

## Abstract of Presentation

Presentation Title:

**Ferroic materials and novel functionalities**

Abstract :

Ferroic materials, which show simultaneous ferroelectric and magnetic ordering, exhibit unusual physical properties and promise new device applications as a consequence of the coupling between their dual order parameters. The talk is a review of recent progress in ab initio description and microscopic understanding of high-quality thin-film oxides, which allow tailoring of their properties through epitaxial strain, atomic-level engineering and interfacial coupling. This is a prerequisite for their incorporation in practical devices.

On the basis of first-principles electronic-structure calculations we predict that epitaxial multiferroic films fabricated as ultrathin Fe films deposited on TiO<sub>2</sub>-terminated (001) surfaces of ATiO<sub>3</sub> perovskites (A = Pb, Ba) exhibit an unexpected change of their magnetic structure with increasing Fe-film thickness. The magnetic order changes from ferromagnetic, with a magnetization of about 3  $\mu_B/\text{atom}$  for the 1-monolayer system, to ferrimagnetic with almost vanishing magnetization upon deposition of a second Fe layer. Ferromagnetic order is restored for thicker Fe films but with significantly reduced magnetization as compared to Fe bulk. The effect is understood in terms of hybridization of electronic states and geometric structure. The magnetoelectric coupling affects the size of the magnetic moments moderately, a spin-reorientation transition is not found.