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Spontaneous polarization in one-dimensional $Pb(ZrTi)O_3$ nanowires[1] IVAN NAUMOV, HUAXIANG FU, Department of Physics, University of Arkansas — Formation of spontaneous polarization in one-dimensional structures is the key phenomenon that reveals collective behaviors in systems of reduced dimension, but has remained unsolved for decades. Here we report *ab initio* studies on finite-temperature structural properties of infinite-length nanowires of $Pb(Zr_{0.5}Ti_{0.5})O_3$ solid solution. Whereas existing studies have ruled out the possibility of phase transition in 1D chains, our atomistic simulations demonstrate an unambiguous otherwise. We show that phase transitions in 1D wires occur on a remarkable macroscopic length scale, but not necessarily on an infinite length scale as assumed in the general theories of 1D phase transition. Such phase transitions are chracterized by large longitudinal d_{33}, χ_{33} responses and a large c/a strain. The long rang ordering in PZT nanowires is explained by use of depolarizing effects associated with finite thickness of wires. Our results suggest no fundamental constraint that limits the use of ferroelectric nanowires and nanotubes arising from the absence of spontaneous ordering.

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