Usage Report for Fiscal Year 2021

Project Title:

Atomic database for X-ray astrophysics

Name:
○Liyi Gu (1)
Laboratory at RIKEN: (1) **Tamagawa high energy astrophysics laboratory**

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

Atomic constants are central to the accuracy of the X-ray spectroscopy of the hot plasma in astrophysical objects. 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 run a large calculation of the atomic constants (levels, energies, transition probabilities, collision strength, charge exchange rates, etc) for astronomically relevant ions using the flexible atomic code (FAC, a free open source code).

A part of the calculations focus on the L-shell transitions of Mg, Si, S, Ar, Ca, Cr, Mn, Fe, and Ni.
We also worked out the uncertainties of the charge exchange rate coefficients for cosmic abundant elements from H to Zn.

3. Result

The L-shell transition data of Mg, Si, S, Ar, Ca, Fe, and Ni are verified and implemented in the atomic database of the SPEX software.

The new calculation will improve the line emission accuracy of the plasma model to a level of 10-30%. The update model will pave the way to high precision measurements of the temperature and element abundances of the cosmic hot plasmas.

The charge exchange line emission are found to be uncertain on a level of 60%.

4. Conclusion

We have performed the theoretical calculation of X-ray spectrum of the L-shell emission of Mg, Si, S, Ar, Ca, Cr, Mn, and Ni, following the successfully example of Fe. We have delivered the new calculation to the SPEX code, which will significantly improve the interpretation of the upcoming XRISM data. We have also estimated the uncertainties on the present charge exchange model in SPEX.

5. Schedule and prospect for the future

A follow-up project is proposed in FY2022 to continue the theoretical calculation of the atomic constants.
We plan to spend the computing time on the innershell ionization and the transition from the meta-stable levels. If there are spare time, we will also calculate the E- and B- dependent transition rates.

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

Fiscal Year 2021 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

Gu, L., Shah, C., Zhang, R. Uncertainties in Atomic Data for Modeling Astrophysical Charge Exchange Plasmas, 2022, Sensors, 22, 752. doi:10.3390/s22030752

[Conference Proceedings]

[Oral presentation]

Gu, L., SPEX status of spectral model development, 50 years astronomical X-ray spectroscopy, Jan 2022

[Poster presentation]

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