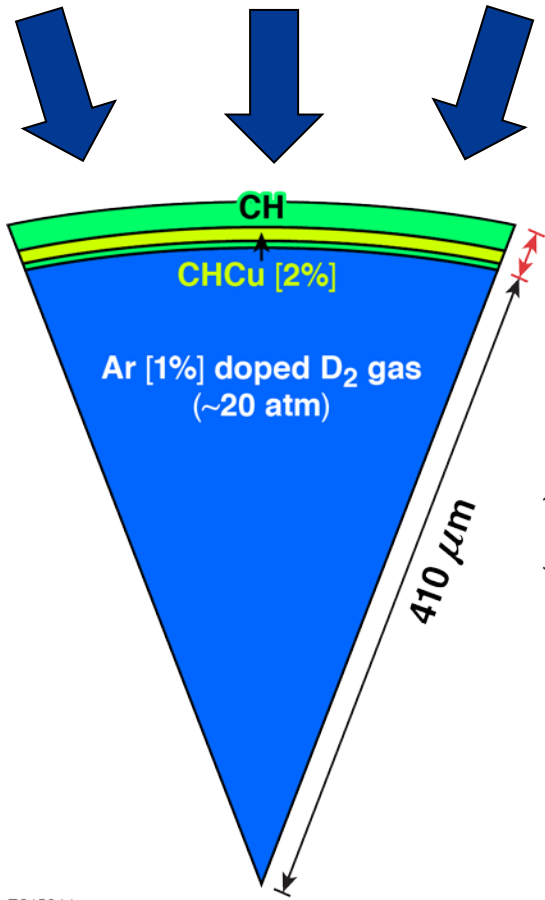
How atomic physics might be altered at extreme HED conditions remains to be understood

- Traditional continuum-lowering models have been called into question from both experimental measurements[1,2] and first-principles calculations[3,4]
- The opacity of iron is found to be higher than any model prediction in experiments for dense plasma conditions[5,6]
- A self-consistent picture between the measured K_α and K_β emission/absorption and atomic-physics modeling is still lacking[7]

[1]O. Ciricosta *et al.*, Phys. Rev. Lett. 109, 065002 (2012).
[2]D. J. Hoarty *et al.*, Phys. Rev. Lett. 110, 265003 (2013).
[3]S. X. Hu, Phys. Rev. Lett. 119, 065001 (2017).
[4]S. B. Hansen *et al.*, Phys. Plasmas 25, 056301 (2018).
[5]J. E. Bailey *et al.*, Nature 517, 56 (2015).
[6]T. Nagayama *et al*., Phys. Rev. Lett. 122, 235001 (2019).
[7]S. X. Hu *et al.*, "Extreme Atomic Physics at Peta-Pascals Probed by Time-Resolved Spectroscopy," to be submitted to Nature Physics.

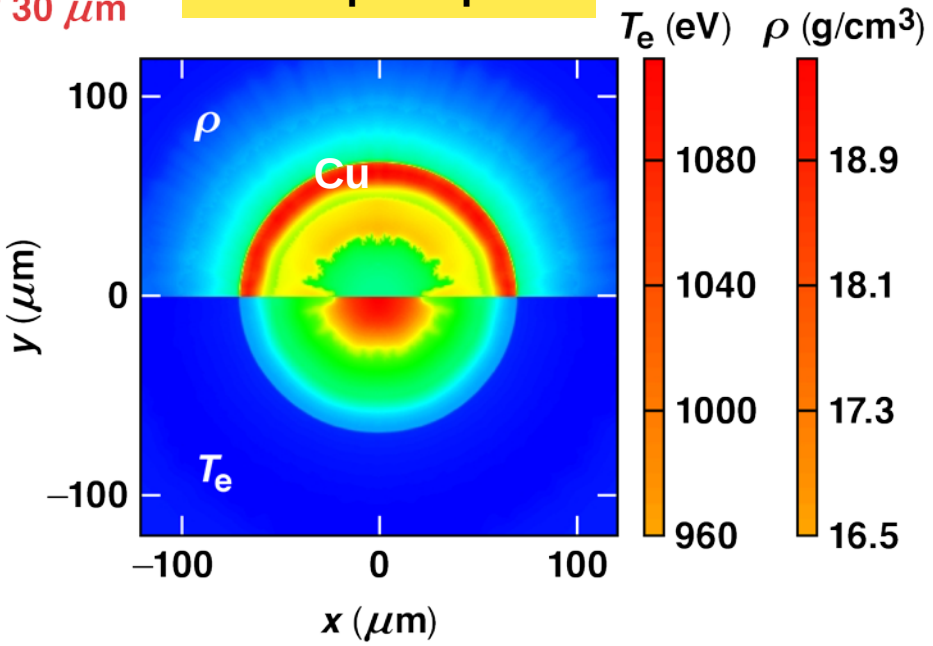
Experimental campaigns using time-resolved spectroscopy have been performed on OMEGA with spherical implosions to understand extreme atomic physics up to ~10 Gbar

