Usage Report for Fiscal Year 2018

Project Title:

Identification of the excitation in the strongly correlated material

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

In the strongly correlated material, the charge, spin, orbital, and lattice degrees of freedom couple with each other and affect a variety of macroscopic response. Recently, researchers are interested in the excited state when the various degrees of freedom are related. Not only a basic quasi-particle, such as a phonon and magnon, but also quasi-particles related to two or more degrees of freedom draw attention. For understanding these coupled quasi-particles, we have investigated excited states in strongly correlated materials by using neutron, synchrotron X-ray, and visible light. In order to interpret the experimental results obtained by these tools, we need to perform theoretical calculation. In particular, first-principle calculation is expected to provide us the useful information, since we don't have to assume the artificial parameters. In this project, we clarify the phonon dispersion in spinel-type oxide MnV_2O_4 based on the first-principle calculation.

2. Specific usage status of the system and calculation method

We installed the first-principle calculation software called "Abinit". Using this software, we calculate the band structure of the spinel-type oxides. After that, we perform the phonon dispersion by using the software "Phonopy".

3. Result

There are no results shown here.

4. Conclusion

The project is under the progress and thus we cannot conclude the project.

5. Schedule and prospect for the future

We finished installing the required software to perform the first-principle calculation. As a test, we tried performing the band structure calculation of $MgCr_2O_4$ using the source code provided by Dr. Shang Gao in CEMS. Now we confirmed that the calculation could be done without any problem. Therefore, as a next stage, we will try to perform the calculation of MgV_2O_4 and MnV_2O_4.

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

We have just tried several band calculations at this stage, since the project has just started since October last year. We need to optimize the calculated condition.