Speaker: Sophie F. Weber

Title: "Surface Magnetization in Antiferromagnets from Symmetry Considerations and First-Principles Calculations"

Abstract: We use a combination of symmetry analysis and density functional theory calculations to examine how a finite magnetization density on certain surface planes can arise in materials which have bulk antiferromagnetic order. The theoretical prediction and subsequent experimental verification of a roughness-insensitive magnetization on the (001) surface of magnetoelectric chromia has already attracted a great deal of attention in recent years. The magnetoelectric effect allows a bulk antiferromagnetic domain to be switched using electric fields in a constant magnetic field, and the surface magnetization, the sign of which couples directly to the bulk domain, serves as a readily detectable probe of the magnetization state. In some cases, surface magnetisation can even occur on planes which appear to be magnetically compensated, via a ferromagnetic canting or an imbalance in sublattice magnetization. However, an equilibrium surface magnetization is not limited to magnetoelectric antiferromagnets with broken inversion and time-reversal symmetries. Expanding on previous arguments [K.D. Belashchenko, PRL 105 (2010)], we provide a detailed symmetry categorisation of antiferromagnets which can posses equilibrium magnetisation on certain surfaces, as well as distinguishing properties of the surface magnetization based on bulk symmetries. We discuss potential bulk symmetry indicators for surface magnetization which can be calculated via first-principles. We then present density functional theory calculations for magnetically compensated surfaces using slab geometries and constrained magnetism; these calculations support the symmetry analysis that such crystal planes, although compensated in the bulk, develop a finite magnetic moment when a vacuum-terminated surface is introduced.