Laboratory measurements as calibration benchmarks for astrophysical X-ray spectroscopy

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May 23, 2022

Thanks to Many other people from many institutions
NASA/GSFC, MPIK, Stanford, SAO…others

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC
LLNL-PRES-835633

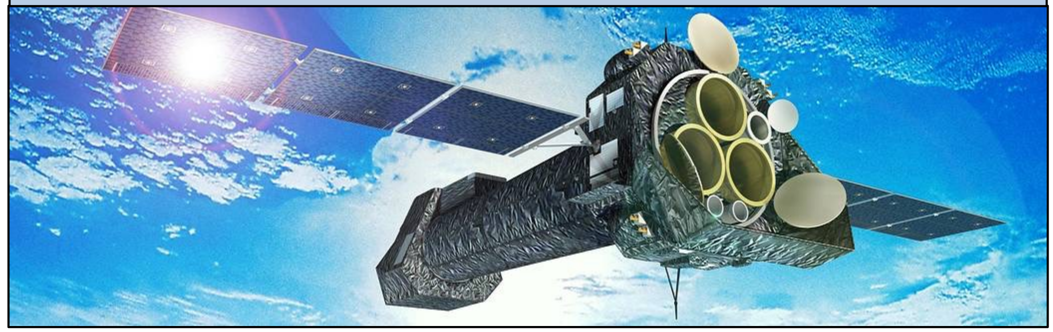
Background/History

- **Laboratory astrophysics:** Began in ~ 1993 at LLNL when S. Kahn realized the Fe L-shell was complex even if resolved by *XMM-Newton's* RGS. Same issue would arise for *Chandra*.

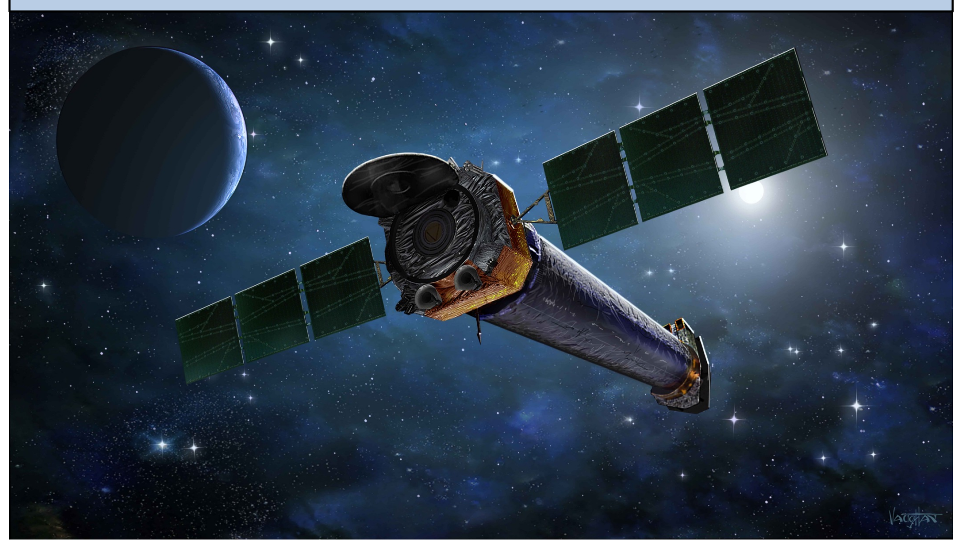
- Contacted P. Beiersdorfer to measure the wavelengths and work with D. Liedahl and M.F. Gu to identify the lines.

- Lines from Fe L-shell were measured between 1993 and 2007 (Brown et al 1998, 2002, Chen et. al, 2007).

XMM-Newton: Launch Dec 1999



Chandra: Launch July 1999



High resolution instruments in orbit helped uncover the need for laboratory astrophysics and measurements are being conducted at multiple facilities worldwide.

Fe L-shell Wavelengths

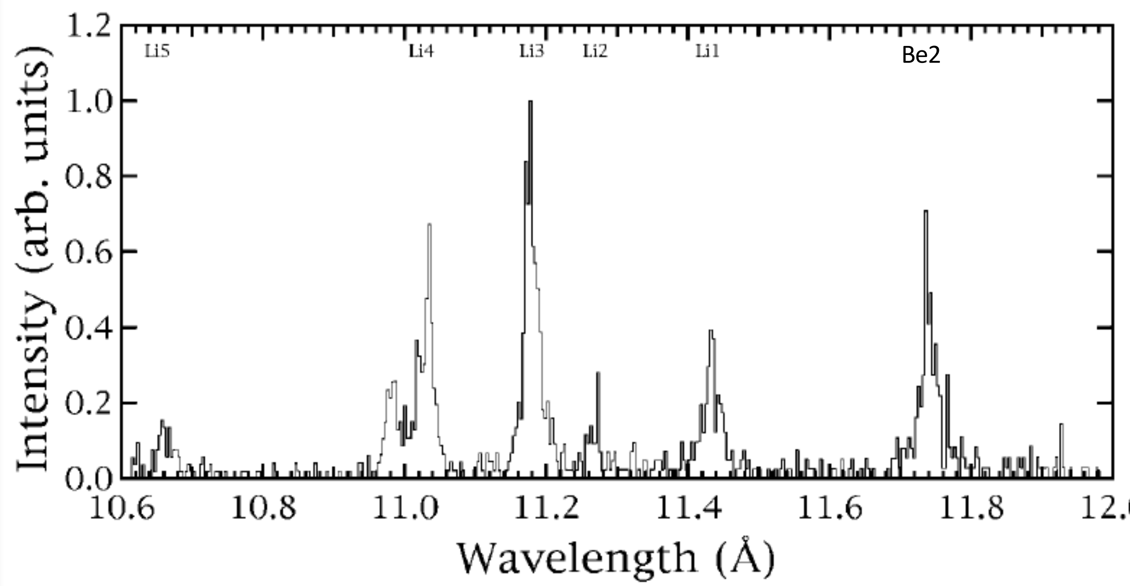
- Measurements of X-ray emission from Fe L-shell lines:
  Brown et al 1998: Fe XVII
  Brown et al 2002: Fe XVIII – Fe XXIV
  Chen et al 2007 : Higher-n Fe

- Initial results used HULLAC for identification. M. F. Gu then built the Flexible Atomic Code.

