Laboratory Astrophysics Needs for X-ray Grating Spectrometers

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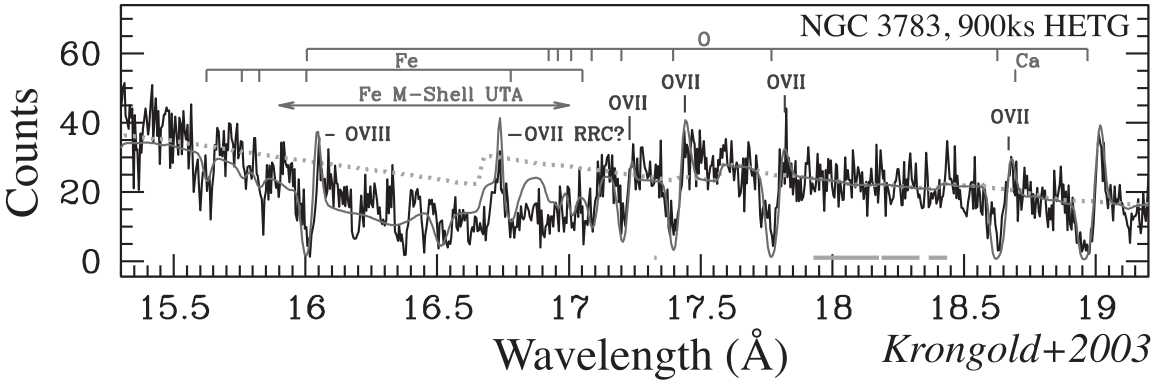

A selected bandpass from the 900 ks Chandra HETG spectrum of NGC 3783

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Abstract

The current generation of X-ray grating spectrometers on Chandra and XMM-Newton has modest sensitivity, largely due to a combination of modest resolution (typically 300-1000) and low efficiency ($\lesssim$ 10%). The next generation of X-ray gratings, however, has already demonstrated far higher resolution and efficiency, capabilities that will transform the field. These gratings are planned for use on Explorers, Probes, and Flagship missions, so the time is right to prepare for the high-quality spectral data that will be returned by these missions. The highest-resolution grating data available, from the Chandra gratings, have already shown the limitations of existing atomic data for modeling; improvements are needed in laboratory measurements of wavelengths, radiative and collisional transition rates, as well as ionization and recombination cross-sections. To prepare for these proposed missions, significant progress needs to be made in understanding the theoretical atomic physics as well. This white paper, in concert with a paper focusing on microcalorimeter missions, will summarize the work that has been done thus far in the field of laboratory X-ray astrophysics, with the goal of identifying the most critical tasks that are still outstanding. This includes tracing science requirements from missions such as Arcus, XGS-P, and Lynx and identifying the laboratory measurements needed to achieve them. We discuss long-term methods to prioritize these needs, along with our initial assessments, and indicate new facilities that will be required.

1. Key Science Goals and Objectives

The next generation of X-ray gratings and optics promises both high-resolution and high-quality spectra for sources ranging from stars and the interstellar medium to supermassive black holes (SMBH) and galaxy halos. This white paper will focus on spectroscopy in the soft X-rays ($6\ \text{Å} < \lambda < 120\ \text{Å}$ ($0.1<E<2$ keV), where the next generation of X-ray microcalorimeters (XRISM/Resolve, Athena/X-IFU and Lynx/LXM) provide resolutions of order R~100-1000, while gratings reach 1000-10000. For organizational simplicity, we will discuss the requirements on theoretical and experimental atomic, molecular, and optical (AMO) physics in this bandpass here, while requirements for energies above 2 keV will be covered in a companion white paper, “Laboratory Astrophysics Needs for X-ray Calorimeter Observatories.”

