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Interaction between ferroelectric nanodots: a first-principles-based study S. PROSANDEEV[1], I. PONOMAREVA, I. NAUMOV, I. KORNEV, L. BELLAICHE, UNIVERSITY OF ARKANSAS TEAM — We have performed Monte-Carlo simulations within a first- principles-based effective Hamiltonian approach to investigate the consequences (if any) of the interaction between nanodots made of lead titanium zirconate. We found that two dots under open circuit electrical boundary conditions weakly interact with each other, implying that they both adopt a vortex structure for their dipoles that is very similar to the one occurring in a single isolated dot. The situation is dramatically different if the first dot is polarized (e.g., by being under an external field) while the second dot is still under open circuit condition. In that case, the dots interact stronger, with this interaction causing the development of a relatively small spontaneous polarization in the second dot and, more importantly, being able to influence the direction of the toroid moment in this second dot – which is of technological importance. We further show how this last interaction, and its consequences, depend on the geometry and shape of the two dots, and reveal that all the striking features can be well understood within a multipole expansion of the field produced by the lattice polarization vortex in the free dot. This work is supported by DOE grant DE- FG02-05ER46188, by ONR grants N00014-01-1-0365, N00014-04-1- 0413 and N00014-01-1-0600, and by NSF grants DMR-0404335 and DMR-9983678.

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