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Ab initio study of ferroelectricity in quantum-confined nanostructures GHANSHYAM PILANIA, RAMAMURTHY RAMPRASAD, University of Connecticut — In the present ab initio study, we have employed density functional theory to investigate the size dependence of ferroelectric properties of BTO quantum wires and quantum dots. In the case of quantum wires, the ferroelectric well depth was calculated as a function of size. We find that the ferroelectric well depth corresponding to bulk BTO is recovered in quantum wires with diameters larger than 1 nm. Analysis of the decomposed density of states indicates that the central BTO unit behaves bulk like, whereas the peripheral units result in defect states in the band gap (with density depending on facet terminations). Complex polarization patterns were also observed, and were strong functions of the surface termination of the nanostructures. For instance, in non-stoichimetric quantum wires with all surface facets terminated with TiO2, strong axial polarization was dominant. However, in BaO terminated quantum wires, polarization in the "shell" region is radial, while in the "core" region the polarization is axial. The BTO quantum dots that were studied displayed even more complex polarization patterns, reminiscent of the "vortex" patterns anticipated earlier based on effective hamiltonian calculations.

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