MAR13-2012-020537

Abstract for an Invited Paper for the MAR13 Meeting of the American Physical Society

Proper, improper and hybrid improper ferroelectricity in oxide perovkites and related compounds PHILIPPE GHOSEZ, University of Liège

Ferroelectricity in oxide perovskites and related compounds has been a topic of intensive research for more than 60 years. Recently, the coupling of the ferroelectric mode with other structural distortions has attracted an increasing interest since it offers promising and still widely unexplored possibilities to couple ferroelectricity with other functional properties and even to produce unusual phenomena. In this context, the trilinear coupling between ferroelectric and oxygen rotational modes in naturally occuring and artificial layered perovskites appeared as a practical way to produce unusual dielectric properties or achieve enhanced magneto-electric coupling. Here, I will first briefly reintroduce the concepts of proper, improper and hybrid improper ferroelectricity, highlighting how to rationalize better the concept of improper ferroelectricity. I will contrast the intrinsic behavior of these three classes of compounds in ferroelectric capacitors. Taking then the prototypical example of BiFeO3/LaFeO3 superlattices, I will illustrate how hybrid improper ferroelectricity and trilinear mode coupling is a promising route to potentially achieve electric switching of the magnetization. Finally, considering the case of PbTiO3/SrTiO3 superlattices, I will discuss how to access from first-principles the phase-transition sequence and finite temperature properties of complex systems combining various structural instabilities, which still remains a challenging issue.