- Wavelengths accurate to ~ 5 mÅ

- K-shell lines from He-like and H-like O, F, & Ne were used for calibration. Calculated wavelengths from Drake (1988), Garcia & Mack (1965).

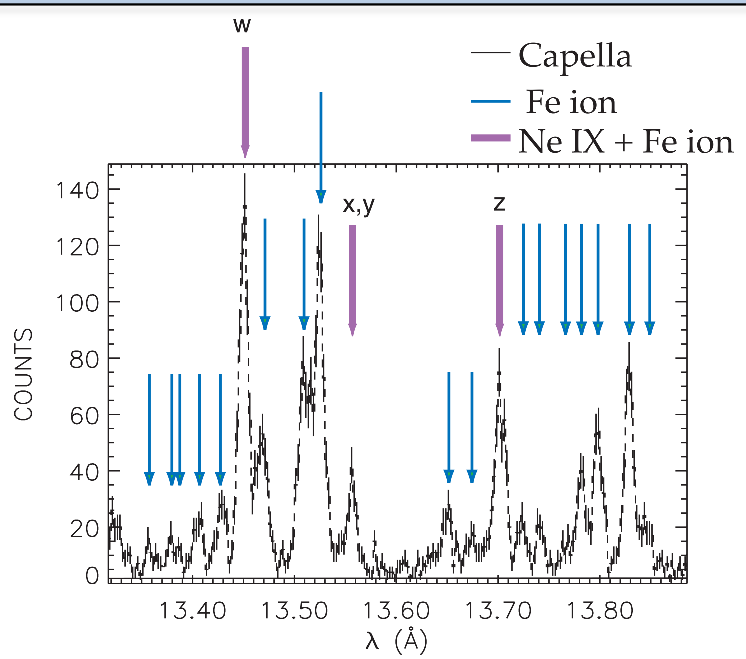
Li-like Fe XXIV spectrum measured at LLNL EBIT-I



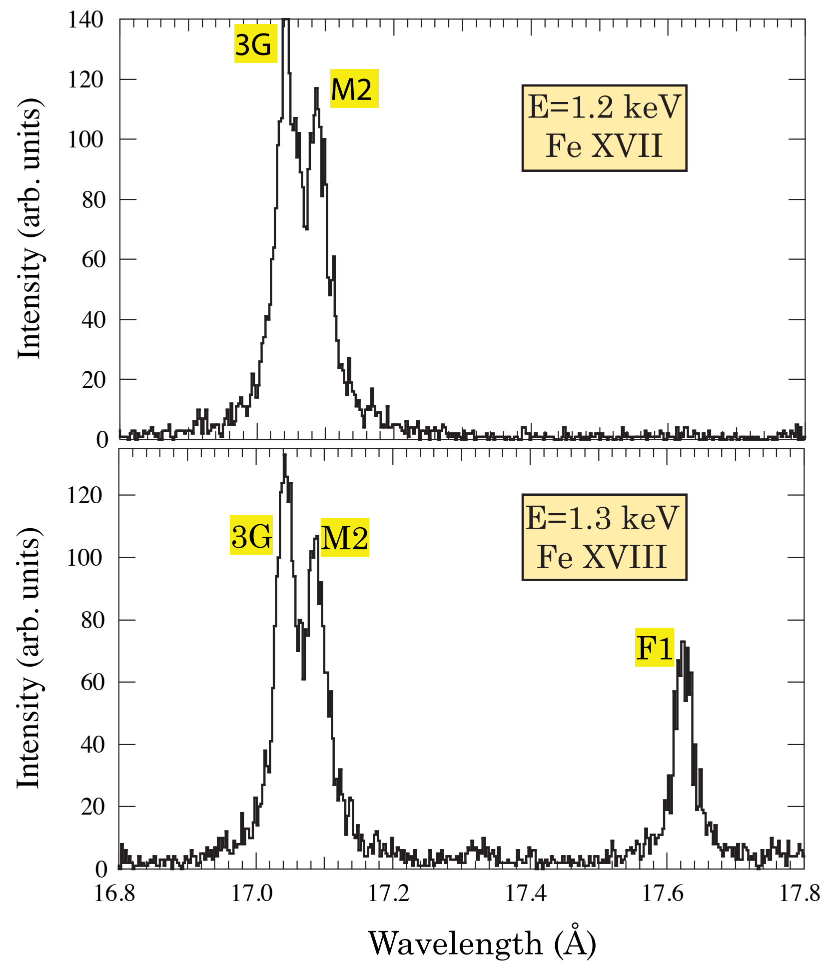
Fe L-shell Wavelengths

- Results greatly improved modeling of HETG and RGS spectra.
- Able to positively ID previously mis-identified, i.e., the F1 line (Drake et al., ApJ , 1999).
- Demonstrated importance for K-shell diagnostics, i.e., must be aware of blends.

Capella spectrum near He-like Ne IX



Mono-energetic electron beam energy allows positive ID with charge state

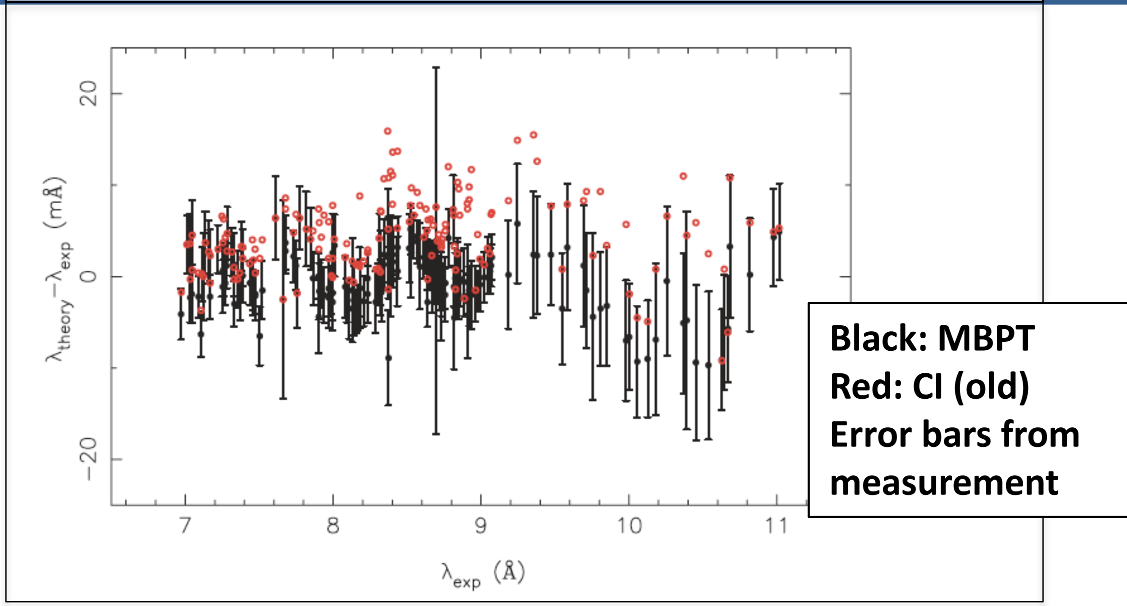


Measurements help to put analysis of spectra measured with *Chandra* and *XMM-Newton* on sound footing

