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Configuration Interaction in Statistically Complete Hybrid-Structure Atomic Models

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with thanks to:

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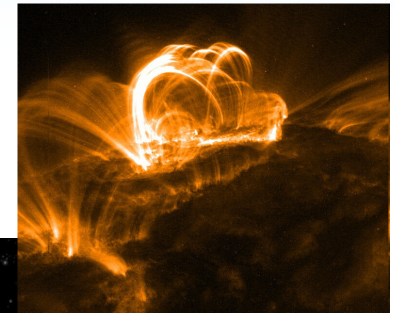
Outline

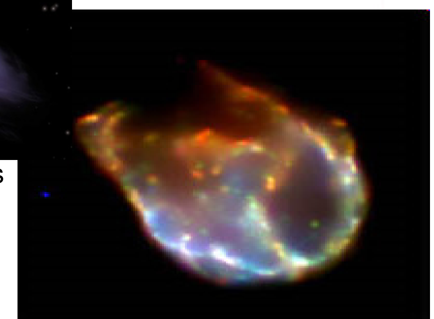
- **Collisional-radiative models and synthetic spectra:** balancing detail, completeness, and tractability

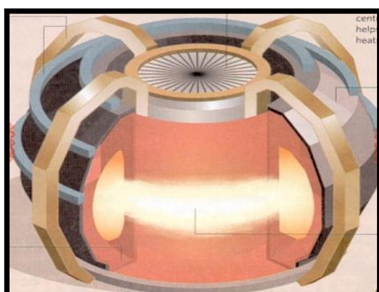
- **Hybrid-structure atomic models:** supplement fine structure data with configurations and superconfigurations

- **M-shell tungsten emission spectra and L-shell iron absorption spectra:** fine structure for spectroscopic accuracy, supplemental levels for satellites and CSDs


stellar opacities


black hole accretion disks


supernovae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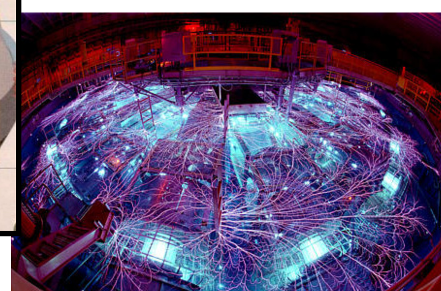
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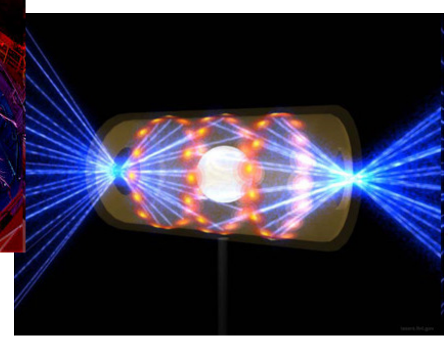
NIF

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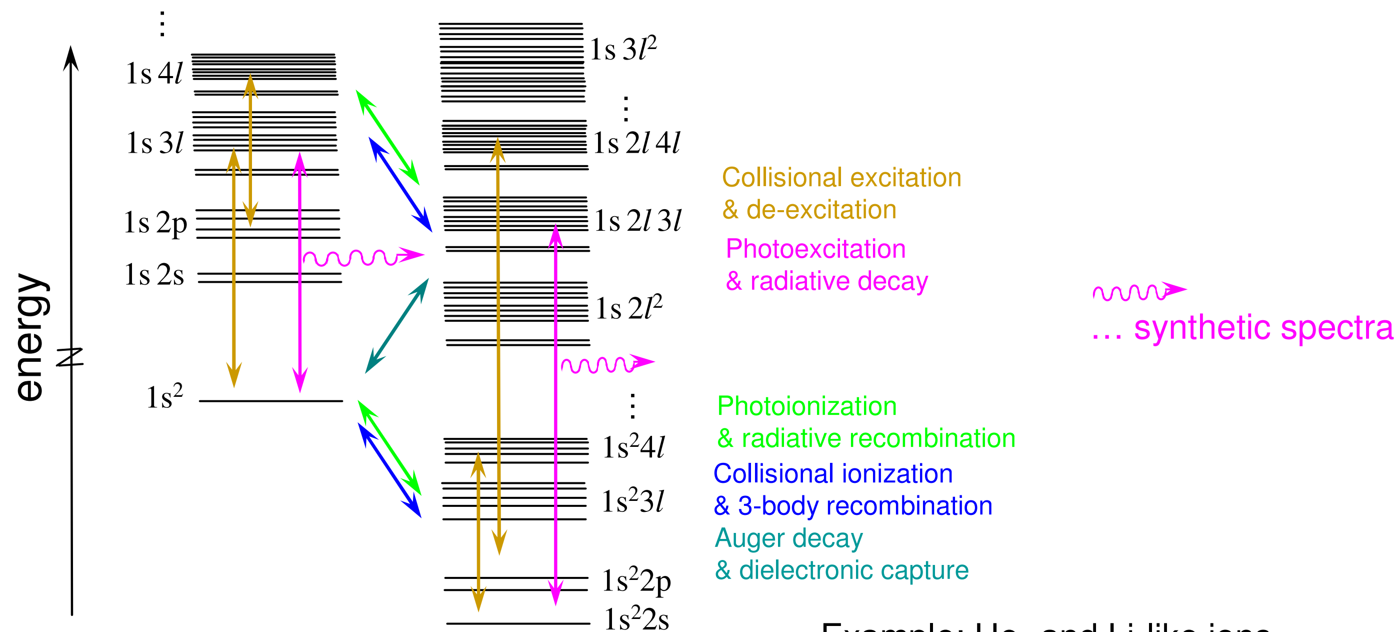
Collisional-radiative models: atomic levels (states) coupled by atomic processes (rates)



Example: He- and Li-like ions

A variety of codes, (RATS, FAC, Cowan…) databases, (NIST, ATOMDB…), and approximations (screened hydrogenic, Lotz…) provide energy level structure and rate data – with various degrees of detail and accuracy.

