Laboratory astrophysics for high-resolution X-ray spectroscopy

Natalie Hell
LLNL

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Lawrence Livermore National Laboratory

Why laboratory astrophysics

Problem of transitions missing in databases: Fe L

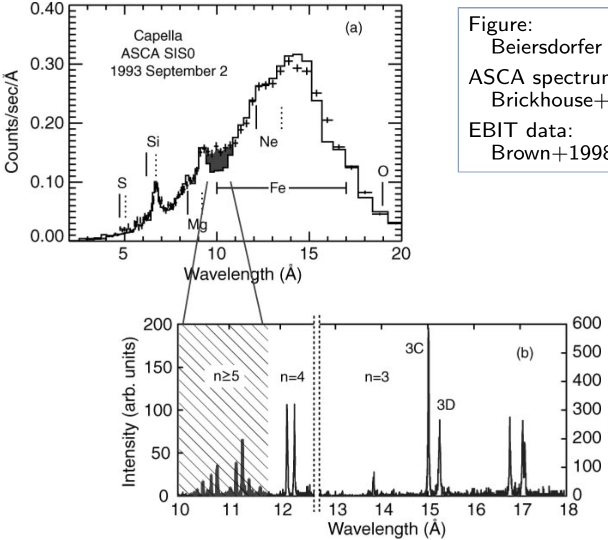


Figure:
Beiersdorfer 2003, ARAA 41, 343

ASCA spectrum:
Brickhouse+2000, ApJ 530, 387

EBIT data:
Brown+1998, ApJ 502, 1015

Weak lines are important:

Model fit to Capella: only strong $n = 3, 4 \rightarrow 2$ transitions in Fe XVII and XVIII.

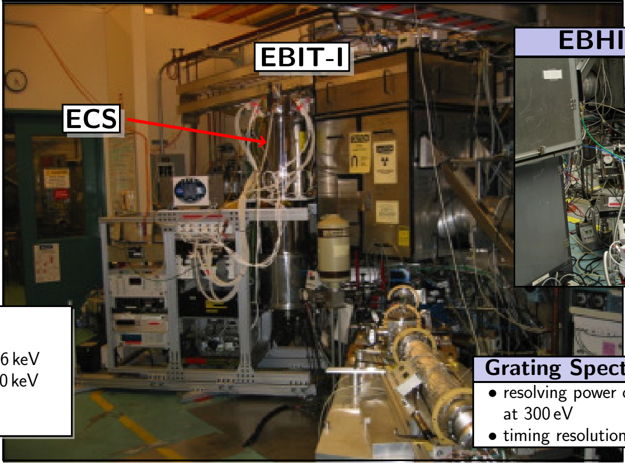
EBIT data: sum of weak $n \geq 5 \rightarrow 2$ transitions contributes $> 10\%$ of total flux

Labastro helps us make our models reliable

The LLNL Electron Beam Ion Trap Facility

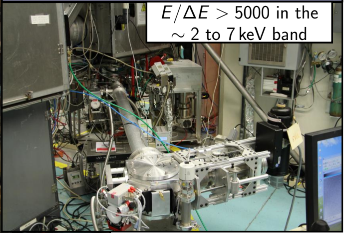
Properties of EBIT-I
- Monoenergetic beam: FWHM$\sim$ 20–50 eV
- $\sim$ 60 μm beam diameter
- $E_{\rm beam}$ =100 eV to > 100 keV
- $n_e \sim 10^{11}$–10^{12} cm^{-3}
- $n_{\rm ion} \sim 10^{10}$ cm^{-3}
- We can sweep the beam
  - linearly
  - quasi-Maxwellian

LLNL EBIT-I and a few EBIT spectrometers



Properties of the ECS:
- calorimeter spectrometer
- energy resolution of $\sim$ 5 eV 6 keV
- broadband $\sim$ 100 eV to > 60 keV
- 65 hour integration times
- large collection area

EBHIX (crystal spectrometer)



$E/\Delta E > 5000$ in the $\sim$ 2 to 7 keV band

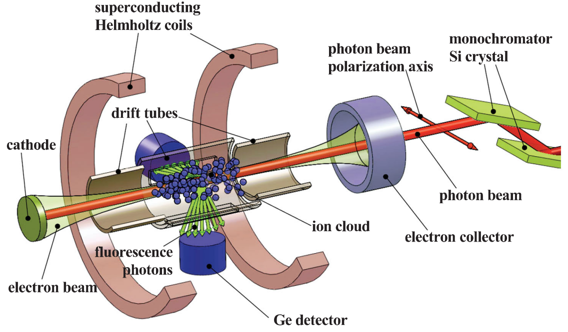
Grating Spectrometer
- resolving power of $\sim$ 3000 at 300 eV
- timing resolution of 40 ns

User-friendly lab-astro research facility;
also available as calibration facility (Brown+2010, SPIE 7732, 77324Q).

