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Thermodynamic stability and band alignment at SrTiO3/GaAs(001) interface[1] JOELSON COTT, RAVI DROOPAD , BYOUNGHAK LEE, Texas State University, TX 78666, USA. — The successful epitaxial growth of SrTiO3 on Si showed that it is possible to integrate the functional oxides with semiconductors incorporating unique multifunctional properties of oxides into various existing semiconductor technologies. While SrTiO3 has been also deposited on GaAs without amorphous interfacial layers, the exact interface structure has been controversial; On one hand, scanning Transmission Electron Microscopy (STEM) shows As atoms at the interface. X-ray photoelectron spectroscopy (XPS) measurements, on the other hand, do not show peaks associated with As-O bonding, indicating that the GaAs/STO interface does not involve an As/oxide layer, contradicting to STEM observations. Using ab initio calculations, we determine the interfacial structure of a SrTiO3 film on a GaAs substrate to help clarify the apparently discrepancy between the XPS and the STEM measurements. The calculations reveal that, under the condition that allows atomically abrupt interfaces, the energetically most stable interface is As/Sr/TiO2 structure, in accordance with both XPS and STEM measurements. We discuss the band offsets and the possibility of in-gap states of various interface structures.

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Joelson Cott
Texas State University, TX 78666, USA.

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