MERIT Long-term Overseas Dispatch Report

Period of stay: 2023/1/7~2023/3/17

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Overview

I had the opportunity to stay with Prof. Philipp Werner's group at the University of Fribourg in Switzerland from January 7th, 2023 to March 17th, 2023. This report provides some background information on the dispatch and highlights of my research activities during my stay.

Background information on the dispatch

During my master's program, I conducted a theoretical study on the photoinduced topological phase transition in an organic conductor α-$(BEDT\text{-}TTF)_2I_3$. While my theoretical predictions were based on some approximations such as neglecting interaction terms, I recognized the need to explore new methods like dynamical mean field theory to predict new physical phenomena more precisely. This is why I plan to collaborate with exceptional researchers in computational physics, such as Prof. Philipp Werner, who has expertise in dynamical mean field theory and density functional theory. Such a collaboration would be invaluable for my future research prospects.

Research activities during my stay

Photoinduced phase transitions are attracting intensive interest due to the significant advances in laser technology in recent years. By using Floquet theory, it was shown that a honeycomb lattice irradiated with circularly polarized light undergoes a photoinduced topological phase transition to the Chern insulator [1]. After this pioneering theoretical study, researchers around the world have vigorously conducted theoretical studies on photoinduced topological phase transitions in various materials, such as silicon, transition-metal dichalcogenides, and α-$(BEDT\text{-}TTF)_2I_3$ [2-4].

Theoretical studies on photoinduced topological phase transitions often start with a tight-binding model and consider the effects of light by multiplying the transfer integral

with a Peierls phase. However, it has been shown that in systems with transfers between different orbitals, the contribution from the dipole excitations is also necessary in addition to the effect expressed by the Peierls phase. Most previous studies have ignored this effect, but calculations of transport coefficients using the dynamical mean field theory suggest that the contribution from the dipole excitations is not negligible [5]. Therefore, we investigated the effect of the dipole excitations on photoinduced topological phase transitions in materials with transfers between different orbitals.

We conducted a study on a basic model of monolayer BC_2N, a material of interest in connection with shift currents. Using the model provided by Prof. Michael Schueler, we calculated the Floquet band structure and various physical quantities, including Berry curvature and Berry curvature dipoles, under different driving conditions, both with and without dipole excitations. However, the complete analysis of the model, especially regarding the shift current, has not yet been finished, so we plan to continue this project.

Acknowledgements

After a two-month stay at the University of Fribourg, I gained a deeper understanding of my research topic and had the valuable experience of being in an internationally diverse environment. I am grateful to my supervisor, Professor Masao Ogata, for giving me the opportunity for a long-term overseas assignment, the Japan Society for the Promotion of Science for supporting my travel expenses, Professor Philipp Werner and Assistant Professor Michael Schueler, my collaborators who provided me with assistance and guidance, and to the members of the Werner group and the MERIT program for their hospitality and support.

References

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