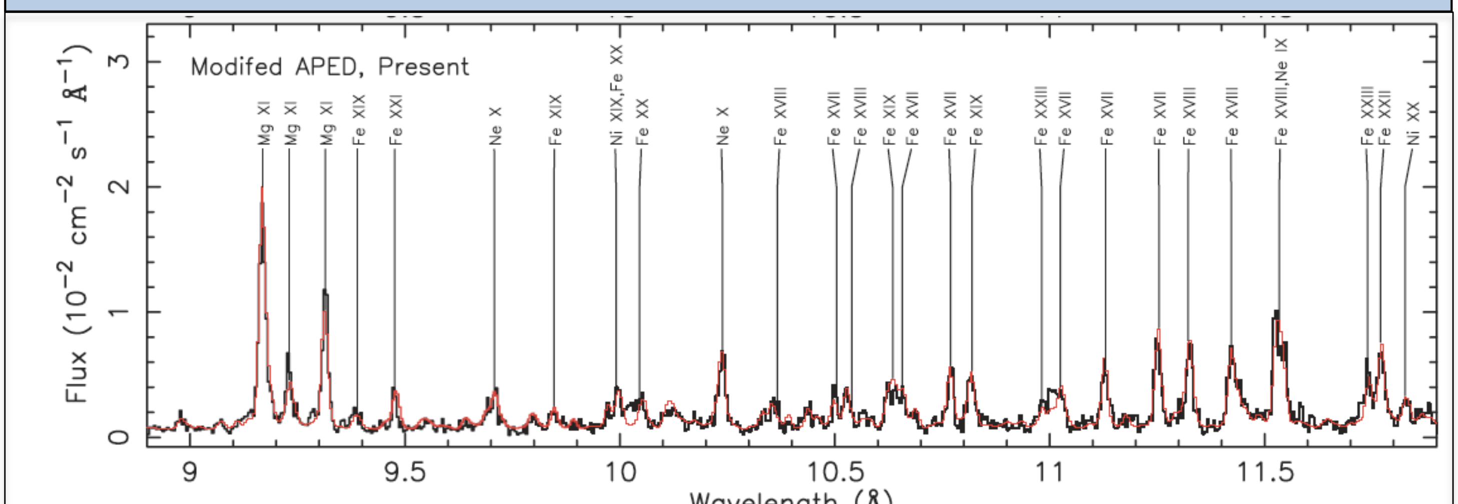
Benchmarking Models

- In parallel to the wavelength measurements, M. F. Gu built the Flexible Atomic Code (FAC).
- M. Gu also developed a MBPT approach to calculating wavelengths. (available as part of FAC).
- Benchmarked using the LLNL EBIT results.
- Available as Modified APED table (MAPED).
- Improved fit to Capella

