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Review of the 10th non-LTE code comparison workshop

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Radiative Properties of Hot Dense Matter
21-26 October, 2018

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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The non-LTE code comparison workshops aim to help the HEDP community assess model reliability

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- Non-LTE models are widely used in the HEDP community:
  - To help interpret spectroscopic measurements & diagnose plasma conditions
  - To inform radiation-hydrodynamic models that are used to design experiments
  - To inform detailed analysis of exotic plasma states
- Non-LTE models are complicated and difficult:
  - Use rates for tens of processes to couple many electronic states
  - Z* and radiative loss rates: hundreds of averaged states
  - Detailed spectra: hundreds of thousands of detailed states
  - Dense & photoionized plasmas require extensive multiply excited & core-hole states; density effects require additional theory; time-dependence is computationally intensive
- Non-LTE workshops have been held every two years since 1996 to help understand the necessary components of and appropriate confidence in these models
  - Traditions of anonymized results & restricted participation foster open discussion and help prevent convergence to popular models

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- Non-LTE model
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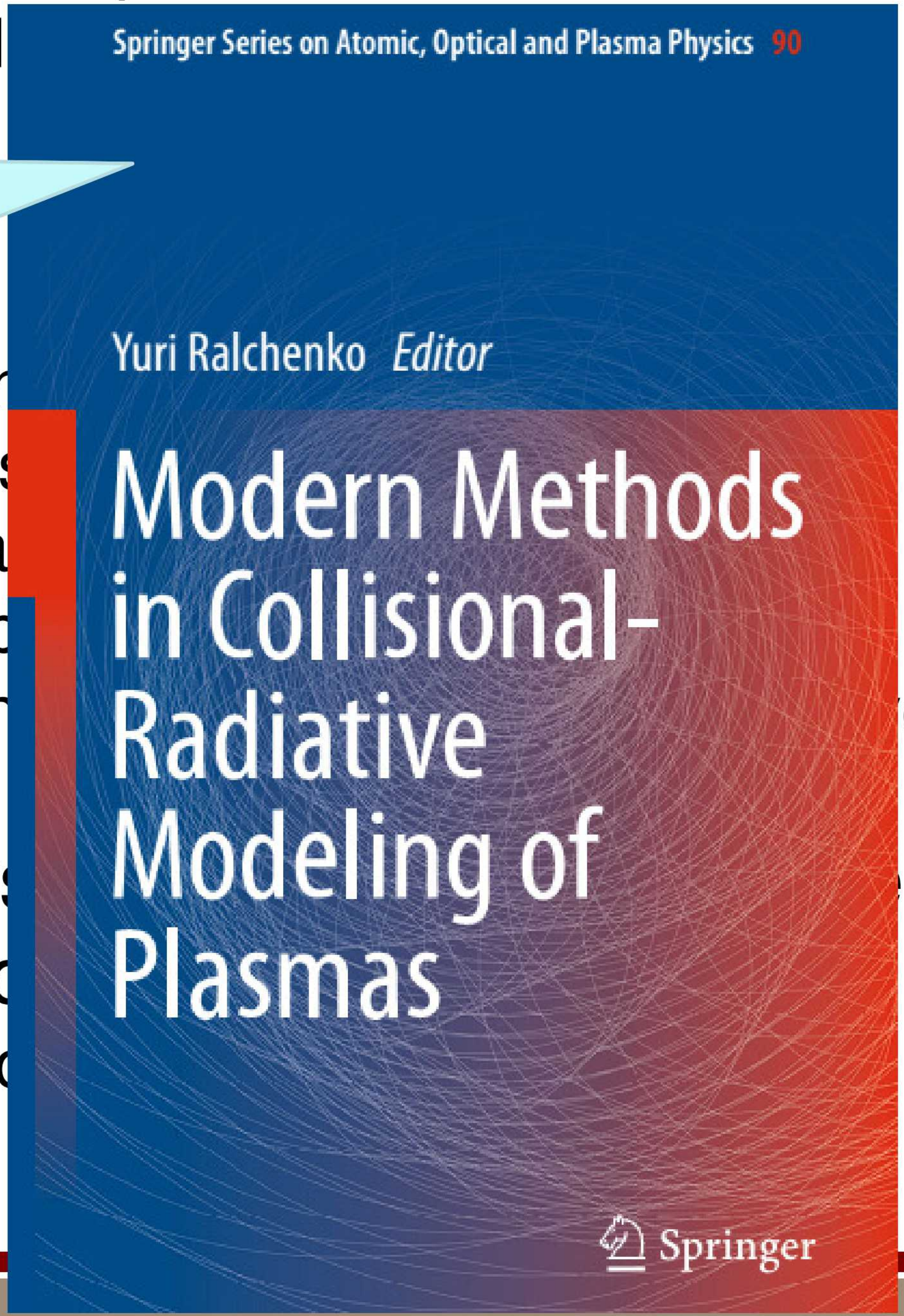
We wrote a book!



The 10th Non-LTE code comparison workshop was held at the UCSD Faculty Club in December 2017

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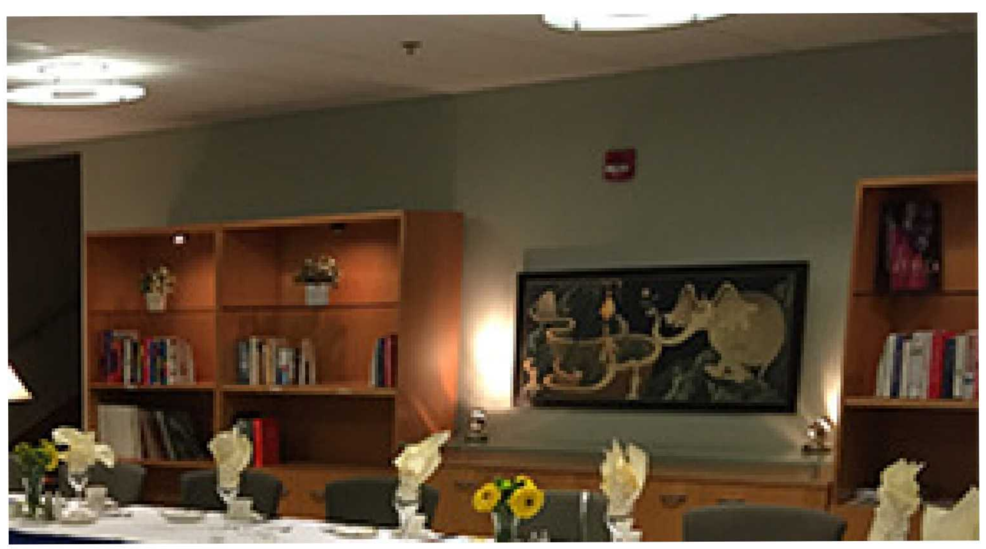

Thanks to local organizers Farhat Beg and Meghan Murphy
and to Michael MacDonald, Guillaume Loisel, and Ed Marley for experimental talks

36 participants from 6 countries and 11 institutions contributed results from > 26 variations of 17 independent codes

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Code	Contributors	Institute	Country	Ne	Al	Si	Cl	Ne-TD	Al-TD
ACRE	Richard Abrantes	UCLA	USA				X		
ABAKO	R. Florido, J.M. Martin-Gonzalez, M.A. Gigosos	ULPGC	Spain	X					
ATLANTIS	M.A. Mendoza, J.G. Rubiano, R. Florido, J.M. Gil, R. Rodriguez, P. Martel, A. Benita, E. Minguez	ULPGC	Spain	X	X	X	X		
ATOMIC	Chris Fontes, James Colgan, Mark Zammit	Los Alamos	USA	X	X	X	X	X	
CORD	Michel Poirier	CEA	France	X			X		
CRAC	Evgeny Stambulchik	Weizmann Inst Sci	Israel	X	X	X	X	X	X
CRETIN	Howard Scott, Paul Grabowski, Hai Le	Lawrence Livermore	USA	X	X	X	X	X	X
DEDALE	Frank Gilleron, Robin Piron, Maxime Comet, Jean-Christophe Pain	CEA	France	X	X		X		
DLAYZ	Gao Cheng, Zeng Jiaolong, Yuan Jianmin	NUDT	China	X	X	X	X	X	X
DRACHMA2	Nicholas Ouart	Naval Research Lab	USA				X		
NOMAD	Dipti, Yuri Ralchenko	NIST	USA	X		X	X	X	
OPAZ	Christophe Blancard	CEA	France	X	X	X	X		
PrismSPECT	Igor Golovkin	Prism Comp.	USA	X	X	X	X		
SCRAM	Stephanie Hansen, Brian Kraus	Sandia	USA	X	X	X	X		X
SCSF	Stephanie Hansen	Sandia	USA	X	X	X	X	X	X
SEMILLAC	Yechiel Frank	Lawrence Livermore	USA	X	X	X	X		
THERMOS	Ilya Vichev, Dmitri Kim, Anna Solomyannaya	KIAM	Russia	X	X	X	X		

Contributing codes span a wide range of detail, statistical completeness, and "extras"

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~1/4 superconfiguration models: ~10^3 states; g_{tot} ~ **10^9**

Time-dependence

Variations in continuum lowering, n_{max}

~1/4 config-avg. models: ~10^5 states; g_{tot} ~ **10^7**

Reasonably accurate spectra & transport

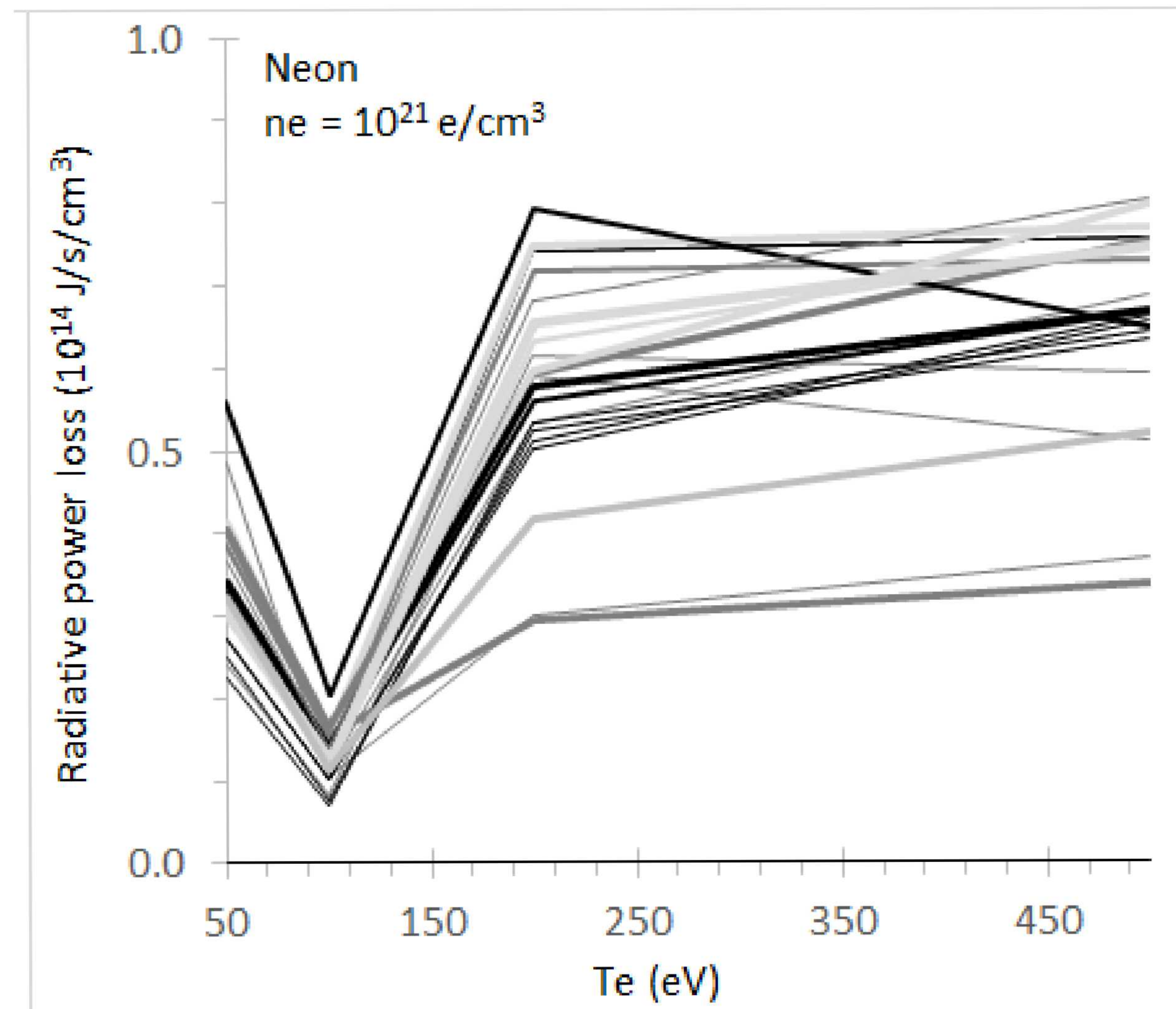
~1/4 fine-structure models: ~10^4 states; g_{tot} ~ 10^3

metastable states

Accurate spectra

sophisticated line broadening

~1/4 hybrid-structure models: ~10^5 states; g_{tot} ~ **10^9**



In this talk, the case results are coded to represent these variations in statistical completeness (line thickness) and detail (line darkness)

We explored cases relevant to plasma diagnostics, density effects, and X-ray free-electron lasers

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Element	Case ID	No. of cases	T_e (eV)	N_e (cm^{-3})	T_{rad} (eV), dilution factor	Plasma radius (cm)	Spectral ranges
Ne	Ne	12	50, 100, 200, 500	10^{19}, 10^{20}, 10^{21}			800-1400 eV, δε=0.3 eV
Ne	Ne-TD	3	$T_e(t)$ for 3 cases in supplemental file*	$N_e(t) = Z^*(t)\times N_i$ with $N_i=10^{18}$	E_{rad}: 800, 1050, 2000		800-1400 eV, δε=0.3 eV
Al	Al	8	10, 30, 100, 300	2×10^{23}, 5×10^{23}			
Al	Al-TD	2	$T_e(t)$ for 2 cases in supplemental file*	$N_e(t) = Z^*(t)\times N_i$ with $N_i=6\times10^{22}$	E_{rad}: 1580, 1650		1400-2400 eV, δε=0.5 eV
Si	Si	12 [24]	30 [60, 100]	10^{19}, 3×10^{19}	T_{rad}: 63 [diluted], multi-Planckian	0.1, 0.3, 1.2	1700-2500 eV, δε=0.25 eV
Cl	Cl	9	400, 500, 600	10^{21}, 10^{22}, 10^{23}			2600-3800 eV, δε=0.15 eV

*Thanks to Hyun-Kung Chung for SCFLY temperature profiles!

