

Abstract Submitted  
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**Role of interface termination in SrRuO<sub>3</sub>/PbTiO<sub>3</sub>/SrRuO<sub>3</sub> capacitors under epitaxial strain**<sup>1</sup> SIMON DIVILOV, MARIVI FERNANDEZ-SERRA, MATTHEW DAWBER, State Univ of NY- Stony Brook — We perform a DFT analysis of (SrRuO<sub>3</sub>)<sub>1</sub>/(PbTiO<sub>3</sub>)<sub>m</sub>/(SrRuO<sub>3</sub>)<sub>1</sub> with varying PbTiO<sub>3</sub> using both LDA and LSDA+U. The goal of the study is to analyze the effects of symmetrical termination along the [001] plane on the magnetic and electric properties of SrRuO<sub>3</sub> and PbTiO<sub>3</sub>, respectively. We observe the electrical polarization of the thin film is highly sensitive to the termination plane, as compared to the bulk. In addition, the termination plane determines the oxygen octahedra tilting (OOT) pattern in the thin film, although the OOT are not coupled to the polarization. Despite having a single layer of SrRuO<sub>3</sub>, we observe a magnetic polarization dependent on the termination. Our results show the importance of *ab initio* calculations in the presence of a rich parameter space to aid experiments in synthesis of superlattice and thin film capacitors.

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