MAR15-2014-020329

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Revealing and understanding the behavior of structural domain walls from first principles[1]

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Ferroelectric and ferroelastic domain walls (DWs) are becoming the focus of renewed excitement. Modern experimental techniques permit an unprecedented control on domain structures, and it is now possible to produce materials with a large volume fraction occupied by the DWs themselves. Also, recent experiments show that DWs can display distinct properties not present in the domains, which suggests the possibility of using the walls themselves as the functional *material* in nano-devices. In this talk I will review recent projects in which we have used theory and first-principles simulation to reveal and explain a variety of DW-related effects. The presentation will include the formation of novel two-dimensional crystals at the DWs of a ferroelastic material, the occurrence of ferroic orders (ferroelectric, ferromagnetic) confined at the DWs of various compounds, and cases in which peculiar (and useful) response and switching properties relie on existence of a multi-domain state. I will also summarize experimental evidence for most of these incredible findings, which clearly ratify domain and domain-wall engineering as a powerful strategy to obtain novel functional nano-materials. // Work done in collaboration with many researchers, the main ones being: J.C. Wojdeł (ICMAB-CSIC), C. Magén (INA at U. Zaragoza), M. Mostovoy (U. Groningen), P. Zubko (U. College London), as well as the groups of Beatriz Noheda (U. Groningen), R. Ramesh (UC Berkeley) and J.-M. Triscone (U. Geneva).

[1]Supported by MINECO-Spain.

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