Generally, only fine structure data includes the configuration interaction effects and detailed transition structure required for spectroscopic accuracy.

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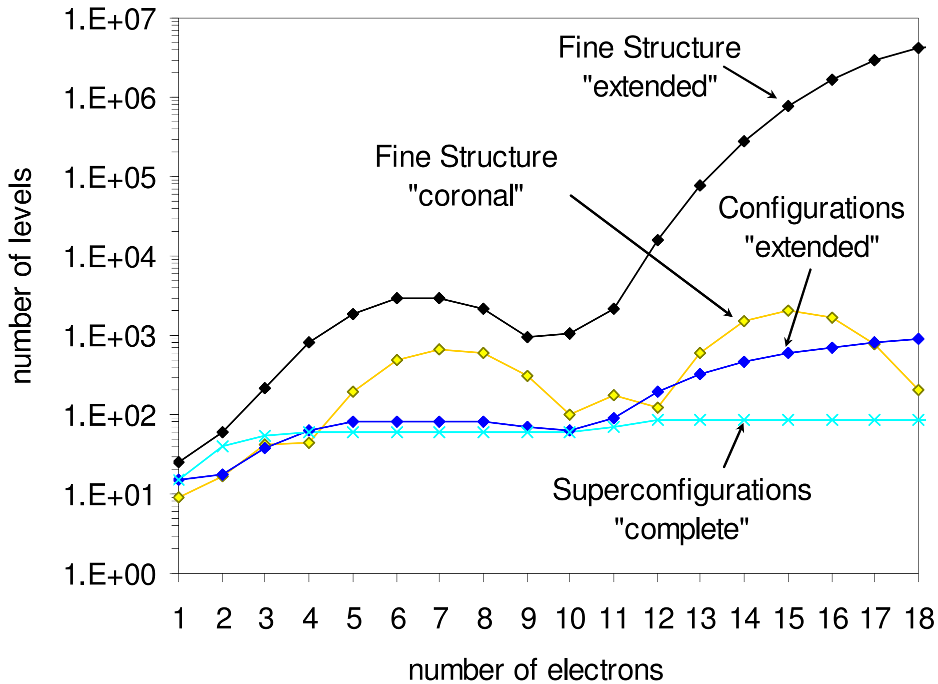
For complex ions, extensive fine structure models become intractable

While the number of singly-excited, “coronal” levels remains reasonable with increasing ion complexity, the number of levels required for an extensive model grows exponentially.

However, only “complete” models with extensive multiply-excited structure can accurately account for dielectronic recombination and satellite emission.



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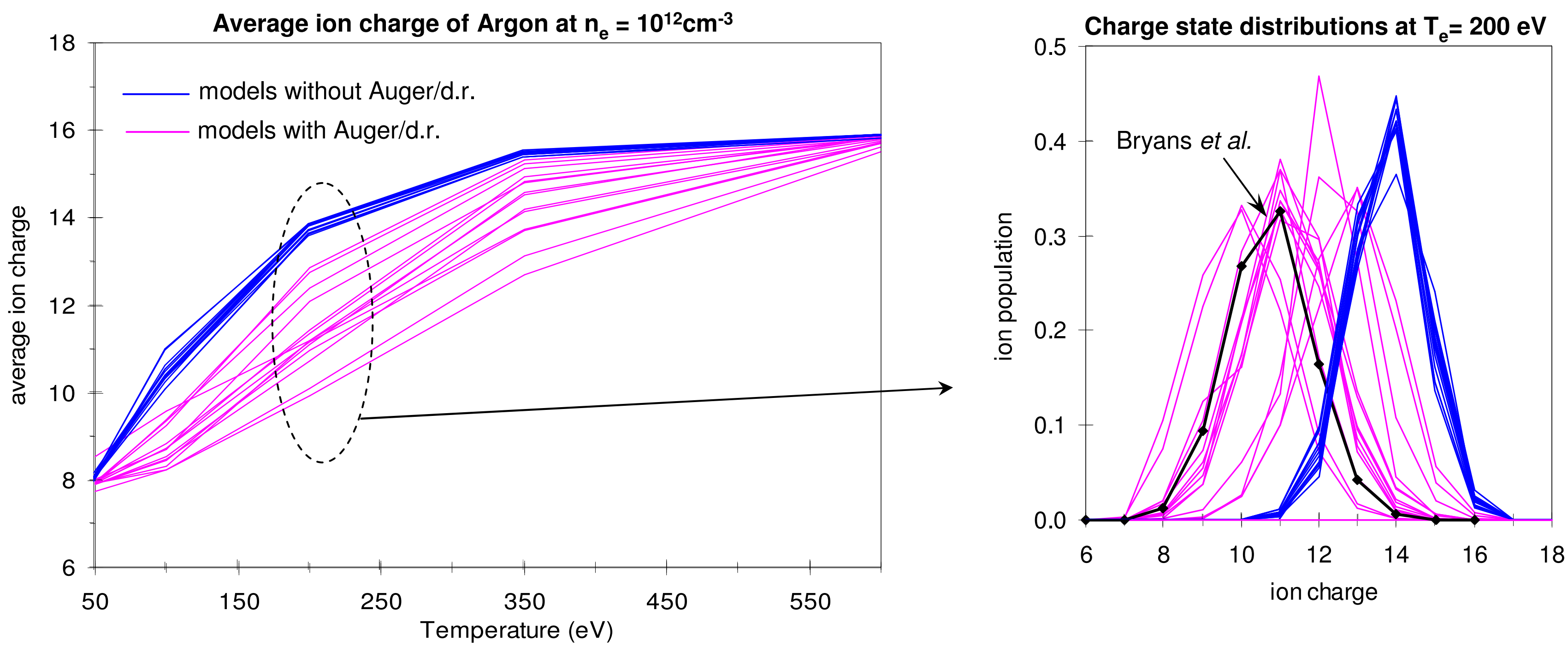
Extensive level structure is critical for accurate modeling of dielectronic recombination

