Interface Energetics and Charge Carrier Density Amplification by Sn-Doping in LaAlO₃/SrTiO₃ Heterostructure

Safdar Nazir, Jianli Cheng, Maziar Behtash, Jian Luo, and Kesong Yang*

Department of NanoEngineering, University of California, San Diego, 9500 Gilman Drive, Mail Code 0448, La Jolla, California 92093-0448, United States

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

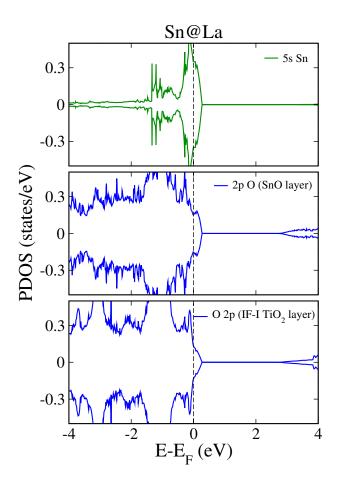


Figure 1S. Calculated spin-polarized partial Sn 5s (at SnO layer) and O 2p (at SnO and IF-I TiO₂ layer) Density of States (DOS) for Sn@La doped (LAO)₆/STO HS system.

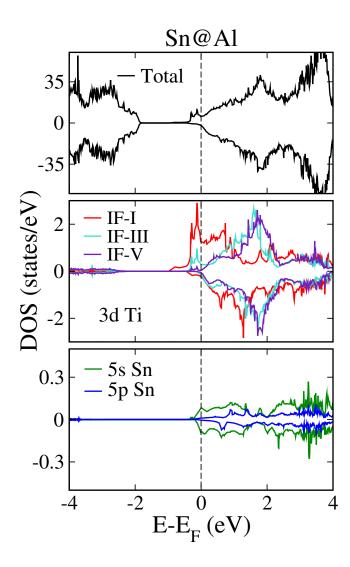


Figure 2S. Calculated spin-polarized total, partial Ti 3d and Sn 5s/5p DOS for Sn@Al doped (LAO)₆/STO HS system. Herein, U=0 eV for Ti 3d orbital and U=7.5 eV for La 4f orbital were used.