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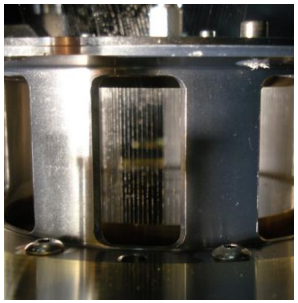

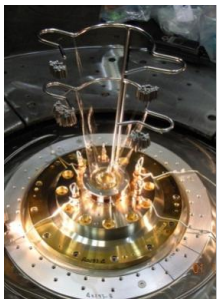

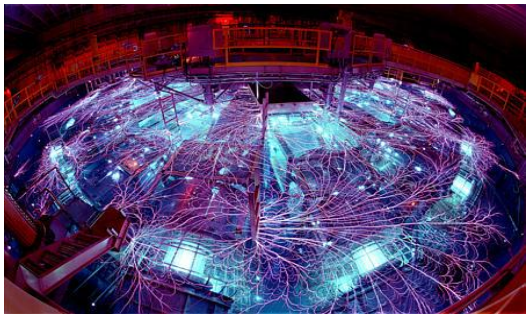

The importance of completeness for NLTE modeling

S.B. Hansen, *Sandia National Laboratories*

Sandia National Laboratories

Exceptional service in the national interest

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“Completeness” in the energy level structure of NLTE models is critical for several reasons

- At low densities, high-n and multiply excited valence states are important for obtaining reliable Auger/D.R. rates
  - D.R. in Ar and its dependence on n_{max}
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  - LTE Fe: comparison with experiment and average atom model
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At NLTE-6, dielectronic recombination was found to be the least consistent process among submitted codes

