Usage Report for Fiscal Year 2025

Project Title:

Atomic database for X-ray astrophysics

Name:
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1. Background and purpose of the project, relationship of the project with other projects

With the XRISM mission now operational, accurate atomic data is vital for interpreting high-resolution X-ray spectra. This research focuses on the SPEX updates to key atomic parameters, specifically inner-shell excitation and dielectronic recombination for major elements. We are moving beyond preliminary testing to perform comprehensive validation against diverse astrophysical data sets. The ultimate goal is to deliver a robust, verified database that ensures the reliability of scientific results from XRISM and future observatories including newAthena from ESA.

2. Specific usage status of the system and calculation method

We performed a systematic suite of calculations to determine the atomic structure, excitation, and dielectronic recombination rates for a broad range of inner-shell and doubly excited levels in cosmically abundant elements. To ensure accurate modeling of the inner-shell atomic structure, we employed the Flexible Atomic Code (FAC), which incorporates relativistic configuration interaction.

3. Result

We have updated both main and satellite transitions for a range of P-like to Li-like ions, utilizing the latest theoretical calculations. These refined atomic data were then applied to XRISM Resolve Performance Verification (PV) observations of supernova remnants in particular for N132D, as well as supermassive blackhole NGC 3783. Incorporating these updates ensures high-accuracy spectral modeling, thereby enhancing the reliability and scientific impact of upcoming results derived from these observations.

4. Conclusion

Utilizing RIKEN's supercomputing resources, we generated a comprehensive set of new atomic data and successfully implemented it into widely used X-ray spectral modeling codes. These updates specifically target inner-shell excitation and dielectronic recombination, providing significant improvements in the accuracy of astrophysical plasma modeling. These advancements are essential for maximizing the scientific return of the XRISM mission, enabling a deeper understanding of physical processes across diverse cosmic environments.

5. Schedule and prospect for the future

Discrepancies in modeling low-charge-state ions within XRISM observations of X-ray binaries and black holes highlight the necessity for improved atomic data. We intend to refine inner-shell energy levels, ionization cross-sections, and transition probabilities essential for high-resolution spectroscopy. By employing the Flexible Atomic Code (FAC) with many-body perturbation theory, we will account for complex electron correlations, thereby enhancing the accuracy of ionization balance calculations and spectral interpretation.

6. If no job was executed, specify the reason.

Fiscal Year 2025 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

L. Gu, H. Yamaguchi, A. Foster, et al., Evidence for charge exchange emission in supernova remnant N 132D from XRISM/Resolve observations, Publications of the Astronomical Society of Japan, 2025.

[Conference Proceedings]

[Oral presentation]

Invited talk, HUBS consortium 2025, June 12-15 Beijing, China

Talk at XRISM consortium 2026 July 1-4 Leiden, the Netherlands

Invited talk at XRISM science meeting 2026 October 20-24 Kyoto, Japan

[Poster presentation]

[Others (Book, Press release, etc.)]