Recent non-LTE workshop results illustrate the importance of d.r. – and the challenge of getting it right.



For coronal plasmas, global d.r. rates can be used (e.g. Mazotta [1], Bryans [2]), but these do not guarantee accurate satellite emission and are only valid at low densities.

[1] Mazotta *et al.*, Astron. Astrophys. Supp **133**, 403 (1998)
[2] Bryans *et al.* Ap J Supp **167**, 343 (2006)

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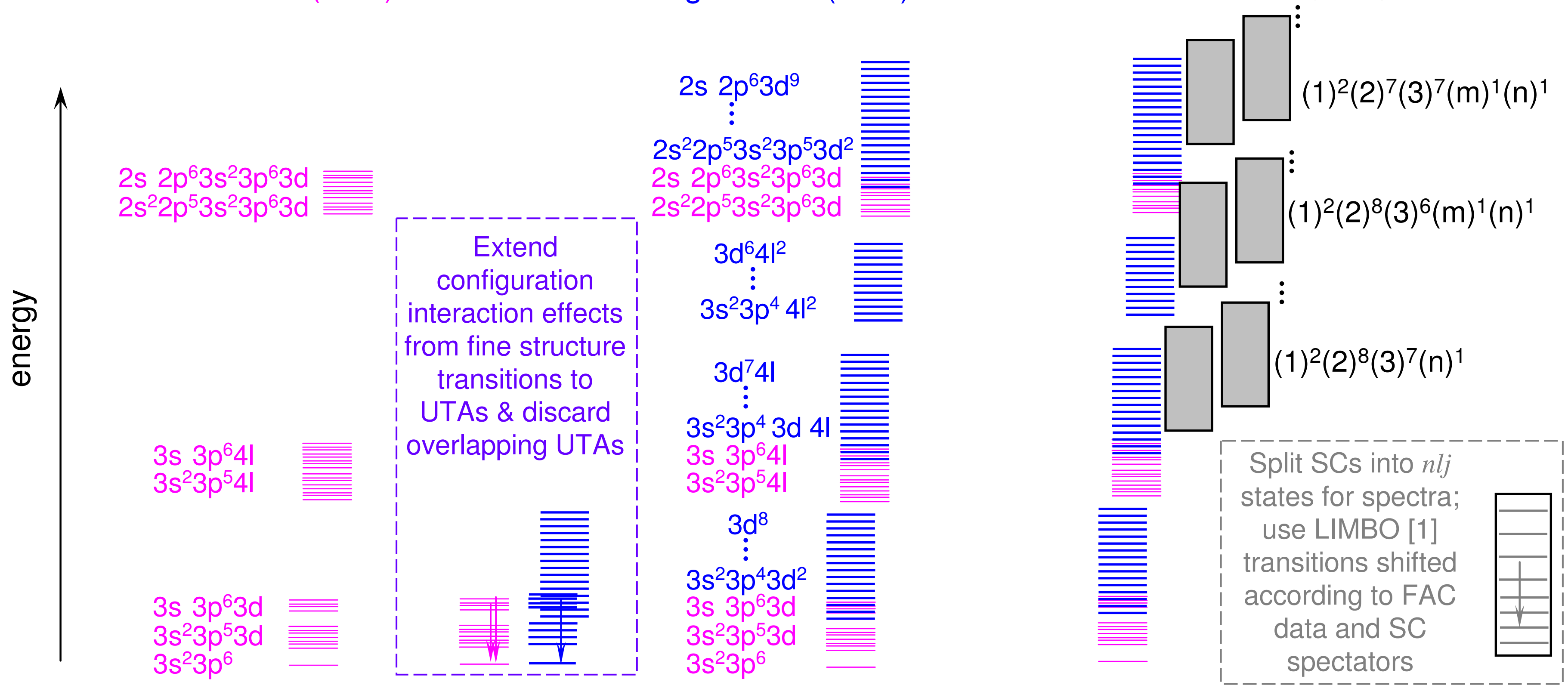
A hybrid-structure approach to collisional-radiative modeling

~200 fine structure "coronal" levels (FAC)

~14,000 (800) rel (non-rel) configurations (FAC)

~100 superconfigurations (screened hydrogenic/LIMBO)



Coronal fine structure captures configuration interaction and metastables.