Neon steady-state cases: explore K-shell plasma diagnostics

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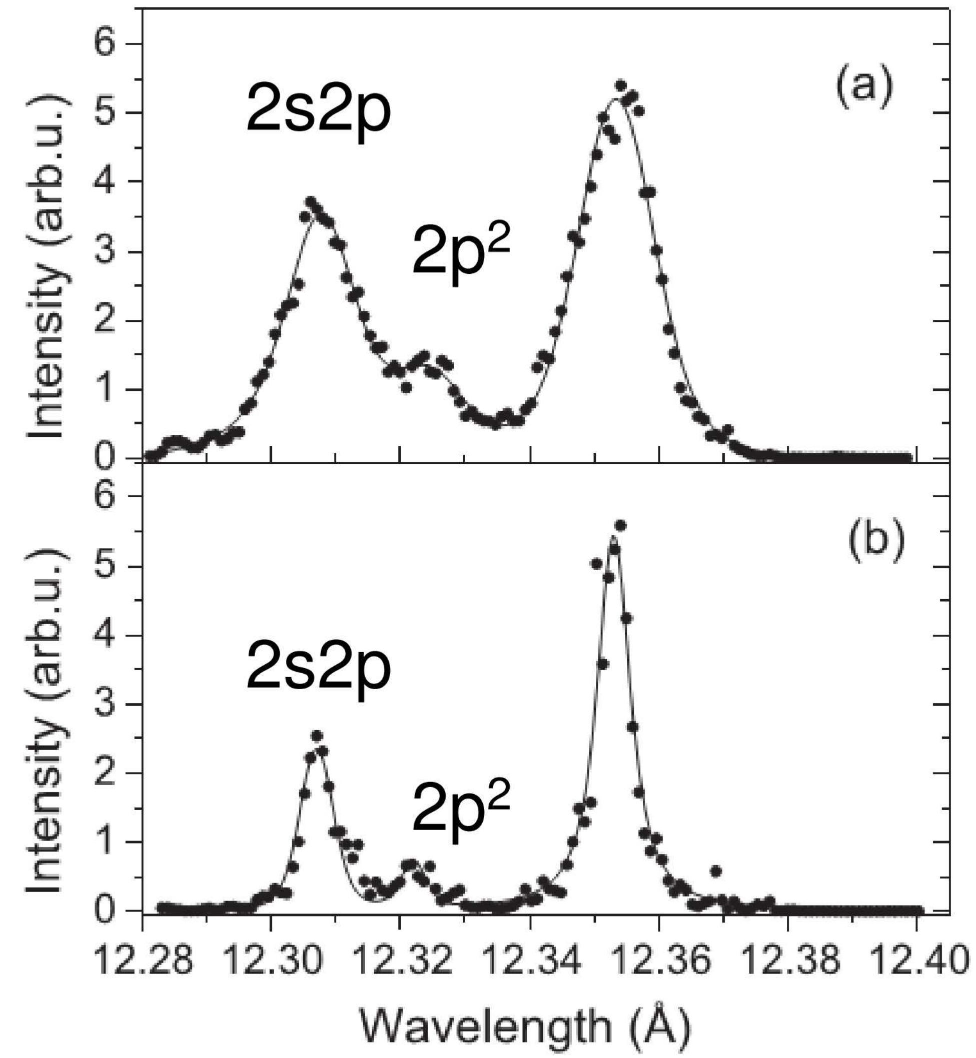
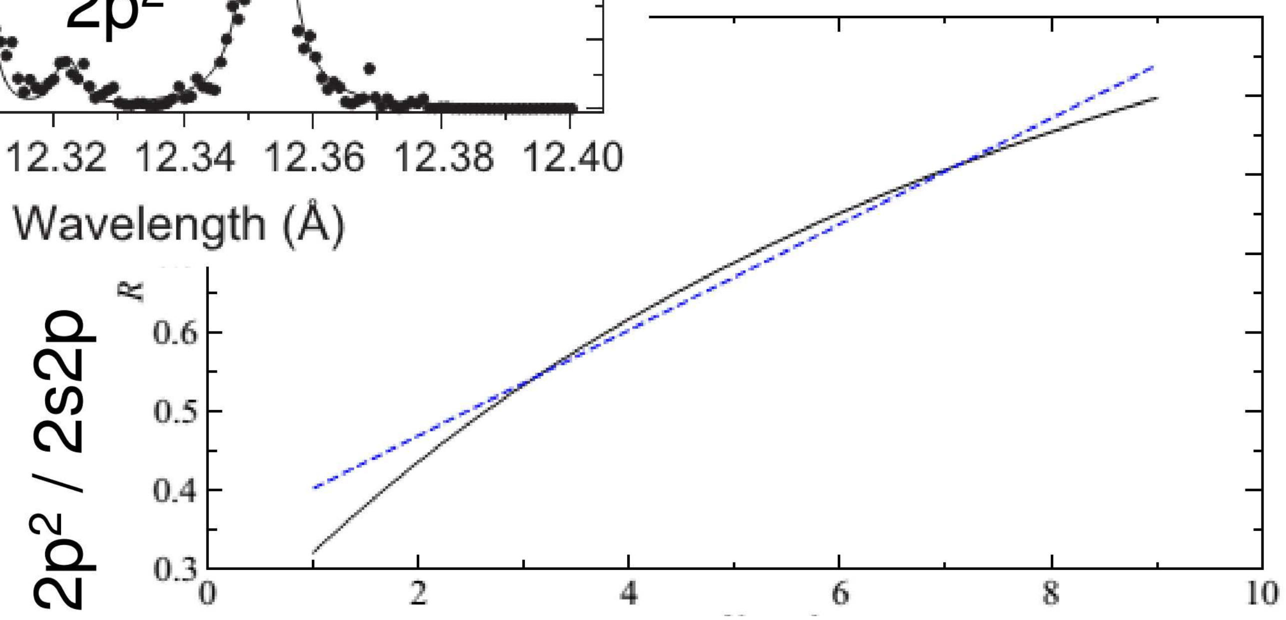
<u>Motivation:</u>

The satellites to neon Lyα have been measured with high spectral resolution from gas puff implosions. Changes in the shape of the satellite features driven by collisional redistribution among $2l\,2l'$ states are used to diagnose density[1], informing analysis of ion kinetic energy[2-3]





1. J. Seeley, *Phys. Rev. Lett.* **42**, 1606 (1972)
2. E. Kroupp *et al.*, *Phys. Rev. Lett* **98**, 115001 (2007)
3. E. Kroupp *et al.*, *Phys. Rev. E* **97**, 103202 (2018)

Ne: Average ion charge (Z*) agrees to within ~0.5

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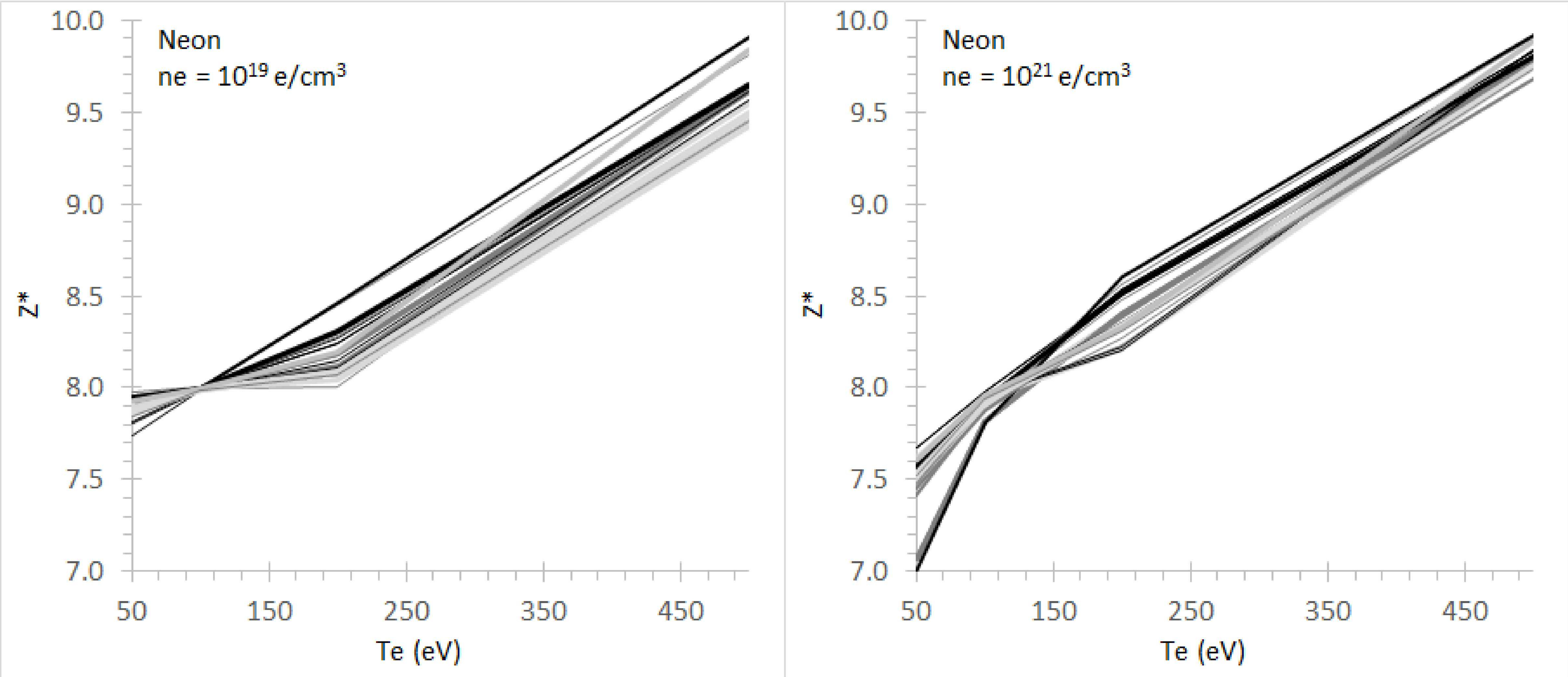
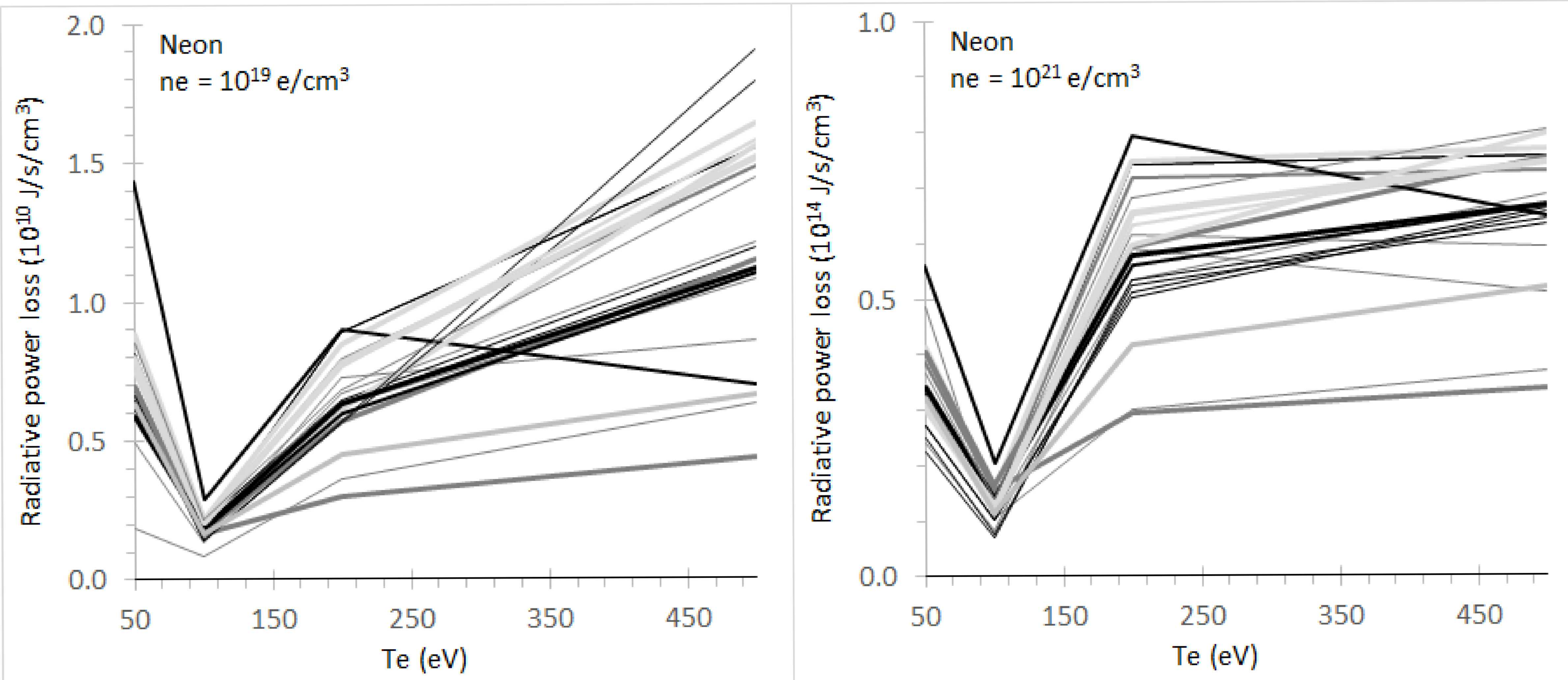


There is a slight trend for more detailed models (darker lines) to be more ionized

Ne: Radiative power losses agree to within 2-3x



There is a cluster of detailed models with RPLs that agree to within ~10%

Ne: Temperature diagnostics from Z*/Z*+1 line ratios

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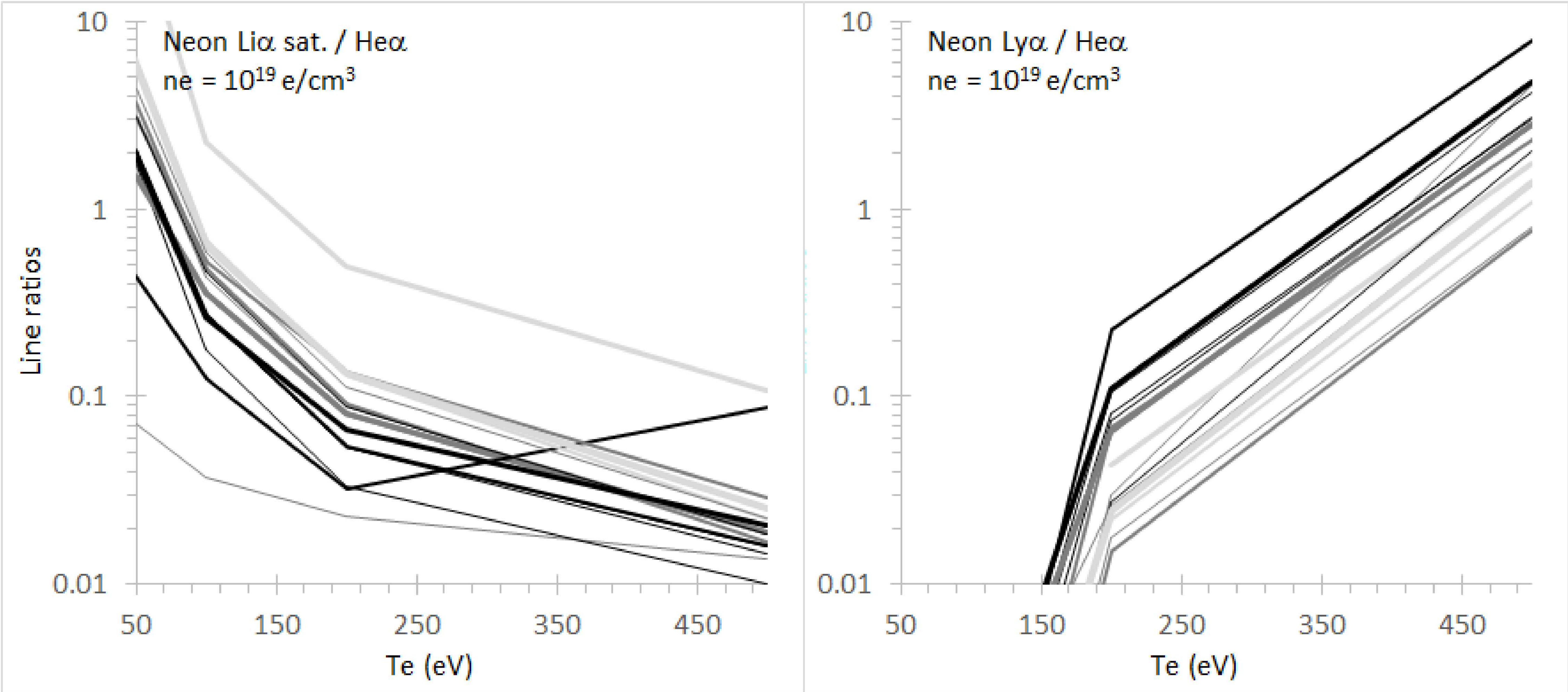
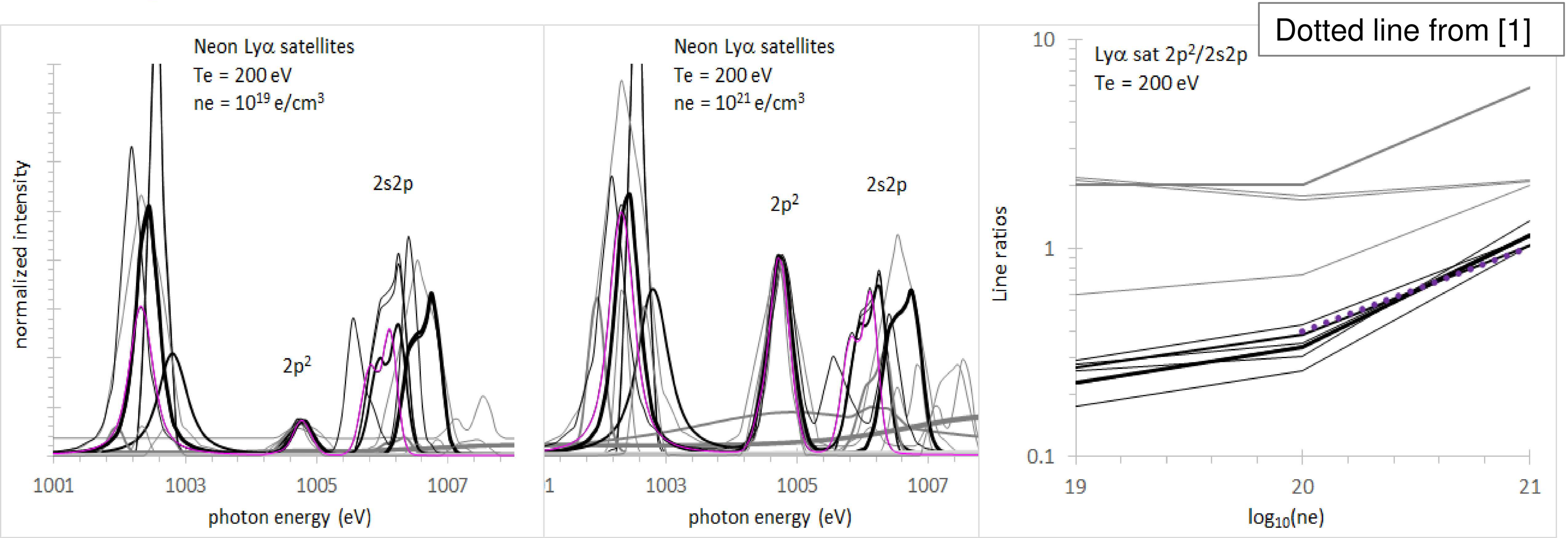