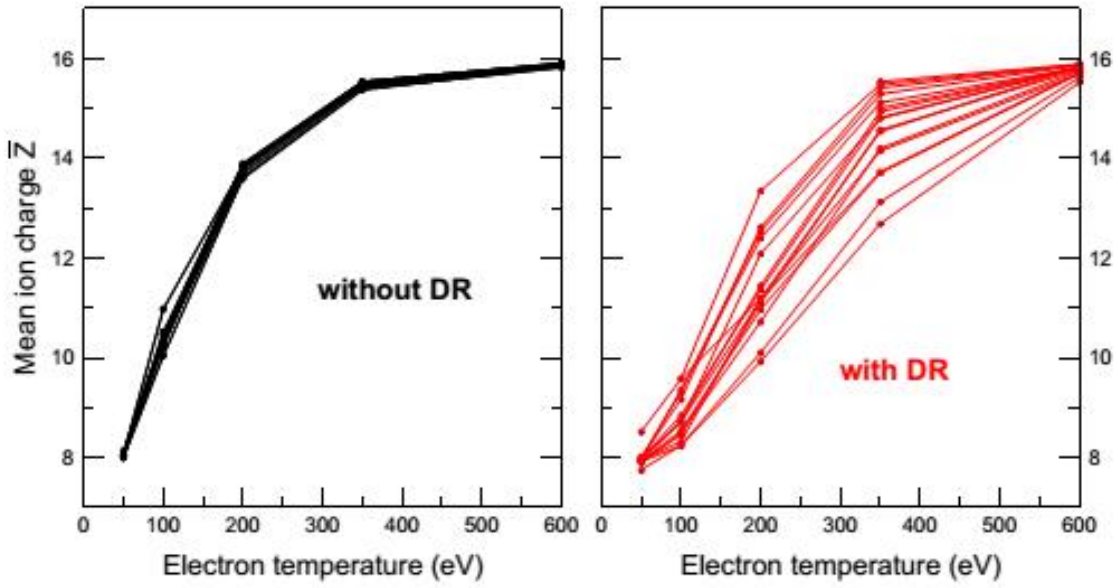


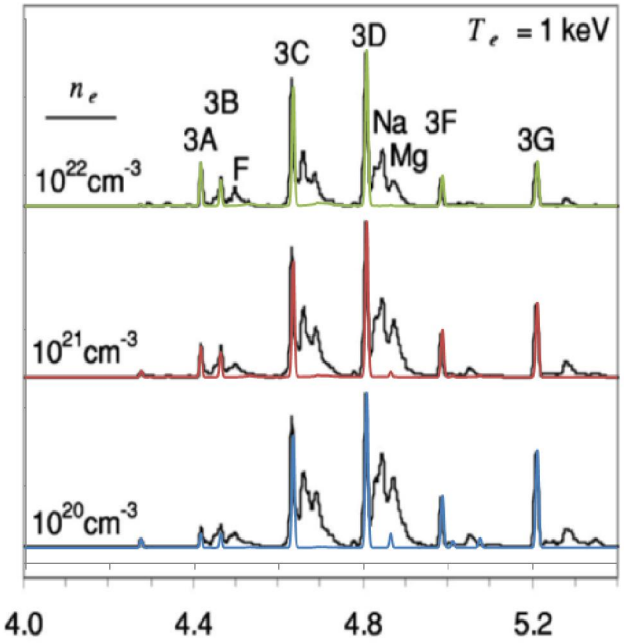
Fig. 4. Mean ion charges $\bar{Z}$ for the NLTE-6 Ar case, $n_e = 10^{12}$ cm^{-3}. Left: without dielectronic recombination, right: with dielectronic recombination.

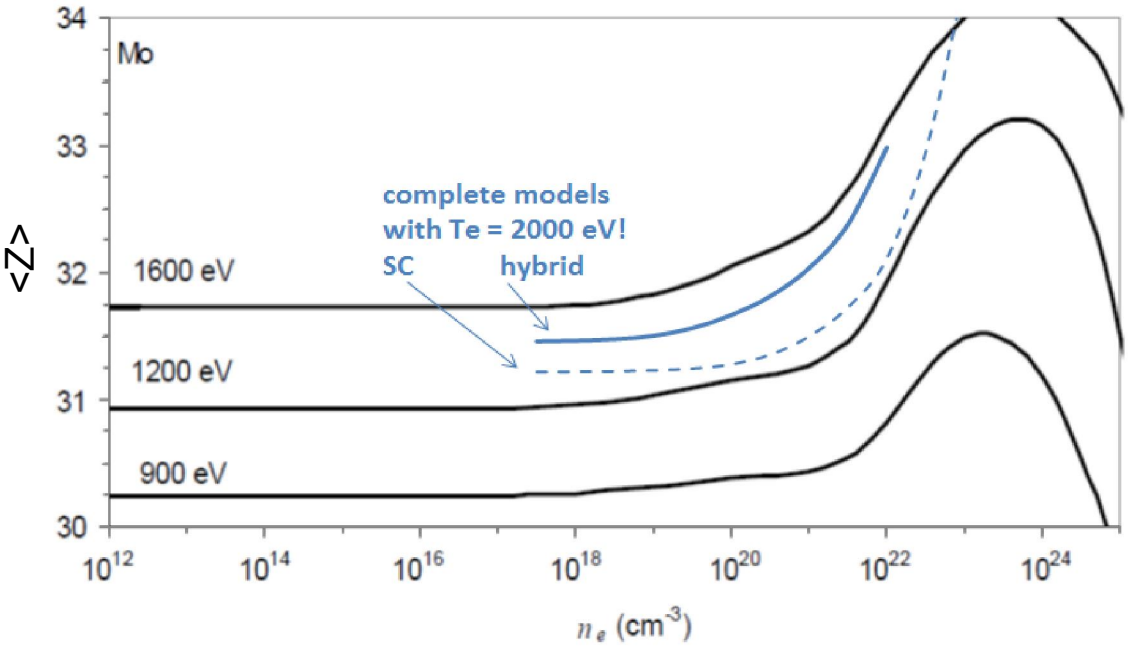
And within a screened hydrogenic model, <Z> varies with n_{max}

n_{max}	<Z>
3	14.3
5	13.0
15	12.8
20	12.8

Chung et al., HEDP **9**, 645 (2013

With supplemental SCs, SCRAM diagnoses significantly lower temperatures from similar spectra





"Complete" models have additional configurations of the kind $1s^2$ $(2l)^6$ nl (nl)'

The more extensive model has very similar predictions for density-sensitive Ne-like line ratios (colors vs. black), but predicts a much smaller <Z> for a given temperature

On LLNL's EBIT, M.May measured significant effects due to "exotic" d.r. resonant with the beam (n_1 ~ 6, n_2 ~11)