Heidelberg Flash-EBIT / PolarX-EBIT at X-ray Light Sources

Resonant photo-excitation in an EBIT

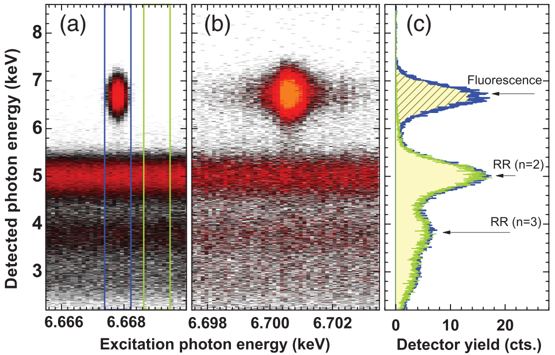
Rudolph+2013



EBIT breeds ions with $E_e <$ excitation threshold

Example: Fe Kα lines

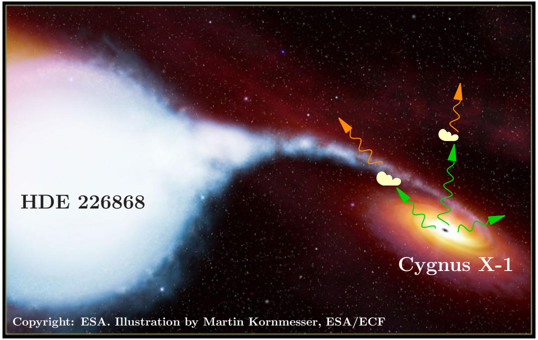
Rudolph+2013, PRL 111, 103002



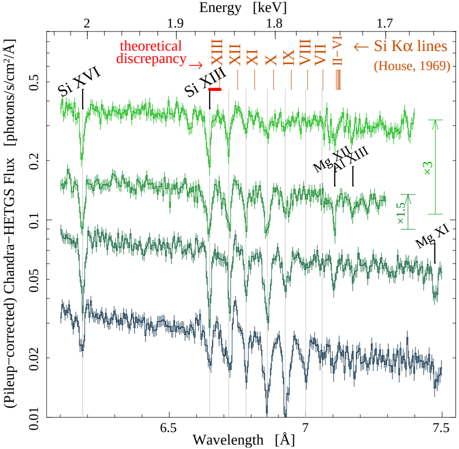
⇒ directly probe atomic structure (e.g., Bernitt+2012, Nature 492, 225)
⇒ Line energies with ∼ 70 meV accuracy (Rudolph+2013, PRL 111, 103002)
⇒ Lifetimes: natural line widths with 10–200 meV accuracy

K-shell transition energies in L-shell ions

Example:
Black-hole high-mass X-ray binary Cygnus X-1



Hanke+2009; Hell+2013; Miskovikova+2016; Hirsch+2019



Miskovicova+2010

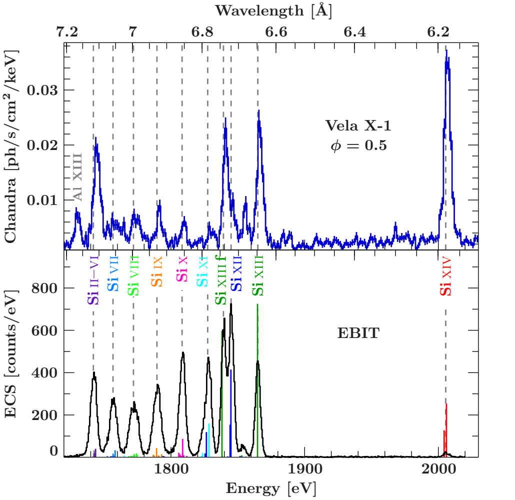
Problem:
- calculations of transition energies vary $\sim$ 2–5 eV
- uncertainty corresponds to several 100 km s^{-1} in Si

$\Rightarrow$ uncertainties on the order of expected Doppler shifts

K-shell transition energies in L-shell ions

Vela X-1 (Chandra-HETG) vs. EBIT-I/Calorimeter: Si

Hell+2016, ApJ 830, 26



K-shell transitions in L-shell ions:

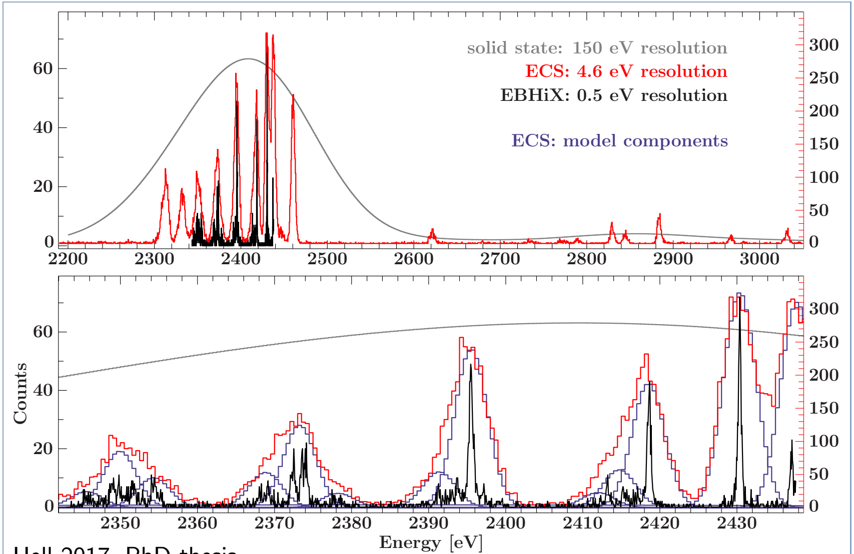
- used to be missing in databases
- seen in many places (HMXBs, AGN, etc)
- seen from Ne, Mg, Si, S

  (e.g., Watanabe+2006; Behar; Hanke+2009; Grinberg+2017)

EBIT-I measurement:

- Resolution: 4.6 eV
- Uncertainties (including systematic):
  < 0.5 eV (strong lines) –
  < 1 eV (weak lines)
  $\lesssim 100\,\mathrm{km\,s^{-1}}$
- comparison to FAC: good to $\sim$1 eV

Improve accuracy with crystal spectrometer: Sulfur Kα



Hell 2017, PhD thesis

Crystal data (EBHiX):

- resolution: $\sim 0.5\,\mathrm{eV}$
- accuracy: $< 0.2\,\mathrm{eV}$ ($< 30\,\mathrm{km\,s^{-1}}$)

Theory:

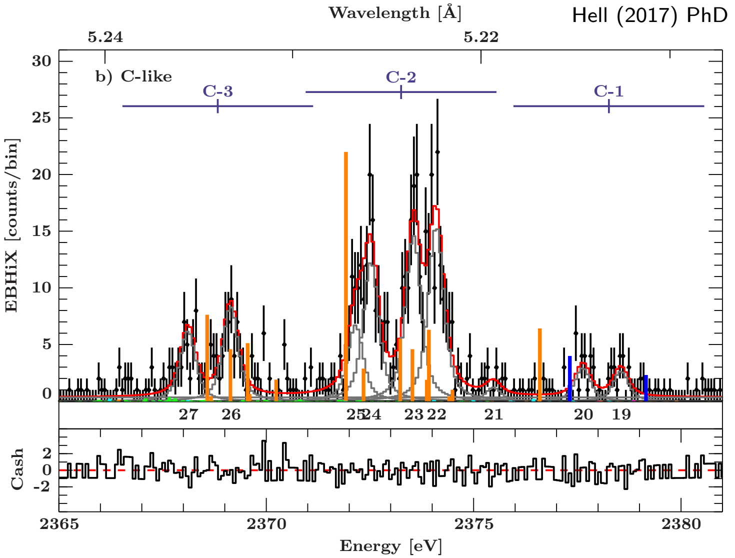
Better agreement for advanced calculations with MRMP

Beiersdorfer+2017, NIMB 408, 67

Good agreement with ECS measurement, but much more detail

Crystal spectrometer fit: $< 0.2\,$eV accuracy

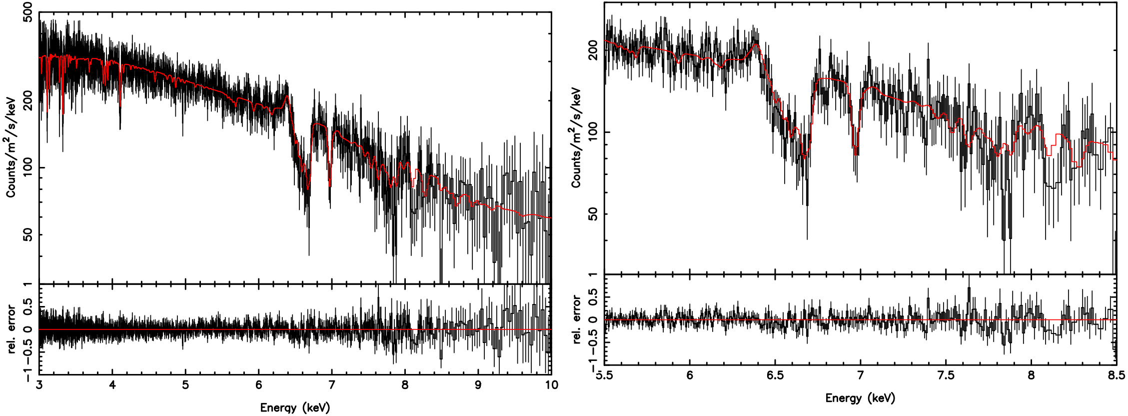
Detailed view of C-like S



Theory accuracy < spectral resolution complicates accurate line ID-ing

$n >= 3$ to 1 transitions in lower charge states

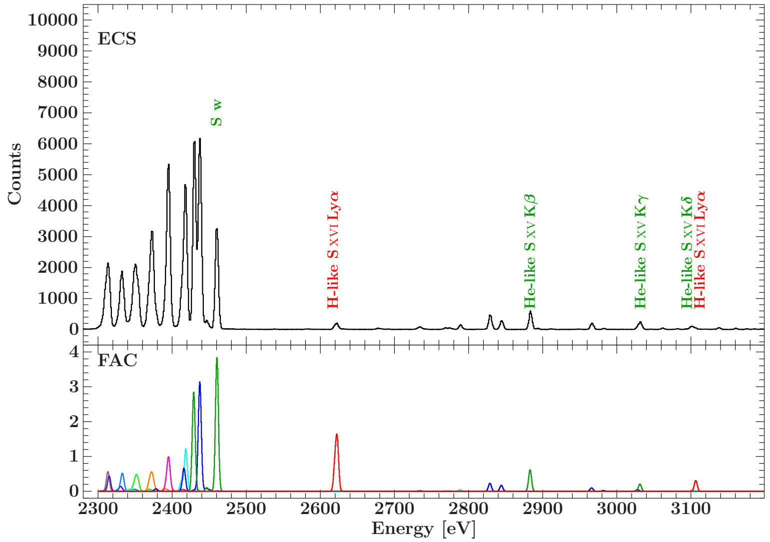
Chandra HETG spectrum of GRS1915+105 entering its obscured state



Miller et al. (2020) Apj 904, 30

Sulfur Kβ for L-shell ions

Measurement with ECS at LLNL SuperEBIT

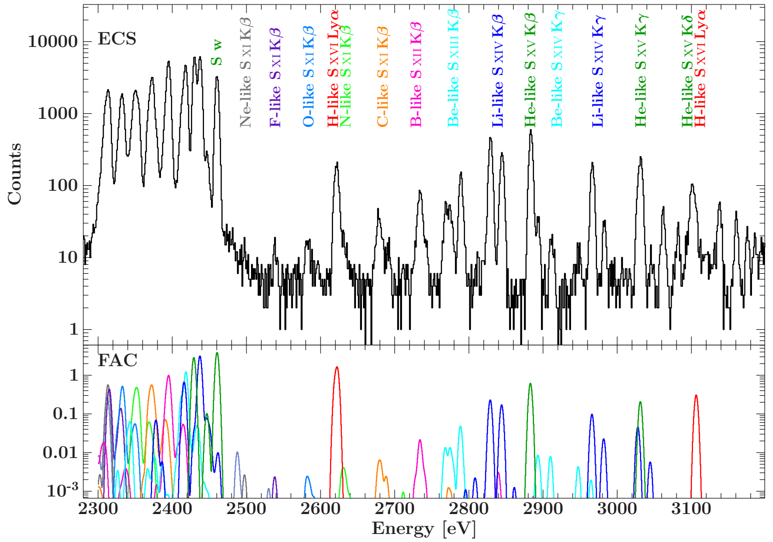


Rahin, Hell, et al. (2023, in prep)

K-shell transitions from $n \leq 3$ states would benefit from some improvements.

