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**Vortex polarization instabilities in $PbTiO_3$ nanowires** GHANSHYAM PILANIA, R. RAMPRASAD, University of Connecticut — The possibility of circular, toroidal or vortex-like ordering (closure domains) of magnetic spin vectors have been considered, and their existence versified, in the past. Recent experimental and computational (based on effective Hamiltonian simulations) work have contributed to the mounting evidence for the presence of such vortex-like domains of electric polarization vectors in ferroelectric nanostructures. Here, for the first time using parameter-free ab initio density functional theory (DFT) based computations, we show the existence of such a vortex polarization state in $PbTiO_3$ [001] nanowires. Our computations involved relaxed and axially strained free-standing $PbTiO_3$ [001] nanowires with varying sidewall terminations and diameters. While stress-free nanowires with their sidewalls terminated by PbO surfaces displayed purely axial rectilinear polarization at all sizes, the $TiO_2$-terminated nanowires, at a critical diameter of 16 Å, display a vortex polarization transverse to the nanowire axis. Moreover, we predict the existence of novel stress-induced phase transitions between the vortex and the rectilinear polarization states in both the PbO- and $TiO_2$-terminated nanowires. Normal mode vibrational frequency analysis of these nanowires further confirms these results.

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