M. Gu (ApJS 2007) MBPT results of compared to lab measurement



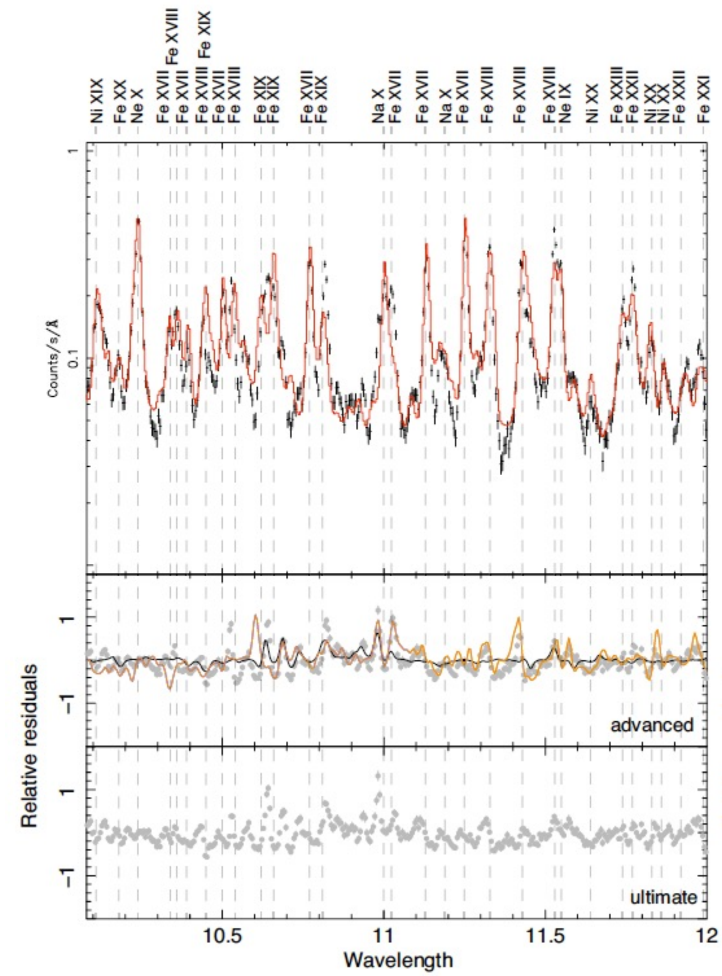
MAPED fit to Capella



More recent study of Fe L-Shell models

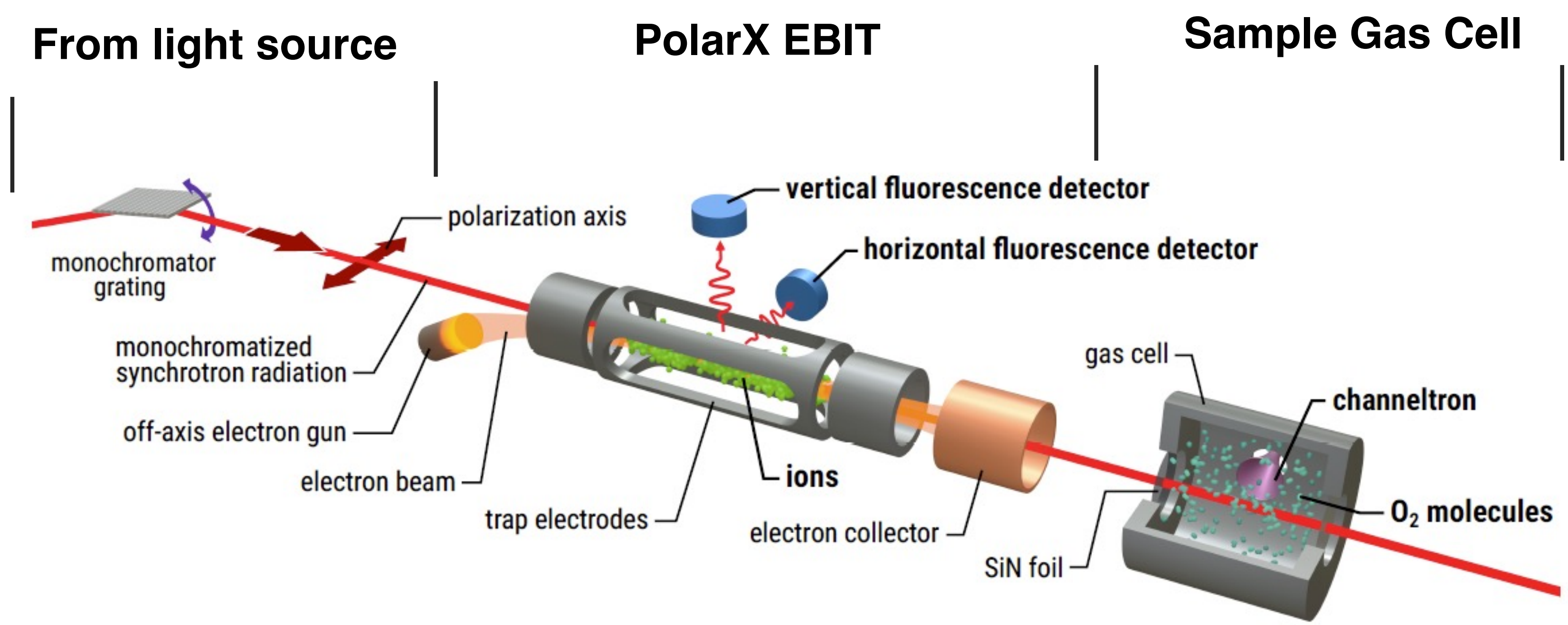
- Recently (since Hitomi), more modeling of the Fe L-shell work has been completed.
- *L.* Gu et al. (A&A 2020), have modeled the Capella spectrum and completed an extensive analysis of Fe data quality.
- Used EBIT data from LLNL and Heidelberg groups for comparison.
- Advanced model includes EBIT data
- “Ultimate” model includes corrected wavelengths from other codes.
- Requests more Lab Astro.

