MAR15-2014-020270

Abstract for an Invited Paper
for the MAR15 Meeting of
the American Physical Society

Emergent Phenomena in Oxide Superlattices from DFT+DMFT[1]

CHRIS MARIANETTI, Columbia Univ

Density functional theory plus dynamical mean-field theory (DFT+DMFT) has proven to be an instrumental tool in describing transition metal-oxides, and DFT+DMFT is well poised to search the rich phase space of oxide superlattices for emergent phenomena. In this talk, we focus on double-perovskite heterostructures of the form $AA'BB'O_6$. Our two separate goals are to design new ferroelectric Mott insulators and high temperature ferromagnetic Mott insulators. In the context of ferroelectric Mott insulators, we demonstrate the ability to design in-plane ferroelectrics based upon transition metal charge transfer and A/A' cation size mismatch, harnessing displacements of both the A-site and B-site. In the context of ferromagnetic Mott insulators, we detail the different mechanisms for obtaining high temperature ferromagnetic Mott states, and we present new candidates for high temperature ferromagnetic insulators. Finally, we discuss the prospect of coupling magnetic and ferroelectric states in addition to potential applications.

[1]The authors acknowledge support from FAME, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA.