

Abstract Submitted  
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**Band offsets of SrTiO<sub>3</sub> thin films grown on Si<sup>1</sup>** KRISTOPHER ANDERSEN, C. STEPHEN HELLBERG, Naval Research Laboratory — SrTiO<sub>3</sub> is a promising material to replace SiO<sub>2</sub> as the gate dielectric in metal-oxide-semiconductor field-effect transistors (MOS-FETs). The advantage of SrTiO<sub>3</sub> is its large dielectric constant: an order of magnitude greater than other promising oxides. However, the negligible conduction band offset found experimentally for heterostructures of SrTiO<sub>3</sub> (001) grown on Si (001) limits the usefulness of SrTiO<sub>3</sub> in devices because of leakage current. Here we present first-principles calculations on Si/SrTiO<sub>3</sub> heterostructures and investigate ways to modify the band offsets. Experimentally motivated structures are considered, and the effects of dopants and defects on the electronic structure are quantified.

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