The 2010 Decadal survey ranked the International X-ray Observatory (IXO) amongst its highest priorities for large space missions. One of IXO’s primary instruments was the X-ray Grating Spectrometer (XGS). The XGS planned to use one of two new grating technologies that showed great promise, either Critical Angle Transmission (CAT) (Heilmann et al. 2019) gratings or Off-Plane Gratings (OPG) (Miles et al. 2018), although both required substantial development in 2010. In the subsequent decade both technologies have made great advances and are now flight-ready. Compared to the gratings on Chandra, both technologies provide more than an order of magnitude greater efficiency and a similar increase in resolution in the 6-60Å bandpass.

The 2010 report identified three key science issues in particular that required the high resolution and sensitivity of the XGS. These were:

1) *Determining how baryons cycle in and out of galaxies*, by measuring the distribution and temperature of the dominant hot gas around galaxies and clusters and maps of the temperature and abundances of gas in our own Galaxy.
2) *Understanding how feedback from a black hole system influences its surroundings*, by determining the mass, energy and momentum in the accretion-driven, outflowing winds from both supermassive and stellar mass black holes.
3) *Examining how stellar systems form and evolve*, by measuring the balance between accretion and outflow and its impact on structure formation on the smallest scales by surveying young accreting stars, evolved coronal stars and exoplanet atmospheres.

As no XGS-like mission was launched in the past decade, it is not surprising that all three remain largely open questions. It seems likely, however, that in the next decade a mission will be started or, hopefully, launched, that can address these issues. Given the substantial time required, it behooves the community to make an early start at identifying and addressing both the theoretical and experimental atomic data needs implied by these science cases, as well as others enabled by these powerful new capabilities.

2. Technical Overview (Specific AMO data needs)

The full X-ray bandpass contains transitions from all abundant metals; in the 0.1-2 keV range this list most notably includes K-shell transitions of C, N, O, Ne, Mg, and Si along with L-shell transitions of Mg, Si, Fe, and Ni. More sensitive spectrometers will add new elements to this less, such as the lower-abundance odd Z elements such as N, Al, and Mn. As we will describe below, the two primary needs are precise and accurate determination of the wavelengths for common transitions as well as the charge state distributions (CSDs) of these ions under a range of thermodynamic and radiative conditions. Additionally important are measurements and calculations of absorption cross-sections as well as collisional and radiative rates for these ions. Some data already exists, but the improved sensitivity of new soft X-ray spectrometers drives the need for improvements in these values. Finally, new types of plasmas, such as those with significant X-ray emission due to charge exchange, are hinted at with existing instruments and improved data will certainly be required to characterize them. As noted below, all of these data must include uncertainties or errors, either from the laboratory measurements themselves or estimated from the theoretical calculations.

2.1 Wavelengths

The current wavelength accuracy goal for the stronger X-ray lines comes from the need to reliably measure Doppler shifts at the resolution provided by the Chandra gratings (R~1000), the highest-resolution spectrometers available. Assuming a line can be centroided to 10% of the resolution, this implies a desired accuracy of 1-2 mÅ. The next generation of X-ray grating spectrometers will achieve R=3000-5000 which would drive this goal to 0.2-0.7 mÅ for the strongest ~10 lines from each ion (including both emission and absorption lines). For fainter but still individually detectable lines - perhaps 50-100 per ion - this can be relaxed to ~50% of the resolution, or ~1-2 mÅ.

Wavelengths can be calculated to <1 mÅ using detailed quantum electrodynamics for H-like and He-like ions (Johnson & Soff 1985; Drake 1988). Lower- to medium-ionization states produce X-ray emission lines either from L-shell transitions in Fe-peak elements (Nahar et al. 2003) or innershell K transitions from lighter elements (Sur et al. 2010). In many cases, only a few laboratory measurements exist, at most, so these wavelengths have been determined using theoretical calculations of the ionic energy level structures, with adjustments to match laboratory data as available. The results vary: extremely detailed calculations can reach accuracies of “a few hundred Kaysers [cm^{-1}]” (Del Zanna & Mason 2018), equivalent to <2 mÅ at 20 Å; however, existing data typically have wavelengths calculated to only ~1% accuracy, or 200 mÅ for a 20 Å line. The strongest lines will need to be created using plasma devices such as electron beam ion traps (EBITs; Brown et al. 1998, 2002) or X-ray free electron lasers (Vinko et al. 2012, Nahar & Pradhan 2015), in conjunction with good spectrometers and calculations to ensure proper line identifications from the laboratory spectra (Kotochigova et al. 2010). These can then benchmark detailed calculations for the remaining lines.