While there would be enormous uncertainty in diagnosed Te if all models were equally trusted, uncertainties are ~20% among a cluster (*sans* outliers) of detailed models

Ne: density diagnostic from collisional redistribution among He-like 2*l* 2*l*' states



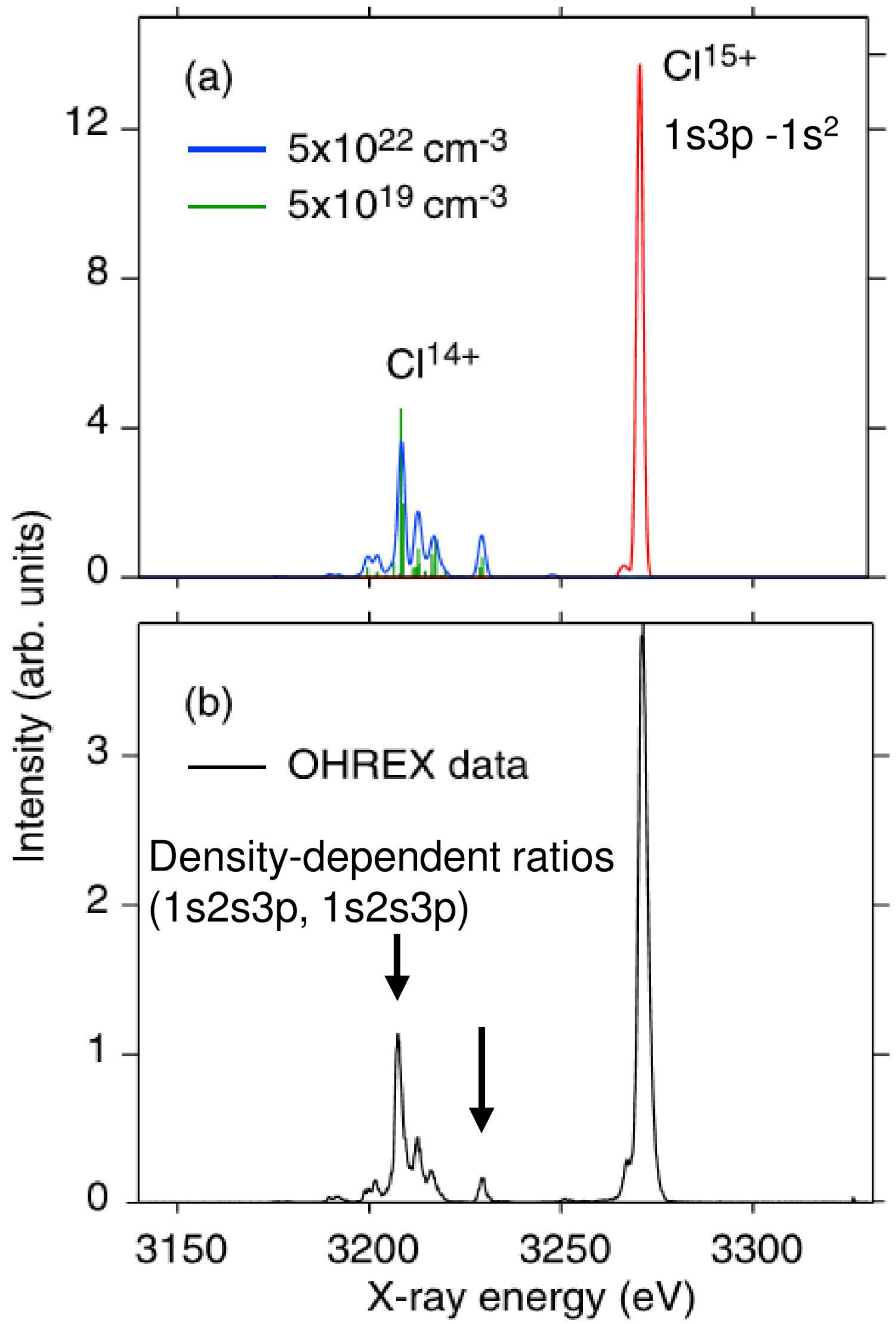
There is fair agreement among models that treat level kinetics (not just spectra) in detail, with implied uncertainties in diagnosed densities of (2 – 3)x above 10^{20} e/cm^3

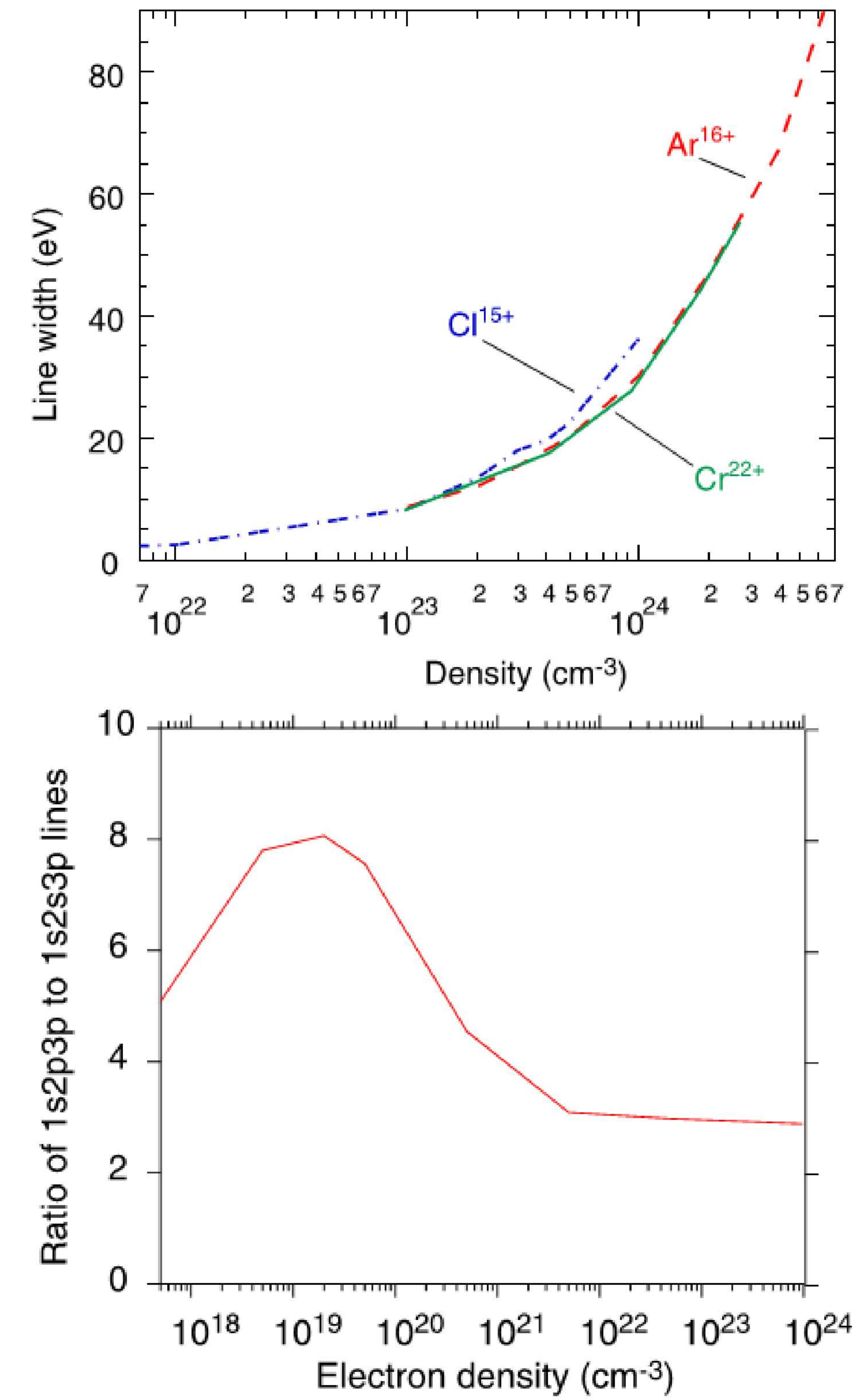
1. E. Kroupp *et al.*, *Phys. Rev. E* **97**, 103202 (2018)

Cl steady-state cases: dense plasma diagnostics

Motivation:

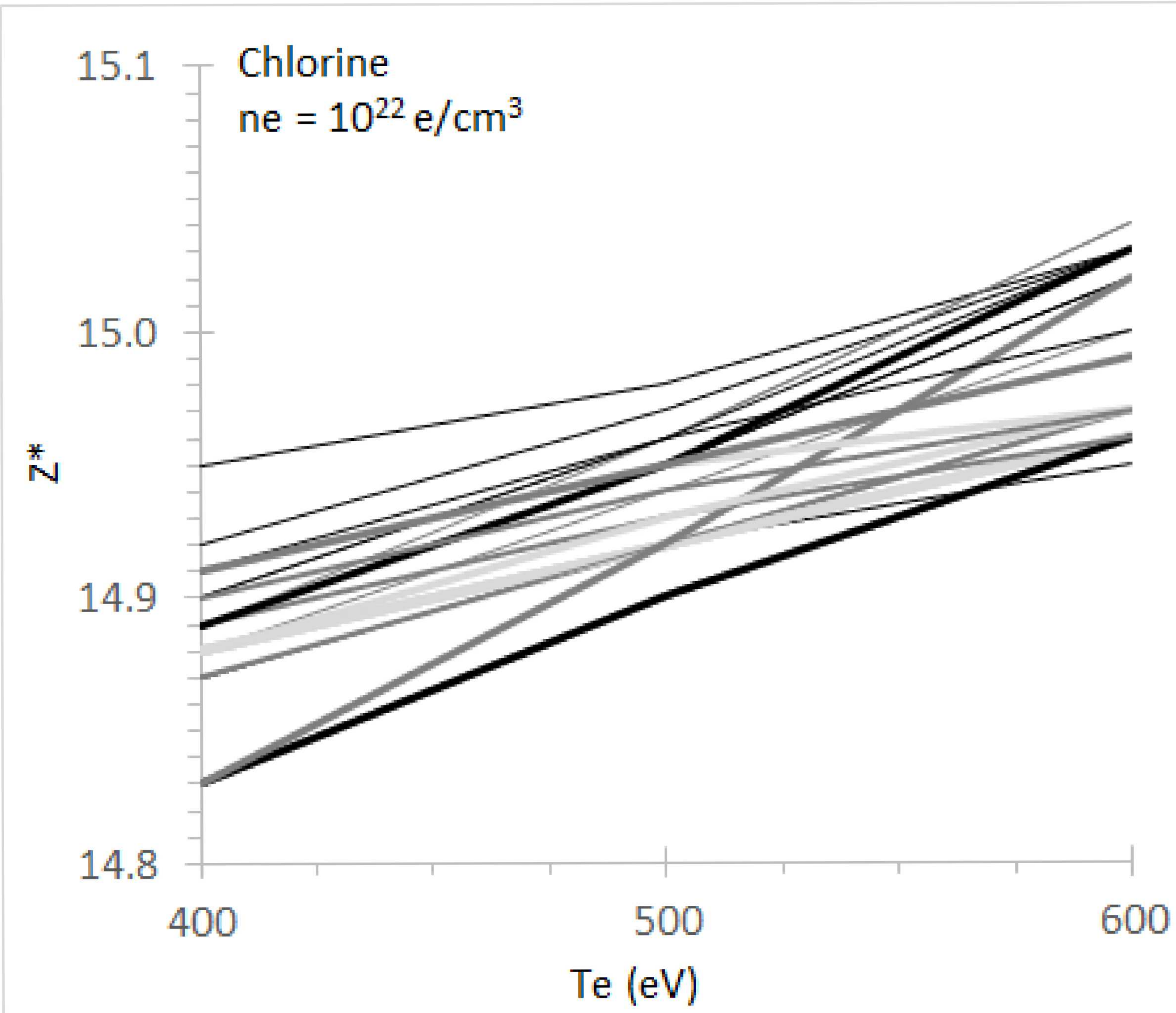
High-resolution OHREX measurements of Cl Heβ and its satellites from chlorinated plastic targets irradiated by both long- and short-pulse beams on ORION: density diagnostics from both Heβ widths and satellite lines sensitive to collisional redistribution among 1s2*l*3*l*'