Sulfur Kβ for L-shell ions

Measurement with ECS at LLNL SuperEBIT



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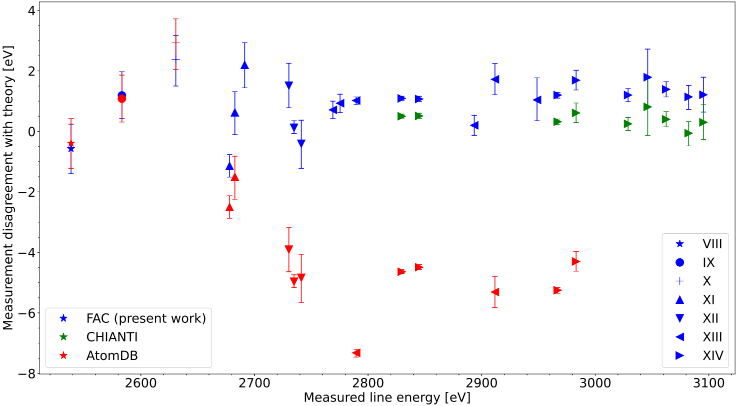
Sulfur Kβ for L-shell ions

Comparison to theory

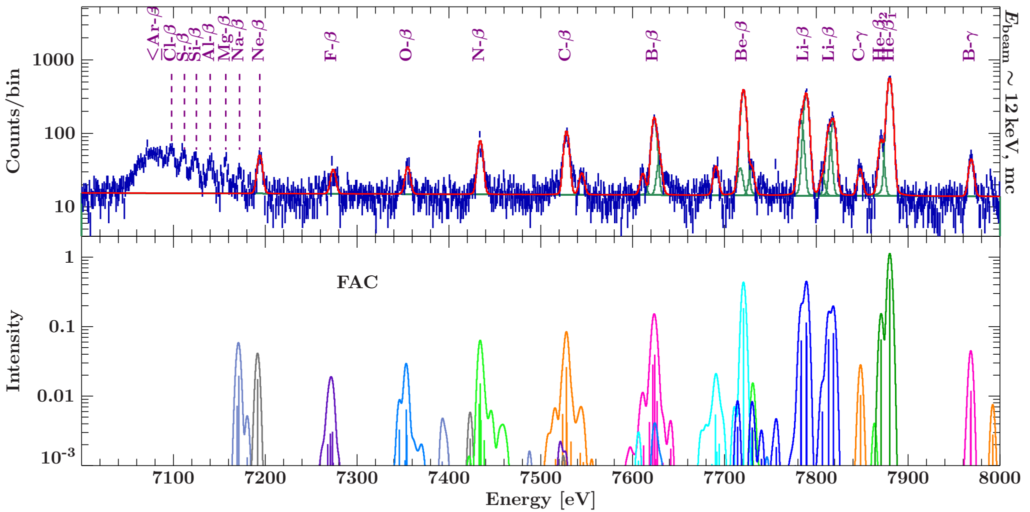


Rahin, Hell, et al. (2023, in prep)

K-shell transitions from $n \leq 3$ states would benefit from some improvements.

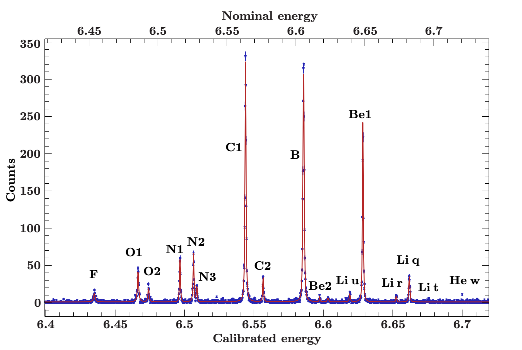
The Fe Kβ spectrum

Measurement with ECS at LLNL EBIT-I, compared to our FAC calculations

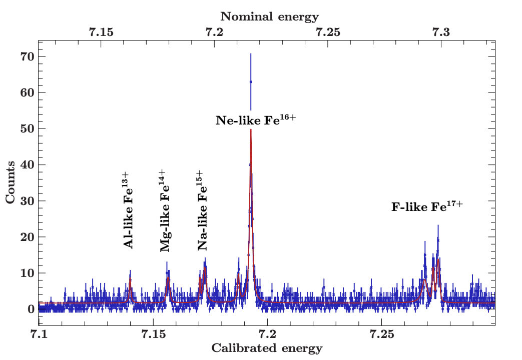


A more detailed view: Fe Kβ at Petra-III

Fe Kα: F- to Li-like



Fe Kβ: Al- to F-like



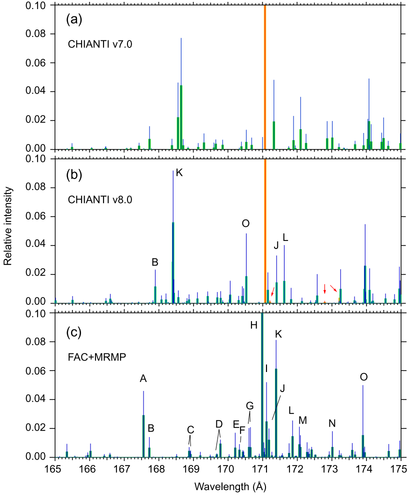
Stierhof, Hell, et al (2023, in prep), with MPIK Heidelberg, GSFC, Erlangen, LLNL