Inner-shell transitions such as the so-called “unresolved transition array” (UTA) of Fe-L shell transitions in Na-like and lower charge states are important in studies of AGN outflows. Calibrating these transitions to the desired sub-mÅ accuracy can best be accomplished using synchrotron soft X-ray beamlines with very high resolution monochromators or X-ray free electron lasers (Vinko et al. 2012, Nahar & Pradhan 2015) to excite the transitions in ion samples created and trapped in portable EBITs (Epp et al. 2007, Simon et al. 2010a,b, Bernitt et al. 2012), while simultaneously detecting both fluorescence and Auger photoionization. For very low charge states, photon-ion merged beam facilities such as the Petra III PIPE experiment can be used (Schippers et al. 2017).

2.2 Charge State Distributions (CSDs)

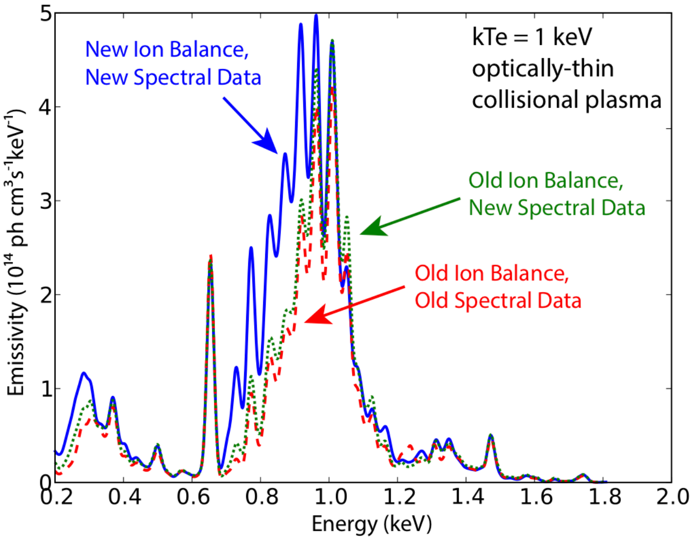

Figure 1: Updating the CSD to the 'new' Bryans et al. (2009) calculation from the 'old' Mazzotta et al. (1998) result led to significantly more Neon-like iron ions, which have strong emission lines in the 0.7-1 keV bandpass; simply changing the spectral data had much less effect. This change led to a complete revision of models for hot gas in elliptical galaxies, as described in Loewenstein & Davis (2012).

An accurate determination of both optically-thin collisional and photoionized plasma CSDs is key to all further analysis. Any systematic errors will have substantial effects on the scientific inferences drawn from the spectra, as notably described in Loewenstein & Davis (2012) in an appendix titled "EVERYTHING YOU KNOW IS WRONG: EFFECTS OF UPDATING THE ATOMIC DATABASE." The cause of this impact can be seen directly in Figure 1 (based on Figure 3 of Foster et al. 2012). The 'new' Iron ion balance used in Figure 1 is from Bryans et al. (2009), which has itself since been updated by Urdempilleta et al. (2017). However, none of these calculations include 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 astrophysical contexts, the density dependence of CSD calculations in a collisional plasma remains another underappreciated problem. This issue was discussed in 1962 by Bates et al., and has been actively addressed for atoms of interest to the fusion community. The CSD calculations developed by and for the astrophysical community - AtomDB (Foster et al. 2012), SPEX (Kaastra et al. 1996), and Chianti (Dere et al. 2019) codes - do not include density corrections. However, the ADAS code (Summers & O'Mullane 2011), developed by the magnetic confinement fusion community, does include density effects. These can appear at densities relevant to stellar coronae or accretion disks; in the case of oxygen, effects appear at densities as low as 5×10^{7} cm^{-3}. Similar calculations have not yet been done for Fe, but typical trends would suggest both the temperature and density range of interest would rise. The approach used by the fusion community is called Generalised Collisional-Radiative (GCR) model (Summers et al. 2006), but it has not yet been extended to heavier metals such as Fe. The effects are complex; Nikolic et al (2013) have demonstrated that dielectronic recombination rates drop at high density as autoionizing states ionize by collision before they can decay. At the same time, collisionally-excited metastable states in Be-like and Mg-like ions will show increases in ionization.