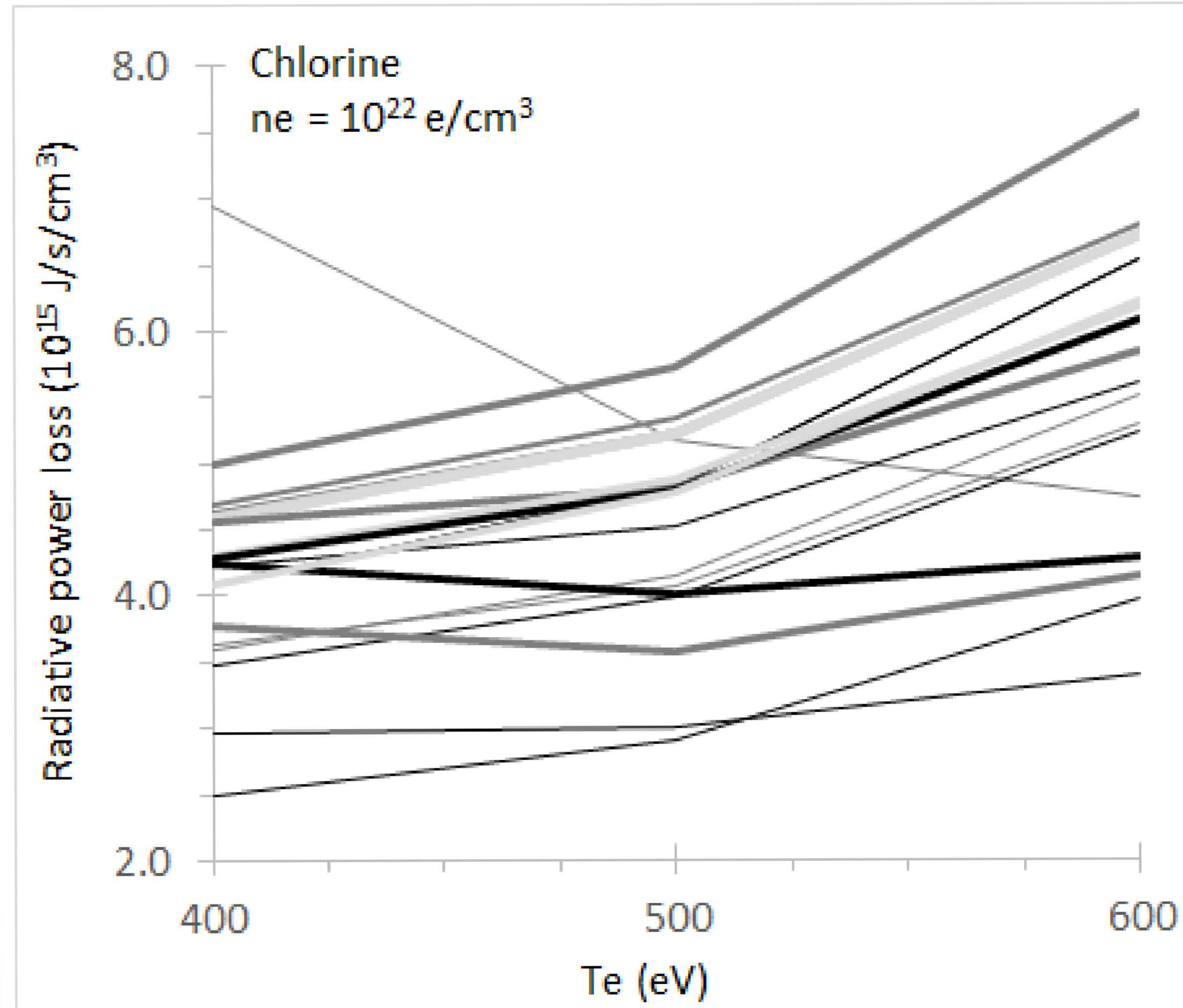




1. P. Beiersdorfer *et al.*, *Phys. Plas.* **23**, 101211 (2016)

Cl: Many codes with extraordinary agreement in Z* and RPL





Z* agrees to within ~0.1 charge state; RPL to within ~20%

Cl: Best fits to measured spectrum

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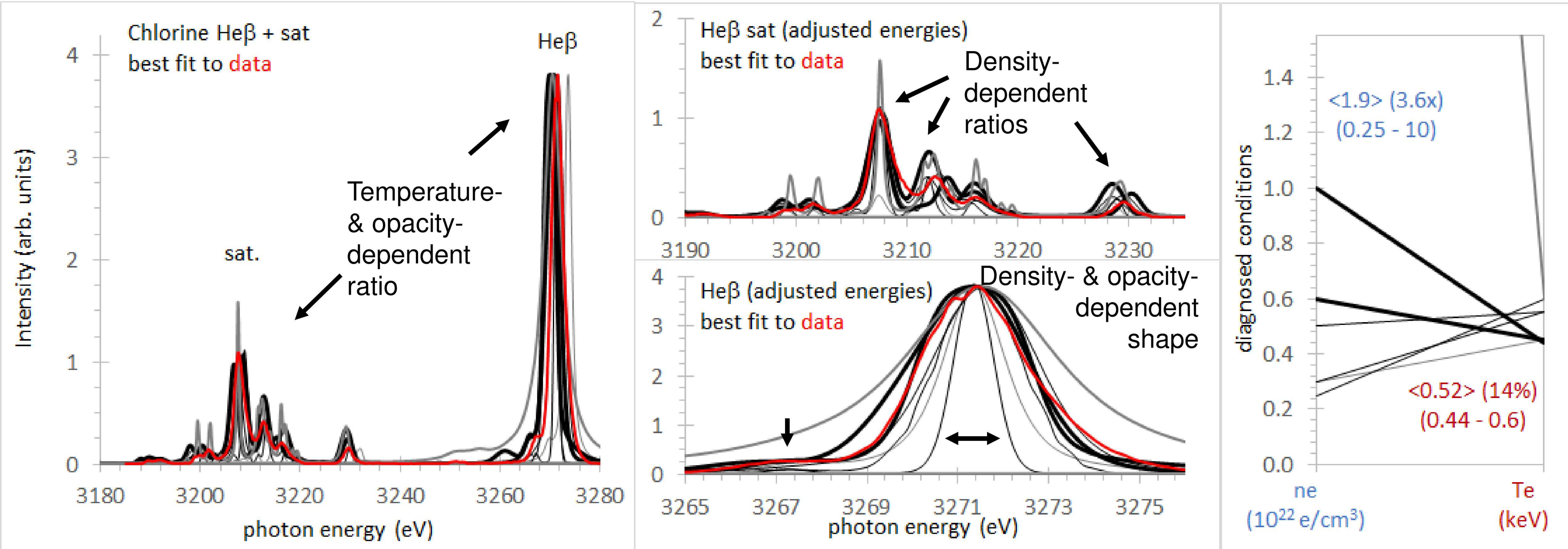
Find Te, ne, [and opacity] by simultaneously fitting Li-like satellite and He-like resonance [and intercombination] line intensities & widths – only one model had detailed Stark profiles



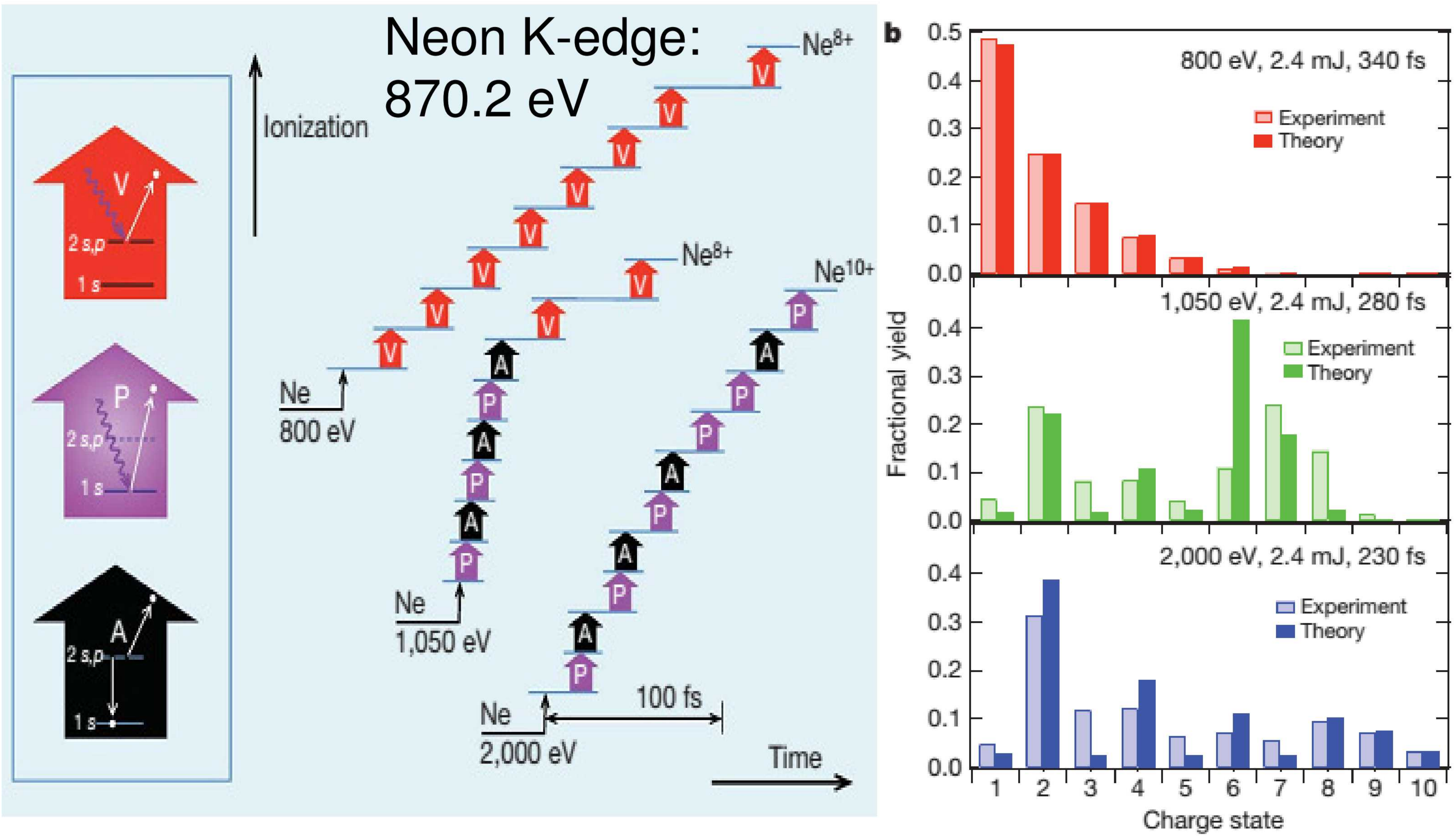
Best-fit temperature variations: σ ~ 15%

Best-fit density variations: σ ~ 200% (60% excluding one code)

Neon time-dependent cases: explore XFEL photoionization

Motivation:

Ions collected from neon gas targets irradiated with XFEL beams at various energies[1] showed either smooth ion yield distributions (E < 870 eV) consistent with sequential L-shell ionization or characteristic deficits in odd-numbered charge states (E > 870 eV) consistent with chains of photoionization followed by Auger decay ($Ne^{X+} \rightarrow Ne^{(X+2)+}$)

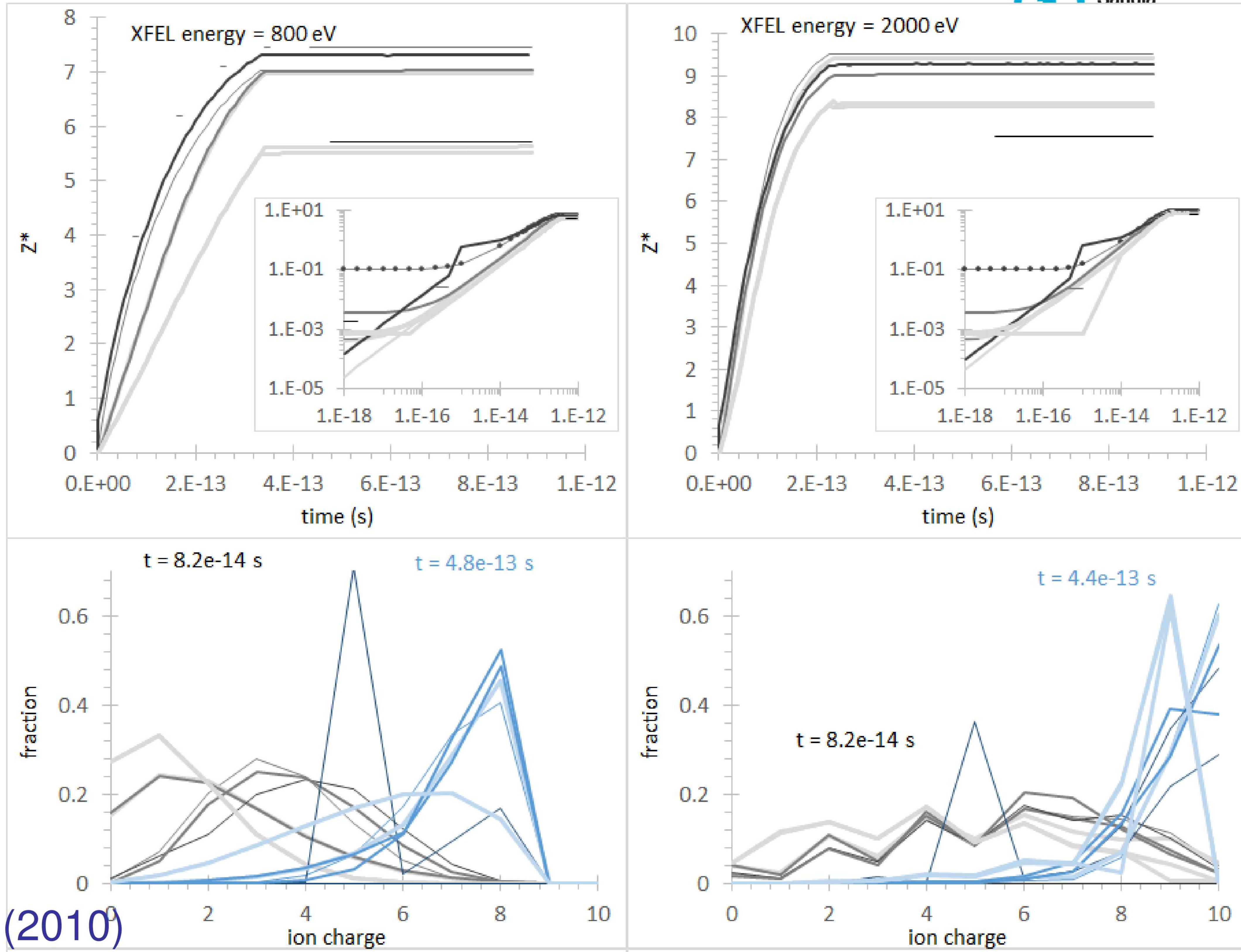


1. L. Young *et al.*, *Nature*. **466**, 56 (2010)

Ne-TD: Z* & CSD

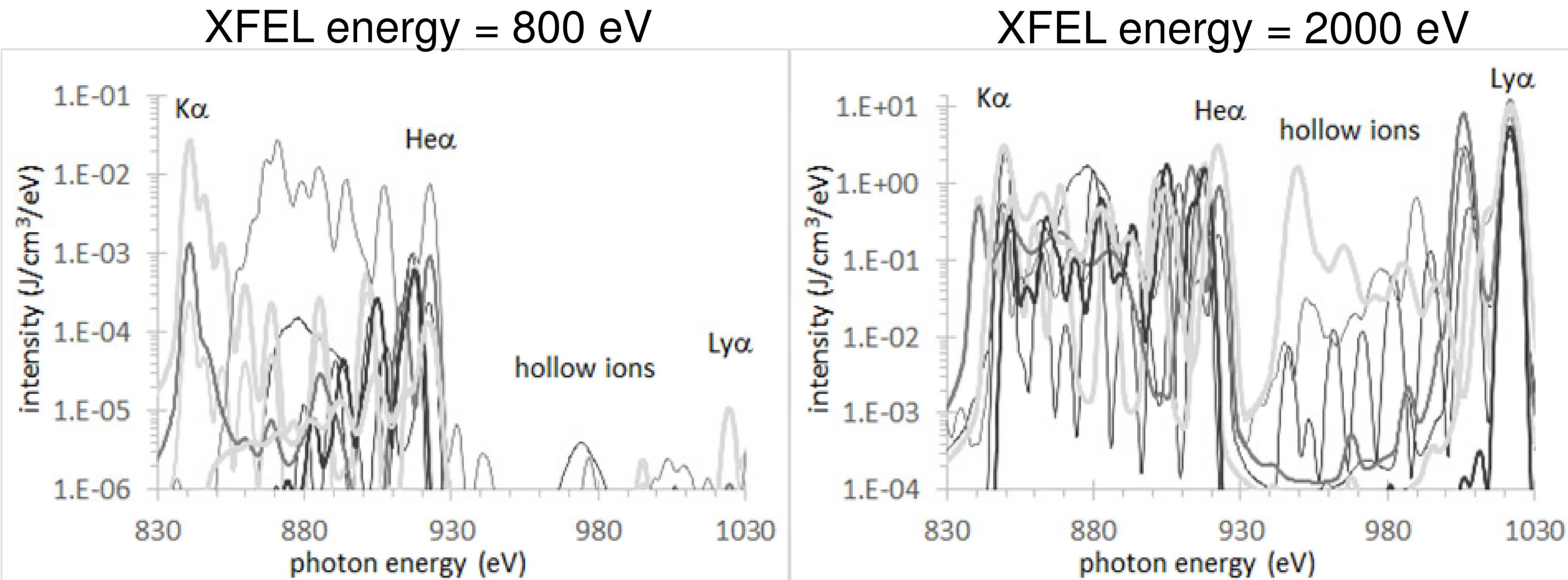
There was significant disagreement in Z* (~2 charge states) for all cases and times

However, all models predicted smooth CSDs for the 800 eV XFEL beam (sequential L-shell ionization) and characteristic deficits in odd charge states for the 2000 eV beam (K-shell ionization followed by Auger ionization), qualitatively reproducing the results of [1].



1. L. Young *et al.*, *Nature*. **466**, 56 (2010)

Ne-TD: Intriguingly, all models predict bright time-integrated fluorescence emission for the 800 eV beam energy



Kα intensities in the 800 eV case are orders of magnitude higher than thermal. With a neutral K-edge energy of 870 eV, no 1s electron can be directly photoionized or photoexcited by an 800 eV photon. The fluorescence intensities here roughly correspond to each model's rate of dielectronic recombination through $(1)^2(n\ldots N)^X + e^- \rightarrow (1)^1(n\ldots N)^{X+2}$ channels.

