Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Vortex-antivortex structures in $PbTiO_3/SrTiO_3$ superlattices[1]
JAVIER JUNQUERA, PABLO GARCíA-FERNÁNDEZ, Universidad de Cantabria, PABLO AGUADO-PUENTE, CIC-Nanogune, JORGE ÍÑIGUEZ, Luxembourg Institute of Science and Technology — When ultrathin ferroelectric layers of $PbTiO_3$ are embedded in superlattices with an incipient ferroelectric, such as $SrTiO_3$, the interplay between elastic, electrostatic, and gradient energies produce complex patterns of the electrical polarization. In particular, nanometer scale of vortex-antivortex arrays have been recently detected,[2] and exotic properties such as the emergence of a negative capacitance have been measured.[3] A realistic atomic simulation of these structures is difficult due to the large number of atoms required and the small differences in energies between the relevant phases. Here we use a recently developed second-principles method [3, 4] that treats all the lattice degrees of freedom with high accuracy at a modest computational cost. The effect of the periodicity, strain, temperature, and external electric fields in the formation of vortex-antivortex pairs is explored. We predict that some of the structures are chiral, that would make them optically active, supporting x-ray circular dichroism.

[1]Financial support from MINECO Grant No. FIS2015-64886-C5-2-P
[2]Yadav *et al.*, Nature **530**, 198 (2016)
[3]P. Zubko *et al.*, Nature **534**, 524 (2016)
[4]J. Wojdel *et al.*, J. Phys.: Condens. Matter **25**, 305401 (2013)

Javier Junquera
Universidad de Cantabria

Date submitted: 12 Nov 2016 Electronic form version 1.4