Laboratory Astrophysics Needs for X-ray Calorimeter Observatories

Activity Consideration Areas: Laboratory Astrophysics, X-ray Astrophysics

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1. Key Science Goals and Objectives

Microcalorimeter spectrographs will revolutionize X-ray spectroscopy. In contrast to X-ray grating spectrometers, whose resolving power is characterized by wavelength (λ/Δλ), microcalorimeters detect photons with fixed energy resolution (ΔE). The *Resolve* calorimeter on board the NASA/JAXA X-ray Imaging and Spectroscopy Mission (XRISM, Tashiro et al. 2018), which is scheduled for launch in early 2022, will have ΔE≈5 eV. This corresponds to a spectral resolving power E/ΔE≈1300 at the important Fe Kα 6.4 keV line, whereas the highest resolution *Chandra* grating has a resolving power λ/Δλ≈150 at the same line[1]. Hence, **XRISM will often be the first instrument to resolve E>2 keV line profiles in many astronomical systems**. XRISM will be followed by the much more sensitive, higher resolution (ΔE<2.5 eV) Advanced Telescope for High Energy Astrophysics (Athena, Barcons et al. 2017) in 2031.

Studies enabled by microcalorimeters include, but are not limited to, characterizing the state of hot gas in galaxy clusters through its turbulent and bulk velocities, determining the impact of accretion disk winds from compact objects on their environments by measuring their energy and mass budgets, and understanding nucleosynthesis from the elemental abundances in supernova ejecta. Notably, X-ray microcalorimeter arrays also operate as integral field spectrographs, providing previously unattainable high-resolution spectra from 0.3-12 keV from extended objects and crowded fields.

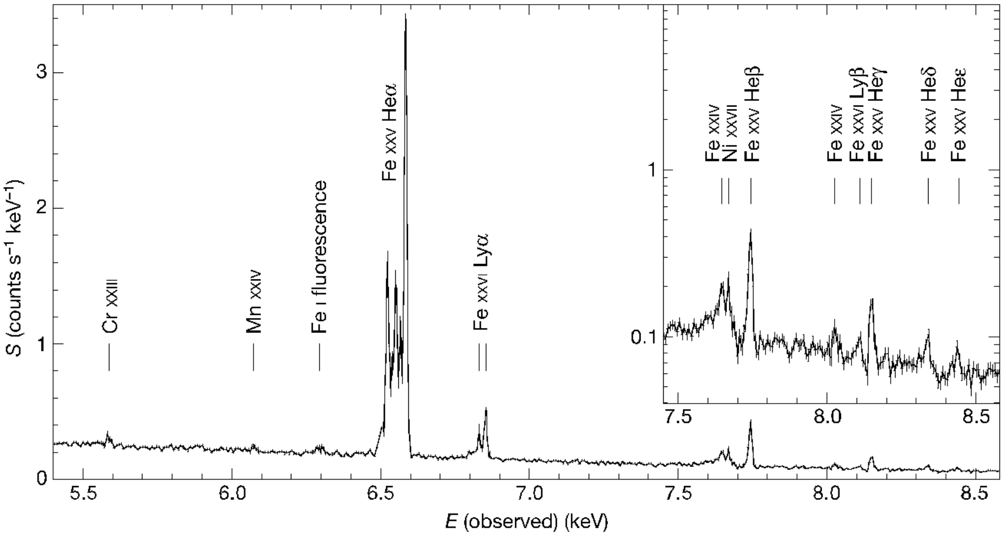

Figure 1: *Hitomi* spectrum of the Perseus cluster showing the strong emission lines from He-like and H-like iron, plus features from highly ionized Cr and Mn. These features tightly constrain the temperature and turbulent velocity in the cluster. (Hitomi collaboration, 2016).

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[1] http://cxc.harvard.edu/proposer/POG/html/chap8.html

Astronomers got a taste of this capability with the short-lived Hitomi mission (Takahashi et al., 2016), which carried a microcalorimeter with ΔE≈5 eV resolution. Its primary observation (338 ks on the Perseus galaxy cluster; Figure 1) produced groundbreaking results, such as characterizing the kinematic and thermal state of the cluster gas, and measuring precise elemental abundances (Hitomi Collaboration 2018a,b,c,d,e,f,g,h).