Al cases: explore continuum lowering in dense plasmas

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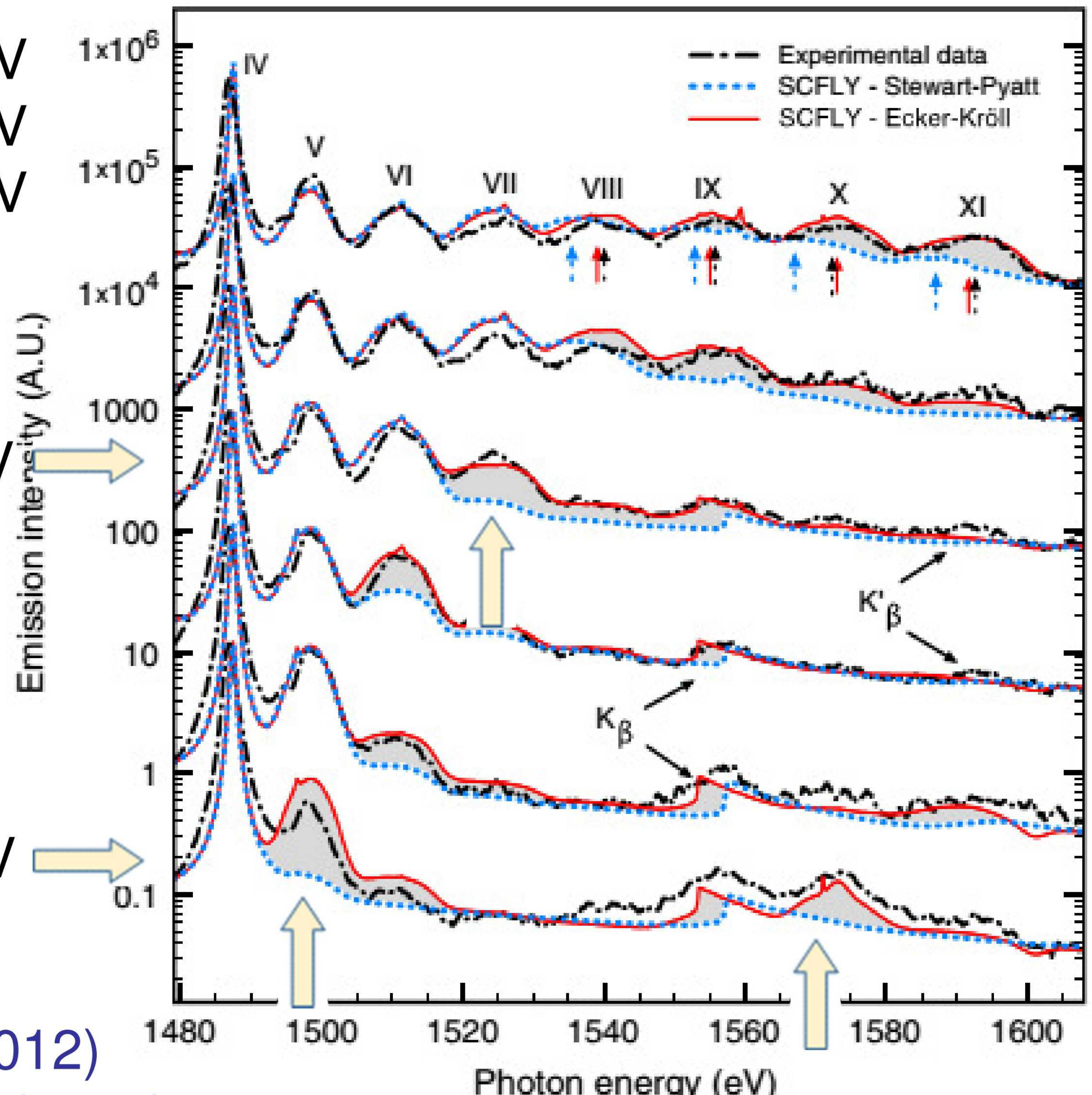
Motivation:

Fluorescence emission spectra measured from Al foils irradiated with a range of XFEL energies[1] showed more emission from high charge states than expected under Stewart-Pyatt continuum lowering (CL) theory, and were fit well with SCFLY[2] using a modification of an older CL theory from Ecker & Kröll.

K-edge:1560 eV
Kα: 1487 eV
Kβ: 1557 eV

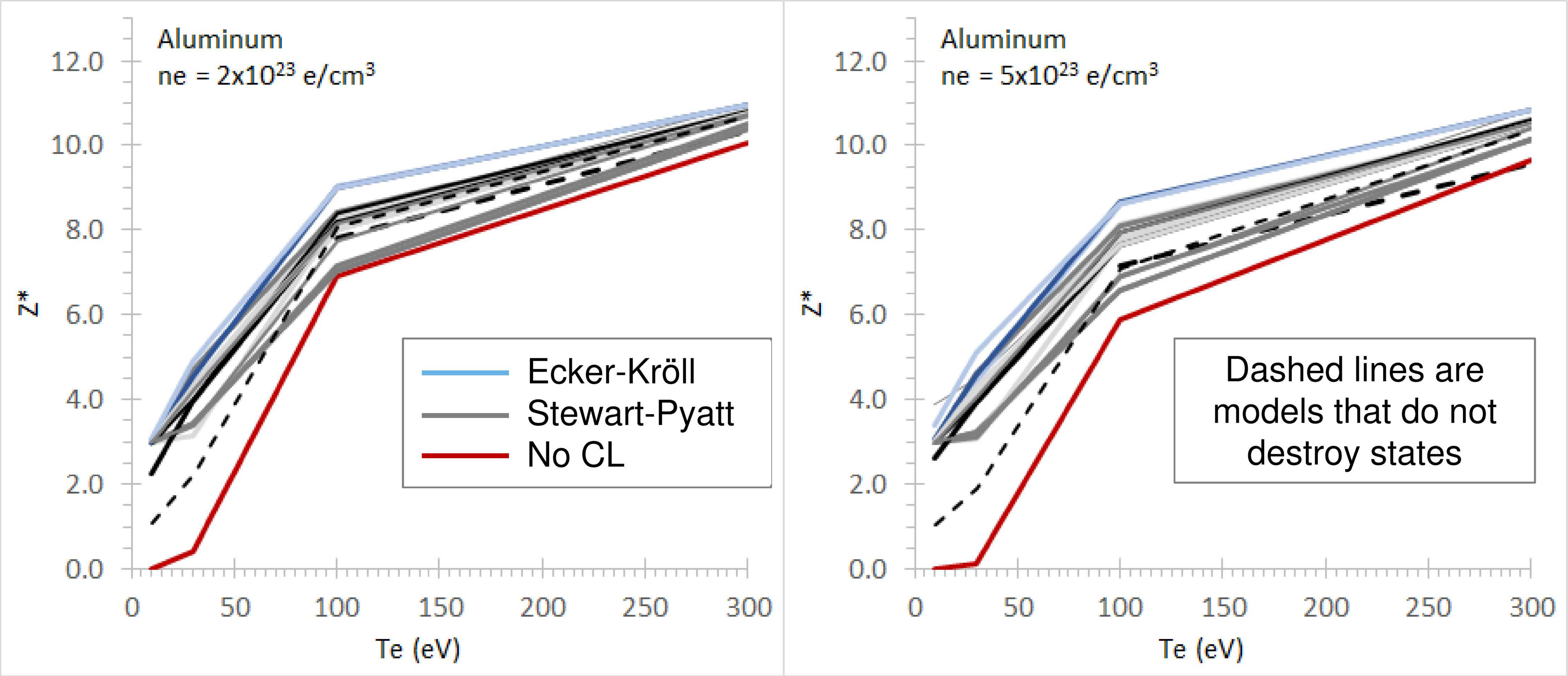
XFEL 1650 eV

XFEL 1580 eV



1. O. Ciricosta *et al.*, *Phys. Rev. Lett.* **109**, 065002 (2012)
2. H.-K. Chung, M. Chen, and R.W. Lee, *HEDP* **3**, 57 (2007)

Al: Steady-state ionization predictions are clearly dependent on the treatment of continuum lowering



Continuum lowering effects can be implemented by reducing ionization potentials (SP, IS, or EK), destroying pressure-perturbed states, or both

Al-TD: Time-dependent ionization is also clearly dependent on continuum lowering

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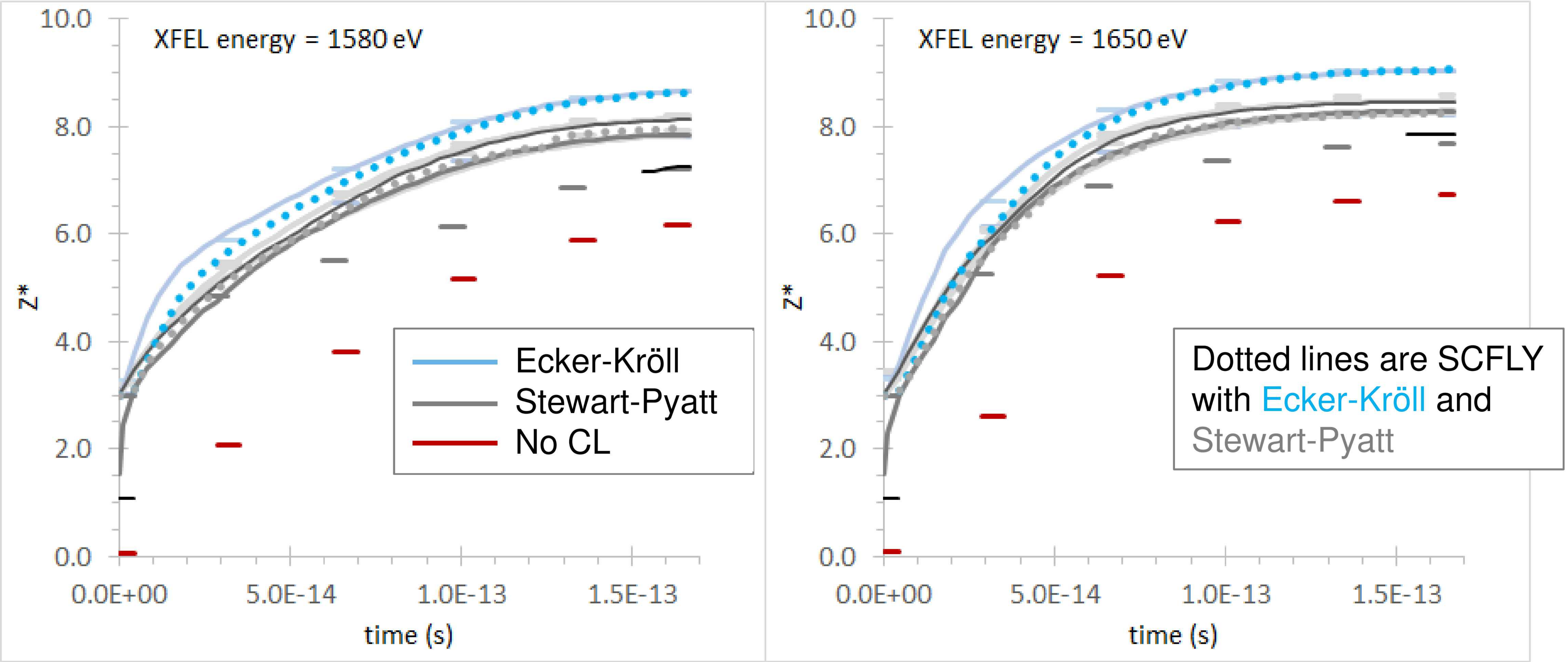
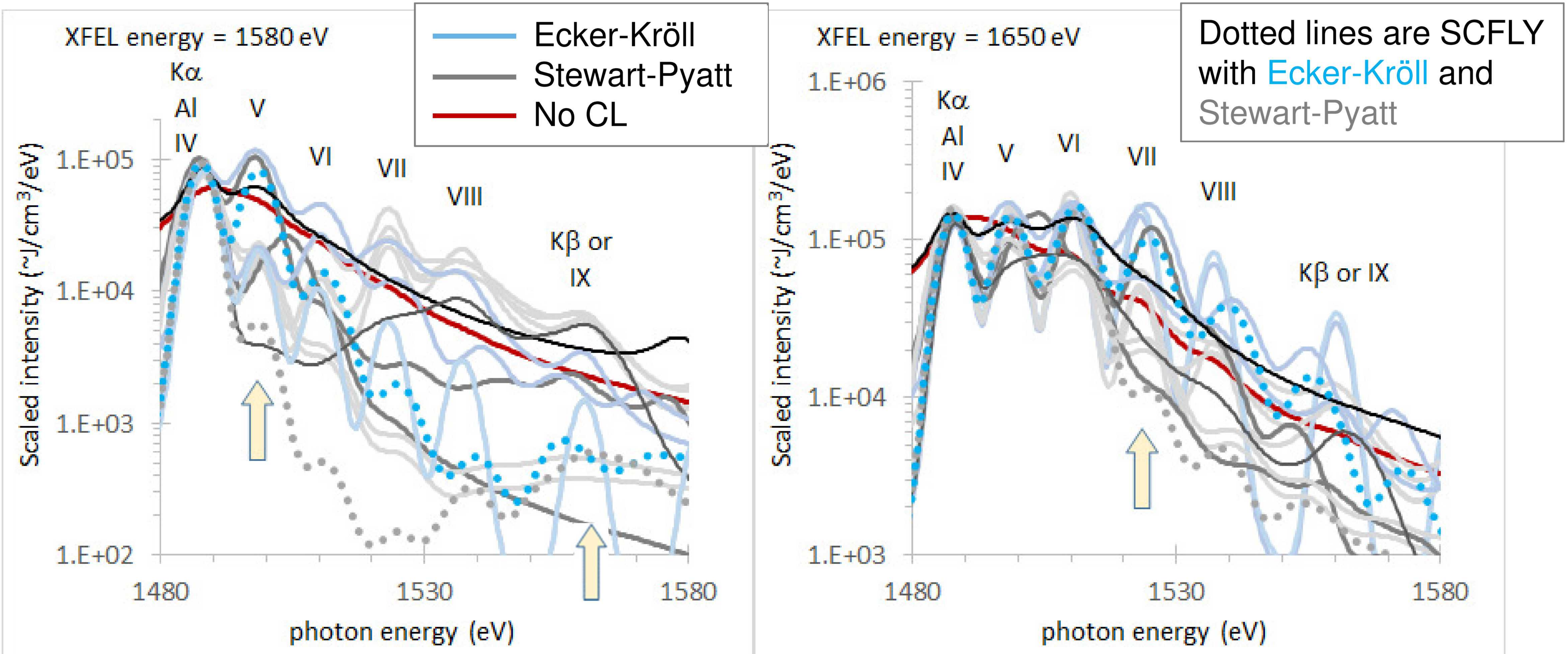


Models using EK CL are most ionized, followed by models using SP/IS and models using IS without state destruction. Models without CL predict the lowest Z*

But continuum lowering does not uniquely constrain spectra



Many models that use SP/IS exhibit intensities similar to SCFLY with EK – though none have yet demonstrated similar fits to data including detailed beam profiles and foil opacity.

Si cases: explore external & internal radiation fields

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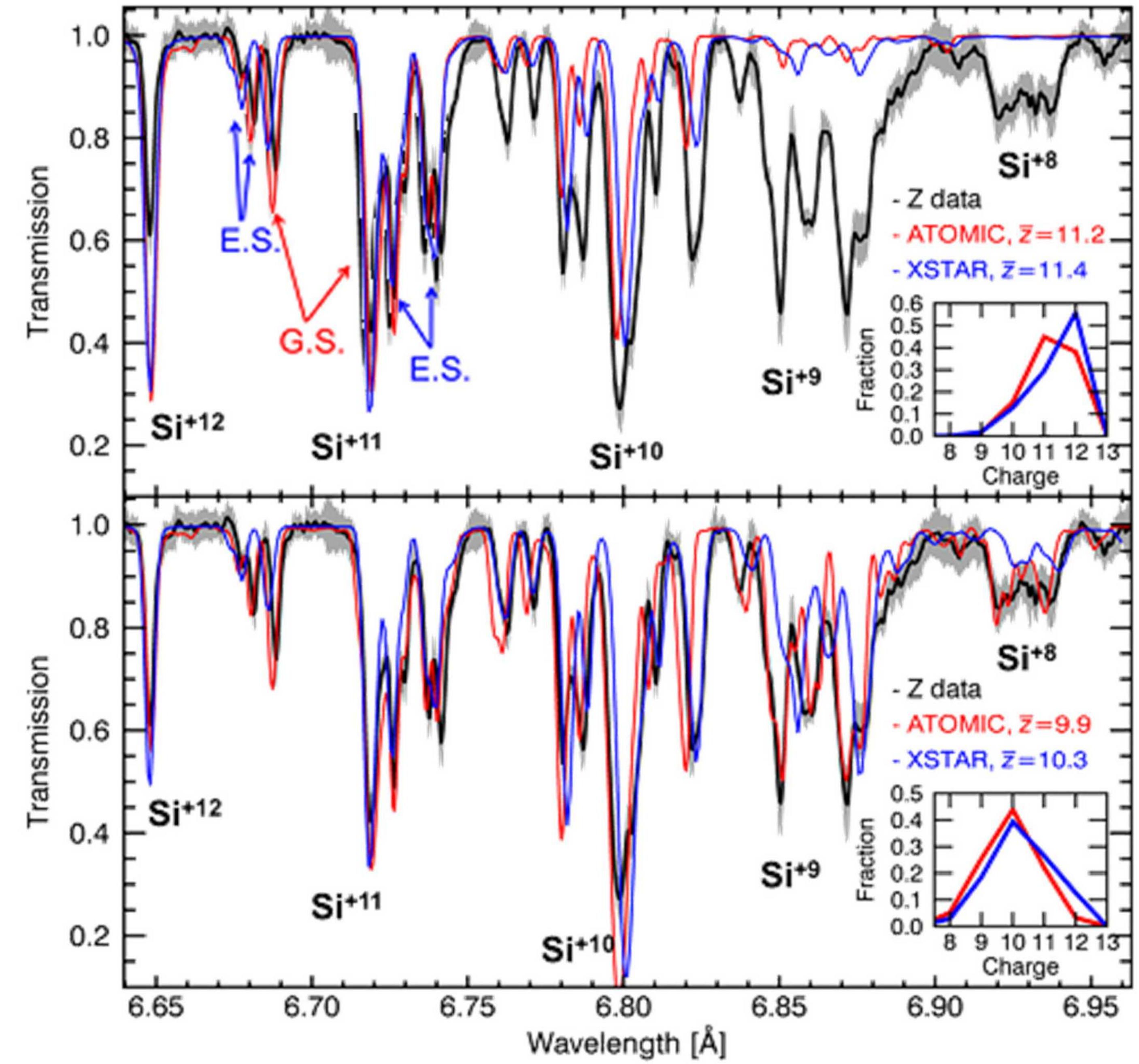
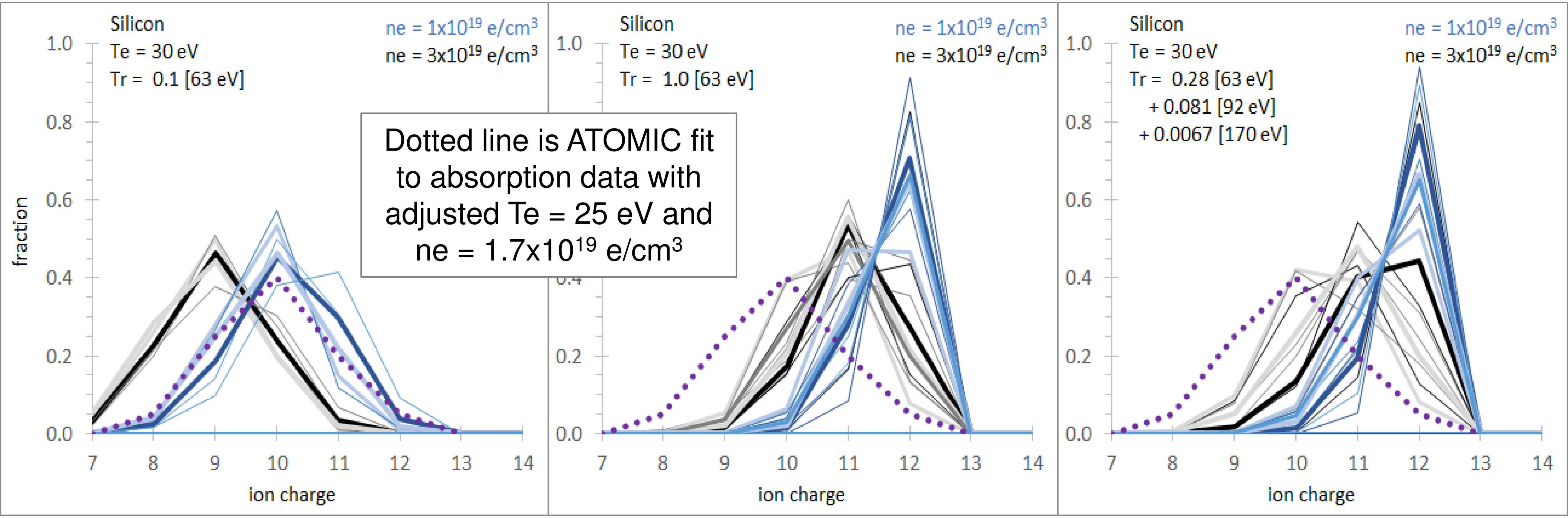
<u>Motivation:</u>

