Usage Report for Fiscal Year 2018

Project Title: **Atomic data for next-generation X-ray astrophysics**

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

Atomic database and plasma radiation modeling form one of the bases for modern astronomy, in particular for X-ray spectroscopy. Characterizing the physical state of cosmic plasma requires an entire set of high quality database and modeling. With the rapid advances in observational techniques, the atomic codes now lag behind, hindering the full potential of the new X-ray missions.

This project aims to perform a necessary update of the current atomic database to the level required for the future X-ray missions, such as XRISM (formerly XARM, a collaboration of JAXA/NASA, launch FY2021), through extensive theoretical calculation of the fundamental atomic data.

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 run uses 106,139.1 core-hours in the past FY year. The calculation time is on the same order as the proposed amount (100,000 core-hour) in the application.

3. Result

The current calculation focuses on the collisional excitation (including pure electron-impact and resonant excitations) and dielectronic recombination for Fe XVI to Fe XXIV, all visible in the X-ray spectrum at the Fe-L complex. The new calculation is substantially more complete than the current database in the SPEX atomic code.

https://www.sron.nl/astrophysics-spex

The new calculations are compared to the existing R-matrix results. The two sets of database are consistent within 10-20% for the main transitions. The discrepancies are much larger for the weaker lines. The uncertainties in the atomic database contribute a main component for the systematics in the science outcome of future X-ray missions.

4. Conclusion

The new calculation obtained through the current project will become an important part of the atomic database in the future SPEX code. However, the calculation still needs to be evaluated through well-calibrated laboratory measurements in electron-beam-ion-trap facilities and most accurate astrophysical observations. Furthermore, the project needs to be expanded to a larger coverage of ions (other Fe, O, Ne, Mg, Si, S, Ar, and Ca) that are prioritized in the X-ray band.

5. Schedule and prospect for the future

A follow-up project is proposed in FY2019 to continue the theoretical calculation of the atomic structure. We plan to spend the computing time in the first half year on the other Fe ions and the late half year on the K-shell (and L-shell when applicable) of O, Ne, Mg, Si, S, Ar, and Ca.

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

Fiscal Year 2018 List of Publications Resulting from the Use of the supercomputer

[Paper accepted by a journal]

Gu, L., I. Zhuravleva, E. Churazov, F. Paerels, J. Kaastra, and H. Yamaguchi. X-Ray Spectroscopy of Galaxy Clusters: Beyond the CIE Modeling. Space Sci. Rev., 214:108, October 2018.

[Oral presentation]

Gu, L. "Theory and observational benchmark of atomic database", Athena workshop 2019, Santander, 2019/01/23

Gu, L. "Atomic data and plasma code needed for XRISM and Athena", AtomDB workshop 2018, CfA, 2018/11/01