Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Influence of quantum confinement and strain on orbital polarization of strained four-layer $LaNiO_3$ superlattices: a DFT+DMFT study[1]
HYOWON PARK, University of Illinois at Chicago, ANDREW MILLIS, CHRIS MARIANETTI, Columbia University — Here we use the combination of density functional theory and dynamical mean field theory to study Ni d orbital polarization in strained $LaNiO_3/LaAlO_3$ superlattices consisting of four layers of nominally metallic NiO_2 and four layers of insulating AlO_2 separated by LaO layers. The layer-resolved orbital polarization is calculated as a function of strain and analysed in terms of structural, quantum confinement, and correlation effects. The overall dependence of orbital polarization on strain in superlattices is qualitatively consistent with recent X-ray absorption spectroscopy and resonant reflectometry data. However, interesting differences of detail are found depending on the sign of strain. Under tensile strain, the two inequivalent Ni ions display orbital polarization similar to that calculated for strained bulk $LaNiO_3$ and observed in experiment. Compressive strain produces a larger dependence of orbital polarization on Ni position and even the inner Ni layer exhibits orbital polarization different from that calculated for strained bulk $LaNiO_3$. The quantum confinement effect is as important as the strain effect and more stronger for tensile strain.

[1]This work is supported by DOE ER-046169 and FAME, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA.

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Date submitted: 06 Nov 2015 Electronic form version 1.4