Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

**First Principles Phases of Sub-Monolayer Sr and La on Si (001)**[1]
KEVIN GARRITY, J.W. REINER, F.J. WALKER, C.H. AHN, S. ISMAIL-BEIGI, Yale, CRISP, CRISP TEAM — The epitaxial integration of complex oxides with semiconductors is a key requirement for many emerging technologies. In the short term, the scaling down of the dielectric layer in current CMOS technology will soon require new materials with higher dielectric constants to prevent quantum mechanical leakage currents. More generally, the epitaxial integration of complex oxides with semiconductors would allow new devices to take advantage of the wide range of oxide properties. To date, the first step of the only known method to grow complex oxides on silicon epitaxially has required 1/2 ML of an alkaline earth metal, usually Sr, to be deposited on a clean silicon surface at about 600 C. Using first-principles density functional theory calculations, we examine the growth of sub-monolayer coverages of both Sr and La on Si (100). For Sr on Si, we report on a novel 1/6 ML structure which explains the complex temperature dependence observed experimentally below 1/2 ML Sr. We compare these results to the case of La on Si and elucidate some differences which hinder the growth of epitaxial oxides on La template layers. Our results predict an experimentally verified low temperature path to epitaxy using a Sr template layer.

[1]Supported primarily by NSF MRSEC DMR 0520495.

Kevin Garrity
Yale

Date submitted: 17 Dec 2008 Electronic form version 1.4