MERIT Internship Program (Domestic) Report

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Host institute

First-Principles Multi-Scale Simulation (FPMS) Team, Research Center for Computational Design of Advanced Functional Materials (CD-FMat), National Institute of Advanced Industrial Science and Technology (AIST)

Outline

I have stayed in Dr. Takashi Miyake's FPMS team in CD-FMat in AIST Tsukuba Central 2 in Tsukuba, Ibaraki for seven weeks. I have never done first-principles calculation before. Therefore, I stayed in this team that has many professional researchers of the first-principles band calculation to learn it. During stay, I acquired skills for the first-principles band calculation and studied strongly correlated electron materials using it.

Research

Strongly correlated electron systems have been intensively studied and there are many kinds of simplified models and their solvers. For quantitative evaluation of each material's functions as practical materials, or for discussion about difference of physical properties between similar materials, however, it is required to perform calculations reflecting materials' detailed features. For this reason, it is suggested that to project band dispersion to low-energy effective models (downfolding method) then to apply solvers to obtained effective models, named MACE (Multi-scale *Ab-initio* scheme for Correlated Electrons).

In this internship program, to acquire skills to elucidate properties of strongly correlated materials by MACE, I learned to use Quantum ESPRESSO, a first-principle band calculation package, Wannier90, a package for calculation of maximally localized Wannier functions from band calculation, and RESPACK, a package for constrained random phase approximation (cRPA) to obtain screened Coulomb interaction and applied these packages to strongly correlated materials and obtained its low-energy effective models. In addition, I introduced

some supporting applications such as WannierTools and cif2cell.

Hereafter I intend to confront obtained models using some solvers and to perform calculation reflecting each material's characters.

Acknowledgement

I really appreciate AIST's acceptation of this internship for seven weeks. Especially I am deeply grateful to Dr. Takashi Miyake for a warm welcome, continuous supports, and band calculation teaching, Dr. Taro Fukazawa, Dr. Nobuya Sato, and Dr. Shotaro Doi for teaching how to use packages, applications and high performance computing such as parallelization, Dr. Hiroki Kato for enjoyable and useful chats and his kindness, Dr. Yoshiyuki Miyamoto, Dr. Seiji Tsuzuki, Dr. Takenobu Nakamura, and Dr. Satoshi Hagiwara for enjoyable lunch time, and Mrs. Harada for continuous supports, procedures, kind guides around AIST. I could have productive and comfortable days in AIST thanks to them. In addition, I would also like to express my gratitude to Prof. Yusuke Kato and Prof. Yukitoshi Motome for agreement with this internship program and introducing me to Dr. Miyake. Finally, I sincerely thank MERIT program and Ms. Asano in MERIT Office for providing this precious opportunity.