The “Z Facility” at Sandia National Laboratory can explore the opacity of highly-ionized radiation-dominated plasmas, providing useful CSD benchmarks. At this facility a so-called `z-pinch plasma’ is imploded, created by running a huge current through a series of parallel wires. This current interacts with a cylindrical foam to create a temporary Hohlraum, which then emits copious photons with E>150 eV, illuminating a metal target (see description in Bailey et al. 2007). Although designed to test solar interior opacities, these experiments can be used to explore astrophysical photoionized plasmas as well (Rochau et al. 2014). In particular, the opacity models include not only the CSD, but also calculations of UTAs (see Gu et al. 2006) as well as a range of ions with multiply excited states and low probability transitions. Comparing the experimental shots with models may not only provide much needed benchmarks for photoionized plasmas (Loisel et al. 2017, Bailey et al. 2015) and their underlying atomic rates, they could also suggest new avenues in atomic physics and spectral modeling worth exploring (e.g. Bailey et al. 2009; Mancini et al. 2009, Nahar & Pradhan 2016).

2.3 Absorption cross sections

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 have high enough resolution for the effects to be observed. The launches of Chandra and XMM-Newton dramatically changed this situation, and substantial theoretical and experimental work has since been completed (see, e.g., Gatuzz et al. 2015 and references therein). This has not, however, addressed all concerns.

McLaughlin et al. (2013), for example, found good comparisons between theoretical calculations and laboratory measurements of the atomic oxygen K edge that disagreed substantially (an energy shift of ~0.6 eV) with observational results from Chandra. This has been challenged by Gorczyca et al. (2013) and Garcia et al (2017) who suggested a number of reasons why the Chandra calibration should be considered more reliable than laboratory measurements, even though its spectral resolution is lower. This debate has not yet been settled in print, however. Issues have arisen with other elements, as Gatuzz et al. (2015) and Juett et al. (2004) advocated for shifting the Fe L cross-section of Kortright & Kim (2000) by 40 mÅ (2 eV). Similar energy shifts are expected depending on the state of the iron-bearing mineral. A similar mismatch exists between the theoretical cross section and the Cyg X-1 grating data (Hanke et al. 2009, Corrales et al. 2016), suggesting the possibility of a more complex dust composition than the simple ferric measurement of Kortright & Kim (2000). Oxygen and iron are two of the most abundant elements after H and He, one of the reasons these disagreements were detectable. As new observatories will have orders of magnitude more sensitivity, such issues will become more common. This requires prioritizing the most scientifically significant photoelectric absorption features, followed by a coordinated theoretical and experimental effort, including precise energy calibration. For ions, this might require the use of an EBIT that can generate and trap a specific ion for hours at a time combined with a synchrotron beam to measure the absorption cross-sections.

