Usage Report for Fiscal Year 2019

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. 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-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

First we calculated the band structure of MnV_2O_4 within LSDA+U model. By assuming the collinear-antiferromagnetic structure of Mn and V ions, the crystal-structure optimization converged.

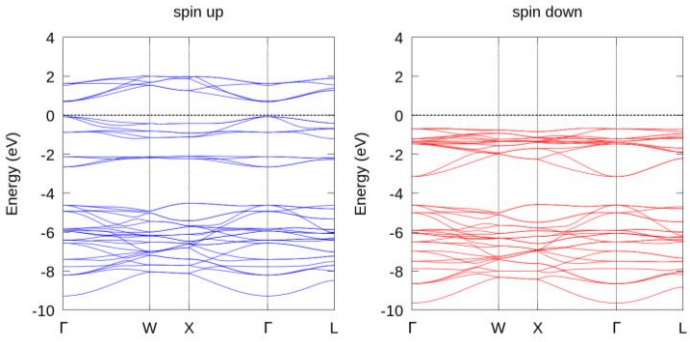

Figure 1: Electronic band structure of MnV_2O_4.

Figure 1 shows that the electronic band structure of MnV_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 proceed to the phonon-dispersion calculation.

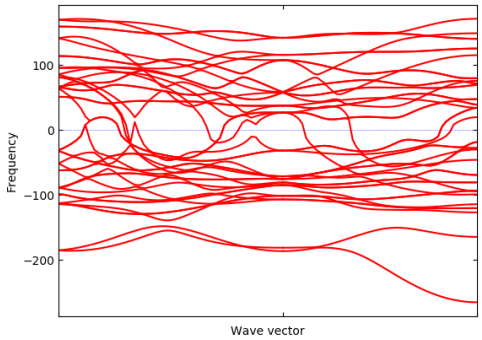

Figure2: Phonon-dispersion of MnV_2O_4

Figure 2 shows the calculated phonon dispersion along X-Γ-L in the present model. At this stage, negative frequencies appear in the phonon dispersion, which indicates that structural instability in our optimized model. In the first-principle calculation, we can get information about the ground state but the ground-state crystal structure of this material is not cubic, thus it might be one of the possibilities in our calculation. We calculate the phonon dispersion for comparing our

calculation with the cubic phase in this material because the assignment of the phonon mode is more easier than the low-symmetry tetragonal phase. But, we need to assume the low-temperature tetragonal phase to exactly perform the first-principle calculation.

4. Conclusion

In the present LSDA+U model in MnV_2O_4, we have not yet succeeded in calculating phonon dispersion, because the negative frequencies appear in the dispersion. This suggests that the present crystal structure obtained in our assumption is unstable.

5. Schedule and prospect for the future

In the next FY, we would like to perform the first-principle calculation assuming the low-temperature tetragonal phase, which should be more stable than the high-temperature cubic phase.