Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First-Principles Prediction of Two-Dimensional Electron Gas Driven by Polarization Discontinuity in Nonpolar/Nonpolar AHfO3/SrTiO3 (A=Ca, Sr, and Ba) Heterostructures[1] JIANLI CHENG, Univ of California - San Diego, SAFDAR NAZIR, University of Sargodha, KESONG YANG, Univ of California - San Diego

— By using first-principles electronic structure calculations, we explored the possibility of producing two-dimensional electron gas (2DEG) in nonpolar/nonpolar $AHfO_3/SrTiO_3$ (A = Ca, Sr, and Ba) heterostructures (HS). Two types of interfaces, AO/TiO_2 and HfO_2/SrO, each with AO and HfO_2 surface terminations, are modeled, respectively. The polarization domain and resulting interfacial electronic property are found to be more sensitive to the surface termination of the film rather than the interface model. As film thickness increases, an insulator-to-metal transition (IMT) is found in all the HS with HfO_2 surface termination: for AO/TiO_2 interfaces, predicted critical film thickness for an IMT is about 7, 6, and 3 unit cells for $CaHfO_3/SrTiO_3$, $SrHfO_3/SrTiO_3$, and $BaHfO_3/SrTiO_3$, respectively; for HfO_2/SrO interfaces, the critical film thickness is about 7.5, 5.5, and 4.5 unit cells, respectively. In contrast, for the HS with AO surface termination, only $CaHfO_3/SrTiO_3$ exhibits an IMT with a much larger critical film thickness about 11 - 12 unit cells. This work is expected to stimulate further experimental investigation to the interfacial conductivity in the nonpolar/nonpolar $AHfO_3/SrTiO_3$ HS.

[1]National Science Foundation and Department of Defense National Security Science and Engineering Faculty Fellowship

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Date submitted: 03 Nov 2016 Electronic form version 1.4