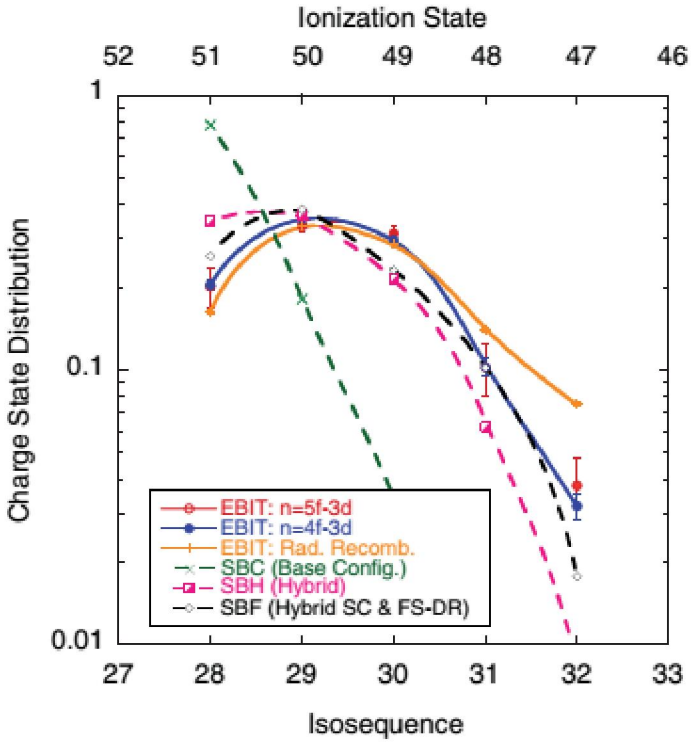


FIG. 5. (Color online) Comparison of the Au charge state distribution at 3.53 keV determined from the $5f \rightarrow 3d$ and $4f \rightarrow 3d$ transitions and radiative recombination emission measured from the EBIT plasma and simulations from SCRAM.

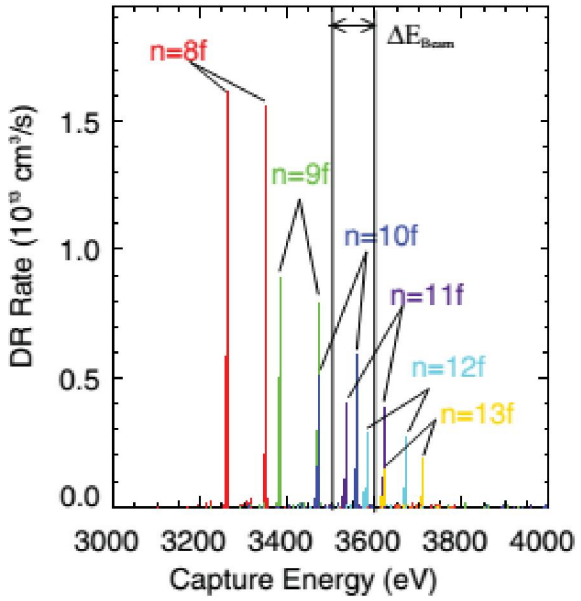
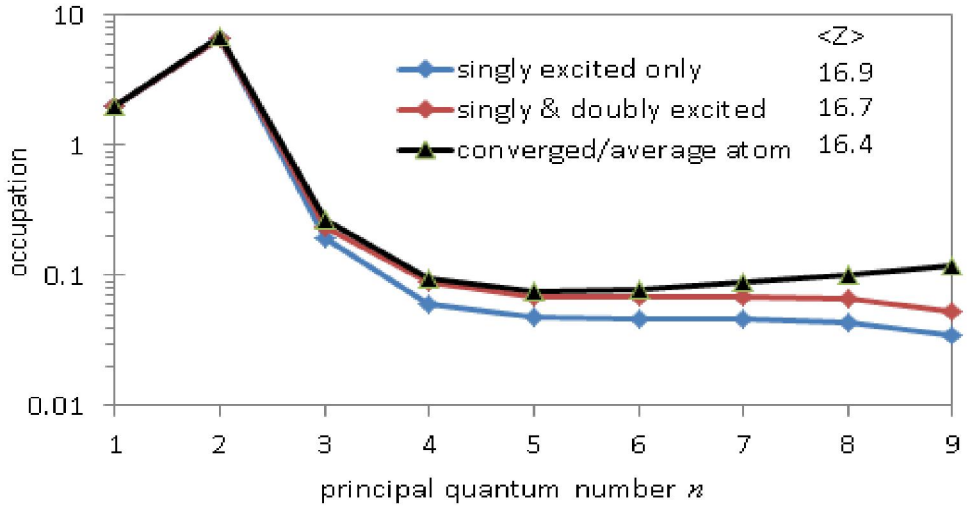


