2020 年度　利用報告書

課題名（タイトル）：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.

In order to understand 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. So far, we succeed in calculating the phonon dispersion by using the shell model, where we use the classical hard sphere model. In particular, first-principles 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-principles calculation.

2．Specific usage status of the system and calculation method

We installed the first-principles calculation software called "Abinit". We optimized the lattice parameters such as lattice constant, atomic coordinates, and so on. Then, we calculate the band structure and move on to the phonon dispersion calculation with the assistance of the software "Phonopy".

3．Result

In the last FY, we tried to calculate the phono dispersion in the spinel-type vanadium oxide MnV_2O_4, but we could not succeed in calculating the phonon dispersion. We consider that this is probably because the orbital degeneracy in V^{3+} ion (S=1) leads to instability of lattice structure. Thus, in this FY, we have calculated the phonon dispersion of $MnCr_2O_4$ by replacing V^{3+} ion (S=1) with Cr^{3+} ion (S=3/2), since Cr^{3+} ion has similar atomic size and thus the phonon dispersion is considered to be close to the MnV_2O_4.

First, we have performed the structural optimization calculation and then have calculated the band structure of $MnCr_2O_4$ within LSDA+U model. By assuming the collinear-antiferromagnetic structure of Mn and Cr ions, the crystal-structure optimization and electronic band-structure calculations have successfully converged.

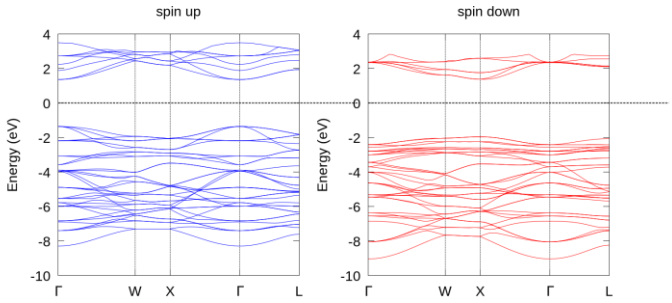

Figure 1: Electronic band structure of $MnCr_2O_4$. Left and right panels show the electronic bands of spin-up and spin-down, respectively.

Figure 1 shows the electronic band structure of $MnCr_2O_4$. The band structure is different between spin-up and spin-down, which suggests that the calculation including electronic correlation successfully works in our calculation.

Next, we proceeded to the phonon dispersion calculation. Figure 2 shows the calculated phonon dispersion with the inelastic x-ray scattering intensity. The negative frequencies never appear in the dispersion, which suggests that the present crystal structure obtained in our assumption should be stable.

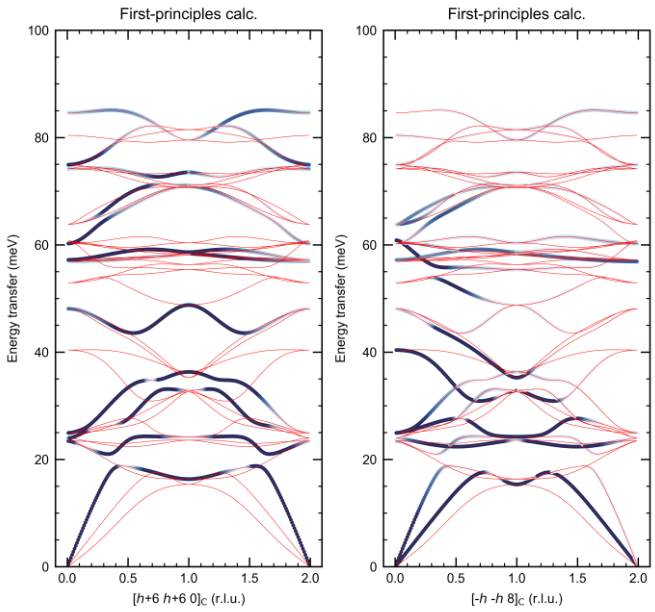

Figure 2: Calculated phonon dispersion of $MnCr_2O_4$. Left and right panels show the phonon bands (red lines) in longitudinal and transverse configurations, respectively. Considering the experimental conditions, the inelastic x-ray scattering intensities (blue) are calculated along [6+h 6+h 0] ($0 \leqq h \leqq 2$) for longitudinal configuration and [-h -h 8] ($0 \leqq h \leqq 2$) for transverse configuration, respectively.

4. Conclusion

We have succeeded in calculating phonon dispersion of $MnCr_2O_4$. We also calculated the inelastic x-ray scattering intensity and inelastic neutron scattering intensity, which can be compared with the experimental results.

5. Schedule and prospect for the future

In the next FY, we would like to challenge the first-principle calculation of MnV_2O_4, using the several software for first-principle calculations. We will compare the present theoretical calculation with the obtained experimental results in more detail. We are also planning to writing the manuscript.