

Polarization Effects on the Interfacial Conductivity in the LaAlO₃/SrTiO₃ Heterostructure: First-Principles Study

Maziar Behtash, Safdar Nazir, Yaqin Wang, and Kesong Yang*

*Department of NanoEngineering, University of California, San Diego, 9500 Gilman
Drive, Mail Code 0448, La Jolla, CA 92093-0448, USA*

*E-mail: kesong@ucsd.edu, Tel: +1-858-534-2514

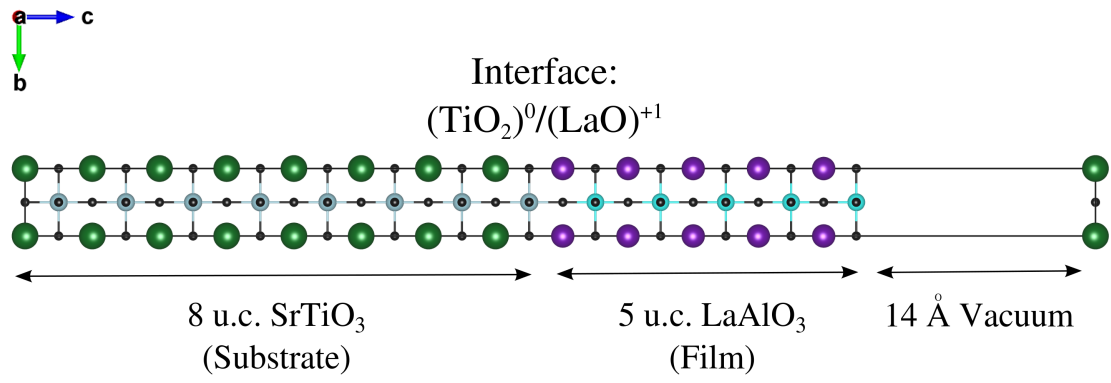


Figure S1: Structural model of the $\text{LaAlO}_3/\text{SrTiO}_3$ (LAO/STO) heterostructure (HS)-based slab system.

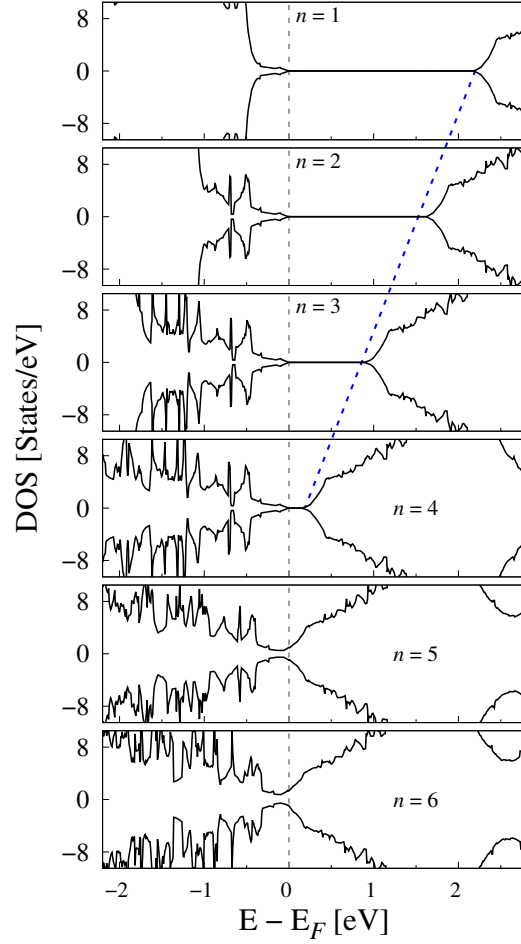


Figure S2: Calculated total DOS of the unstrained (LAO)_{*n*}/STO (*n*=1-6) HS-based slab systems. The vertical black dashed line indicates the Fermi level at 0 eV. The dashed blue line is plotted as a guide of eye.

