

**Subject:** MS Colloquium- 12/1/05-Wu 212/A-157  
**From:** Nancy Sanchez <sanchez@anl.gov>  
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**Corrected Posting**

**MATERIALS SCIENCE COLLOQUIUM**

**SPEAKER:** Professor Ruqian Wu  
University of California, Irvine

**TITLE:** Density Functional Studies of Innovative Magnetic Materials

**DATE:** Thursday, December 1, 2005

**TIME:** 11:00 a.m.

**PLACE:** Building 212, Room A157

**HOST:** David Keavney

Refreshments will be served at 10:45 a.m.

**Abstract:** It has been increasingly recognized in many fields of materials science that state-of-the-art ab initio electronic structure calculations based on the density-functional theory have been enormously successful. Synergistic applications of theory and experiment have been demonstrated repeatedly to become a "must" to further advance our microscopic understanding in anomagnetism. I will discuss results of our recent work on magnetic systems, including magnetic surfaces, magnetic semiconductors and nanoentities, particularly, using x-ray absorption and magnetic circular dichroism. High-quality agreements with experimental data indicate the reliability of DFT calculations for the determination of many physical properties.