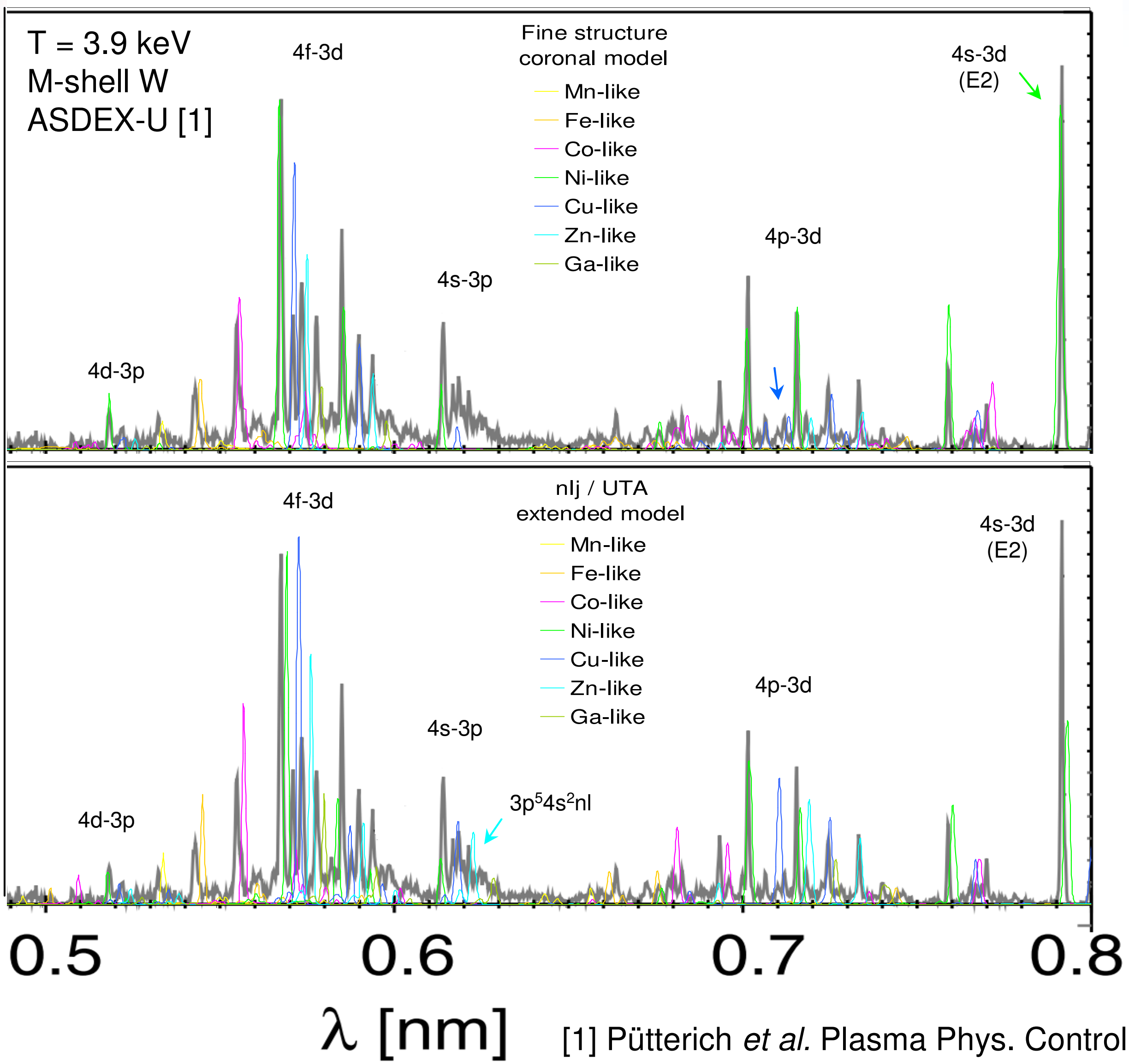
Supplemental configurations/UTAs provide continuity at moderate densities.

Supplemental superconfigurations ensure statistical completeness and exhaustive d.r. channels

Hybrid-structure models are computationally tractable even for complex ions.

[1] Liberman, Albritton, Wilson, & Alley, Phys. Rev. A **50**, 171 (1994)

Fine-structure and UTA models have different strengths



Fine structure model with restricted (coronal) level structure generally has more accurate wavelengths and relative intensities.

UTA model with extensive level structure includes many doubly excited states; captures satellites and low-level background emission.

[1] Pütterich *et al.* Plasma Phys. Control. Fusion **50**, 085016 (2008)

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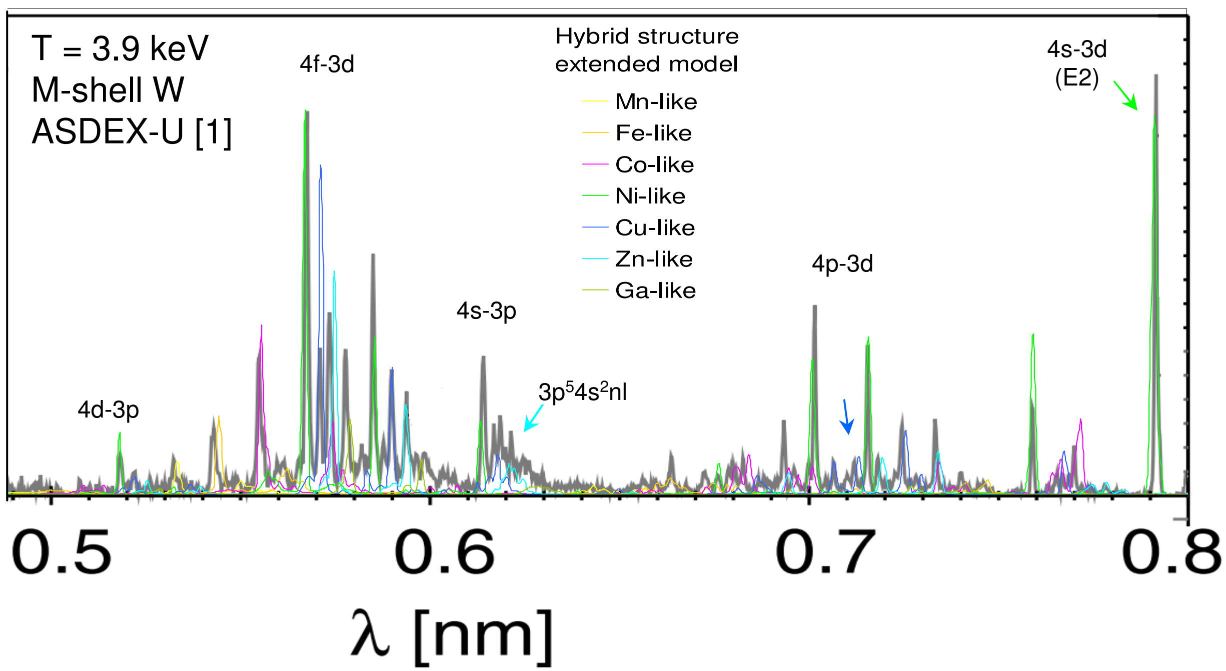
Hybrid-structure models combine those strengths

A comparison of the common transitions gives configuration interaction shifts and strength transfers for each $nlj \rightarrow (nlj)'$ transition type in each ion:

$$\delta E^{CI} = \left(\frac{\sum_{ul} g_{ul} A^{rad}_{ul \rightarrow ll} \Delta E_{ul \rightarrow ll}}{\sum_{ul} g_{ul} A^{rad}_{ul \rightarrow ll}} \right)_{\text{fine structure}} - \left(\frac{\sum_{ul} g_{ul} A^{rad}_{ul \rightarrow ll} \Delta E_{ul \rightarrow ll}}{\sum_{ul} g_{ul} A^{rad}_{ul \rightarrow ll}} \right)_{\text{UTA}}$$

$$f^{CI} = \left(\sum_{ul} g_{ul} A^{rad}_{ul \rightarrow ll} \right)_{\text{fine structure}} \Big/ \left(\sum_{ul} g_{ul} A^{rad}_{ul \rightarrow ll} \right)_{\text{UTA}}$$

These corrections are applied to all UTAs, regardless of spectator.



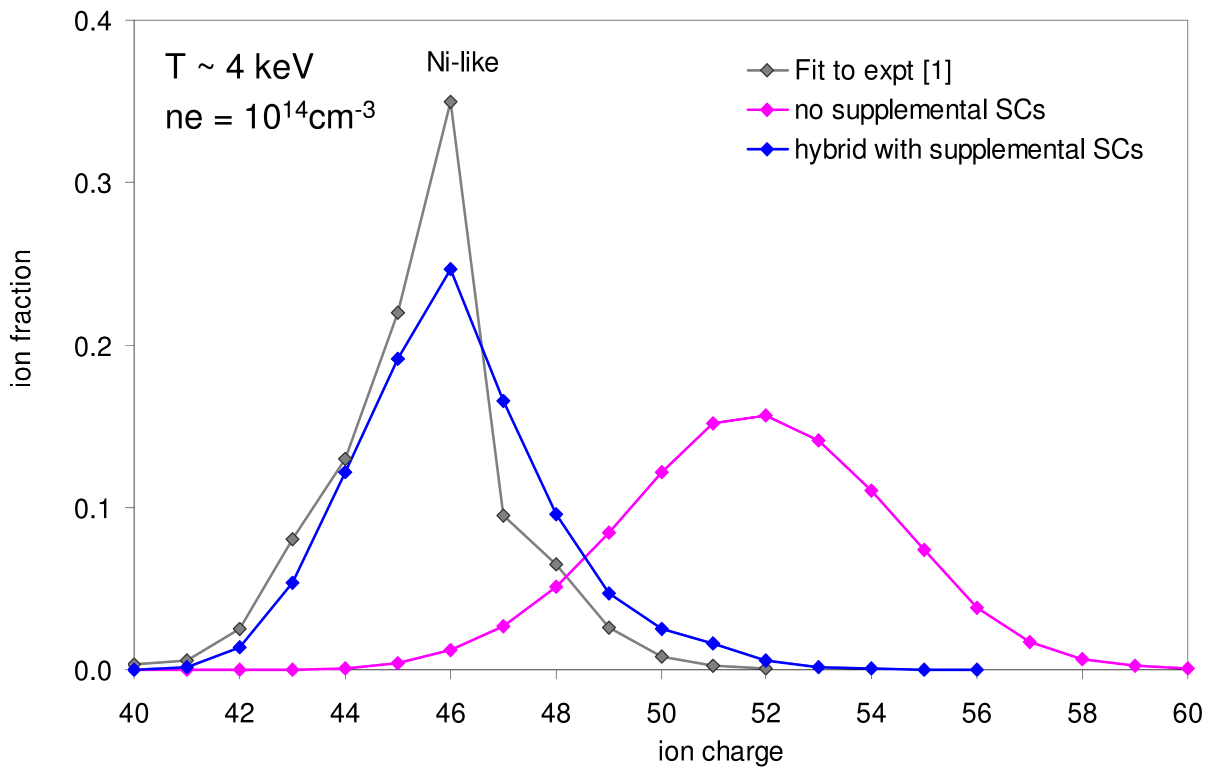
Hybrid-structure models with CI corrections applied to excitation and decay rates seamlessly combine the accuracy of fine-structure models with the extensive level and line structure of UTA models.

