

Abstract Submitted
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Structure of SrTiO₃ thin films grown on Si¹ C. STEPHEN HELLBERG, Naval Research Lab, KRISTOPHER ANDERSEN, Naval Research Lab — Although SrTiO₃ films on Si have been extensively studied, the structure of the interface is not yet known. We present first-principles density-functional calculations of the energetics of the numerous proposed structures for the interface. We find that the energetically favored structure is one that has not been previously considered. The structure is consistent with x-ray and TEM probes of the interface. We discuss the implications of the interface for device applications.

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