Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Magnetic order and structural phase transition in strained ultrathin $SrRuO_3/SrTiO_3$ superlattice[1] MINGQIANG GU, XIAOSHAN WU, Nanjing University, GUOPING ZHANG, Indiana State University — Strain is one of the key parameters to control the properties of functional materials in fabrication. With first-principles simulations, we find for the first time that $SrRuO_3/SrTiO_3$ superlattice undergoes robust phase transitions with the in-plane lattice strain ranging from -4.5% to 6%. In the high tensile strain region, the magnetic ordering among neighboring Ru ions changes from a ferromagnetic to an antiferromagnetic phase, together with a metal-to-Mott-insulator transition, a unique character in our superlattice which is absent in the bulk. On the other hand, in the low strain region, the suppression of the octahedra tilting was also observed. The driving force of the suppression of tilting was investigated and found to be the charge redistribution in the Sr-O plane. All of these are important to the strategy of controlling the structural, electronic and magnetic properties in Ru-based perovskite systems.

[1]This work was supported by NKPBRC (2010CB923404) and NNSFC (Nos. 10974081,10979017).

Mingqiang Gu
Nanjing University

Date submitted: 11 Nov 2011 Electronic form version 1.4