[1] Pütterich *et al.* Plasma Phys. Control. Fusion **50**, 085016 (2008)

Supplemental superconfigurations ensure statistical completeness

Without extensive dielectronic recombination channels, collisional-radiative models tend to predict overionized charge state distributions.

With supplemental SCs, hybrid-structure models give reliable charge state distributions *at any density*.



[1] Pütterich *et al.* Plasma Phys. Control. Fusion **50**, 085016 (2008)

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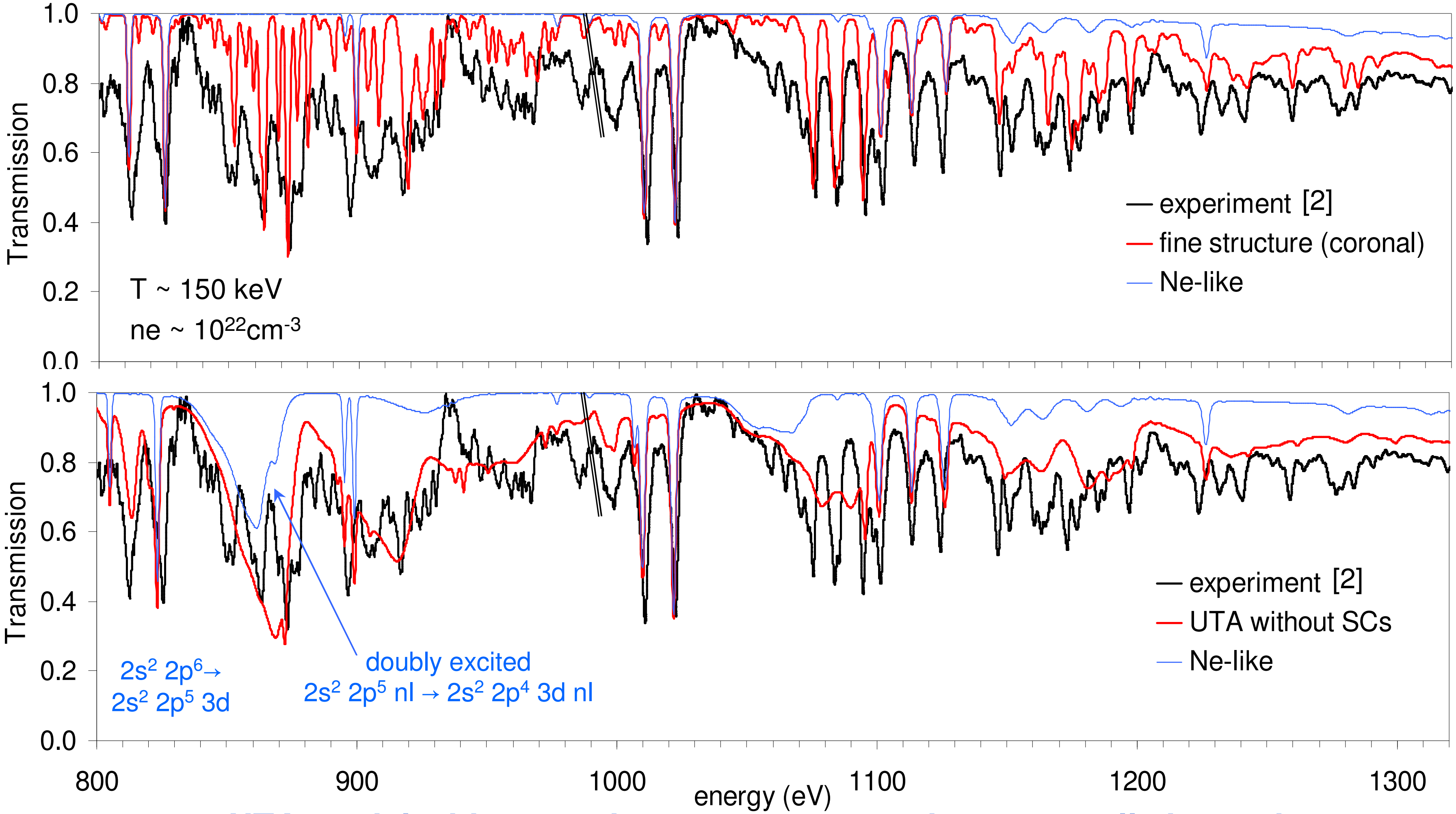
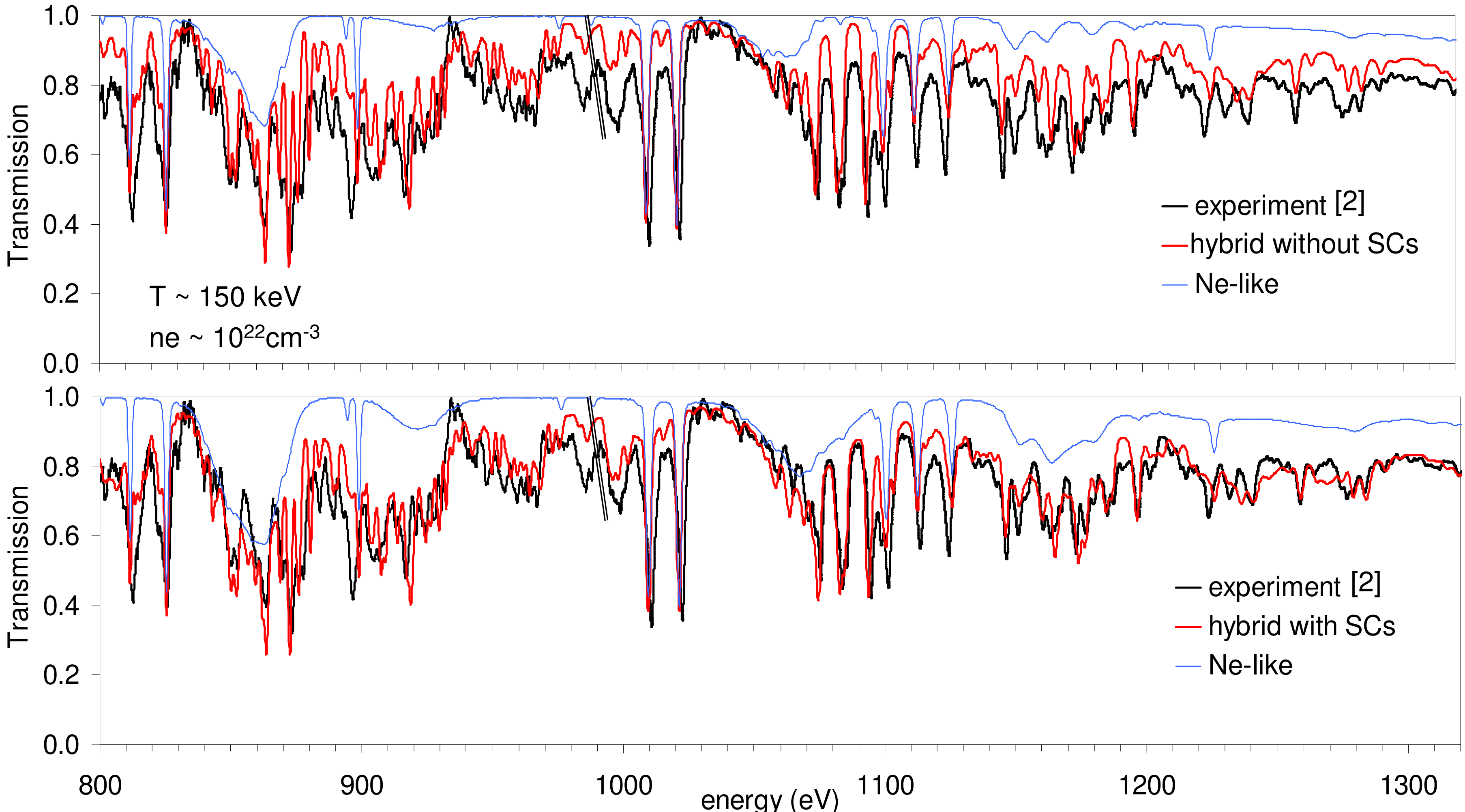
Extensive level structure is critical for high-density absorption spectra