Powerful laser beams

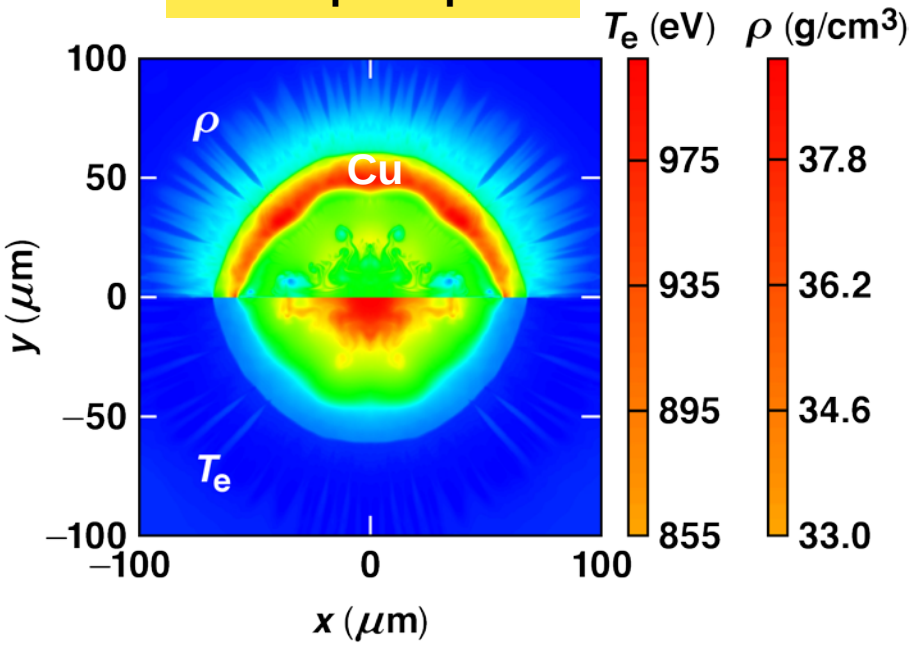


Varying the laser power, one can create HED matters at different densities and/or temperatures (5 to 100 Gbar pressures!).

