MAR11-2010-001414

Abstract for an Invited Paper
for the MAR11 Meeting of
the American Physical Society

Ferroelectric vortices from atomistic simulations[1]

LAURENT BELLAICHE, University of Arkansas

In 2004, the use of a first-principles-based effective Hamiltonian [1] led to the prediction of a novel structure in zero-dimensional ferroelectrics, in which the electric dipoles organize themselves to form a vortex [2]. Such structure exhibits the so-called spontaneous toroidal moment, rather than the spontaneous polarization, as its order parameter [2]. Subsequently, various original phenomena, all related to vortices, were predicted in ferroelectric nanostructures. Examples of such phenomena are: (i) the existence of a new order parameter, denoted as the hypertoroidal moment, that is associated with many complex dipolar structures (such as double-vortex states) [3]; (ii) the possible control of single and double vortex states by electric fields, via the formation of original intermediate states [4-8]; (iii) the discovery of a new class of quantum materials (denoted as incipient ferrotoroidics), for which zero-point vibrations wash out the vortex state and yield a complex local structure [9]; (iv) the existence of chiral patterns of oxygen octahedral tiltings that originate from the coupling of these tiltings with the ferroelectric vortices [10]. The purpose of this talk is to discuss some of these striking phenomena, as well as, to reveal others (if time allows). These studies are done in collaboration with A.R. Akbarzadeh, H. Fu, I. Kornev, I. Naumov, I. Ponomareva, S. Prosandeev, Wei Ren and D. Sichuga.

[1] L. Bellaiche, A. Garcia and D. Vanderbilt, Phys. Rev. Lett. 84, 5427 (2000).
[2] Ivan I. Naumov, L. Bellaiche and Huaxiang Fu, Nature (London) 432, 737 (2004).
[3] S. Prosandeev and L. Bellaiche, Phys. Rev. B 77, 060101(R) (2008).
[4] S. Prosandeev, I. Ponomareva, I. Kornev, I. Naumov and L. Bellaiche, Phys. Rev. Lett. 96, 237601 (2006).
[5] I. Naumov and H. Fu, Phys. Rev. Lett. 98, 077603 (2007).
[6] S. Prosandeev and L. Bellaiche, Phys. Rev. Lett. 101, 097203 (2008).
[7] S. Prosandeev, I. Ponomareva, I. Kornev, and L. Bellaiche, Phys. Rev. Lett. 100, 047201 (2008).
[8] I. Naumov and H. Fu, Phys. Rev. Lett. 101, 197601 (2008).
[9] S. Prosandeev, A. R. Akbarzadeh and L. Bellaiche, Phys. Rev. Lett. 102, 257601(2009).
[10] David Sichuga, Wei Ren, Sergey Prosandeev, and L. Bellaiche, Phys. Rev. Lett. 104, 207603 (2010).

[1]These works are supported by the NSF grants DMR 0701558 and DMR-0080054 (C-SPIN), DOE grant DE-SC0002220, and ONR grants N00014-08-1-0915 and N00014-07-1-0825 (DURIP).