Contribution ID : **34** Type : **not specified**

Rational design of multiferroic superlattices

Multiferroics, materials that typically display ferroelectricity and magnetism, have generated a tremendous flurry of interest in recent years due to their fundamental complexity and potential for applications in nano-electronics and energy conversion. Finding in nature single-phase compounds with those properties, however, has proved extremely difficult. Such a scarcity of bulk multiferroic materials has motivated researchers to investigate oxide-based materials in thin film and superlattices geometries where i) the properties of the ferroelectric can be tuned almost at will by choosing an appropriate substrate lattice parameter, (ii) the electrostatic coupling between different oxide layers can be exploited, and iii) interfaces, rather than the oxide itself, can show novel multi-functional properties which are absent in either of the bulk constituents. In the development of this field first-principles simulations have played a major role, leading to the present situation in which theory often leads the way to new devices.

In this talk, I will present a general first-principles approach to predict the behavior of perovskite oxide superlattices based exclusively on the properties of their individual bulk constituents. Such a formalism combines constrained electric displacement strategies with a rigorous description of interface polarity. As a result, a clear separation between genuine interface and bulk effects is possible. Crucially, the present method allows one to quantify straightforwardly the impact that interface polarity has on the equilibrium (and metastable) phases of a superlattice. As a proof of concept I apply this formalism to [PbTiO3]m/[BiFeO3]n heterostructures and show that (i) earlier first-principles predictions obtained in ultrashort-period superlattices with explicit supercell simulations are accurately reproduced, and (ii) by assuming interface terminations with different nominal charge, radical changes in the overall ferroelectric properties of the superlattice are disclosed that lead to the stabilization of otherwise inaccessible bulk phases.

Primary author(s) : Dr CAZORLA, Claudio (School of Materials Science and Engineering, UNSW Australia)

Presenter(s) : Dr CAZORLA, Claudio (School of Materials Science and Engineering, UNSW Australia)