Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics. This journal is © the Owner Societies 2016

Supporting Information

High-Mobility Two-Dimensional Electron Gas in SrGeO₃- and BaSnO₃-Based Perovskite Oxide Heterostructures: *Ab-initio* Study

Yaqin Wang, a, b Wu Tang, Jianli Cheng, Safdar Nazir, and Kesong Yang*b

^aState Key Laboratory of Electronic Thin Films and Integrated Devices, University of Electronic Science and Technology of China, Chengdu 610054, P. R. China.

^bDepartment of NanoEngineering, University of California, San Diego, 9500 Gilman Drive, La Jolla, California, 92093-0448, United States

*E-mail: <u>kesong@ucsd.edu</u>. Tel: +1-858-534-2514.

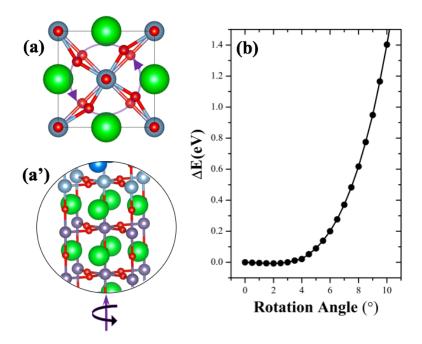


Figure S1. Scheme of LaAlO₃/SrGeO₃ heterostructure with GeO₆ and AlO₆ rotations from (a) top view and (a') slide view, and (b) calculated total energy difference ΔE as a function of the rotation angle. ΔE is calculated relative to the total energy of non-rotated structure. All AlO₆ cages in the film and two GeO₆ cages near the interface are rotated.