As astronomical X-ray grating spectrometers become more sensitive, comparisons with results from other bandpasses will become important. Pradhan (2000) demonstrated that UV and X-ray lines of the same O VI ion may be used as diagnostics and abundance determination. Mathur et al. (2017) compared measurements of O VI in the UV (from the 1032 Å,1038 Å doublet) and the soft X-ray (from the 22.032 Å Kα transition in O VI), and noted that “the column density inferred from the X-ray line was consistently larger than that from the UV line.” They suggested that one cause - although not the entire solution - was blending with the O II Kβ line at 22.04 Å, leading to a significant overestimate of the O VI column density when measured in X-rays. Gatuzz et al. (2019) explored this possibility using Chandra observations of 13 X-ray binaries and 29 AGN to measure O I-O III and O VI-O VIII, finding that the O II blending contributes <30%. They suggest new atomic data may be required, or exploring potential line saturation and/or radiative excitation, admitting this “remains as an open question,” but see also Mathur et al. (2019, in preparation). Again, this example arises in part because existing spectrometers are only sensitive to the large column densities found with oxygen; new facilities will reveal new problems.

2.4 Collisional and radiative rates

Substantial work remains to be done in this area, such as the need for more accurate data are the w,x,y, lines of He-like ions and dielectronic satellite lines, which are often used as diagnostics in both transient and non-transient plasmas. In addition to transition probabilities, the modeling requires accurate level-specific photoionization cross-sections and recombination rates for the constituent ions. However, in the interests of space and as the issues are largely similar this discussion is left for the companion white paper, “Laboratory Astrophysics Needs for X-ray Calorimeter Observatories.”

2.5 Charge Exchange (CX)

CX, an inherently non-equilibrium process, occurs when a neutral atom (or molecule) interacts with an ion, ‘exchanging’ one (or more) electrons from the neutral to the ion, often in an excited state. Depending upon the ion, the resulting radiative cascade can include X-rays, typically < 2 keV. This was first identified in cometary X-rays (Lisse et al. 1996, Cravens 1997) and since has been detected or suggested as occurring in solar system planets (Dennerl 2010), supernova remnants (Katsuda et al. 2011), and starburst galaxies (Zhang et al. 2014). The next generation of X-ray spectroscopy missions will seek to address the following science goals with regard to CX:

1) Characterize heliospheric foreground CX in order to correct for it in observations of extended sources, as well as to probe the solar wind itself.
2) Measure CX in the solar system (solar wind interactions with comets and planet exospheres) to measure the composition of the neutral target and the interaction velocities.
3) Search for contributions from CX to X-ray emission in the wide variety of astrophysical sources with ionized/neutral interfaces (galaxy clusters, circumgalactic medium, star-forming regions, etc.).

CX from abundant ions, such as oxygen, leads to emission in many of the same lines produced by collisionally ionized or photoionized gas, but with different line ratios. Since a hot or ionized plasma is a prerequisite for CX, both will often contribute to diagnostic emission lines in CX sources. Accurately measuring the CX contribution therefore requires high quality models. Current model accuracies are limited to 100-200% uncertainty in the CX fraction because most cross-sections remain poorly known. The uncertainties in the predicted emission spectra already limit our ability to determine how important CX is in many phenomena, such as starburst galaxies, and may hobble attempts to make detailed measurements of ionized gas with next-generation spectrographs. Hence, both new laboratory experiments and theoretical calculations are urgently needed. This will require a dedicated and sustained effort, as both are technically challenging.

On the experimental side, in cosmic plasmas, atomic H usually dominates neutral CX interactions. Atomic H is the easiest neutral target for calculations, as only one electron can be captured. Multi-electron targets must include calculations of multi-electron capture, a major complication. However, experiments with atomic H are very challenging because the atomic H must be prevented from reforming into H_2 and there is always a mixture of targets from residual H_2 and background gases. Thus, a method to identify the neutral in each collision event is required.

CX theory has issues as well. The most widely used theoretical method (multi-channel Landau-Zener, or MCLZ) cannot distinguish the degenerate levels of hydrogenic ions, and thus is incapable of predicting the angular momentum state of the captured electron from CX onto bare ions. Alternative methods, such as quantum molecular orbital close coupling (QMOCC) are computationally expensive, especially for systems with multiple electrons. Charge exchange between atomic H and H-like ions, producing X-ray emission from He-like ions, should be easier to calculate with MCLZ, since the levels are not degenerate.

