

Abstract:

**From Large Spin Hall Metal to Topological Chern Insulator, Materials Discovery
through First Principles Calculations**

Guang-Yu Guo (郭光宇)

Department of Physics, National Taiwan University, Taipei 10617, Taiwan

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.

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Brief Bio :

Guang-Yu Guo is currently a Distinguished Professor of National Taiwan University (NTU) and also a National Chair Professor of the Ministry of Education. He received his PhD from Cambridge University, UK in 1987. He joined the NTU Physics Faculty in 1998 after working in Daresbury Laboratory, UK for eleven years as a postdoc, higher and senior staff scientist. He also worked in National Chengchi University as a chair professor and the founding director of the Graduate Institute of Applied Physics during 2009-2013. He has been vigorously conducting research in condensed matter and materials physics in the past twenty-nine years, publishing over 200 journal papers with nearly 5000 citations and h-index of around 40. He has won several academic awards and honors including the National Science Council Outstanding Research Awards (1998, 2004, 2009) as well as the Ministry of Education 57th Academic Award (2013) and 19th National Chair Professorship (2015). He is an elected Fellow of the PSROC (2005), APS (USA) (2005) and Institute of Physics (UK) (2013).