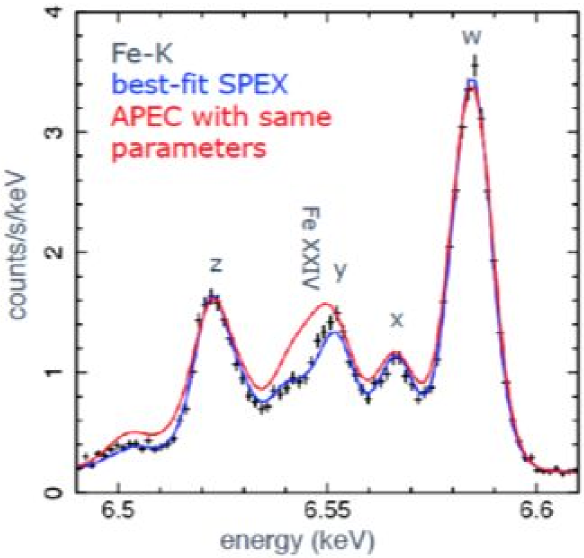

Figure 2: The Hitomi SXS spectrum in the Fe Heα band (black) with the best-fit SPEX (blue; Kaastra et al., 1996) model compared with APEC (Foster et al, 2012) model with the same parameters(red). APEC can achieve a comparably good fit to SPEX with differing parameter values, in which case the sense of the discrepancy is reversed.

However, this observation also demonstrated that the atomic databases on which astronomers rely to interpret the data are inadequate (Hitomi Collaboration 2018d). Many lines had incorrect transition energies and line strengths prior to an intensive effort to gather and calculate accurate atomic data. The level of disagreement between the models used to interpret such spectra is illustrated in Figure 2, which shows the discrepancy between two widely used coronal emission models fitted to this spectrum.

Knowledge of the uncertainties in the atomic data (and a framework to incorporate them into modeling software) is also important to prevent misinterpretation of discrepancies between models and measured spectra, since X-ray spectral models are calculated from first principles and atomic data. Atomic data are equally important for complex models and measurements that focus on a single transition.

The key quantities include transition energies, collision strengths, oscillator strengths, and fluorescent yields. Experiments and calculations are also needed to understand the charge state distribution of astrophysical plasmas and charge transfer within them. A given measurement, such as the optical depth via resonance scattering in the hot gas in galaxy clusters, typically relies on multiple quantities (e.g., energy, collision strength, and charge state distribution). Each of these must be known well enough that observational uncertainties, rather than laboratory ones, limit measurements.

These issues are urgent and must be addressed in the coming decade to fulfill the scientific promise of XRISM and Athena. Here we describe the atomic data needed and the current state of the art for measuring or calculating these quantities. A companion white paper, "Laboratory Astrophysics Needs for X-ray Grating Spectrometers," describes the corresponding quantities and priorities for next-generation X-ray grating spectrometers, which have superior resolution at E<2 keV.

2. Technical Overview (Specific Data Needs)

In the 2-10 keV X-ray bandpass the most commonly studied lines are K-shell transitions of Si, S, Ar, Ca, Fe, and Ni (along with transitions from odd-Z elements with Z<30). The primary data needs include precise and accurate determinations of the energies for these transitions, the charge-state distributions (CSD) of these ions under a range of thermodynamic and radiative conditions, measurements and calculations of absorption cross-sections, and collisional and radiative rates for these ions. Hitomi showed that existing data may not be adequate for microcalorimeters, and the science drivers for XRISM and Athena can be traced to needed improvements in these values. More work is also needed to characterize charge transfer, which will be an increasingly important topic with sensitive spectrometers. Finally, all of these data must include uncertainties or errors from laboratory measurements or estimated from theoretical calculations.