- resonance excitation with high-resolution photon beam
- disentangle line blends by selective charge state breeding
- Measurements for Fe^{9+} (Ar-like) to Fe^{23+} (Li-like)
- analysis in progress (lead: J. Stierhof)

EUV line surveys

Comparison of theory line lists: Fe IX

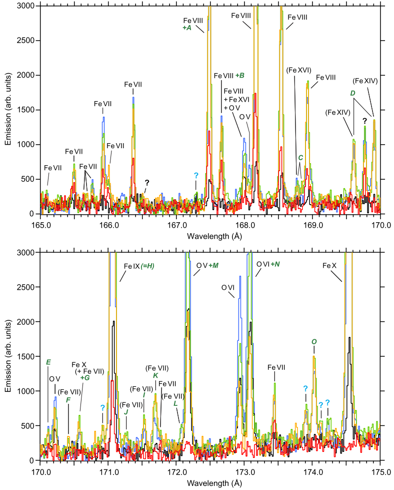
Beiersdorfer&Träbert (2018)



orange/red: lines considered verified

EBIT-I measurements

Beiersdorfer&Träbert (2018)



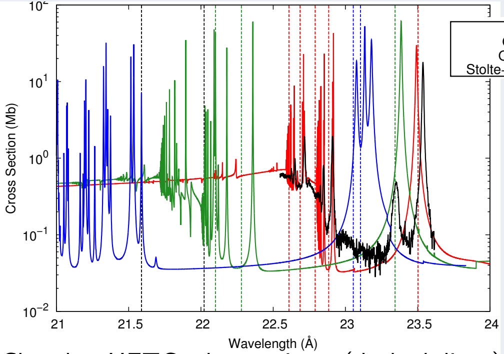
different colors at different beam energies, i.e., varying charge balance

Line content differs between database versions and different calculations. Laboratory benchmarks are needed.

Photoionization resonance energies

Lab-astro with Chandra-HETG

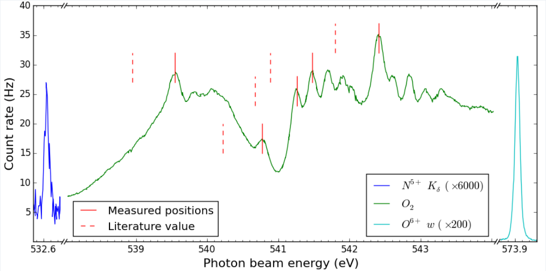
Gatuzz+2013, ApJ 768, 60; Garcia+2017, AIP CP 1811



Chandra HETG observations (dashed lines) disagree with resonance energies of theoretical photoionization cross sections of O ions and with lab measurements that were calibrated on O_2.

EBIT simulatenous with gas chambers at BESSY synchrotron

Leutenegger+2020, PRL, 125, 243001



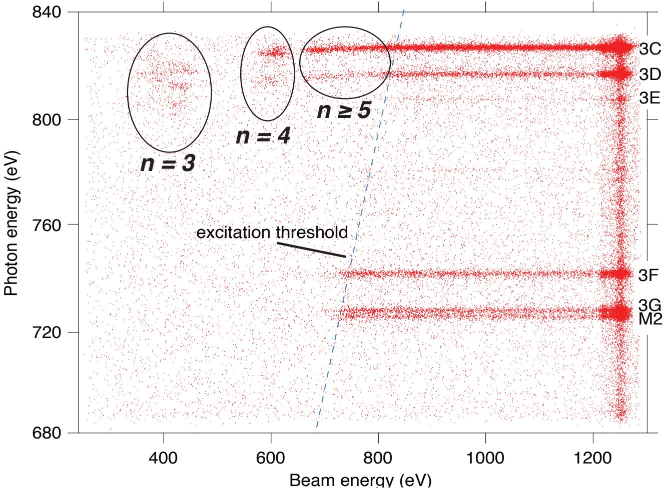
achieve 30 meV precision in calibrating the O_2 Rydberg spectrum against He-like N VI
'old' O_2 calibration standard is off by ∼500 meV

Measurement at BESSY resolves the problem identified with Chandra-HETG

T_e-dependent dielectronic satellites of Fe XVII

Spectral emission as function of electron energy

Beiersdorfer+2017, AIP CP 1811, 040001



Circles: satellites with spectator electrons in $n = 3, 4, \geqq 5$

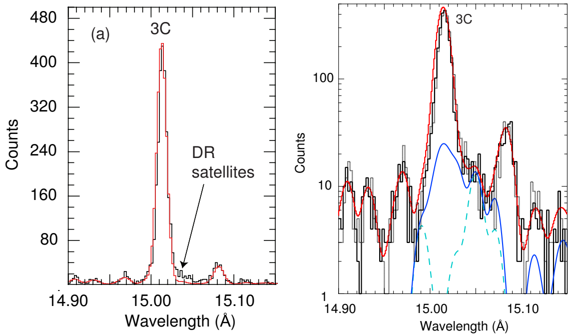
Linear sweeps of electron beam energy at EBIT-I. Spectra recorded with high-resolution crystal spectrometer
$\Rightarrow$ select line formation process, separate collisional excitation from dielectronic recombination

All DR satellites associated with 3C and 3D of Ne-like Fe XVII
(Beiersdorfer+2015, JPCS 583, 012022)

No DR satellites associated with 3F, 3G, or M2
(Beiersdorfer+2017, AIP CP 1811, 040001)

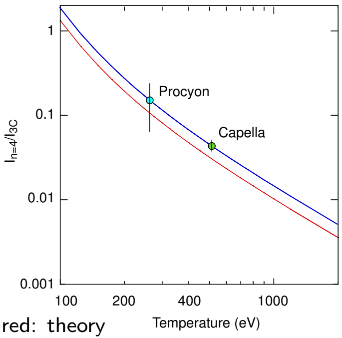
DR temperature diagnostic for stellar coronae

Chandra HEG spectra of Capella



Beiersdorfer+2018, ApJ 864, 24

Coronal temperatures of Procyon and Capella



red: theory
blue: scaled to EBIT-I results

Would be even better resolved with Arcus!

