Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Metal-insulator transition and emergence of spontaneous polarization in $(La_{1-x}Sr_xMnO_3)_m/(LaNiO_3)_n$ superlattices constructed from metallic building blocks[1] SAURABH GHOSH, Vanderbilt University, Oak Ridge National Laboratory, USA, ROHAN MISHRA, Washington University in St. Louis, USA, JASON HOFFMAN, ANAND BHATTACHARYA, Argonne National Laboratory, USA, ALBINA Y. BORISEVICH, Oak Ridge National Laboratory, USA, SOKRATES T. PANTELIDES, Vanderbilt University, USA — $La_{0.7}Sr_{0.3}MnO_3$ and $LaNiO_3$ are metallic oxides. However, short-period superlattices of the form $(La_{0.7}Sr_{0.3}MnO_3)_m$ $/(LaNiO_3)_n$ show insulating behavior depending on m and n. In particular, the insulating property is robust when $m = n = 2$ (SL 2/2). Here, using first-principles density functional theory (DFT) and DFT+U (static $d - d$ Coulomb interaction), we explain the experimental observation and discuss a general mechanism that underlies such metal-insulator transition for different m and n. The general mechanism is based on the finding that disproportionation on Ni sites is the key. Further, we predict that insulating SL 2/2 is ferroelectric with large spontaneous polarization. The ferroelectric distortion persists in the cases where the superlattices are metallic, which leads to the possibility of designing a new family of 'polar metals'. Finally, we discuss the origin of such polar distortion and its coupling with the magnetic properties (by considering spin-phonon coupling) of the material.

[1]This work is supported by DOE Grant number DE-FG02-09ER46554 and DOE BES DMSE

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Date submitted: 02 Dec 2015 Electronic form version 1.4