UTA model with extensive structure reproduces overall absorption but misses detailed features

[2] Bailey *et al.* PRL **99**, 265002 (2007).

Hybrid model with supplemental SCs describes experimental absorption data well



Fine structure, UTAs, and supplemental SCs all contribute to good data fit with only ~10^5 lines (vs. ~ 10^7 for fully fine structure model)

[2] Bailey *et al.* PRL **99**, 265002 (2007).

Summary

Hybrid structure models:

- highly accurate rates and wavelengths (configuration interaction)
- complete dielectronic recombination channels
- extensive energy level structure for satellite features
- computationally tractable even for complex ions

include all the lines; include all the channels

Useful for modeling spectra from the coronal to the LTE regime…
and everything in between

[1] Hansen, Bauche, Bauche-Arnoult, and Gu, HEDP **3**, 109 (2007) – fine structure + UTA

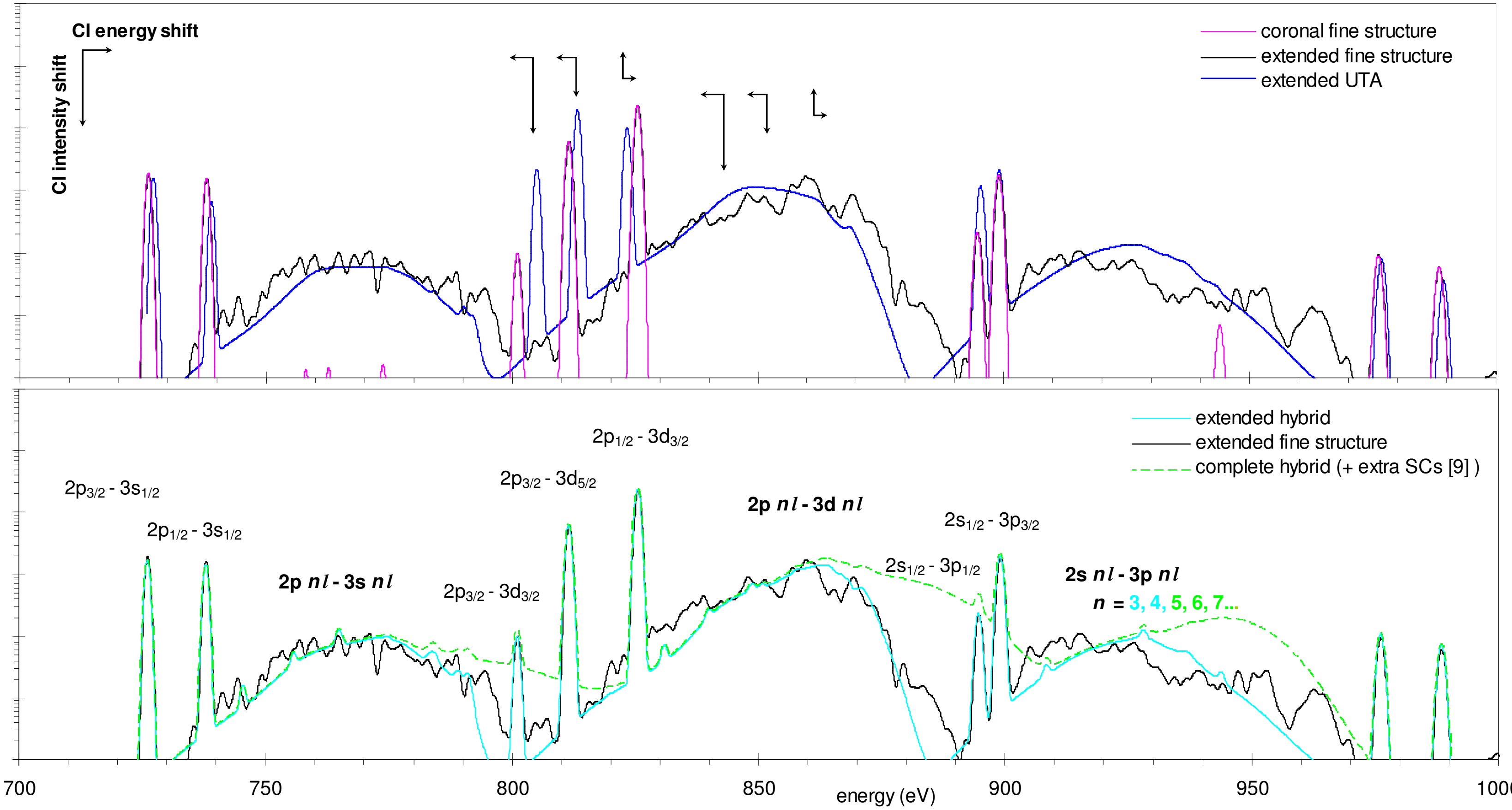
[2] Brown, Hansen *et al.* PRE **77**, 066406 (2008) – CI shift and supplemental SCs

