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Vortex polarization, strain induced phase transitions and dielectric response in ultra-thin $PbTiO_3$ nanowires from first principles[1] GHANSHYAM PILANIA, R. RAMPRASAD, University of Connecticut — Nature of ferroelectricity in nanostructures and the resulting dielectric response are of both fundamental and applied interest. Here, using density functional theory (DFT) based computations, we investigate polarization configurations as a function of axial strain in ultra-thin $PbTiO_3$ [001] nanowires. Our computations involved relaxed and axially strained free-standing nanowires with varying sidewall terminations and diameters. While stress-free nanowires with their sidewalls terminated by PbO surfaces displayed purely rectilinear axial polarization at all sizes, the TiO_2-terminated nanowires, at a critical diameter of 16 Å, display a non-rectilinear vortex polarization transverse to the nanowire axis. We discuss the origins of such behavior. We also predict the existence of novel stress-induced phase transitions between the mutually exclusive vortex and the axial polarization states in both the PbO- and TiO_2-terminated nanowires. Normal mode vibrational frequency analysis of these nanowires further confirms these results. Furthermore, by employing density functional perturbation theory in combination with effective medium dielectric theory we calculate dielectric permittivity of the ferroelectric nanowires and compare it with the corresponding bulk results.

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