FIG. 8. (Color online) Dielectric capture rate vs capture energy (eV) for $3d6fnf$ with $8 \leqslant n \leqslant 13$ for Ni-like Au into Cu-like Au in the $E_{beam} = 3.53$ keV monoenergetic beam EBIT plasma.

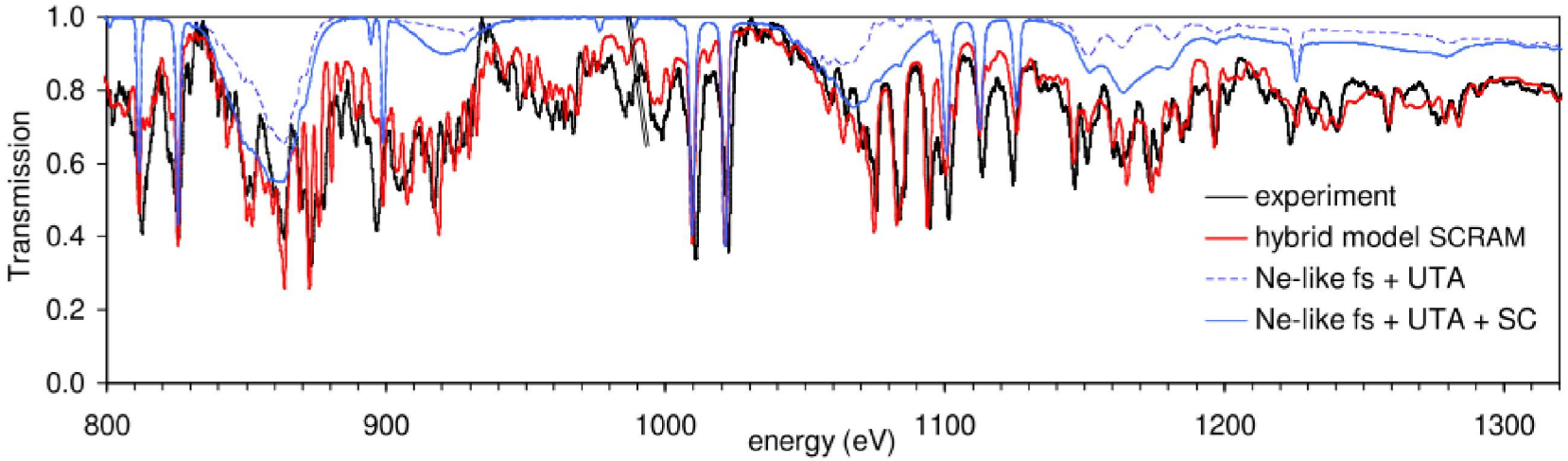
Models need extensive multiply excited structure including high-n states

M. May et al, PRE 84, 046402 (2011)

At high densities, IPD destroys some of the high-n states, but collisions make many-times-excited states accessible