[3] Scott and Hansen, HEDP **6**, 39 (2010) – SC models and nlj transitions

[4] Hansen, Bauche, and Bauche-Arnoult, to be published in HEDP – finite-width SCs in hybrid models

Supplemental slides

Extending configuration interaction (CI) from fine structure transitions to UTAs is key



Each nlj – nlj transition in each ion has its own CI corrections obtained from the overlapping sets of fine structure transitions and UTAs [1]

[1] Brown, Hansen *et al.* PRE **77**, 066406 (2008)

[9] Scott and Hansen, HEDP **6**, 39 (2010)

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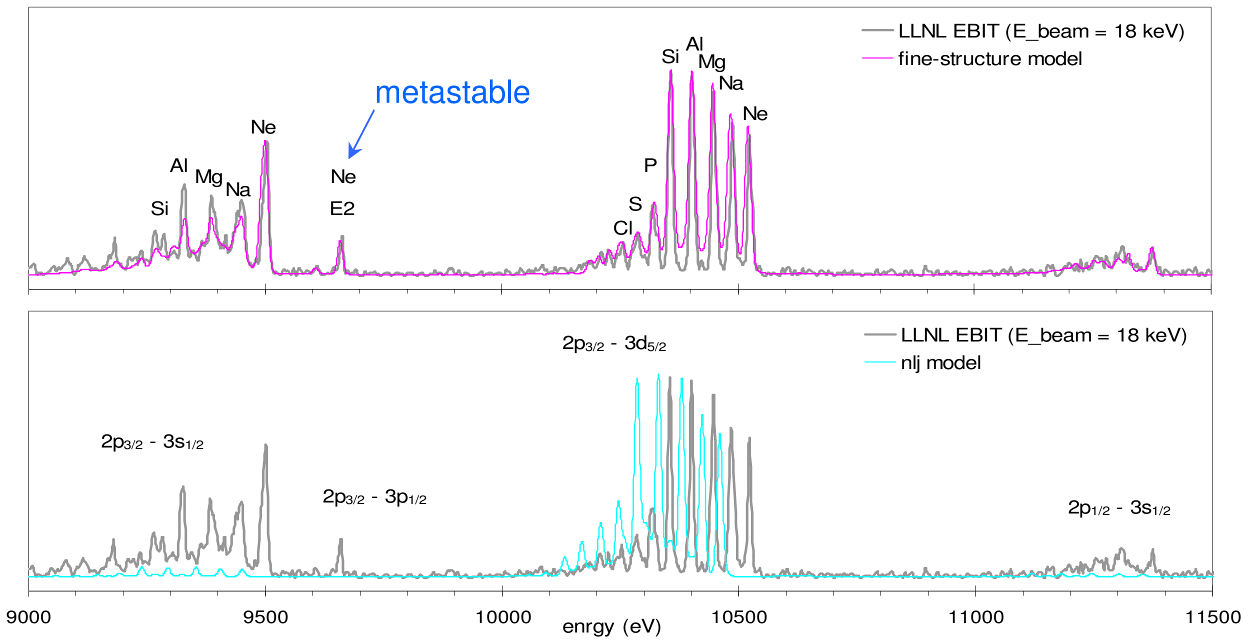
Low-density "coronal" models generally use high-accuracy atomic data

Coronal atomic models are widely used for EBIT, tokamak, and astrophysical sources, where low densities ensure that population is concentrated in ground states

Example:
L-shell Au emission
from LLNL EBIT [1]



Low-density emission spectra are well-modeled by fine-structure models with only singly excited (coronal) states. Less accurate models generally do not capture the effects of metastable levels or configuration interaction.

[1] Brown, Hansen *et al.* PRE **77**, 066406 (2008)