1-ns-square pulse



2-ns-square pulse

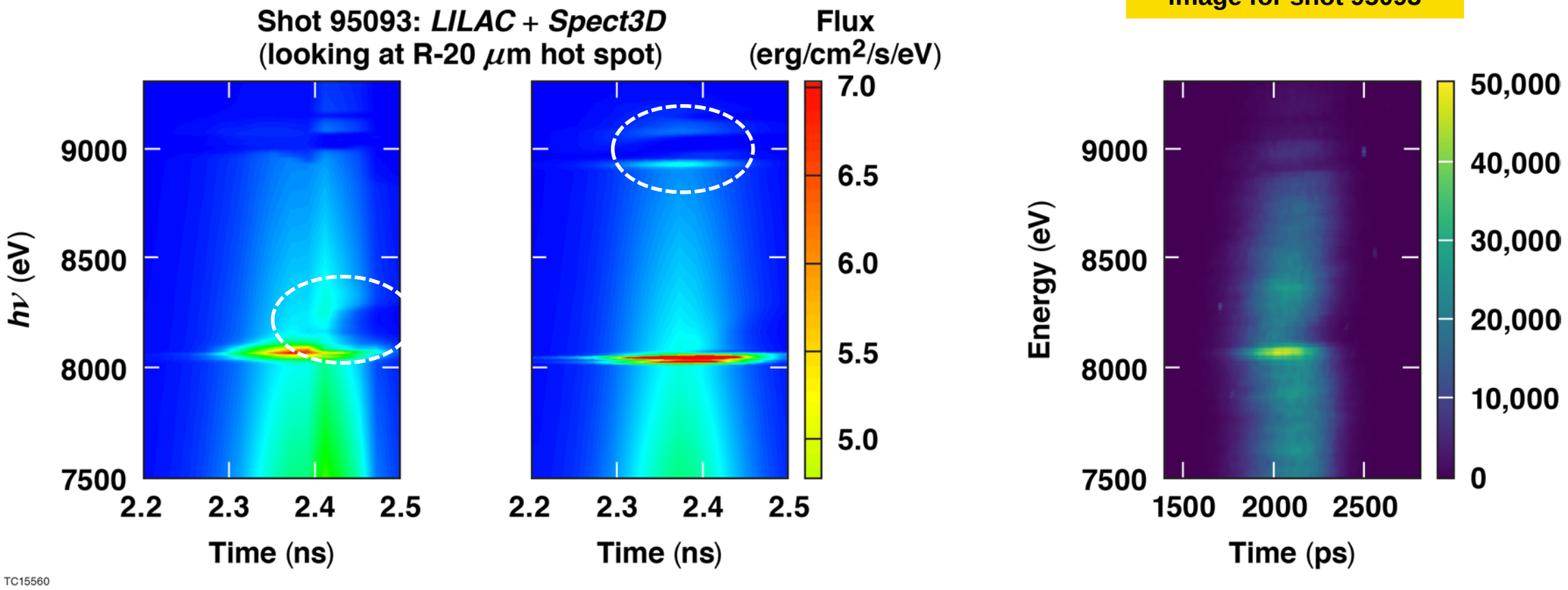


We have applied *Spect3D* to post-process hydro-simulations with different atomic-physics models to compare with experiments

The Ecker–Kroll model

The Stewart–Pyatt model

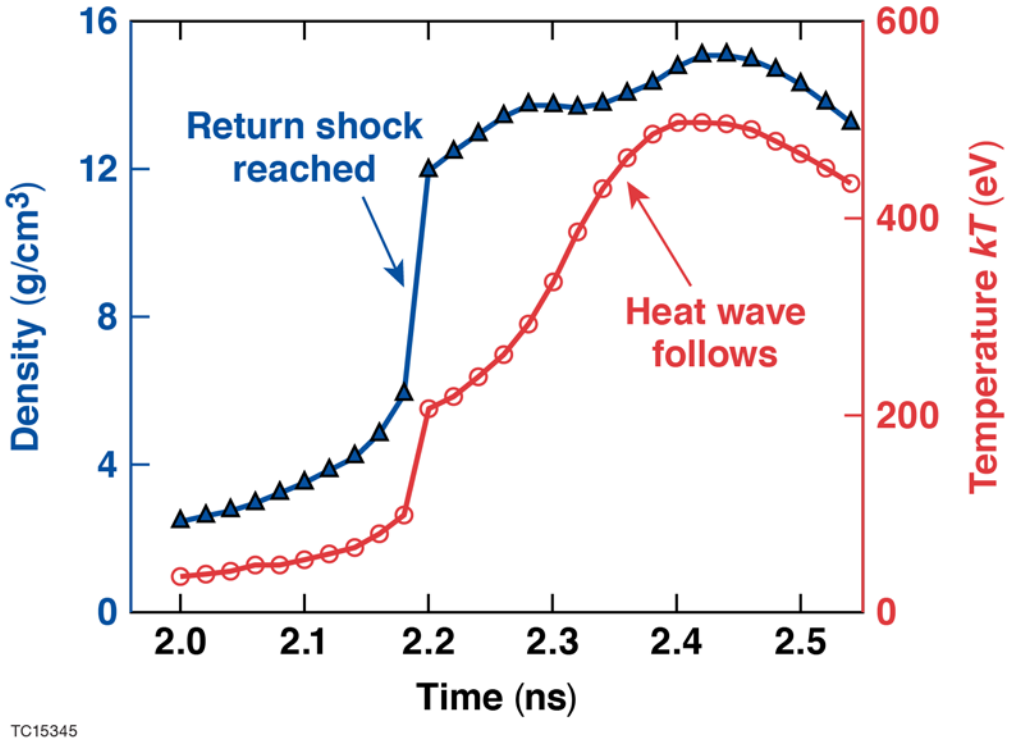
Preliminary experimental image for shot 95093