Simultaneous measurements of highly resolved and reproducible absorption and emission spectra from well-characterized photoionized plasmas indicate lower ionization than predicted by ATOMIC and XSTAR:
ne = 8.5×10^{19} e/cm^3 (expansion and Z*)
Te = 33 +/- 7 eV (ratios of absorption from Li-like states that should follow Boltzmann statistics: absorption ~ $X_i f_{ij}$ with $X_i = g_i e^{-Ei/Te}$)



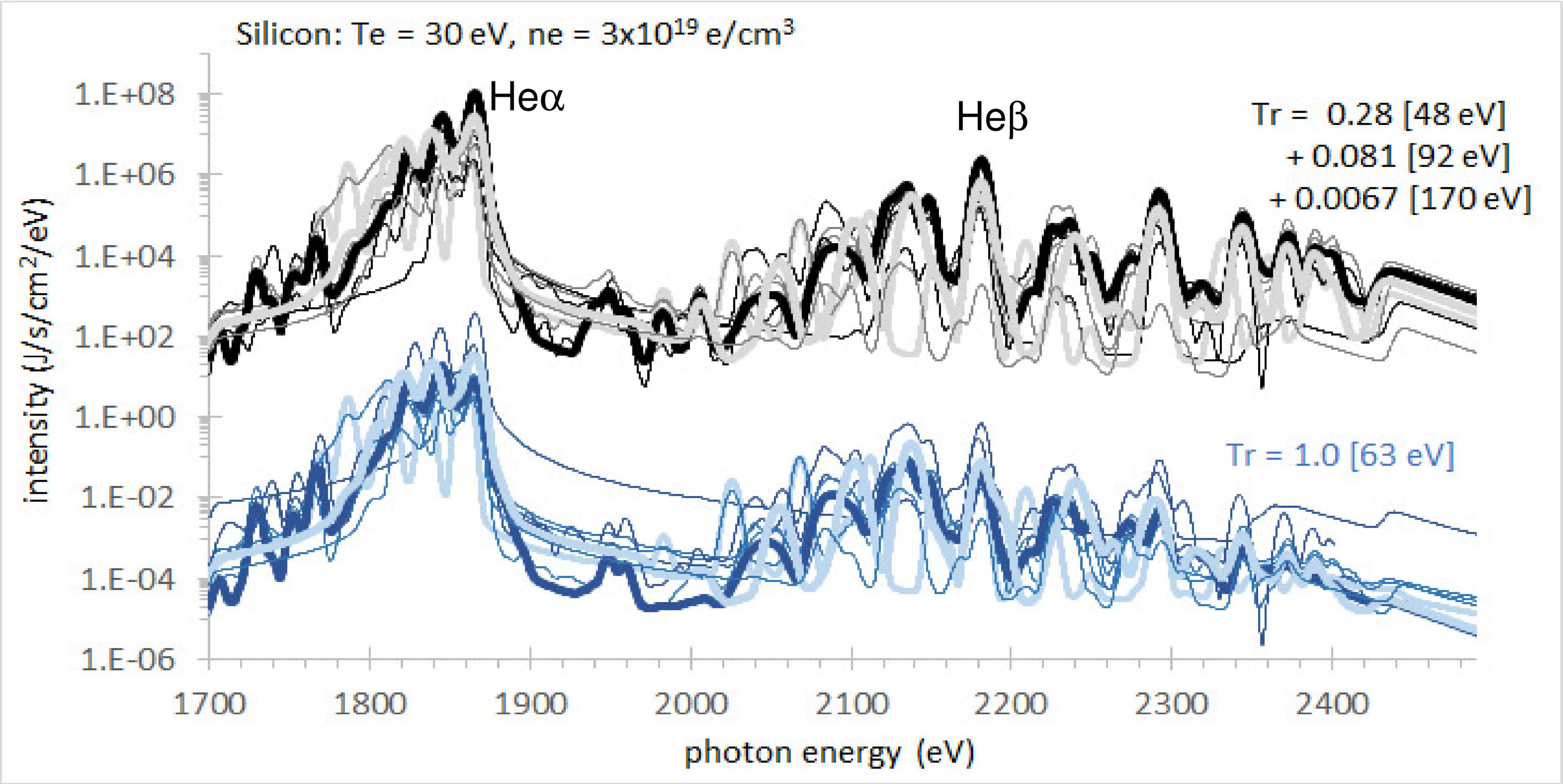
G. Loisel *et al.*, *Phys Rev. Lett.* **119**, 075001 (2017)
C. Fontes *et al.*, *J. Phys. B* **48**, 144014 (2015)
T. Kallman and M. Bautista, *Astrophys. J. Suppl. Ser.* **133**, 221 (2001)

Si: with significant external radiation, all models predict higher ionization than observed in the experiment



Increasing the external radiation field (single or multi-Planckian with similar total energies) increases Z* by ~2 in all models, and all models show decreasing ionization with increasing densities as collisional recombination increases relative to photoionization.

Si: Emission spectra from all models reliably reflect the underlying charge state distribution



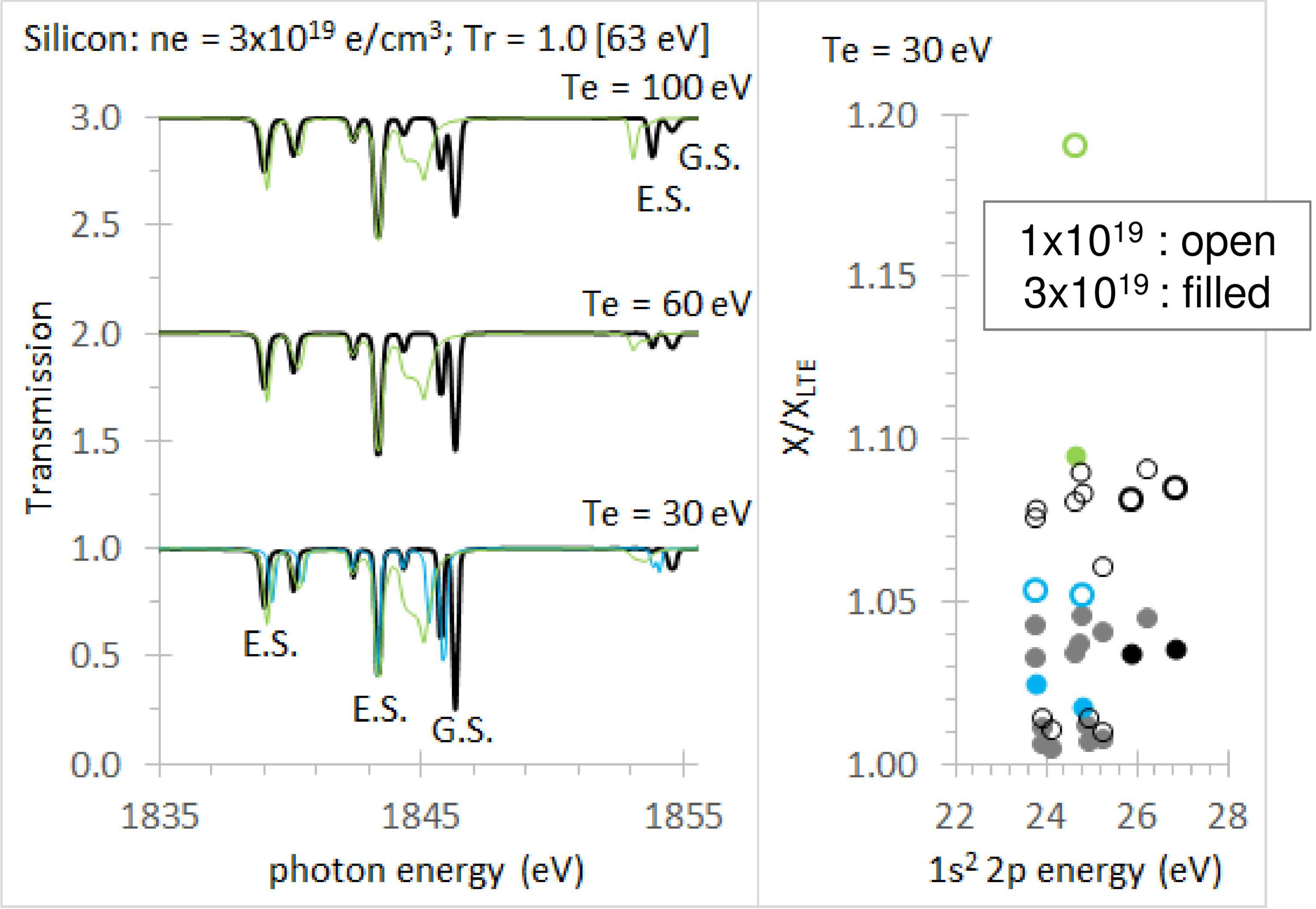
Emission spectra (artificially broadened) also have fair agreement in absolute intensities, with the multi-Planckian enhancing intensity by ~10^6 over Tr = 63 eV.

Si: Many models have Li-like $1s^2 2l$ populations higher than LTE, potentially supporting lower temperatures

We invited additional Te, rad. field, and opacity data in the post-workshop call for resubmissions

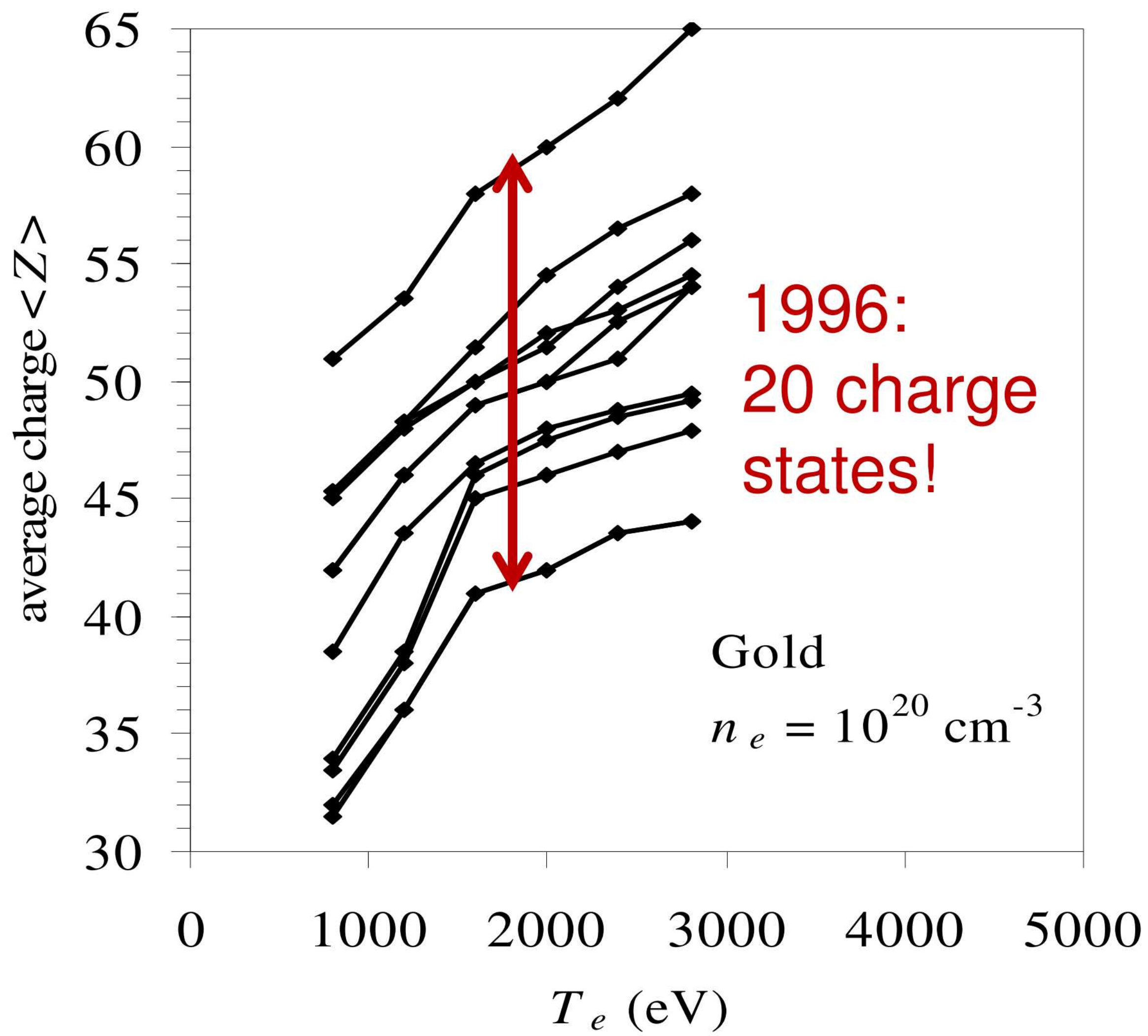
Among three codes, there were significant differences (line shape, energies, and intensities) in the Li-like absorption lines that were used for the experimental thermometer

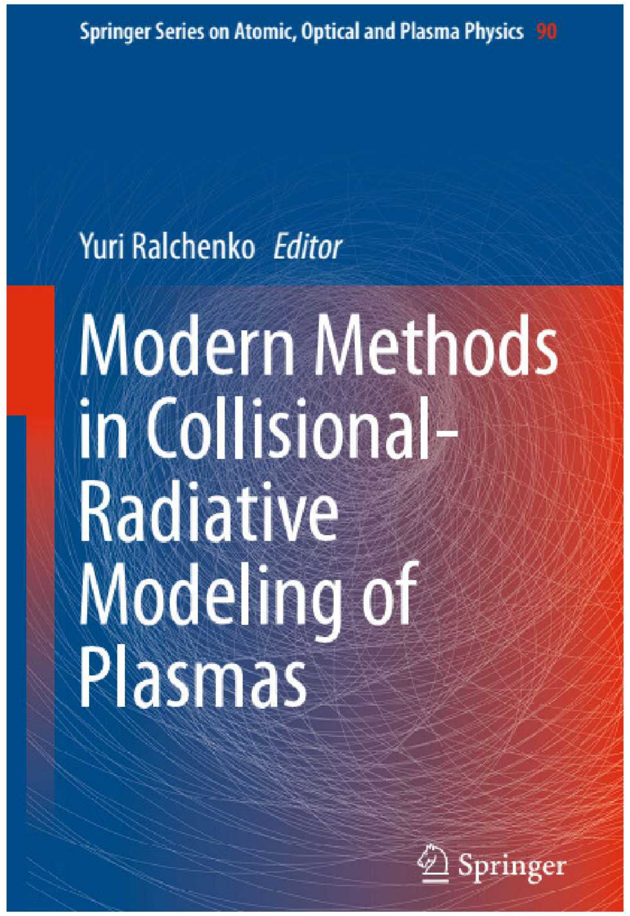
All contributing codes had higher-than-Boltzmann excited state populations, especially at the lower density, which could lead to overestimated temperatures

