Usage Report for Fiscal Year 2020

**Project Title:**

Atomic database for X-ray astrophysics

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

Science outcome from spectra of the X-ray emitting astrophysical objects rests crucially on accurate modeling of the underlying atomic processes. The advent of precision astronomy, to be allowed by the high-resolution X-ray spectrometer on-board XRISM (to be launched in FY2022, JAXA/ISAS), is making the demand for robust modeling of the atomic spectrum more stringent than ever. The **goal** of the research is to bridge the gap between requirement and current quality of the plasma modeling, through systematic improvement, extension, and validation of the atomic data and software of the SPEX code. These new developments will result in a fundamental improvement of our capability to perform frontline science with the new challenging data obtained with XRISM.
This project and its successors are a part of the RIKEN pioneering project "evolution of matters in the universe".

2. Specific usage status of the system and calculation method

We calculate atomic data of the basic atomic structure (level energies, transition probability) and collision cross sections (electron-impact collision excitation, dielectronic recombination, radiative recombination, Auger auto-ionization, innershell ionization/excitation) using the flexible atomic code (FAC, a free open source code).

The current calculation focuses on the L-shell line emission from cosmic abundant elements, including Fe, Mg, Si, S, Ar, Ca, and Ni.

The current run has used 105786.7 core-hours in the current fiscal year. The calculation time is on the same order as the proposed amount in the application.

3. Result

In FY 2019, we ran successfully the calculation on collisional excitation (including pure electron-impact and resonant excitations) and dielectronic recombination for Fe XVI to Fe XXIV. This calculation continued in FY 2020 to the L-shell processes of other abundant elements, on the order of Ni, Mg, Si, S, Ar, and Ca. The new calculations will be substantially more complete than the available data in the best existing atomic code.

The new data of the Fe L-shell are compared to the existing results with the R-matrix method, as well as to the controlled laboratory measurements obtained with the EBIT experiments, and the stellar corona grating spectrum of Capella. The comparison reveals difference of 10-20% for the main emission lines. The discrepancies are much larger for the weaker lines. We expect that the same level of uncertainties should be applied to the calculations of other abundant elements.

4. Conclusion

We are now performing the theoretical calculation of X-ray spectrum of the L-shell emission of Mg, Si, S, Ar, Ca, and Ni, following the successfully example of Fe. We will deliver the new calculation to the SPEX code, which will significantly improve the interpretation of the upcoming XRISM data.

## ５. Schedule and prospect for the future

A follow-up project is proposed in FY2021 to continue the theoretical calculation of the atomic structure. We plan to spend the computing time in the first half year on finishing the cosmic abundant series (Mg, Si, S, Ar, Ca, and Ni) while spending the late half year on the less abundant elements (Al, Ti, Cr, and Mn).

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

## Fiscal Year 2020 List of Publications Resulting from the Use of the supercomputer

### [Paper accepted by a journal]

Gu, L., Shah, C., Mao, J., Raassen, A. J. J., de Plaa, J., Pinto, C., Akamatsu, H., Werner, N., Simionescu, A., et al. X-ray spectra of the Fe-L complex. II. Atomic data constraints from the EBIT experiment and X-ray grating observations of Capella, Astronomy & Astrophysics, 2020, 641, 93

### [Conference Proceedings]

### [Oral presentation]

**Gu, L.** SPEX update and uncertainties on atomic data, AtomDB workshop 2020, US, CfA, 2020-08-04

### [Poster presentation]

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