2.1 Transition Energies

Accurate and precise energies underpin dynamical and redshift measurements, and have obvious importance for line identification and deblending. For example, the line centroid of neutral Fe Kα from white dwarf systems constrains the gravitational redshift at the surface of the white dwarf, and thereby the stellar mass (Mukai et al, 2014). Likewise, Fe Kα observations of light echoes from Sgr A* coming from nearby molecular clouds can be used to measure the rotation curve of the inner Galaxy (Koyama et al., 2014). Both of these require centroiding the lines to better than 30 km s^{-1}. With good signal, centroids can be measured to an accuracy ~10x higher than the nominal detector resolution, corresponding to 10-20 km s^{-1} for Athena and XRISM, respectively. This measurement is therefore in reach for both, if we know the transition energy to better than 0.25 eV ($\Delta E/E \sim 4 \times 10^{-5}$).

The energies of many of the strongest lines have been measured in the laboratory to a fractional accuracy of $\Delta E/E \sim 10^{-5}$ (3 km s^{-1}). Lines from hydrogenic ions can be calculated to $\Delta E/E \sim 10^{-6}$.

However, conventional configuration-interaction codes can calculate line energies for more complex ions with $\Delta E/E \sim 10^{-3}$ at best. Techniques such as many-body perturbation theory can improve this to $\sim 10^{-4}$, but this has not been demonstrated for many types of transitions of interest, such as K lines.

Sufficiently accurate energies exist for most of the strong lines of cosmically abundant elements from highly ionized ions. However, this is not the case for trace elements, such as Cr or Mn; many K line energies for low- and medium-ion stages are known only to within $\Delta E/E \sim 10^{-2}$. These are important since their abundances relative to iron provide insight into nucleosynthetic processes, such as in Type Ia SN explosions (Yamaguchi et al. 2015). The transition energies are important because displaced lines can lead to poor fits, which for weak lines can lead to abundance errors of up to 100%, and velocity shifts between various elements is important for supernova structure.

Other lines for which the current measurements are not sufficiently accurate include the inner-shell lines (K lines) from near-neutral ions, such as Fe II - Fe X, which are important in strongly irradiated gas and active galactic nucleus (AGN) “reflection” (i.e., emission from the X-ray illuminated accretion flow close to the black hole), and are likely important in the example of the white dwarf given above. These have uncertainties $\Delta E/E \sim 10^{-2}$, which potentially limits the ability to make measurements such as the rotation curve of the inner Galaxy. Neutral elements have very precise measurements, though often measured in a metallic or solid form which may differ from isolated atoms in their valence structure.

2.2 Charge State Distribution (CSD)

Many science goals for XRISM and Athena depend on modeling knowledge of the emissivity or opacity in a given atomic transition. These depend in turn on several atomic quantities: generally the charge state distribution (CSD) or ionization balance determines the ion fractional abundances, and a collisional or radiative excitation rate determines the excitation or population of the relevant atomic levels.

The prototypical calculation of CSD is for coronal plasmas in which the dominant processes are electron-impact collisional ionization and radiative and dielectronic recombination. In spite of active work for more than 50 years, there is still divergence between recent compilations of rates, e.g., by Bryans et al. (2009), vs. the collection by Urdampilleta et al. (2017).

Furthermore, none of these calculations includes usable error estimates. In the case of CSD calculations, this will require propagating errors (or their equivalent in the case of theoretical calculations) from the rates to the final population estimates. Some work has been done in related areas (e.g., Bautista et al. 2013), but much more remains. Ideally, error estimates - including correlations between rates - would be available for all atomic data. However, a practical first step would be to include error estimates for CSD calculations, where there are only tens or hundreds of rates to consider rather than the millions or billions when all possible bound-bound transitions are included. Additionally, while many different calculations of time-dependent collisional and photoionized non-equilibrium ionization (NEI) exist, few experimental tests or even critical evaluations of theory have been performed.

In order to best prioritize the atomic data needs, numerical experiments are needed, utilizing models to determine the sensitivity of the emissivity or opacity to the atomic rate or cross-section for ionization, recombination, excitation or decay. This topic is described in more detail in the companion white paper "Laboratory Astrophysics Needs for X-ray Grating Spectrometers."

2.3 Absorption cross sections

X-ray absorption in bound-bound and bound-free transitions at E>2 keV provides key diagnostics of outflows from AGN and X-ray binaries, measurements of the abundances in the interstellar medium, and has the potential to constrain the geometry in galaxy clusters. Microcalorimeters will have superior resolution near the Fe and Ni line complexes above 6 keV (notably, absorption from ionized species is important), and will also be sensitive to absorption in the Kα lines of noble gases such as Ar and Ne.

