Abstract Submitted
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Ab initio study of a symmetric SrRuO3/PbTiO3/SrRuO3 ferroelectric capacitor[1] SIMON DIVILOV, Stony Brook University, JUDITH GABEL, University of Wuerzburg, MATTHEW DAWBER, MARIVI FERNANDEZ-SERRA, Stony Brook University — We performed a density functional study of the free standing capacitor $(SrRuO_3)_1/(PbTiO_3)_m/(SrRuO_3)_1$ using local density approximation and Hubbard U to study the effects of $SrRuO_3$ [100] surfaces on the bulk properties of $PbTiO_3$. In addition we analyze how the thickness, epitaxial strain and termination plane of $PbTiO_3$ modify its bulk behavior. We observe different rumpling patterns for both paraelectric (PE) and ferroelectric (FE) phases, based on the termination plane. For the FE phase, we observe oxygen octahedra tilting dominated by in phase and out of phase tilts around the [100] axis. In all our simulations the $SrRuO_3$ layers remain metallic, even those at the open surfaces.An analysis of Schottky barriers and coupling between magnetism and ferroelectricity will be presented.

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