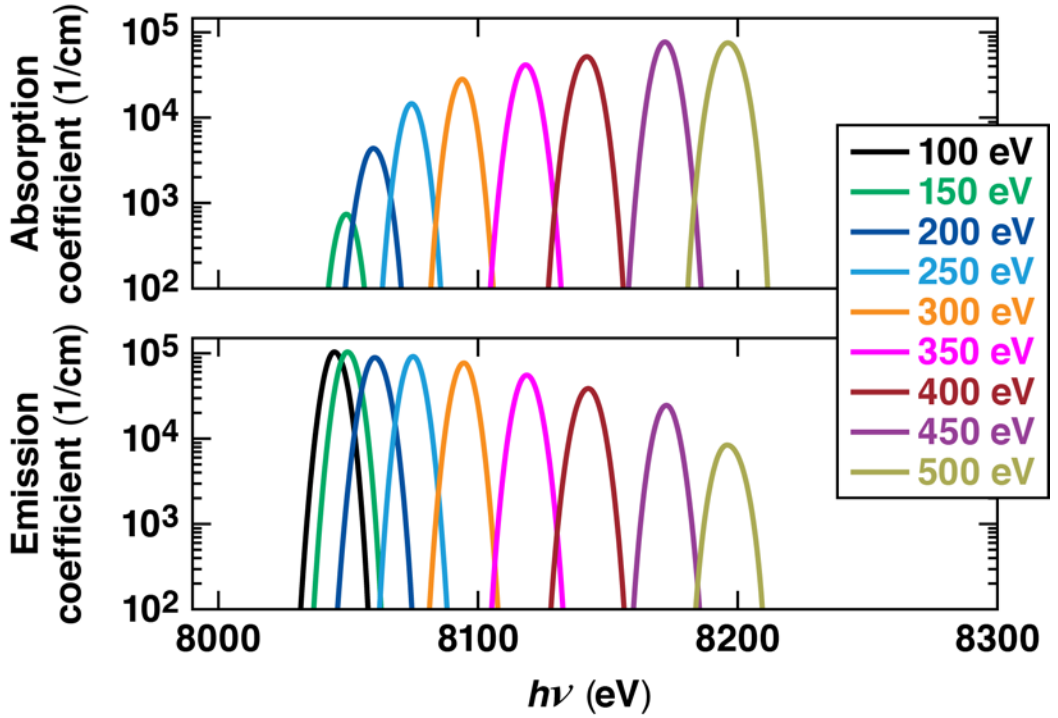
No single model gives all of the K_α/K_β emission and absorption features observed in experiments!

Ab-initio simulations using DFT have been performed to understand the experimental observations