The first X-ray absorption cross-sections for astrophysical use (Bell & Kingston 1967; Morrison & McCammon 1983) used data for neutral atoms only with step-function edges taken from the Bearden (1966) or Henke et al. (1982) compilations. Although the potential impact of ions, molecules, and even grains was understood (Ride & Walker 1977), the X-ray spectrometers then available did not require them. However, the gratings aboard *Chandra* and XMM-Newton demonstrated the inadequacy of these edges and spurred on both theoretical and laboratory work, especially at the low energies where the gratings have the best resolution (nevertheless, much more work is needed at low energies; see the companion gratings APC white paper). Work is now especially needed for highly ionized species.

One of the best ways to measure cross-sections for ions is through using a synchrotron beam with an Electron Beam Ion Trap (EBIT) that can generate and trap a specific ion for hours at a time (Epp et al, 2007, Simon et al., 2010ab, Silver et al 2011). Studies of dust composition through the fine structure in the O, Si, and Fe absorption edges are also of great interest, and rely on connecting laboratory measurements of grains with different structures (e.g., crystalline vs. amorphous) to line/edge features measured against X-ray binaries. A larger library of absorption measurements from "astronomical" dust will be important to determining the interstellar dust composition. Both endeavors imply prioritization, which can be traced to the XRISM and Athena science cases.

2.4 Collisional and radiative rates

Many astrophysical sources radiate line-dominated spectra resulting from mechanical heating of diffuse gas. In such a plasma, ionic levels are excited by collisions with thermal electrons, which then decay through radiative transitions. A key example is supernova remnants, in which the shocks resulting from the supernova propagate through the pre-supernova stellar envelope or winds, ejecta from the explosion, and interstellar material. Typical shock speeds in young supernova remnants are ≥1000 km/s, corresponding to electron temperatures in the ~keV energy range and thus X-ray emission. Key quantities include the elemental abundances in the stellar progenitor, mass of elements synthesized in the supernova, the total energy in the shocks, and the density distribution of the circumstellar gas. Another example is galaxy clusters, in which X-rays are emitted by hot gas in the cluster potential well, and where one wants to understand the influence of heating by AGN and the enrichment of heavy elements in the cluster medium by galaxy stripping and feedback.

Both examples infer quantities of astrophysical interest from observed line strengths. This requires modeling of the CSD and of the rates for collisional excitation into excited states, for which the atomic rates for electron-impact collisional excitation are a key ingredient. These rates are derived from cross-sections that can be measured in the laboratory or calculated using theoretical atomic physics code packages.

Calculations are necessary because models used for astrophysical X-ray spectra must include many transitions, and experiments cannot provide accurate data in the needed volume. The calculation workhorse is the distorted-wave (DW) technique (Bhatia 2000); more computational detail is provided by the R-matrix technique (Bautista 2000). Calculations of electron impact excitation must contend with the fact that highly-ionized, heavy ions imply the importance of relativistic effects, while for near-neutral, heavy ions the structure is complicated and large calculations are needed. Cross-section calculations must also resolve the complicated resonance structure. Many transitions are ‘damped’, i.e. the lifetimes of the states are affected by decay through channels other than the channels of interest, due to eg. spontaneous radiative decay or Auger decay. Excitation of ion states with inner shell vacancies are particularly challenging, but are important, particularly in non-equilibrium situations. Recent improvements in the scaling properties of the R-matrix codes now permit cross-section calculations that include these effects on a large scale (Ballance 2013).

Measurements are crucial for testing and benchmarking the calculations, and also easing some of the modeling complexity. The required precision varies between ions, but much of the need is just for additional benchmark measurements. Cross-sections can be directly measured with an electron-beam or merged-beam apparatus, such as the Lawrence Livermore National Laboratory EBIT measurements of Fe^{17+} - Fe^{23+}, in which the cross sections were determined by measuring line strengths and normalizing to recombination emission (Chen and Beiersdorfer 2002). Meanwhile, measurements of energies will lead to an accurate model of the energy-level structure in a given ion, which greatly improves the accuracy of calculated collision cross-sections.

