

786th ASRC Seminar

Date: June 25 (Thursday), 13:30~14:30

Location: Meeting room 103, ASRC bldg.

Speaker: Dr. Guang-Yu Guo

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CEMS,RIKEN Center)

Title: From Large Spin Hall Metal to Topological Chern Insulator:
Materials Discovery through First Principles Calculations

Abstract:

Today, quantum-mechanics-based first-principles calculations have become a powerful tool in materials research, thanks to advanced theories, numerical algorithms and modern computers. In particular, they prove indispensable to understand intricate phenomena occurring in materials, to search for new materials and to design novel functional materials. In this talk, I will present our own discoveries in solid state and materials physics, through development and application of first-principles calculations. These discoveries include (a) theoretical finding and experimental confirmation of the sophisticated iron *d*-orbital ordering in magnetite [1-2], thus solving a seventy year old classical problem in solid state physics, (b) demonstration of no exact cancellation of spin and orbital Hall conductivities in hole-doped semiconductors [3], (c) finding of the largest intrinsic spin Hall effect in platinum metal [4] which is now widely used as generator and detector of spin current in spintronic research, (d) proposal of multi-orbital Kondo effect in iron-doped gold whose resonant skew scattering leads to the gigantic observed spin Hall angles [4-5], and more recently, (e) discovery of exotic quantum topological Hall phase [an unconventional quantum anomalous Hall (or Chern insulating) phase] caused by nontrivial topology of the magnetic structure in chiral antiferromagnetic potassium rhodium dioxide [6], instead of the conventional one by the simultaneous occurrence of relativistic spin-orbit coupling and ferromagnetism.

[1] H.-T. Jeng, G. Y. Guo, and D. J. Huang, Phys. Rev. Lett. 93, 156403 (2004).

[2] D.J. Huang et al., Phys. Rev. Lett. 96, 096401 (2006).

[3] G. Y. Guo, Y. Yao and Q. Niu, Phys. Rev. Lett. 94, 226601 (2005).

[4] G. Y. Guo et al, Phys. Rev. Lett. 100, 096401 (2008).

[5] G. Y. Guo, S. Maekawa, and N. Nagaosa, Phys. Rev. Lett. 102, 036401 (2009).

[5] B. Gu et al., Phys. Rev. Lett. 105, 086401 (2010).

[6] J. Zhou et al., Phys. Rev. Lett. 116, 256601 (2016).

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