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Ferroelectric instabilities in $CaTiO_3$ nanoparticles from first principles SHEN LI, KARIN RABE, Department of Physics and Astronomy, Rutgers the State University of New Jersey, Piscataway, NJ 08854, USA — Ferroelectric instabilities of nanoparticles are expected to be markedly different from those of the bulk material. In many cases, ferroelectricity could be weakened or suppressed, although there is no clear reason why this should always be the case. Previous first-principles studies have shown that in bulk cubic CaTiO3, the polar instability is suppressed by the stronger oxygen octahedron-rotational instabilities, yielding a nonpolar ground state. To investigate the possibility that the nanoparticle configuration could weaken or eliminate the octahedron rotation, we performed first-principles calculations for a single-unit-cell cluster, containing one oxygen octahedron, using a real-space pseudopotential density-functional-theory method (PARSEC). For an electrically isolated cluster, the symmetric nonpolar state is found to be stable. However, if the depolarization field produced by a polar distortion of the cluster is screened, a lower-symmetry polar distorted structure becomes more favorable, so that the cluster can be considered ferroelectric. Our results are consistent with the recent findings regarding the central importance of compensation of the depolarization field in the ferroelectricity of perovskite oxide thin films and nanostructures.

Shen Li
Department of Physics and Astronomy, Rutgers the State University
of New Jersey, Piscataway, NJ 08854, USA

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