Sample of L. Gu (A&A, 2020) SPEX fit to Capella



Continued focus on Fe L-shell helps prepare for future high-resolution missions

Evolution of wavelength standards: EBITs and HCIs at advanced light sources

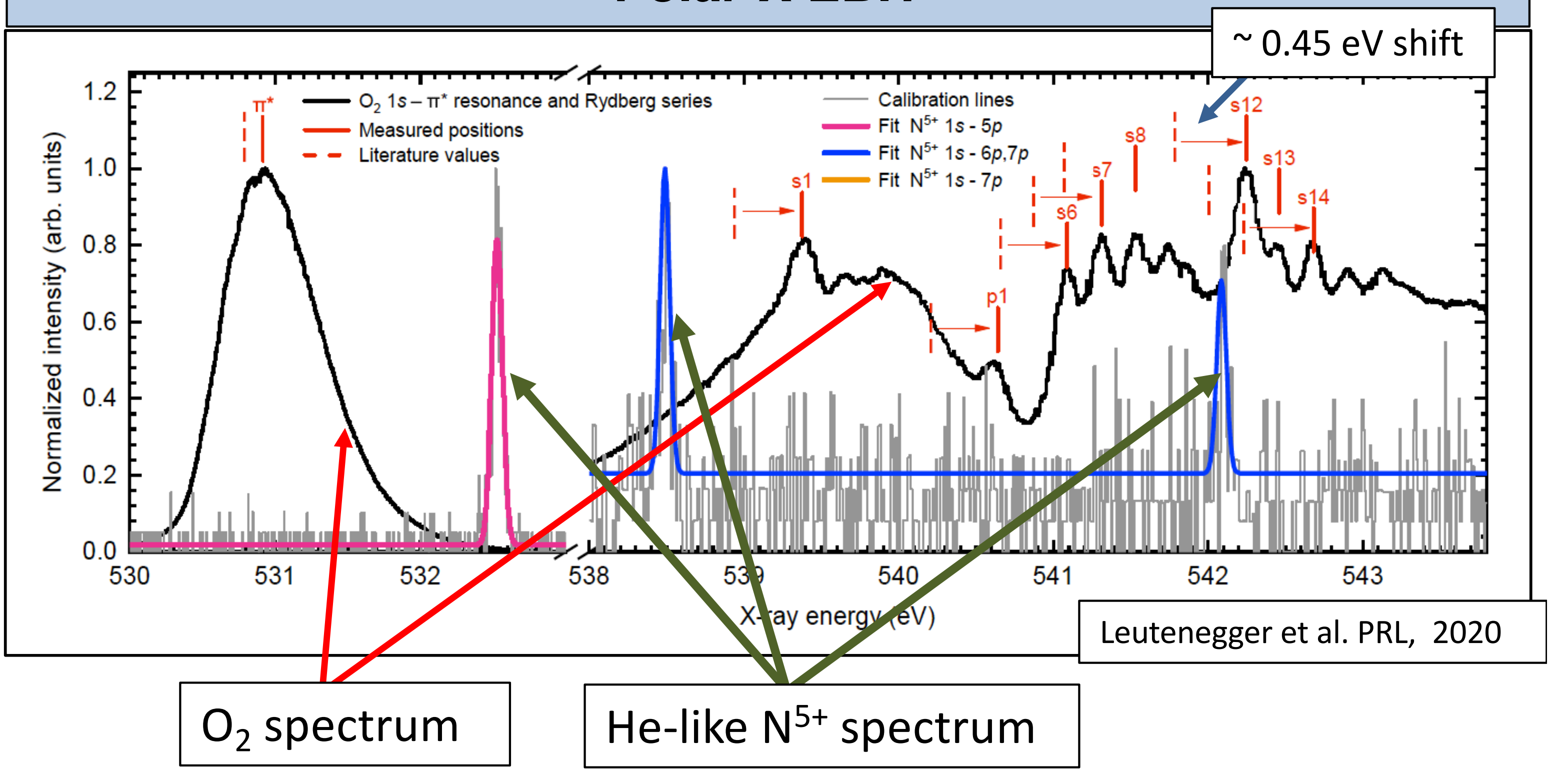


EBITs at advanced light sources enable high accuracy measurements of transition energies

Example Results: Recalibrate molecular and atomic oxygen

- Wavelength of atomic O absorption measured by *Chandra & XMM-Newton* in *ISM* did not agree with lab measurement.
- Old lab measurement calibrated using O_2 absorption based on EELS measurements.
- Using Polar-X EBIT at BESSY-II, the O_2 spectrum was recalibrated against He-line N^{5+} line emission.

O_2 and He-like N^{5+} spectra measured at BESSY-II using Polar-X EBIT



New measurement Polar-X EBIT at BESSY-II update the O_2 standard and bring the O absorption feature into (near) agreement with theory and lab measurement.

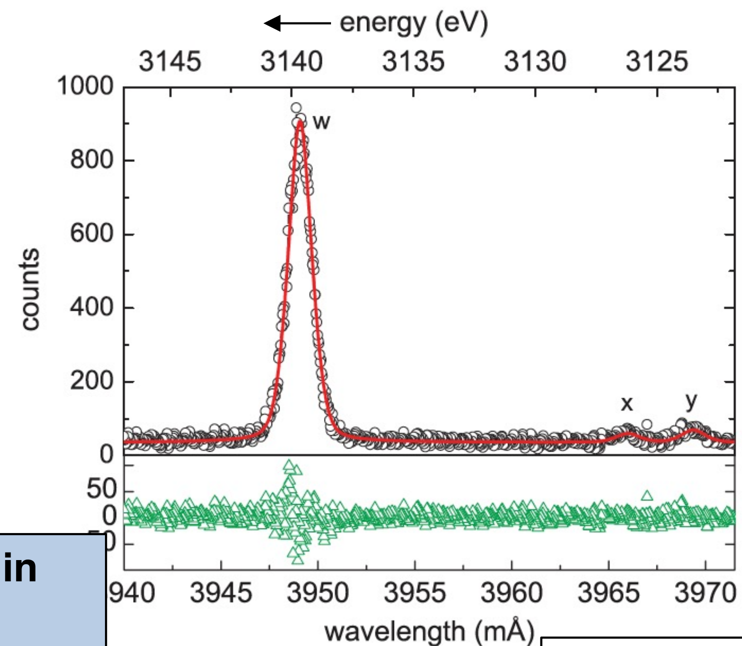
K-shell standards

- K-shell emission from helium-like and hydrogenic ions are the standard reference lines for energy-scale calibration for ground-based experiments and X-ray observatories.
- Early measurements were conducted using beam foil techniques, laser experiments, vacuum spark devices, or measured from tokamaks.
- In the late 1980s and early 1990s, EBITs were used as the new standard source for generating highly charged ions and measuring emission wavelengths.
- More recently, using EBITs at advanced light sources.
- He-like systems have been measured absolutely or against H-like systems.
- H-like systems have been measured absolutely.

K-shell measurements

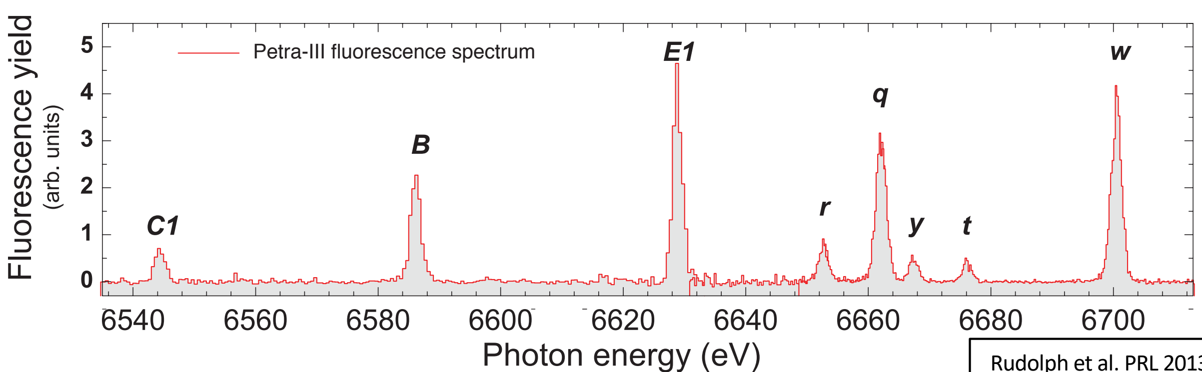
- Most He-like systems have been measured relative to H-like transition energies.
- Some absolute measurements have been made to high accuracy, e.g.:
  - Ar^{16+} :Kubicek et al., 2012 (MPIK-Heidelberg EBIT) with accuracy of 5 meV.
  - Ar^{16+} :Machado et al., 2018 (NIST ECR) with accuracy of 8 meV (agrees with Kubicek.)
  - Fe^{24+} : Rudolph et al., PRL (2013) w/ accuracy of 70 meV

MPIK EBIT absolute wavelength measurement of He-like Ar^{16+}



Kubicek et al. RSI 2012

Absolute wavelength measurements of K-shell transitions in highly charged Fe using FLASH-EBIT at Petra-III

