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### **Unusual phenomena in ferroelectric nanostructures<sup>1</sup>**

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First-principles based computations are nowadays capable of tackling really complex challenges of fundamental and technological importance. For example, a dipole vortex structure has been discovered, by means of these methods, in isolated nanoparticles of ferroelectrics –which may lead to a new generation of efficient nanoscale memory devices [1]. Here, we use first-principles-based approaches to address the following issues: (i) what are the elastic signatures and field characteristics of dipole vortices in isolated ferroelectric nanodots? (ii) how to control the chirality of such dipole vortices (which is an important challenge to solve for future applications)? and (iii) what are the possible ground states of arrays of ferroelectric dots embedded in a crystal lattice? Regarding item (i), we found that the tetragonal axial ratio in the vortex state is lower than 1 (unlike in “normal” ferroelectric or antiferrodistortive phases), and that the electric field produced by the dipole vortex outside the dot oscillates in space when changing the polar angle of the cylindrical coordinate system. Such features can serve as fingerprints of the vortex state to experimentally confirm the existence of such unusual state. Moreover, we demonstrate that, and explain why, using inhomogeneous electric fields is an efficient solution to item (ii) [2]. Finally, it is predicted that array of embedded dots can adopt new phases, depending on the temperature and difference in polarizability between the dots and medium [3]. Atomistic details of such phases, as well as their governing mechanisms, will be provided.

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[1] I. Naumov, L. Bellaiche, & H. Fu. “Unusual phase transitions in ferroelectric nanodisks and nanorods,” *Nature* 432, 737 (2004).

[2] S. Prosandeev, I. Ponomareva, I. Kornev, I. Naumov, & L. Bellaiche. “Controlling toroidal moment by means of an inhomogeneous static field: an ab initio study,” *Phys. Rev. Lett.* 96, 237601-1-4 (2006).

[3] S. Prosandeev & L. Bellaiche. “Properties of ferroelectric nanodots embedded in a polarizable medium: atomistic simulations,” *Phys. Rev. Lett.* 97, 167601 (2006).

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