$n = 4$ DR satellite to 3C intensity ratio provides very accurate measure for coronal temperatures:
Procyon: 264^{+142}_{-51} eV (3 photons!) and Capella: 514^{+27}_{-25} eV
$\Rightarrow \sim 5\%$ uncertainty dominated by counting statistics

Method pioneers the possibility to infer temperature of stellar coronae from DR satellite lines.

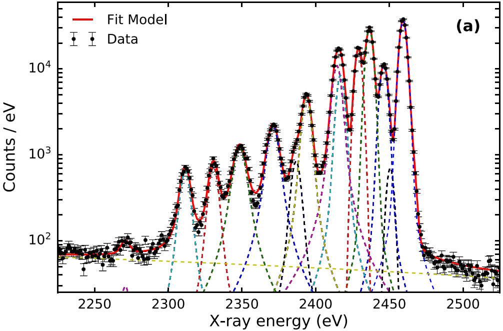
Line formation contributions: cross section measurements

Shah, Hell, et al. (2021), ApJ 914, 34

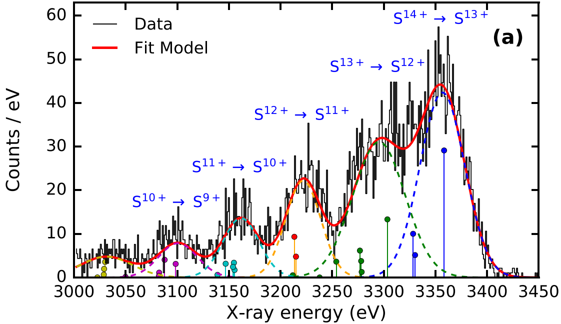
Collisional excitation cross sections: normalize CE to RR

Sulfur Kα measured with ECS @ LLNL EBIT-I:

Collisional excitation (CE):



Radiative recombination (RR):

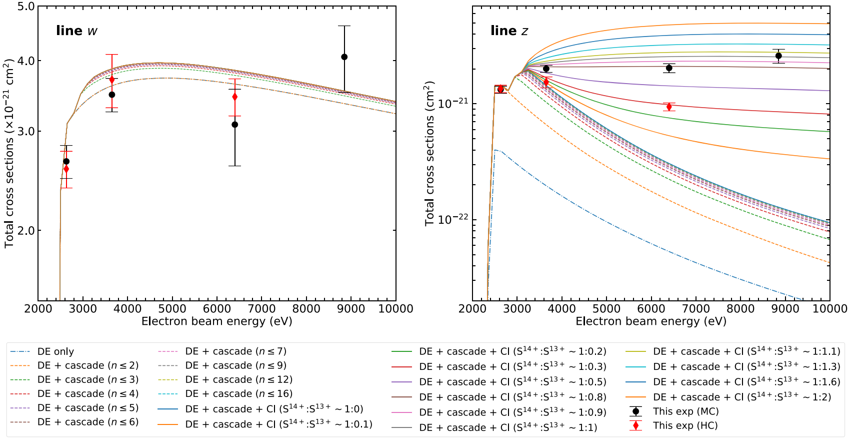


Cross section measurements at different charge balances allow probing contributions from collisional (inner-shell) ionization

Line formation contributions: cross section measurements

Shah, Hell, et al. (2021), ApJ 914, 34

S K cross sections at different charge balance



black:
Li- / He-like
$\sim 1/1$;

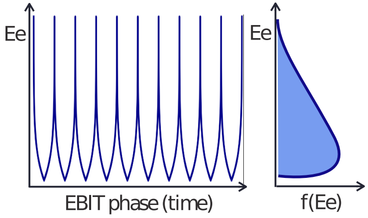
red:
He-like
dominant

Cross section measurements at different charge balances allow probing contributions from collisional (inner-shell) ionization

The EBIT Maxwellian simulator

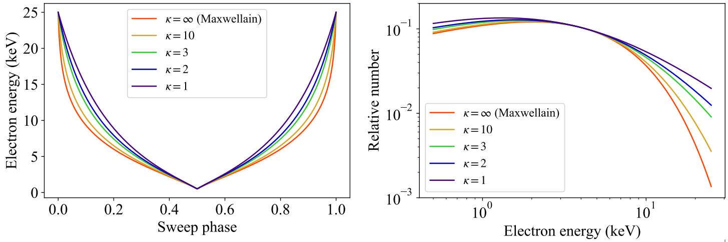
Time-averaged E_e distribution

Savin+2000, RSI 71, 3362



Non-maxwellian distributions: κ distribution

M. Sawada, priv.comm.



ionization timescales $n_e t$:

		SNR	EBIT
n_e	(cm^{-3})	~ 1	$\sim 10^{12}$
t	(s)	$\lesssim 10^{12}$	$\lesssim 1$
$n_e t$	$(\mathrm{s\,cm}^{-3})$	$\lesssim 10^{12}$	$\lesssim 10^{12}$

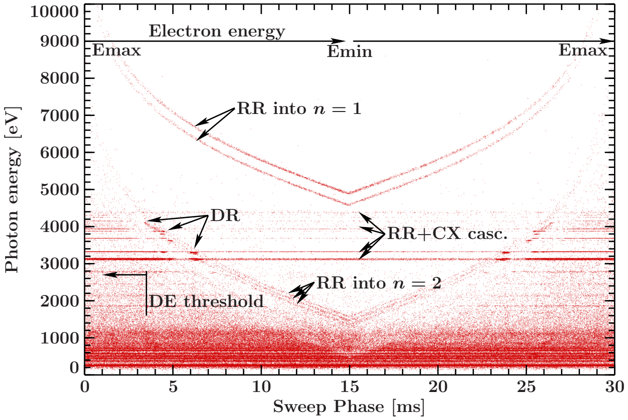
Electron-energy distributions can be simulated as a time-average by “sweeping” the EBIT electron beam energy

Ionization timescales in EBIT match those of SNR.

