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Atomic and Electronic Structure of SrTiO₃/GaAs Hetero-Interfaces¹ QIAO QIAO, WERONIKA WALKOSZ, SERDAR OGUT, ROBERT KLIE, University of Illinois at Chicago — Metal-oxide semiconductor interfaces have received much attention in recent years due to their potential applications in metal-oxide-semiconductor field-effect transistors. In this study we examine the atomic and electronic structures of epitaxial SrTiO₃[100] thin films on GaAs[001] using atomic-resolution Z-contrast imaging and electron energy loss spectroscopy in combination with first principles calculations to develop a fundamental understanding of the interfacial structure-property relationships. We will demonstrate that it is energetically favorable for SrO layer of SrTiO₃ to be in direct contact with the terminating As layer of GaAs, as opposed to the TiO₂ layer. However, the model with the simplest 1x1 surface unit cell is not in agreement with the photoemission data.² First principles total energy calculations will be used to consider how different GaAs(001) surface reconstructions are modified in the presence of SrTiO₃ to find the low-energy semiconducting interface. ²Y. Liang et al., *Appl. Phys. Lett.*, **86** (8), 082905 (2005).

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