Usage Report for Fiscal Year 2024

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

This research focuses on improving the accuracy of atomic data crucial for interpreting high-resolution X-ray spectroscopic data from current and future missions. With XRISM operational, the SPEX team is actively updating atomic data, prioritizing inner-shell excitation and dielectronic recombination cross-sections for cosmically abundant elements. While these updated data have undergone preliminary testing in single-temperature calculations, comprehensive validation against diverse astrophysical observations is essential. The delivery of accurate database will ensure the reliability of scientific results derived from XRISM.

2. Specific usage status of the system and calculation method

A systematic suite of calculations was undertaken to determine atomic structure, excitation, and dielectronic recombination rates for a broad selection of inner-shell and doubly excited levels in cosmically abundant elements. The Flexible Atomic Code (FAC), incorporating relativistic configuration interaction, was employed to ensure accurate modeling of inner-shell atomic structure.

3. Result

For a range of P-like to Li-like ions, both main and satellite transitions have been updated based on the latest calculations. These refined atomic data have been applied to the XRISM Resolve Performance Verification (PV) observations of supernova remnants such as Cas A, Kepler, and W49B, as well as a selection of active galactic nuclei (AGNs). By incorporating these updates, we ensure the high accuracy in spectral modeling, thereby enhancing the reliability and scientific impact of forthcoming publications based on these observations.

4. Conclusion

The newly calculated atomic data, generated using RIKEN's supercomputer, have been successfully implemented into widely used X-ray spectral modeling codes, supporting the scientific objectives of the XRISM mission. These updates include significant improvements to innershell excitation and dielectronic recombination components, ensuring more accurate modeling of astrophysical plasmas. These advancements are crucial for interpreting XRISM observations and will contribute to a deeper understanding of astrophysical processes across a wide range of cosmic environments.

5. Schedule and prospect for the future

XRISM observations of X-ray binaries have revealed discrepancies in the modeling of low-charge-state ions, highlighting the need for significant updates to atomic data. In particular, the innershell energy levels, ionization cross sections, and related transition probabilities require refinement to accurately interpret high-resolution spectra. To address this, we will perform a systematic recalculation using the Flexible Atomic Code in its many-body perturbative mode. This approach will

account for complex electron-electron interactions, improving the accuracy of ionization balance and spectral modeling.

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

Fiscal Year 2024 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

[Conference Proceedings]

[Oral presentation]

-XRISM science team meeting series, March 2023, ISAS/JAXS Tokyo, “laboratory astrophysics”
-XRISM science team meeting series, March 2024, Tokyo university of science, “N132D first light”
-RIKEN rEMU workshop, May 2024, online, “Atomic data need for XRISM”
-Netherlands Astronomers' Conference (NAC), May 2024, Egmond aan zee, “XRISM early results and scientific impacts”
-Charge exchange universe conference, June 2024, Volos Greece,
“Charge exchange model in SPEX”, invited
“Charge exchange with XRISM/Resolve”, invited
-Highly charged ions (HCI-21) conference, September 2024, Egmond aan zee, “Hot and energetic Universe with XRISM and TES on EBIT”
-XRISM science team meeting series, September 2024, Tokyo metropolitan university, “SPEX code update”

[Poster presentation]

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