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

Although AMO physics remains an active field, many practitioners have moved into areas not relevant to soft X-rays, such as ultra-cold plasmas. This is of particular concern for laboratory astrophysics, as funding for the experimental equipment has not traditionally come from NASA or NSF astrophysics budgets. Most astrophysical projects rely on baseline funding from other sources, only providing the additional funding required to run specific measurements.

A modest number of experimental groups remain, however. EBITs that create a plasma dominated by a single ion and then probe it with an electron beam have been used for astrophysical measurements at institutions including NASA's GSFC, LLNL, SAO, NIST, and Clemson. These are used to measure wavelengths and collision strengths and potentially collisional ionization and recombination rates. For photoionized plasmas, Z-pinch machines described in S2.1 can create conditions similar to those found in astrophysical photoionized plasmas.

Measurements of transition rates, opacities, and wavelengths of inner-shell transitions can most easily be done with an EBIT designed to be permanently positioned at a synchrotron ring (e.g. Micke et al. 2018). Bernitt et al. (2012) demonstrated the power of this approaching using a portable EBIT at the Stanford LCLS to measure X-ray transition rates in Fe XVII. On the theoretical side, as noted in S2.2, high-quality calculations of X-ray transitions can be done but require substantial investments of computer time. A number of results exist for EUV transitions from low-lying levels (see, e.g., S5.6 of Del Zanna & Mason 2018); extending these to the higher energy levels and including inner-shell transitions that exist in the soft X-rays are possible but would require even larger calculations.

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 state-selective charge exchange cross sections (e.g., Cumbee et al. 2018), each method has a range of limitations and the overall accuracy of the results are 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 AMO theorists - as well as the funding agencies that support them - has always been identifying specific data needs and prioritizing them. This overall problem includes a number of smaller issues:

- Identifying and connecting data needs to the experimental or theoretical group 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.' 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 PATR (Program Annual Technology Report)." [cite https://apd440.gsfc.nasa.gov/tech_gap_priorities.html]. In the case of astronomical spectroscopy, the data archives - e.g., HEASARC for high energy observations - are the obvious place to host an equivalent "High Energy Lab Astro Needs" (HELAN) board. We note that although this white paper focuses on X-rays, equivalent boards could be hosted at the other NASA archives. Similar to the TMB, this board could meet annually to review data needs submitted by the community. These could be for existing missions, or for 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. Ideally, this effort should be coordinated internationally, as laboratory astrophysics facilities (and AMO theorists) exist around the world.

5. Schedule

This work would address existing observations from the Chandra HETG/LETG and the XMM-Newton RGS, as well as prepare for new missions such as Lynx or smaller missions such as an X-ray grating probe or MIDEX (e.g., Arcus, which if proposed at the next opportunity could launch in 2028). Although focused on grating missions and soft X-rays here, the atomic data issues remain relevant to missions such as XRISM (launch 2022) and Athena (launch 2031) for spectra over the whole X-ray band.

6. Cost Estimates:

Funding for X-ray laboratory astrophysics primarily comes from the NASA APRA program. The APRA lab astro 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 but of course only includes US efforts, while this endeavor is intrinsically international. Addressing the “US share” of the needs identified above and in the companion white paper “Laboratory Astrophysics Needs for X-ray Calorimeter Observatories” for confirmed missions such as XRISM and Athena, as well as a hoped-for X-ray grating mission, will require a modest increase of $1.5M/year. This will support ~4 experimental groups ($250k/year each) using existing facilities as well as the placement of one new EBIT at a light source (estimated cost $2M, or $200k/year over a decade). It will also support ~5 graduate students or postdocs ($60k/year each) doing theoretical work.

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