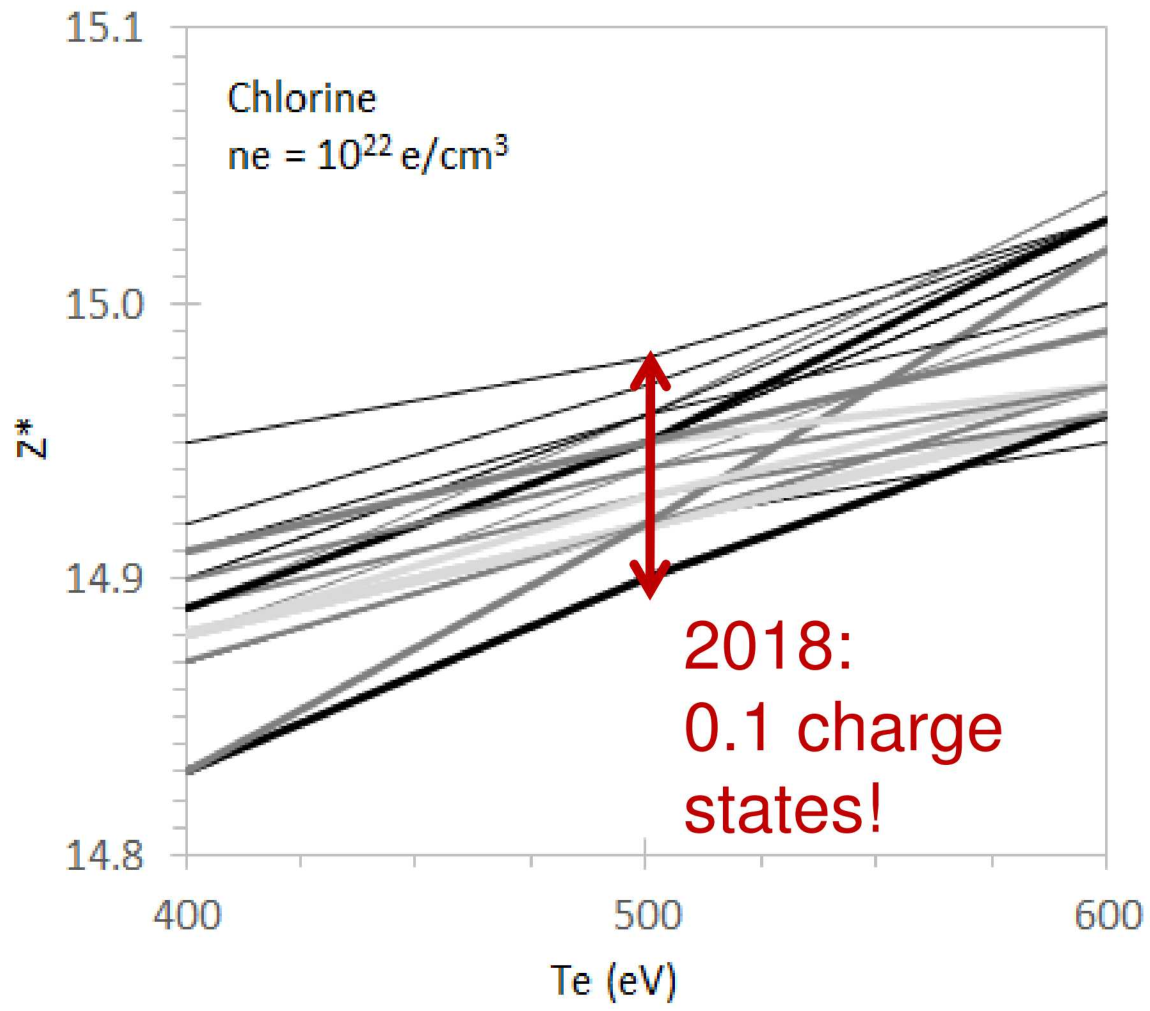


Conclusion: the non-LTE code comparison workshops aim to help the HEDP community assess model reliability

- Helps set confidence in simulations, diagnostics, and conclusions drawn from data
- We've come a long way from 1996 – dense plasmas are the new frontier
- We welcome new contributors and ideas for next year's cases



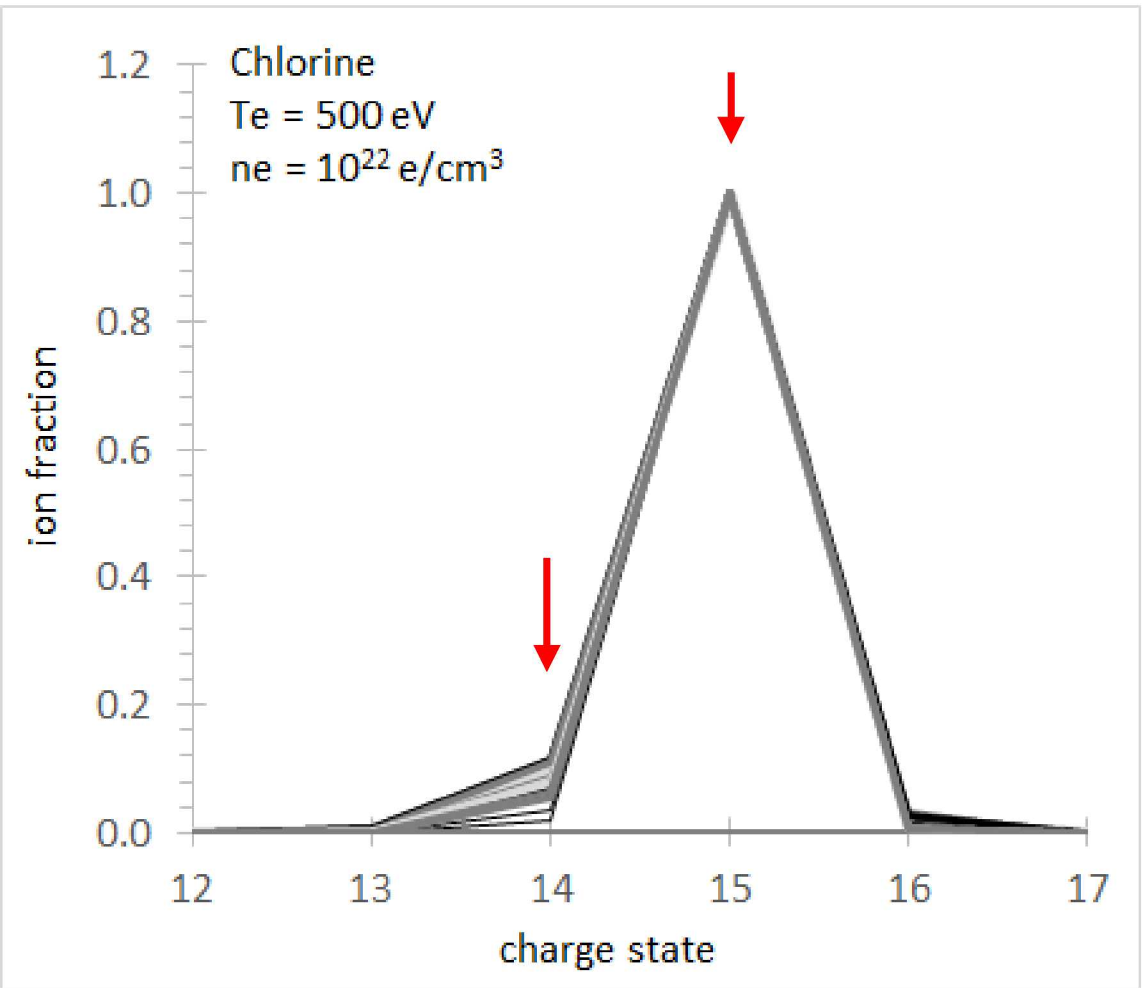


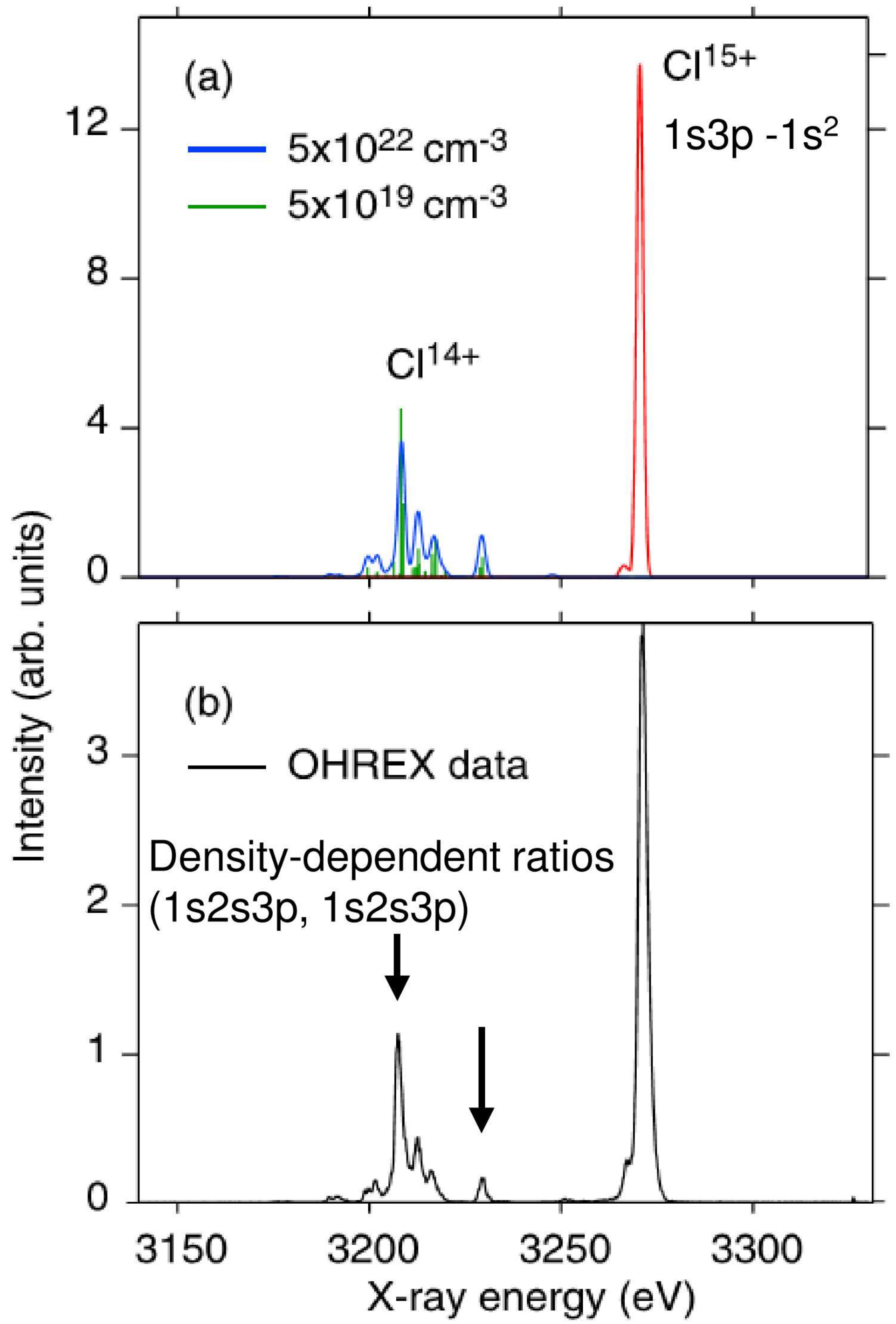


Backup slides

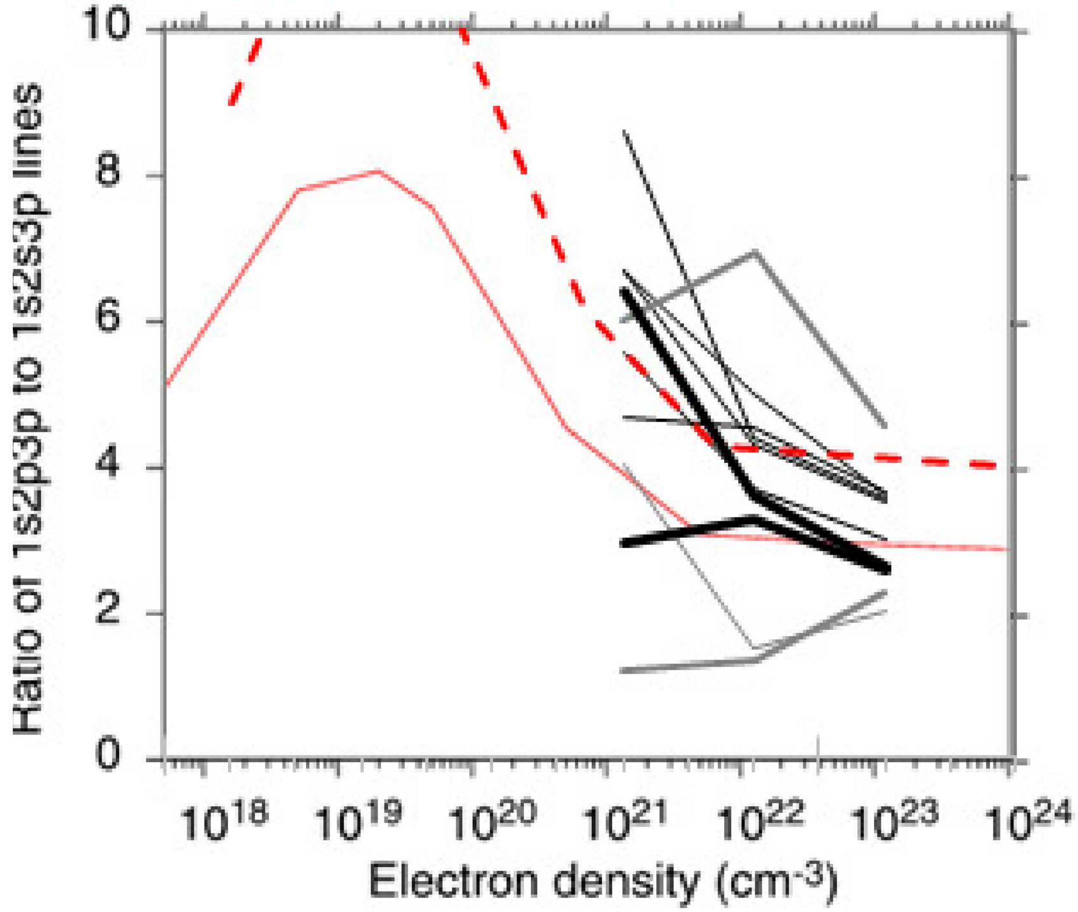
Cl: density-diagnostics are sensitive to charge state distibutions