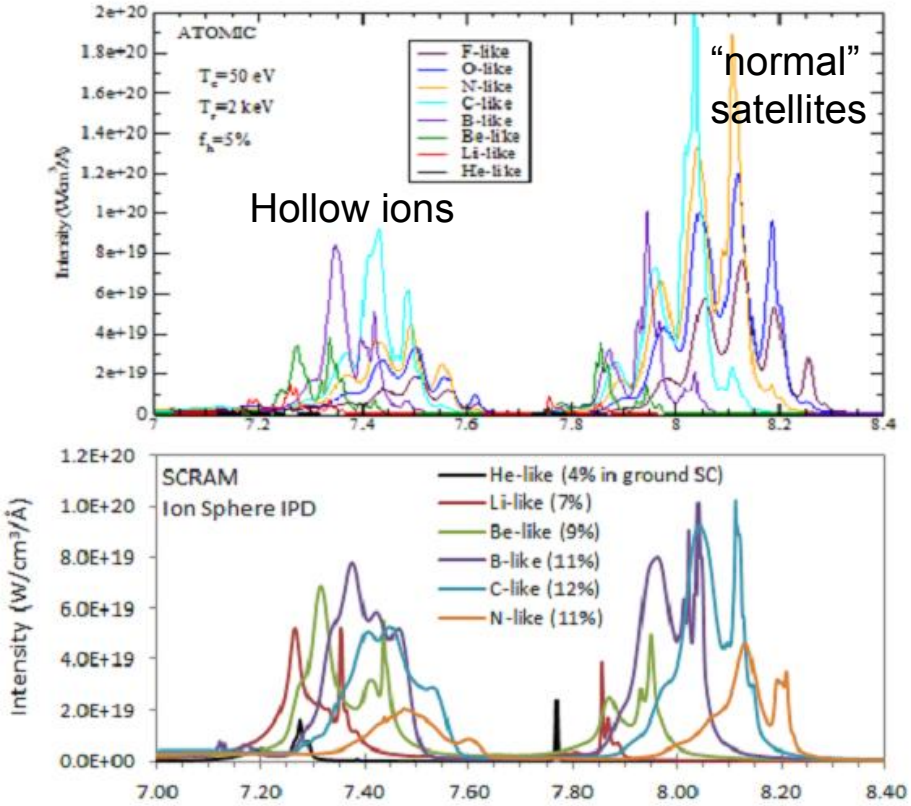


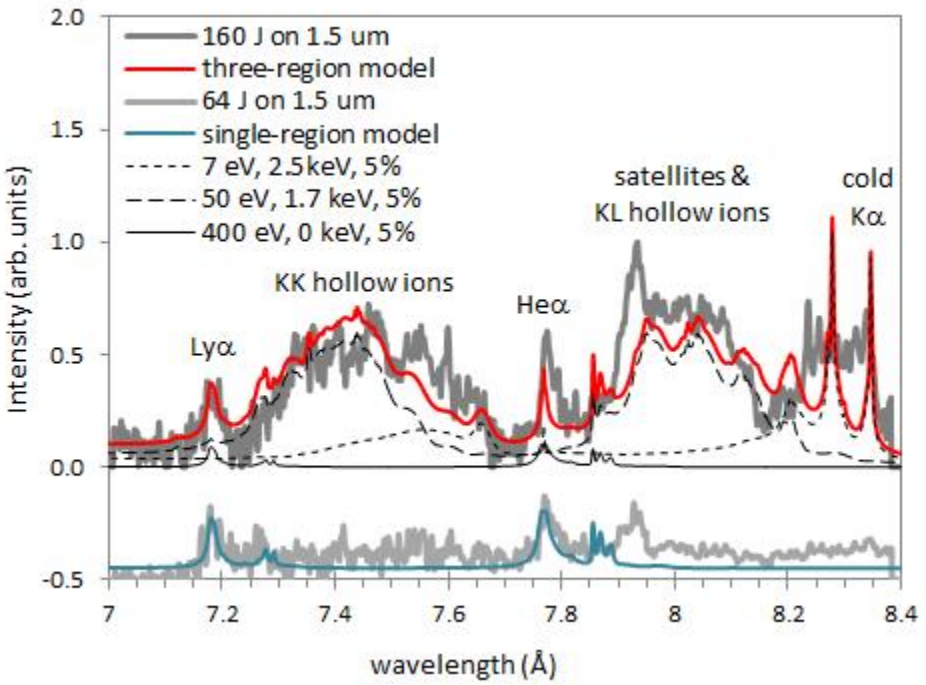
A model's degree of completeness is reflected in both its CSD/<Z> and spectrum



Bailey et al., Phys. Rev. Lett. 99, 265002 (2007)

When high density plasmas have suprathermal electrons or photons, states with inner shell holes must be modeled





Models need extensive multiply excited valence structure for statistics (e.g. $1s^2\ (5l)^6$), and each such configuration must be paired with ones that have 1 & 2 K-shell holes