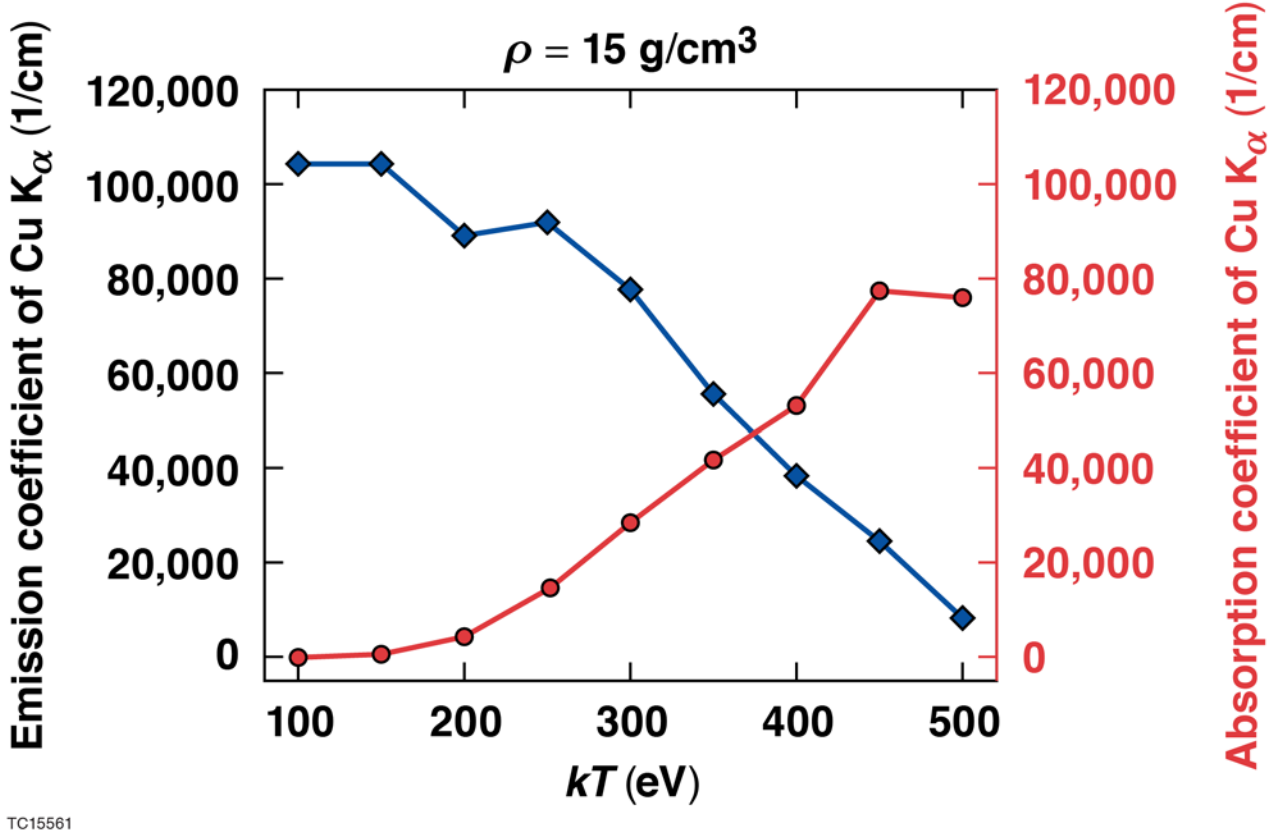
ρlT seen by the Cu-doped CH layer



Thermal-DFT predictions on Cu-K_α emission/absorption spectral changes



DFT calculations indicate both K_α-shifting and K_α-feature changes from emission to absorption during the heat-wave propagation into the CHCu layer



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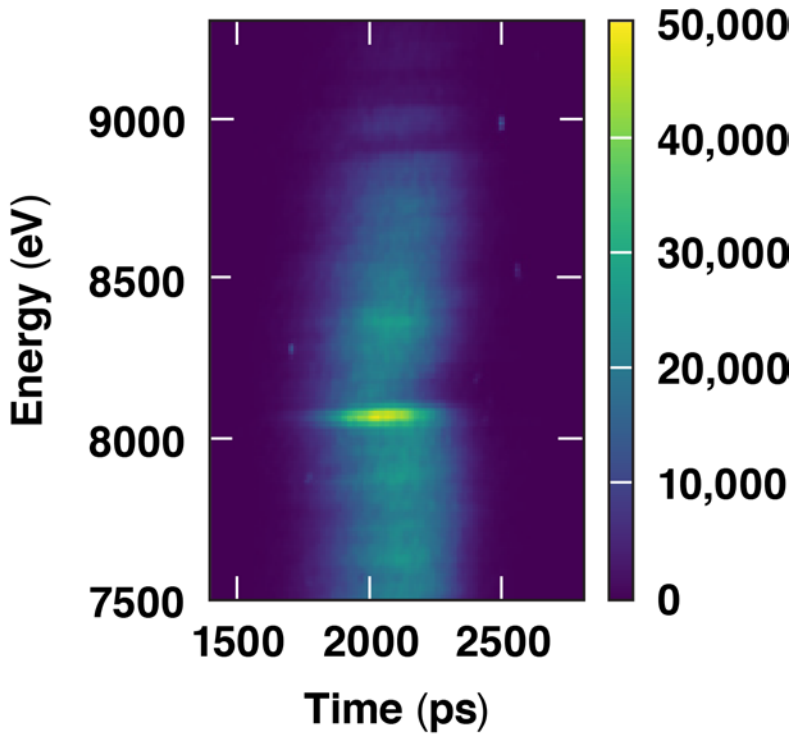

A DFT-based multi-band non-LTE modeling code ("*VERITAS*") is under development to gain a self-consistent understanding of extreme atomic physics at HED conditions

$$\begin{cases} -n_i \sum_{j\neq i}^{N_L} W_{ij} + \sum_{j\neq i}^{N_L} n_j W_{ji} = 0, \text{ (steady state)} \\ \mu \dfrac{dI(r,n,v)}{dz} = \eta(r,n,v) - \chi(r,n,v) I(r,n,v) \end{cases}$$

- The above coupled NLTE kinetic modeling can be solved for the self-consistent radiation field and state populations
- Instead of using a traditional atomic-physics model to calculate the Einstein coefficients (rates W_{ij}) for bound-bound and bound-free transitions, we extract them from DFT simulations!

Outlook for future work

- **Refining the experimental analyses to obtain calibrated timing and spectral resolution while making the DFT-based multiband NLTE-code "*VERITAS*" operational**

- **Using *VERITAS* to post-process LILAC/*DRACO* simulations to obtain time-resolved x-ray spectra and image for direct comparison with experiments, thereby helping to identify the deficient in traditional atomic-physics models**

- **Designing future experiments to probe the recently DFT-predicted interspecies radiative transitions* with a double-shell platform****

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***S. X. Hu *et al.*, Nat. Commun. 11, 1989 (2020).**
****S. X. Hu *et al.*, Phys. Rev. E 100, 063204 (2019).**

Summary/Conclusions

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Thank You