Disentangling spectral contributions

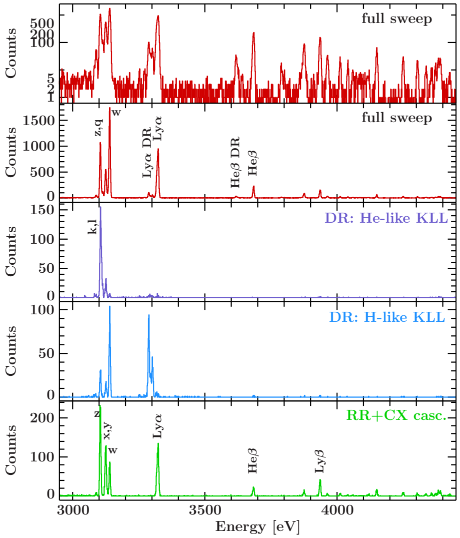
Hell, Sawada, et al

Sweep-phase resolved emission



Event mode allows us to also extract spectra from different sweep phases, and thus separate different emission processes

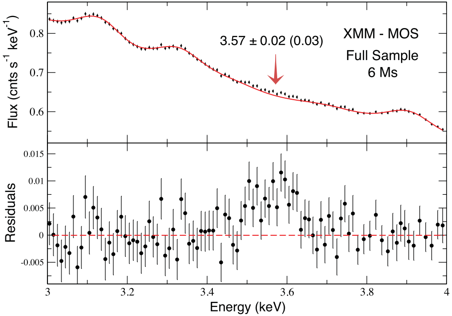
Spectra of select components



EBIT-I Maxwellian simulator benchmarks: the 3.5 keV line

Unidentified line in galaxy clusters

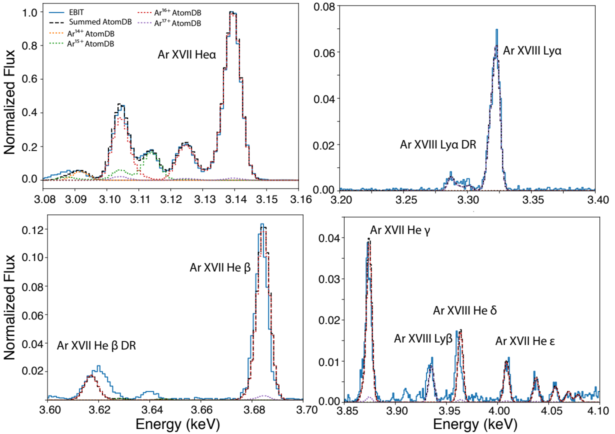
Bulbul+2014, ApJ 789, 13



- DR to non-DR parent flux ratio underpredictd by up to a factor 2.3, too small to explain 3.5 keV line
- Other possible explanations: charge exchange on S (Betancourt-Martinez+2014, PRA 90, 052723; Shah+2016, ApJ 833, 52)

EBIT-I Ar spectra at $kT_e \simeq 1.74$ keV

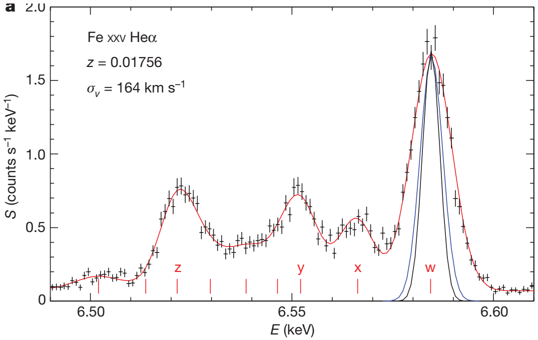
Bulbul+2018, ApJ 870, 21



Testing models against "known" laboratory spectra are important

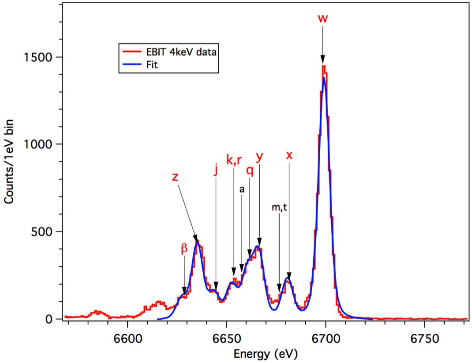
Calibrating SXS Perseus spectrum with EBIT-I Fe spectrum

Perseus spectrum with Hitomi-SXS



Hitomi Collaboration (2016), Nature 535, 117
Line centers from Beiersdorfer+1993, ApJ 409, 846

EBIT-I spectrum at $kT_e \sim 4\,\mathrm{keV}$



Leutenegger+2016, SPIE 9905, 99053U
Data from Gu+2012, CJP 90, 351

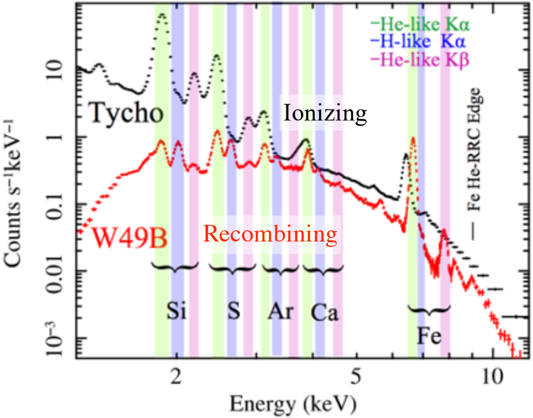
Hitomi-SXS was not fully in thermal equilibrium and calibrated yet during Perseus observation

An empirical model gained from an EBIT-I spectrum similar to Perseus together with knowledge from extensive ground calibration was used to correct the SXS differential gain shift.