[9] Colgan, Faenov Phys. Rev. Lett. 110, 125001 (2013)

[10] Submitted to Phys Plasma

XFELs provide extremely transient and non-thermal radiation; require extensive time-dependent modeling

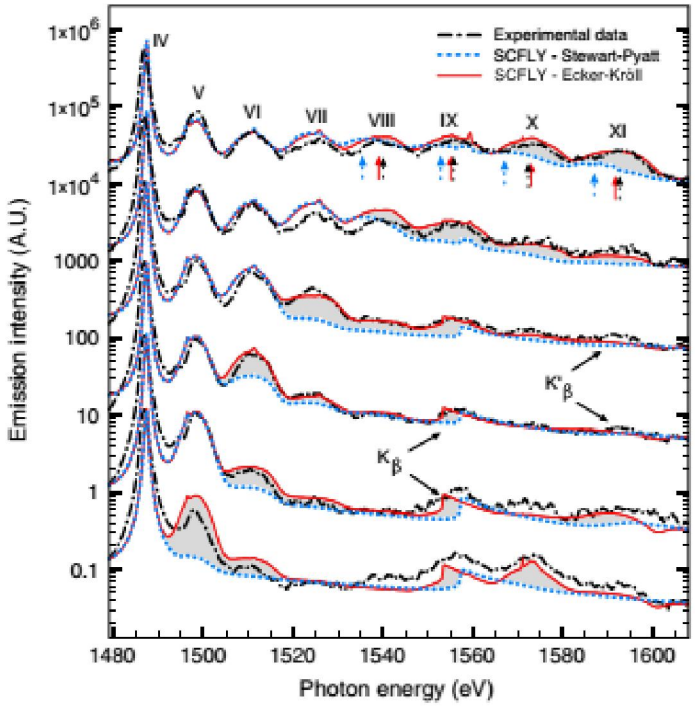


FIG. 1 (color online). Experimentally recorded K-α emission spectra from hot solid-density aluminum. SCFLY simulations with different IPD models are compared with the experimental data for a subset of the x-ray laser photon energies. From the bottom, the spectra corresponding to 1580, 1600, 1630, 1650, 1720 and 1830 eV pump photon energies are shown. The spectra have

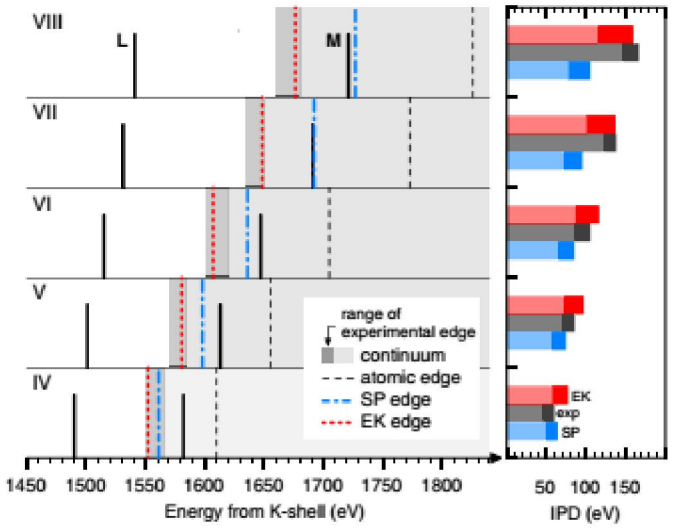


FIG. 2 (color online). Left—The grey region shows the continuum for different charge states, as determined from the experimental spectra in Fig. 1, with the dark grey region corresponding to the observed range of the K edge. The values given by the SP and EK calculations correspond to the edges calculated at the time of maximum emission for each associated K-α line. The calculated energy to pump a K-L and K-M transition (for the same number of L shell electrons in the final state) is also indicated. Right—IPD values; the darker colored zones of the histogram correspond to the IPD variation detected, for the experimental bars, and to the total IPD variation during the

On the LCLS experiment, the onset of photoionization-driven fluorescence occurred at significantly lower photon energies than predicted by standard Stewart-Pyatt IPD

Ciricosta et al, Phys. Rev. Lett. 109, 065002 (2012)

SCFLY: Chung, Chen & Lee HEDP 3, (2007)

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