2.4 Fluorescence Yields

Among the most commonly observed lines in X-ray spectra are inner-shell fluorescence lines, such as the Fe Kα line near 6.4 keV. In many cases, these are excited by the decay following the removal of an inner-shell (K-shell) electron. The line intensity then depends on the ion fraction (charge state distribution), the K-shell ionization rate, and on the fluorescence yield, i.e., the fraction of K-vacancy ions which emit a line as opposed to decaying by the Auger process.

These lines are important diagnostics of compact sources containing a strong source of continuum X-rays capable of creating inner shell vacancies, such as X-ray binaries, in which the Fe Kα line is generally the strongest single feature in the X-ray spectrum. Fe Kα is also observed at the Galactic Center from Sgr A*, and in reflection-dominated AGN. The line intensity, which depends on the fluorescence yield, can be used to determine a combination of the iron abundance and the geometrical covering of the line emitter relative to the continuum X-ray source. The lines may come both from neutral atoms and near-neutral ions (Fe II-X).

Fluorescence yields have been measured to an accuracy of a few percent for neutral atoms by X-ray illumination of laboratory samples (Bambynek et al., 1972). However, fluorescence yields for *ions* depend almost entirely on calculations. These are challenging for near-neutrals owing to the large dynamic range between the valence shell and inner-shell energies, and the need to include many states for an accurate computation (Palmeri et al, 2003). Current estimates for the accuracy of these calculations is 10-20%, at best. This limits the interpretation of astrophysical spectra, as high signal-to-noise spectra can achieve percent-level *statistical* uncertainties in astrophysical model parameters.

2.5 Charge Exchange (CX)

CX is a collision between an ion and a neutral atom or molecule, in which one or more electrons are transferred from the neutral to the ion, often into an excited state. X-rays (and other photons) are then produced in a radiative cascade. CX has been observed in our Solar System due to the solar wind interacting with neutrals in the heliosphere, planetary atmospheres, and comets. There are also hints that it is important in supernova remnants, star forming galaxies, and galaxy clusters. CX is typically discussed in the context of lines associated with medium-Z elements such as C and O, since in the heliosphere the most abundant projectiles after H and He are ions of these elements. These needs are discussed in our companion white paper, "Laboratory Astrophysics Needs for X-ray Grating Spectrometers."

However, there is no a priori reason to exclude charge exchange with ions from heavier elements, such as Si, S, and Fe, which will fall in the spectral band where the calorimeters excel, and these will be of great astrophysical interest (Shah et al. 2016). Nominal detections of CX with S and Fe were even observed with *Hitomi*. This will produce emission in many of the same lines produced by collisionally or photoionized gas, but with different line ratios. Thus, improved calculations and benchmark experiments must not be neglected for heavy elements.

The following table summarizes what we consider to be the most important atomic data needs from these categories and the lab astro activities needed to prepare for X-ray calorimeters.

Atomic data category	Most important need	Tool/technique
Transition energies	Near-neutral ions, inner shells	Experiment, light source + ion trap
Charge state distribution	Experimental benchmarking, error propagation	Experiment (eg. ebit) + simulation
Absorption cross sections	Absorption from compounds and dust	Light source experiment
Collision cross sections	Large scale application of current code packages	Computation, experimental benchmarks
Fluorescence yield	Near-neutral ions, inner shells	Light source experiment
Charge exchange	Ion + atomic H	Dedicated beam experiment

3. Technology Drivers (new experiments, theories, etc.)

Owing to the funding levels required, most projects to measure atomic quantities relevant to X-ray astrophysics rely on baseline funding from other sources, and use funding from the NASA Astrophysics Research and Analysis (APRA) program to provide the additional funding required to run specific measurements. Thus, at least in the next decade, we envision additional experiments with existing technologies, up to and including commissioning a new EBIT.

Experimental groups at institutions including NASA's GSFC, LLNL, SAO, NIST, and Clemson are carrying out relevant measurements with EBITs that create a plasma dominated by a single ion and then probe it with an electron beam. These are used to measure energies, collision strengths, collisional ionization and recombination rates, and charge transfer cross sections. For photoionized plasmas, Z-pinch machines can create conditions similar to those found in astrophysical photoionized plasmas.

