CQSE Special Seminar

Weekly Seminar
Sep. 11, 2014 (Thursday)

TIME   Sep. 11, 10:30am
TITLE   Anisotropic multipolar exchange interactions in systems with strong spin-orbit coupling
SPEAKER   Mr. Shu-Ting Pi
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PLACE   Rm716, CCMS & New Physics Building, NTU

Abstract

We introduce a theoretical framework for computations of anisotropic multipolar exchange interactions found in many spin-orbit coupled magnetic systems and propose a method to extract these coupling constants using a density functional total energy calculation. This method is developed using a multipolar expansion of local density matrices for correlated orbitals that are responsible for magnetic degrees of freedom. Within the mean-field approximation, we show that each coupling constant can be recovered from a series of total energy calculations via what we call the "pair-flip" technique. This technique flips the relative phase of a pair of multipoles and computes the corresponding total energy cost associated with the given exchange constant. To test it, we apply our method to uranium dioxide, which is a system known to have pseudospin J=1 superexchange induced dipolar, and superexchange plus spin-lattice induced quadrupolar orderings. Our calculation reveals that the superexchange and spin-lattice contributions to the quadrupolar exchange interactions are about the same order with ferro and antiferromagnetic contributions, respectively. This highlights a competition rather than a cooperation between them. Our method could be a promising tool to explore magnetic properties of rare-earth compounds and hidden-order materials.

Reference:

Phys. Rev. Lett. **112**, 077203