# Theoretical and numerical study on novel quantum phenomena in spin-orbit coupled materials

Yukitoshi MOTOME
*Department of Applied Physics,*
*The University of Tokyo, Bunkyo, Tokyo 113-8656*

We have theoretically studied a variety of intriguing phenomena in correlated electron systems with strong spin-orbit coupling. During this fiscal year, we have been making substantial progress on the following topics (project numbers: H30-Ca-0064 and H30-Cb-0014). We have also devoted our efforts to a closely related topic on the Kitaev-type quantum spin liquids (project number: H30-D-0005). We summarize the main achievements for each topic below.

(i) *Magnetielectric effect*: We have performed a systematic study of the magnetic phase diagrams and magnetoelectric responses for a simple model that we constructed for a family of compounds composed of low-symmetric square cupola of Cu $S$=1/2 spins. We compared our theoretical results and the experimental data in collaboration with the experimental groups [1,2]. We have also studied a magnetoelectric effect in a heterostructure of band insulator and ferromagnet [3].

(ii) *Nonreciprocal transport*: We have unveiled nonreciprocal spin Seebeck responses in antiferromagnets on noncentrosymmetric lattices [4]. We have also elucidated a nonreciprocal spin transport in monoaxial chiral magnets, which would be useful as a spin-current diode in spintronics devices [5].

(iii) *Materials design by ab initio calculations*: Based on *ab initio* band calculations and model constructions, we have developed a generic theory for the $e_g$-orbital systems on a honeycomb structure. We found a plethora of peculiar band crossings, such as multiple Dirac nodes, semi-Dirac nodes, quadratic band crossings, and line nodes [6]. We have also proposed new candidate materials of $f$-electron systems for the Kitaev quantum spin liquids [7].

(iv) *Magnetic vortices and skyrmions*: We have clarified that both Neel- and Bloch-type magnetic vortices can appear in spin-orbit coupled metals, by using an effective spin model [8]. We extended the study to itinerant electron models and found interesting magnetic textures by a large-scale simulation [9]. We have also clarified the effect of magnetic anisotropy on the magnetic skyrmions with a high topological number of two [10].

(v) *Kitaev quantum spin liquids*: By using the Majorana mean-field theory, we have found successive phase transitions in the antiferromagnetic Kitaev model while increasing an external magnetic field, where the Majorana fermionic states change their topology in the reciprocal space [11]. Also, upon our theoretical results obtained thus far, we have collaborated with several experimental groups for identifying the signatures of Majorana excitations in the Kitaev magnets: thermal Hall effect [12] and its half-quantization [13], Raman scattering [14], and nuclear quadrupole and magnetic resonances [15]. We have published a second article of our review on this topic [16].

## References


[1] Y. Kato, K. Kimura, A. Miyake, M. Tokunaga, A. Matsuo, K. Kindo, M. Akaki, M. Hagiwara, S. Kimura, T. Kimura, and Y. Motome: Phys. Rev. B **99** (2019) 024415.

[2] K. Kimura, Y. Kato, K. Yamauchi, A. Miyake, M. Tokunaga, A. Matsuo, K. Kindo, M. Akaki, M. Hagiwara, S. Kimura, M. Toyoda, Y. Motome, and T. Kimura: Phys. Rev. Mat. **2** (2018) 104415, *Editors' Suggestion*.

[3] K. N. Okada, Y. Kato, and, Y. Motome, preprint (arXiv:1902.04204), accepted for the publication in Phys Rev. B.

[4] R. Takashima, Y. Shiomi, and Y. Motome: Phys. Rev. B **98** (2018) 020401(R).

[5] S. Okumura, H. Ishizuka, Y. Kato, J. Ohe, and Y. Motome, preprint (arXiv:1903.12358).

[6] Y. Sugita and Y. Motome, Phys. Rev. B **99** (2019) 041101(R).

[7] S.-H. Jang, R. Sano, Y. Kato, and Y. Motome, preprint (arXiv:1807.01443).

[8] S. Hayami and Y. Motome: Phys. Rev. Lett. **121** (2018) 137202, *selected as Cover image*.

[9] K. N. Okada, Y. Kato, and Y. Motome: Phys. Rev. B **98** (2018) 224406.

[10] S. Hayami and Y. Motome: Phys. Rev. B **99** (2019) 094420.

[11] J. Nasu, Y. Kato, Y. Kamiya, and Y. Motome: Phys. Rev. B **98** (2018) 060416(R).

[12] Y. Kasahara, K. Sugii, T. Ohnishi, M. Shimozawa, M. Yamashita, N. Kurita, H. Tanaka, J. Nasu, Y. Motome, T. Shibauchi, and Y. Matsuda, Phys. Rev. Lett. **120** (2018) 217205.

[13] Y. Kasahara, T. Ohnishi, Y. Mizukami, O. Tanaka, S. Ma, K. Sugii, N. Kurita, H. Tanaka, J. Nasu, Y. Motome, T. Shibauchi, and Y. Matsuda, Nature **559** (2018) 227.

[14] Y. Wang, G. B. Osterhoudt, Y. Tian, P. Lampen-Kelley, A. Banerjee, T. Goldstein, J. Yan, J. Knolle, J. Nasu, Y. Motome, S. Nagler, D. Mandrus, and K. S. Burch, preprint (arXiv:1809.07782).

[15] Y. Nagai, T. Jinno, Y. Yoshitake, J. Nasu, Y. Motome, M. Itoh, and Y. Shimizu, preprint (arXiv:1810.05379).

[16] 求 幸年, 那須 譲治: 固体物理 **53** (2018) 305.