Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Polar-nonpolar Oxide heterostructures for photocatalysis
HONGLI GUO, Department of Physics, University of Science and Technology of China, JIN ZHAO, Department of Physics, University of Science and Technology of China, The International Center for Quantum Design of Functional Materials, WISSAM SAIDI, Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania, 15261, United States — The discovery of two-dimensional electron gas (2DEG) at the interface of polar $LaAlO_3$ (LAO) and non-polar $SrTiO_3$ (STO) open the research field of layered oxide heterostructures. In this study, we propose new application of oxide heterostructures for photocatalysis. We take a sandwich-like heterostructure STO/LAO/STO as an example and prove it to be a promising photocatalyst which is active for near-infrared light. Because the sandwiched LAO is polarized and generates a build-in electrostatic field, the valance band and conduction band locates on two opposite STO surfaces. First principles calculations prove that the band gap is reduced and the absorption of near-infrared to visible light is improved distinctly. Simultaneously, the build-in electric field in LAO accelerates the electrons and holes into opposite directions, preventing the recombination, and generates an electron doped surface and a hole doped STO surface, which could be used for H_2O reduction and oxidation separately. Our study gives a new perspective into the applications of oxide heterostructures in solar energy conversion.

Hongli Guo
University of Science and Technology of China

Date submitted: 12 Nov 2014 Electronic form version 1.4