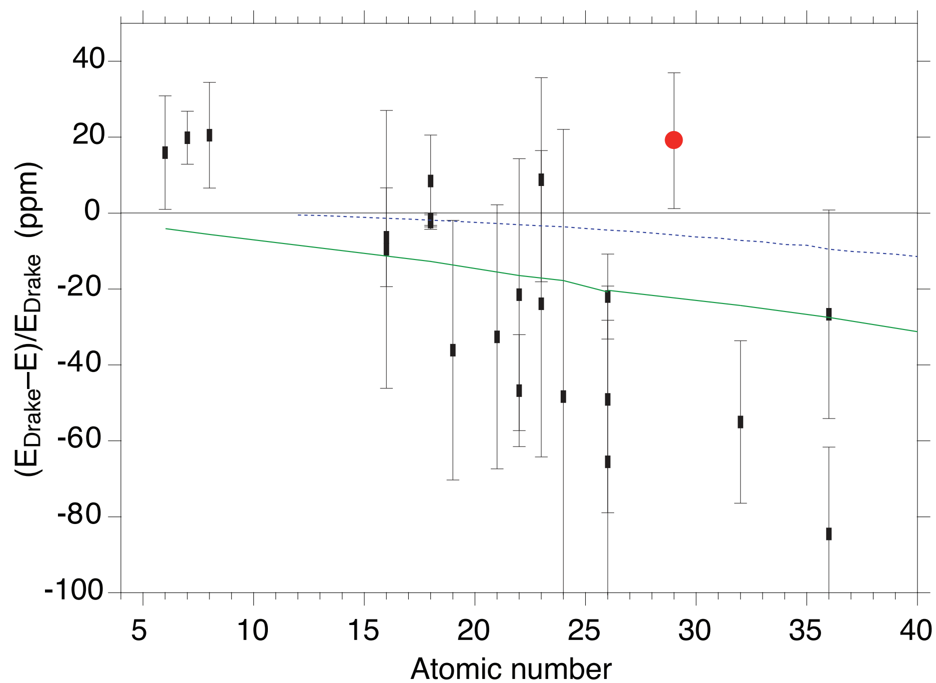


Rudolph et al. PRL 2013

K-shell measurements: He-like Systems

- He-like line lines w is on good footing for most measurements.
- Solid Green : Cheng et al., PRA (1994)
  Dashed Blue: Artemyev et al., PRA (2005)
  Reference: Drake, Can. J. Phys. (1988).

He-like line w versus Z compared to theory



Beiersdorfer et al. PRA 2015

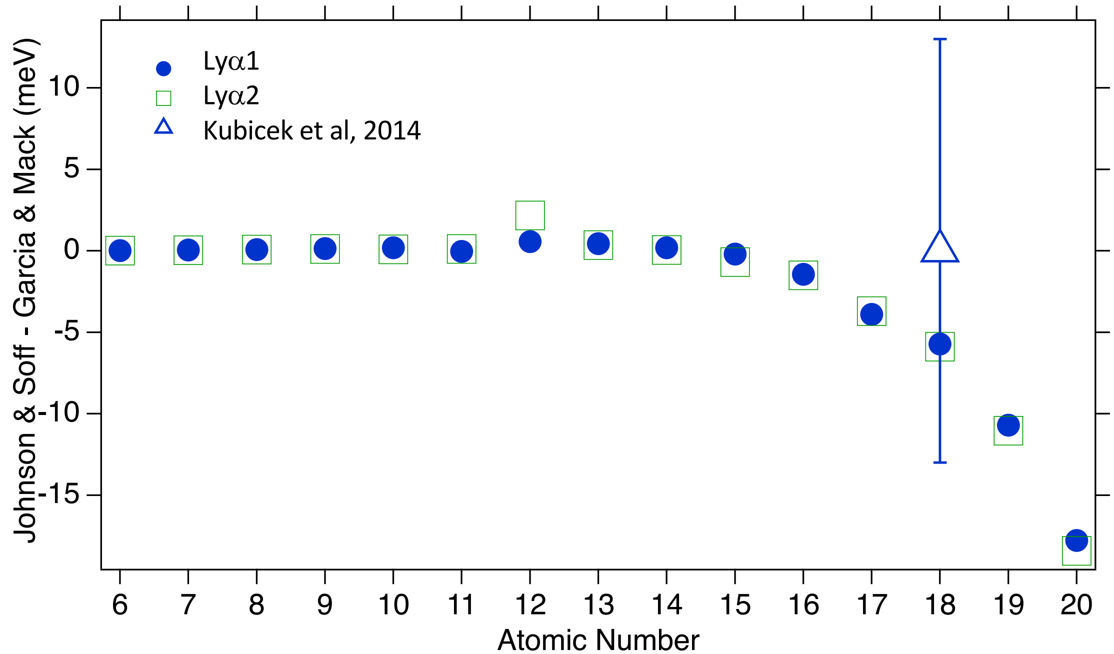
K-shell measurements: H-like lines

- Transitions of H-like K-shell emission is usually taken from:
  - Garcia & Mack, JOSA (1965) (Z = 1 to 20)
  - John & Soff, ADNDT (1985) (Z = 1 to 100)

- Essentially all measurements agree with Johnson & Soff results within error.

- Calculations of Johnson & Soff are the regularly accepted standard.