Non-equilibrium plasma in supernova remnants

Ionizing vs Recombining plasma

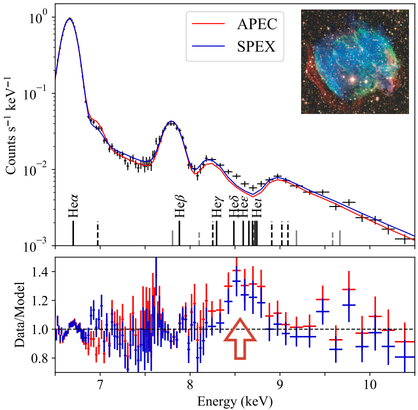
Ozawa+2010, PhD thesis



Ionizing and recombining plasmas have significantly different spectra

Recombining Plasma in W49B

data Ozawa+2009, reanalyzed by M.Sawada

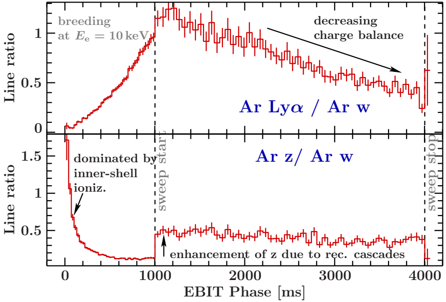


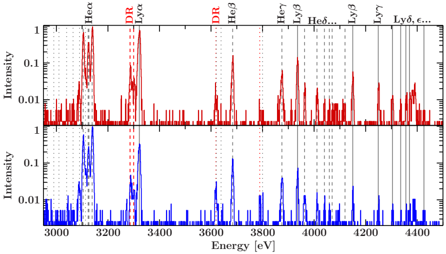
NEI models under-predict flux of high-*n* He-series

Non-equilibrium plasmas at EBIT-I

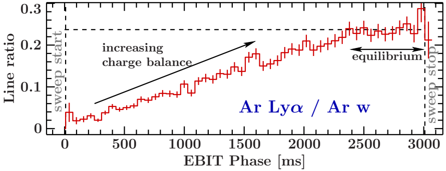
Hell, Sawada, et al.

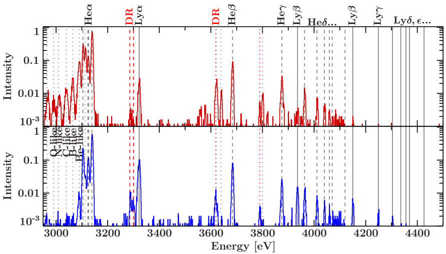
Recombining Plasma





Ionizing Plasma





Recombining:

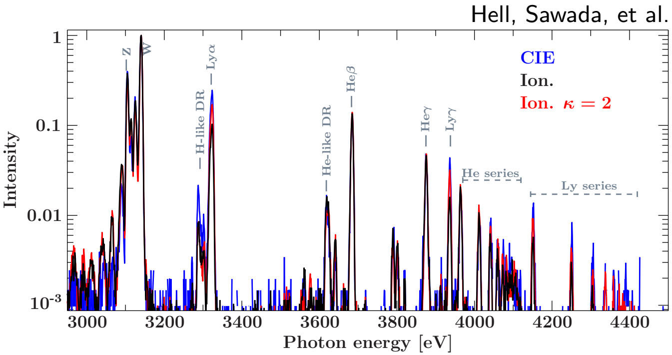
First breed high charge balance, then switch to sweeps at low kT_e ⇒ charge balance decreases

Ionizing:

Start sweeping at high kT_e immediately ⇒ charge balance increases

κ-distribution at EBIT-I: Ar spectra

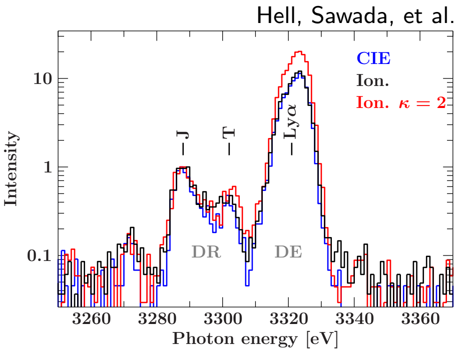
Normalized to Ar w



Charge balance:

- ionizing lower than CIE
- increased by high-energy tail (κ)

Normalized to Lyα DR



DR line ratio:

- unaffected by charge balance
- DE boosted by high-energy tail

Maxwellian simulator allows studying the impact of NEI plasma conditions on line ratios

Conclusions & Outlook

- High-resolution spectroscopy with the Chandra / XMM gratings already faces challenges with atomic data / plasma models
- A lot of work remains to be done (measurements, calculations, databases, models) to bring the atomic reference data into shape for XRISM, Athena, Arcus, LEM, . . .
- next generation X-ray gratings has already demonstrated far higher resolution and efficiency than Chandra / XMM
- Many of the tools are available (both theory and experiments), but need to be used
- Models need well understood test data to be tested on (see, e.g., the Leiden test suite). Some of this data can be from laboratory measurements.
- Challenges exist beyond the shown examples: e.g., charge exchange (CX), dust (fine structure at absorption edges; fluorescence)
- Explore synergies with other fields: solar physics, laser-produced plasmas, fusion, etc, use atomic data and plasma models too.

Talk to us – we are here to help

If you have a problem (e.g., missing data, mis-matching models, new features, insufficient accuracy, . . .) or questions / interests, come talk to the laboratory astrophysics community.