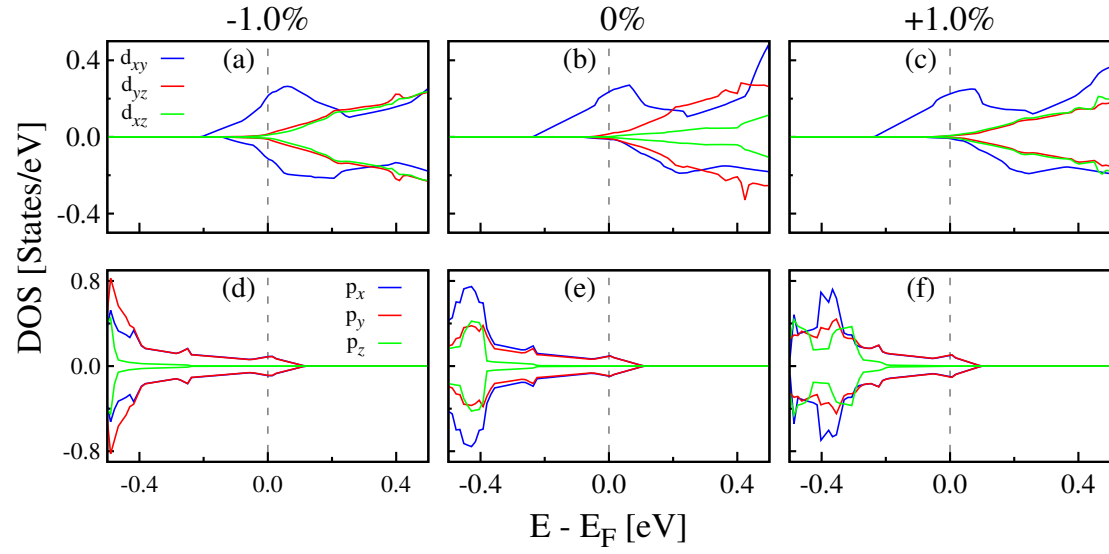


Figure S3: Calculated layer-resolved DOS of the Ti 3d orbitals from interfacial (IF-I) TiO₂ layers in the STO substrate and O 2p orbitals from AlO₂ surface layers for -1%, 0%, and +1% uniaxially strained (LAO)₅/STO HS-based slab systems.

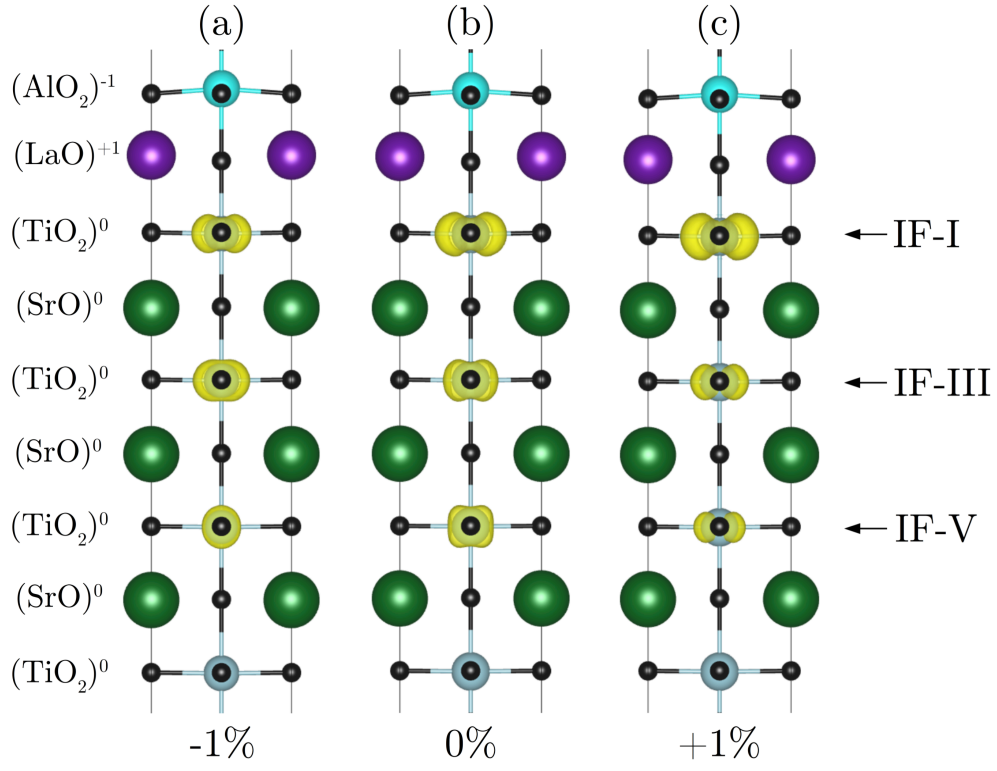


Figure S4: Calculated charge density projected on the bands forming the 2DEG in the $(\text{LAO})_5/\text{STO}$ HS-based slab systems with -1% (a), 0% (b), and $+1\%$ (c) uniaxial strains.