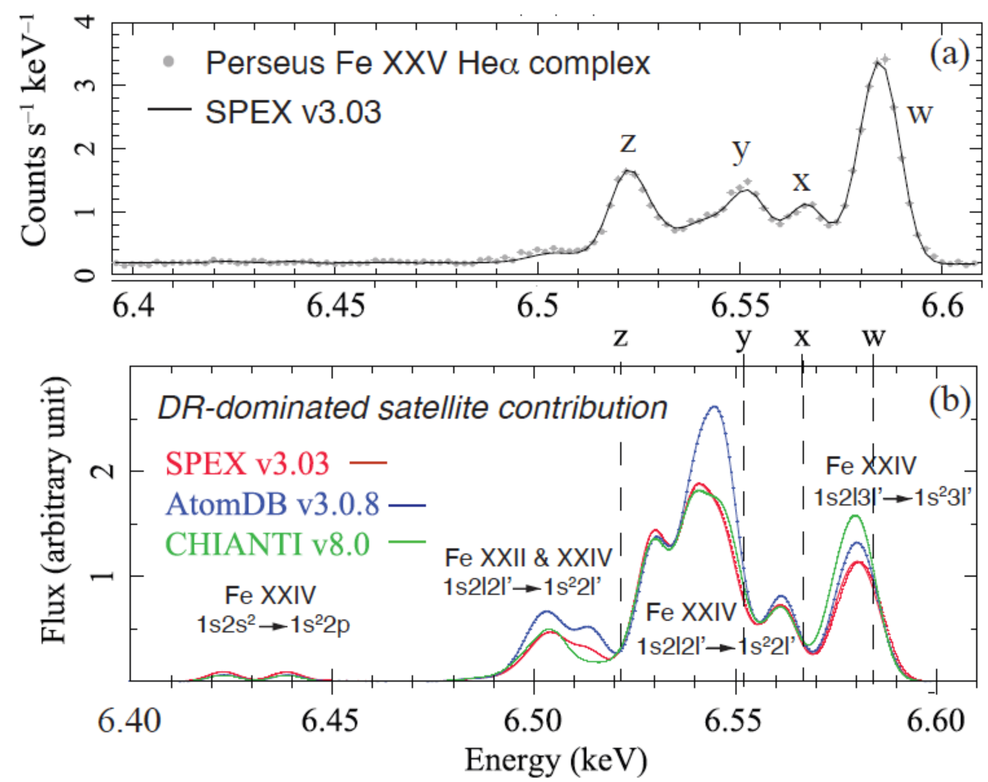
Compare J & S and G & M and MPIK EBIT measurement for Lyα1 and Lyα2



K-shell measurements: Emission energies of DR satellites

- Positions of resonance lines are not the only lines that are important, satellite lines are also important.
- Satellite lines and higher-n lines are not as well tested, although some measurements exist, for example Beiersdorfer et al., (1993).
- Some satellite lines are not resolvable spectroscopically.
- Can be resolved by sweeping beam in an EBIT.

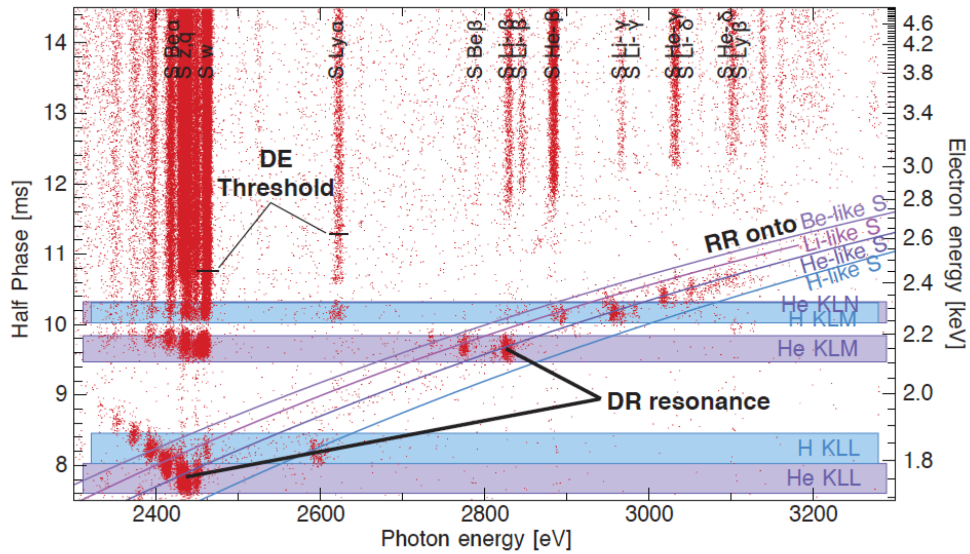
Perseus spectrum measured with Hitomi's SXS with theoretical satellite contribution



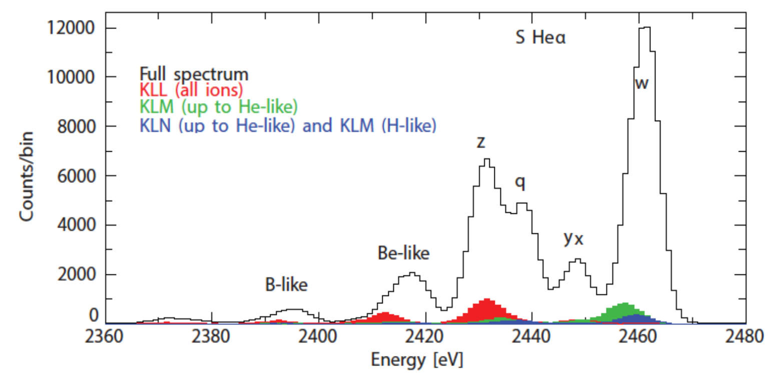
Hitomi Collaboration 2018 PASJ

K-shell measurements: Emission energies of DR satellites

Electron Beam energy versus Photon emission energy for Maxwellian sweep at LLNL's EBIT-I



Corresponding sulfur Heα spectrum with measured DR contribution for kT = 1.1 keV



- Using broad band calorimeter, we can measure the photon emission as a function of electron beam energy.

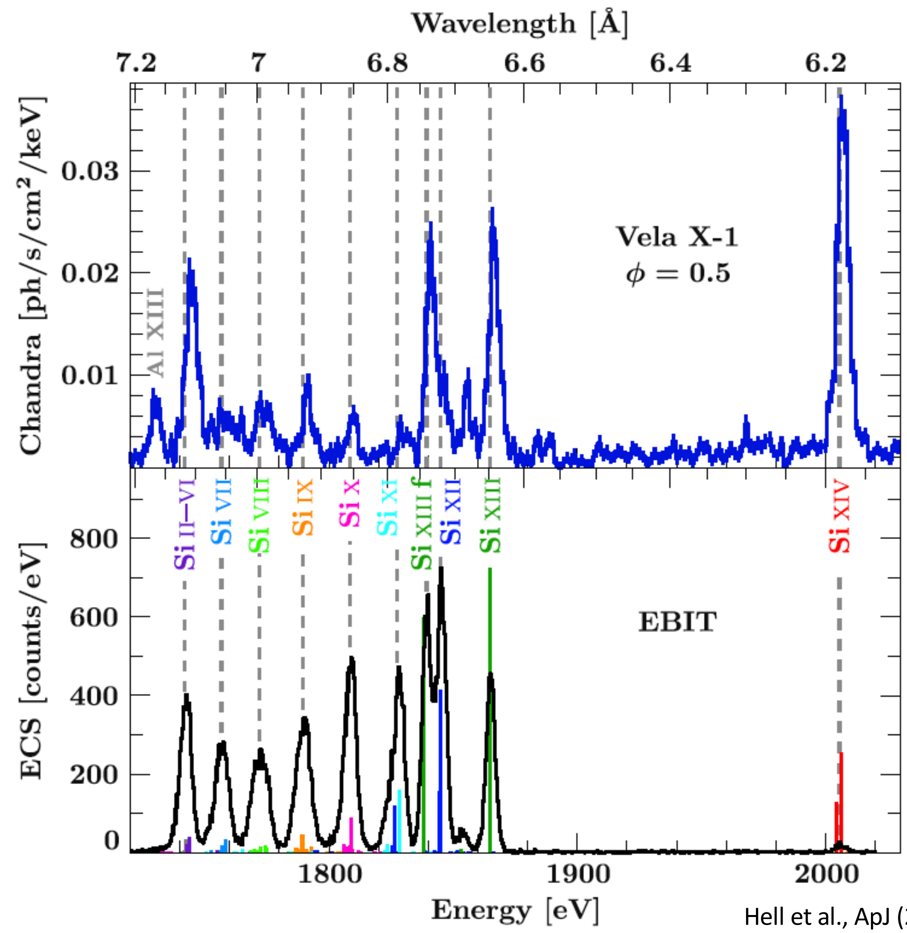
- The photon energy of the DR satellite lines can be resolved by sweeping the beam.