CX experiments are desperately needed that combine a CX beamline with (1) a cold target recoil ion momentum spectrometer (COLTRIMS), capable of distinguishing between H and H_2 collisions via time-of-flight spectroscopy of the recoil products of the collision; (2) a calorimeter in order to use photon spectroscopy to distinguish capture into different angular momentum states; and (3) an atomic hydrogen source. Finally, although a number of approaches exist to calculate CX cross sections (e.g. Cumbee et al. 2018), each method has limits and the overall accuracy is suspect. New approaches to this important problem would be welcomed.

4. Organization, Partnerships, and Current Status:

The primary challenge to developing collaborations among the distinct communities of X-ray astronomers, experimental physicists, and atomic, molecular, and optical physics (AMO) theorists - as well as the funding agencies that support them - has always been identifying specific data needs and prioritizing them. Addressing this problem includes:

- Connecting data needs to the experimental or theoretical groups that can address them.
- Ensuring a plausible timescale, as experimental results typically require a minimum of 2-3 years to complete, while even theoretical calculations often involve a year or more.
- Evaluating the utility of the data to create a usable prioritization, as astronomers can easily identify far more needs than any funding source can meet.

NASA has addressed a similar issue regarding technology needs for new missions within the PCOS/COR program offices via a process of prioritizing identified gaps[2]. In this process, "Each Program's Technology Management Board (TMB) evaluates and prioritizes technology gaps submitted by its community each summer and the results are published in the respective Program Annual Technology Report."

In the case of astronomical spectroscopy, the data archives - e.g. NASA's High Energy Astrophysics Science Archive Research Center (HEASARC) - are the obvious place to host an equivalent "High Energy Lab Astro Needs" (HELAN) board. Although this white paper focuses on X-rays, equivalent boards could be hosted at the other NASA archives. Similar to the TMB,

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[2] https://apd440.gsfc.nasa.gov/tech_gap_priorities.html

this board could meet annually to review data needs submitted by the community. These could be for existing or approved future missions. The board would issue an annual report that would not itself provide any funding, but would indicate to funding agencies where the priorities lie.

We emphasize that the need for this effort is international, owing to the international nature of XRISM, Athena, and other projects. US funding for the efforts described here will motivate funding in Europe and Japan, where many lab astrophysics facilities and AMO theorists reside.

5. Schedule

A key driver for this work is the XRISM launch in early 2022. Any new effort to measure atomic quantities requires time for obtaining funding, planning (and constructing, in some cases) the experiment, as well as carrying out the measurements and analysis. For this reason it is important to prioritize and encourage this work as soon as possible.

6. Cost Estimates

Funding for X-ray laboratory astrophysics primarily comes from the NASA APRA program. The APRA laboratory astrophysics program funds ~25 programs/year at average of $150K/year (in $FY19); grants are typically for three years, allowing for ~8 new proposals per year. This includes all areas of laboratory astrophysics (not just those relevant to X-rays), although it is important to note that groups outside of the US also work on topics relevant to this white paper.

Addressing the "US share" of the needs identified in Section 2 and in the companion white paper, "Laboratory Astrophysics Needs for X-ray Grating Observatories," requires a modest increase in APRA awards of $1.5M/year. This would support ~4 experimental groups using existing facilities (atk/year, each), the placement of one new EBIT at a light source (estimated cost $2M, or $200k/year over a decade), and ~5 graduate students or postdocs ($60k/year each) doing theoretical work.

Atomic data are not tied to a single mission and are essential to diagnostics that underpin much of X-ray astronomy, so this modest investment will have far-reaching consequences. While not all of the desired work could be completed with this budget, it would enable measurements and calculations of high priority quantities, and funding through APRA would allow selection via competitive, peer-reviewed proposals. Sustained, mission-independent funding for X-ray laboratory astrophysics is essential because of the funding structure and schedule for laboratories vs. missions, because new measurement or calculation needs may be discovered at any time during or after a mission (e.g., to enable an astronomical measurement yet to be conceived), and because it is relevant to missions of all sizes (from the *Lynx* Surveyor to the *Arcus* MIDEX).

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