[1] assumed equal He- and Li-like populations for line ratio



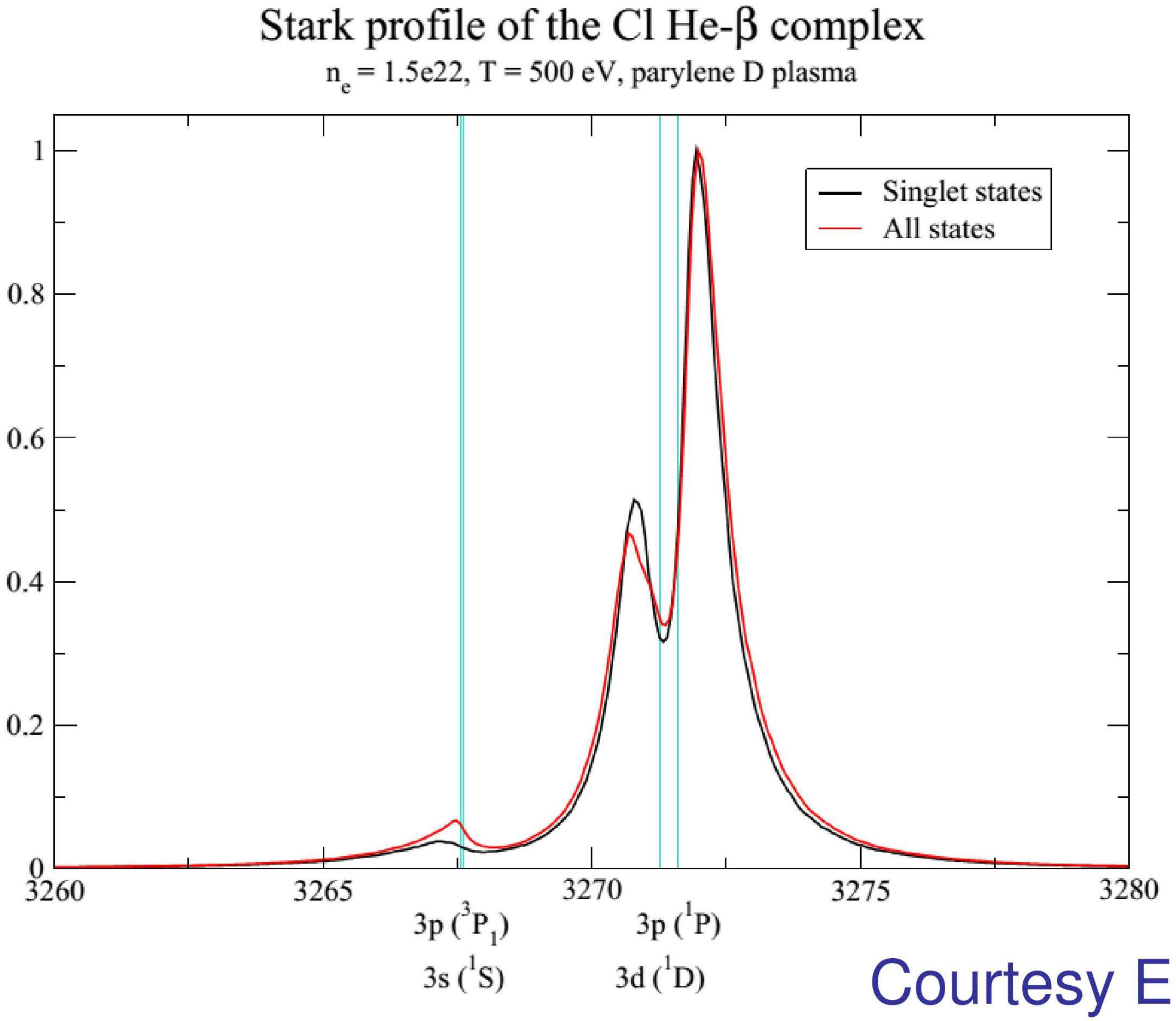


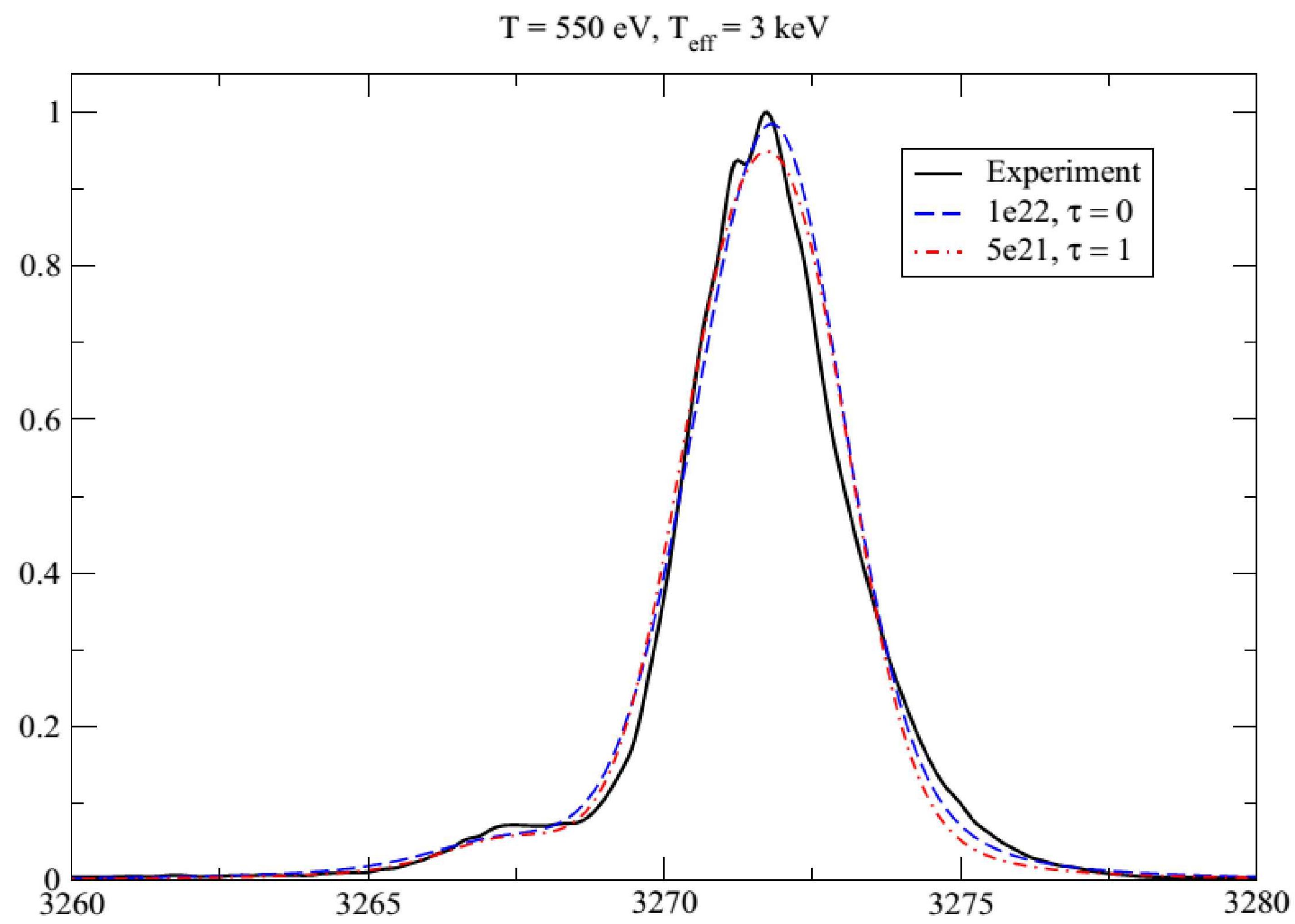
Dashed line excludes 30% intensity in 1s2s3p from direct excitation in Lik-like



1. P. Beiersdorfer *et al.*, *Phys. Plas.* **23**, 101211 (2016)

Cl: Accurately fitting Heb requires actual line shape theory rather than common (and rough) approximations

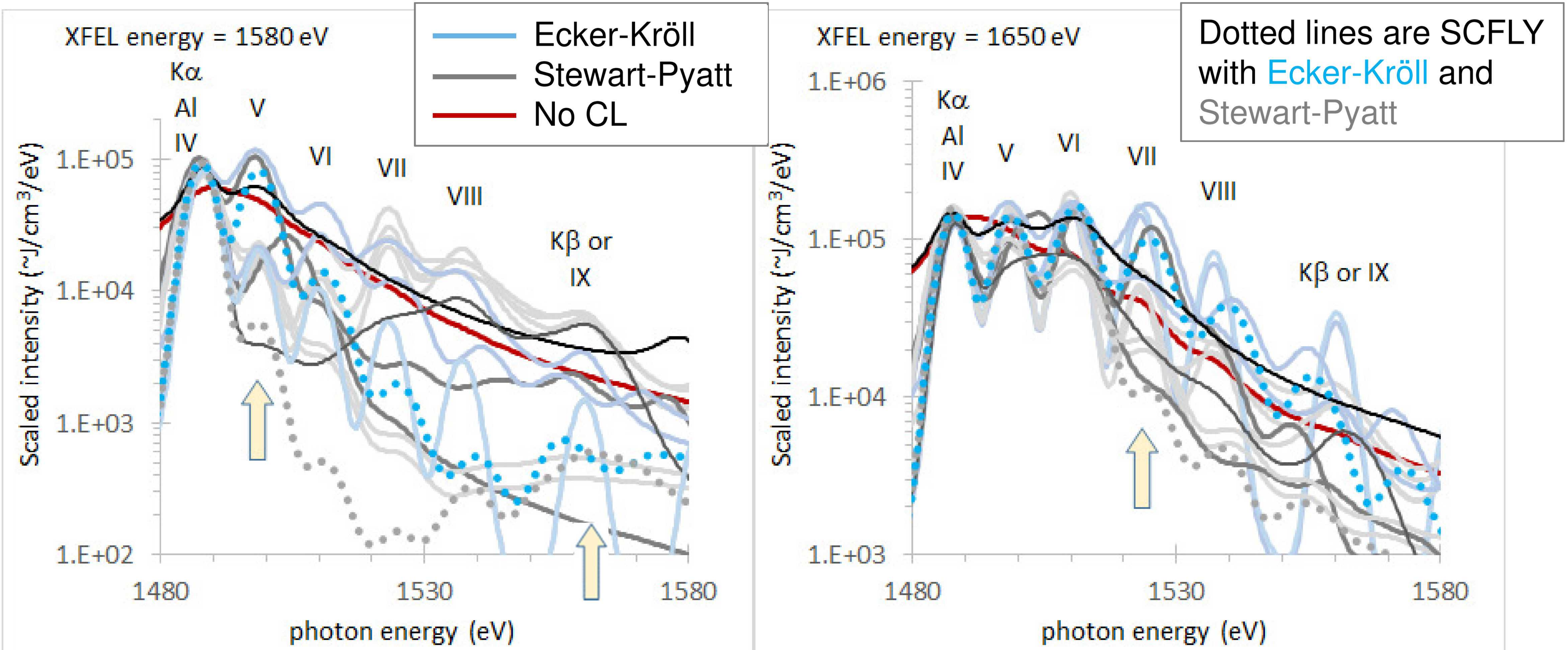




Courtesy E. Stambulchik

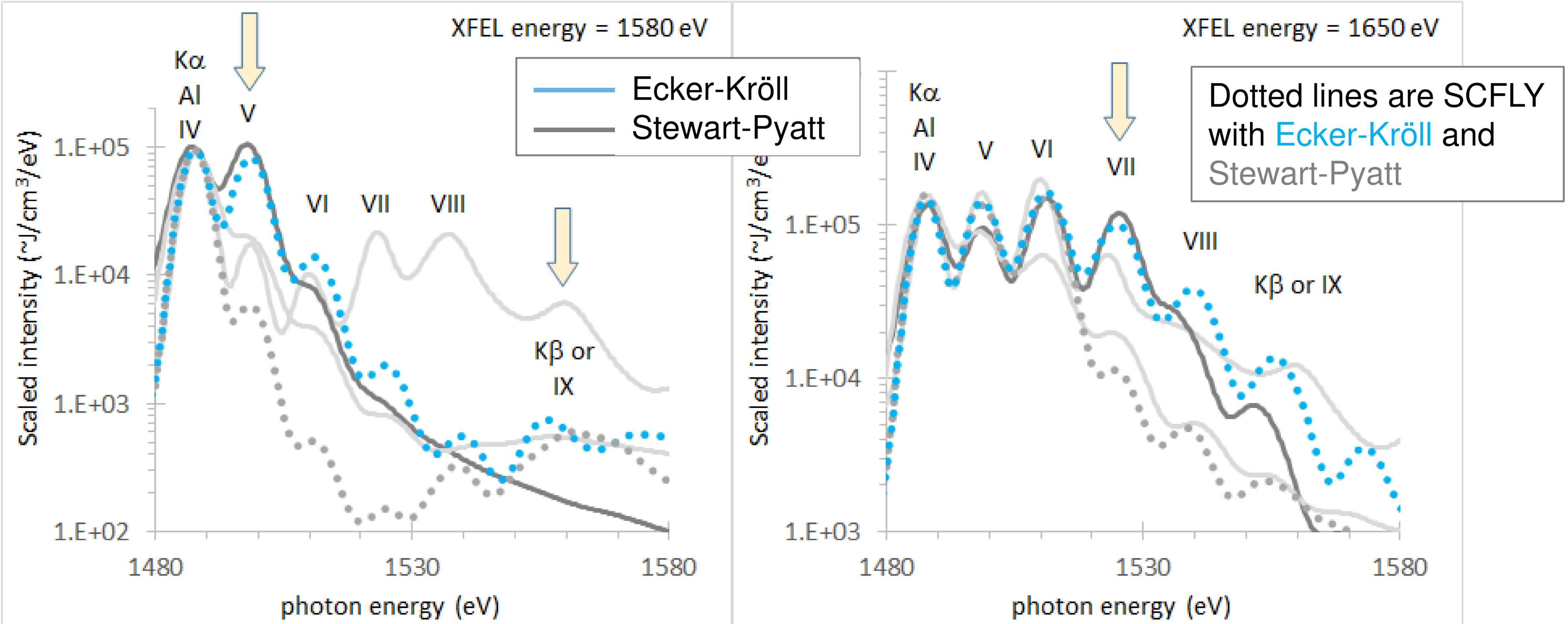
The Heβ line shape depends on opacity, collisional broadening, and Stark mixing with the dipole-forbidden $1s^2$ (^1S) – 1s3s (^1S) transition – few models included all effects!

But continuum lowering does not uniquely constrain spectra



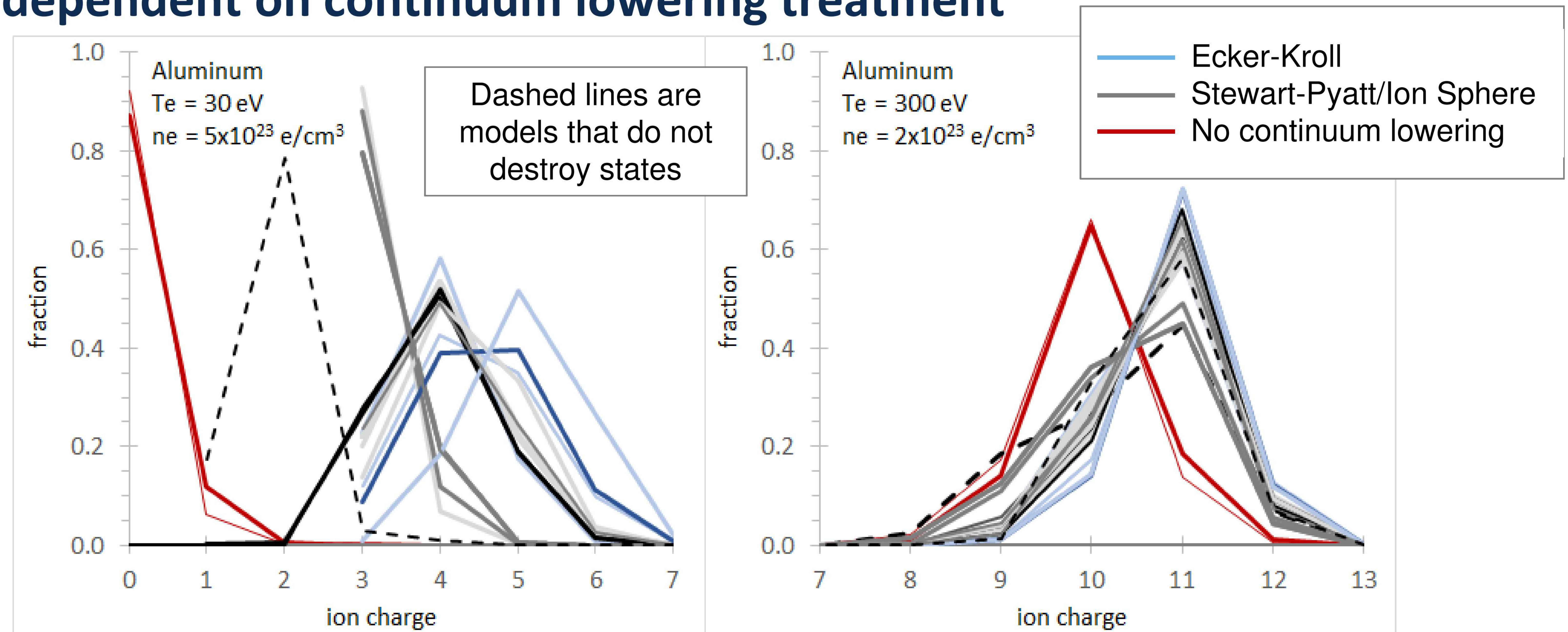
The intensity distributions of the predicted spectra span an enormous range, with ambiguous dependence on the CL theory implemented and other model variations

The fluorescence emission depends on model structure as well as the treatment of continuum lowering



While some models that use SP/IS predict intensity distributions similar to SCFLY/EK, it is not clear that any would fit the experimental data as well with opacity/beam profiles included.

Al: Steady-state charge state distributions are clearly dependent on continuum lowering treatment



Continuum lowering effects can be implemented by reducing ionization potentials, destroying pressure-perturbed states, or both