Joint CQSE and CASTS Seminar

Weekly Seminar
Jun. 15, 2012 (Friday)

TIME	Jun. 15, 14:30 ~ 15:30
TITLE	Spin crossover in Earth materials and complex oxides
SPEAKER	Prof. Han Hsu
	Department of Physics, National Central University
PLACE	Rm716, CCMS & New Physics Building, NTU

Abstract

The total electron spin of a transition-metal ion in a crystalline solid can vary with many factors, including temperature, pressure, and strain. Such a phenomenon, known as spin-state crossover (or spin crossover), has great technological potentials, as it allows artificial control of materials' magnetic properties. Not as widely known, spin crossover also plays a crucial role in geophysics. In the Earth interior, as pressure and temperature increase with depth, the total electron spin of iron incorporated in Earth minerals changes accordingly, which leads to elastic anomalies in the host minerals and suggests a possible source of seismic anomalies in the Earth's lower mantle (660-2890 km depth). While spin crossover in ferropericlase [$(Mg_{1-x}Fe_x)O$], which constitutes ~20 vol% of the lower mantle, is well understood, spin crossover in iron-bearing magnesium silicate ($MgSiO_3$) perovskite, the *major* mineral phase (~75 vol%) in the same region, has been highly controversial.

Complex oxides also exhibit controversial spin crossovers. A classic example is lanthanum cobaltite ($LaCoO_3$). While the thermally induced spin crossover of bulk $LaCoO_3$ has been intensively studied, its detailed mechanism has been unclear and highly debated for more than four decades. Recently, strain-induced ferromagnetism in thin-film $LaCoO_3$ has been discovered. It has also attracted great attention, but its detailed mechanism has been unclear, too.

In this talk, I will present our research on perovskite $MgSiO_3$ and $LaCoO_3$, showing how these long-standing controversies can be clarified via first-principles calculations. I will also show that first-principles calculations, in combination with experimental techniques that probe nuclear quadrupole interactions, such as Mössbauer or nuclear magnetic resonance (NMR) spectroscopy, can solve spin problems in different scientific disciplines.