Integrated Materials Design Centre Seminar

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Ab Initio Design of Multifunctional Perovskite Superlattices

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Date: **Tuesday, 9th June 2015**
Time: **11:00 pm – 12.00 pm**
Venue: Room M10, Chemical Engineering (Building F10)

Abstract
When layers of perovskite oxides are epitaxially stacked to form a periodically repeated heterostructure, new intriguing functionalities can emerge in the resulting superlattice. Such heterostructures can undergo abrupt phase transformations under the application of electric fields, mechanical stresses and temperature variations, and thus are attractive for nanoelectronics and energy conversion applications. The remarkable tunability of superlattices often is rationalized in terms of epitaxial strains, electrostatic coupling, and local interface effects. First-principles methods have been of invaluable help in rationalizing and guiding the experimental efforts towards the synthesis of novel materials with enhanced multifunctionalities. However, *ab initio* modelling of perovskite superlattices remains yet challenging due to the existence of internal varying electric fields and polar discontinuities.

In this talk, I will present a general first-principles approach for predicting the behaviour of oxide-based superlattices in an effective and systematic way. Such a formalism combines constrained electric displacement strategies with a rigorous description of interface polarity. As a proof of concept I apply my formalism to $[PbTiO_3]_m/[BiFeO_3]_n$ heterostructures and show how interface terminations with different nominal charge can radically change the overall ferroelectric properties of the superlattice, leading to the stabilization of otherwise inaccessible bulk phases.

Biography
Claudio Cazorla is an ARC Future Fellow in the School of Materials Science and Engineering in UNSW Australia. Previously, he was a JAE-DOC Fellow in the Institute of Materials Science of Barcelona (Spain). His primary research interest is the application and development of computer simulation techniques to understand and predict new oxide-based and inorganic materials for nanoelectronics and energy applications.