Seminar

Hidden spin polarization in materials with inversion symmetry: causes and consequences

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Abstract

Spin polarization in nonmagnetic materials is a textbook effect associated with spin-orbit coupling and the *global* absence of inversion symmetry. We note, however, that the relativistic spin-orbit interaction is anchored primarily on atomic nuclear sites and should thus be primarily sensitive to *site point-group* asymmetries, rather than *bulk space-group crystal asymmetry*. In centrosymetric crystals the spin bands are degenerate in *E* vs *k* *momentum space*, but this does not mean that the spins are mixed in *position space*. In contrast, we find and validate via first-principles calculations that in centrosymmetric materials with non-centrosymmetric site symmetries (such as MoS_2, $LaOBiS_2$, or Bi_2Se_3) there is a ***nonzero local spin polarization*** even though the ***total*** spin is zero. Such real-space spin-polarizations are normally hidden by compensation effect, rather than being intrinsically absent, and are already verified by upcoming experiments.

This understanding leads to the recognition that a previously overlooked hidden form of spin polarization should exist in a much broader class of 3D bulk solids that own global inversion symmetry, and thus open the possibility to provide new routines for manipulating electron spins. The concept of hidden spin polarization also explains many previously embarrassing observations of apparent polarization noted in centrosymmetric systems that by common understanding should not have existed.

About the Speaker

Dr. Qihang Liu is currently a research associate in University of Colorado, Boulder, working with Prof. Alex Zunger. He received his bachelor and PHD degree in School of Physics, Peking University at 2007 and 2012, respectively. Before joining University of Colorado, Boulder, he was a postdoctoral fellow in Prof. Arthur J. Freeman's group in Northwestern University. Qihang is engaged in the field of theoretical condensed matter physics of real materials, using fundamental, first-principles quantum mechanics. His research mainly includes a two-way approach. One is to understand and predict properties of materials – electrical, optical, magnetic and topological – as they emerge from the defining attributes of materials. The other one is the "inverse problem", i.e., to predict the type of materials that would have the target property being predetermined already.