- EBIT measurements where of DR the electron beam is swept across the resonances have also been completed, for example Beiersdorfer, et al., (2015), and Shah et al., ApJ (2019).

Wavelengths of k-shell transitions in L-shell ions

- Transition energies of innershell transitions are more uncertain and less well studied.
- Can be measured using an EBIT alone or coupled to light sources.
- Innershell lines from more complex M-shell ions have also been measured at both EBIT and using EBITs at advanced light sources.
- Measurements have, for example, helped better understand physics of ``onion”-like structure in clumps around HMXBs.

Silicon K-shell spectrum measured at EBIT-I compared to *Chandra* spectrum from Vela X-1

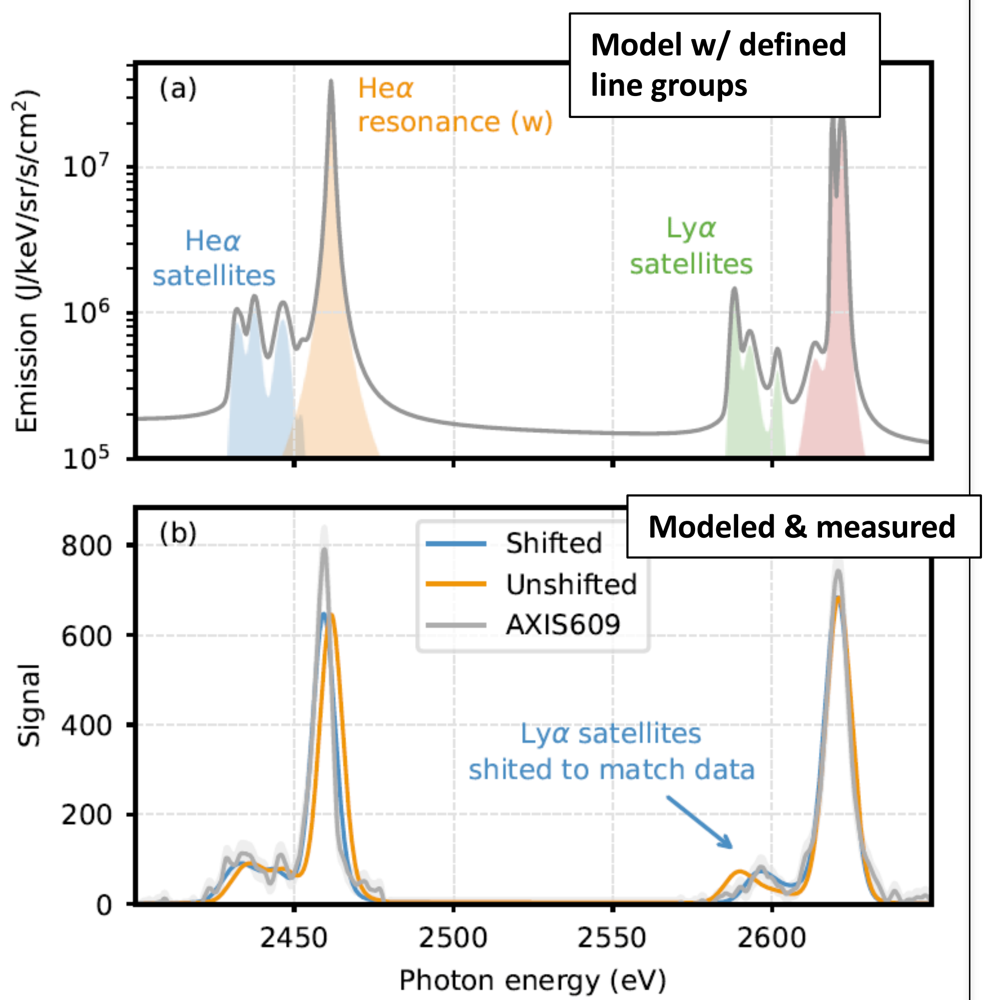


Hell et al., ApJ (2016)

Treating uncertainties in wavelengths

- Uncertainties in wavelengths have been incorporated into APED (see for example, Heuer et al., ApJ 2021).
- Allow lines to move within uncertainty
- One method defines line groups and allows their position to move.
- Can allow for small errors in instrument calibration or model so they do not affect the source physics result.

Modeled and measured He- and H-like sulfur spectra



MacDonald et al., HTPD (2022)

Summary

- Transition wavelengths are important for gleaning the most out of high-resolution spectra.

- Wavelengths of strong Fe L-shell transitions are on sound footing, for now.

- He-like and H-like reference energies are well tested at the meV level.
  Is this good enough?

- More work may be needed for transition energies of innershell transitions, such as K-shell transitions in L-shell ions, and M-shell transitions in L-shell ions.

- Including uncertainties in spectral modeling packages is necesssary to understand limits of atomic data and help uncover where more laboratory data is needed.

- Although He-like and H-like lines are the best references, all the known wavelengths should be used when available to constrain gain scales.

Thank You!

Lawrence Livermore National Laboratory