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First Principles Theory of Sub-Monolayer Strontium on Silicon (001) KEVIN GARRITY, Yale University Department of Physics, JAMES REINER, FREDERICK WALKER, CHARLES AHN, SOHRAB ISMAIL-BEIGI, Yale University Department of Applied Physics — Conventional attempts to continue transistor scaling consistent with Moore's law will soon result in unacceptable quantum mechanical leakage currents across the dielectric oxide layer. One promising solution to this problem is to replace the current silicon dioxide layer with a thicker crystalline oxide with a higher dielectric constant, grown epitaxially on silicon. Although there has been progress in growing high quality epitaxial interfaces for some materials, the initial stages of growth, including the deposition of the initial metal layer, are not well understood. Using *ab initio* density functional theory, we study the initial stages of the deposition of strontium titanate on silicon (001), a good model system due its successful epitaxial growth. We present the binding energies of several new low energy structures with sub-monolayer converages of strontium which differ significantly from the conventional view of this surface. Additionally, to include finite temperature effects, we calculate vibrational free energies. We compare our results to experimental samples grown by molecular beam expitaxy.

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