Abstract Submitted
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A generalized diffraction approach to predict the coupling of interface structure and function with lattice displacements[1] F. J. WALKER, J. W. REINER, A. M. KOLPAK, Y. SEGAL, D. KUMAH, CRISP, Yale University, Z. ZHANG, Argonne National Laboratory, APS, S. ISMAIL-BEIGI, C. H. AHN, CRISP, Yale University — Abrupt changes in symmetry, bonding and structure strongly affect functional behavior at oxide-semiconductor interfaces. In this talk, we consider specific examples of crystalline BaO and $SrTiO_3$ deposited on Si. Charge transfer at the interface between the oxide and semiconductor is found using synchrotron x-ray diffraction. This charge movement couples to optical modes in the BaO and $SrTiO_3$ layers. This effect extends deep into the films because the polarization of the optical mode is not effectively screened in the insulating BaO and $SrTiO_3$ layers. Differences in atomic displacements between the BaO and $SrTiO_3$ thin films result in a polarization that alternates sign in the case of BaO, as opposed to a uniform polarization in $SrTiO_3$. These differences impact on the electronic properties of the system, including how the semiconductor and oxide bands align.

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Fred Walker
CRISP, Yale University

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