Abstract Submitted
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Density functional study of ferroelectric-electrode interfacial effects on the stability of ferroelectricity in thin-films[1] WISSAM A. AL-SAIDI , University of Pennsylvania, ALEXIE KOLPAK, Yale University, ILYA GRINBERG, ANDREW RAPPE, University of Pennsylvania — Ferroelectric (FE) thin-films are very promising materials for various technological applications. The continuous demand of miniaturization of devices based on FE thin-films by the micro-electronic industry demands an understanding of the critical thickness of ferroelectricity in thin films. Using an ab initio density-functional approach, we study the properties of several capacitor-like structures which are based on PbTiO3 and BaTiO3 ferroelectric materials. Different electrodes are used in our study to gain a thorough understanding of the electrode-ferroelectric interfaces, and the role of the interfacial chemical bonding and charge transfer in stabilizing the FE polar phase. We finally used our ab initio results to develop a phenomenological predictive model based on a Landau-Ginzburg-Devonshire functional.

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