Electronic mechanism for ferroelectricity and strong magneto-electric coupling in charge-ordered multiferroics

GERARDO ORTIZ, LEONID ISAEV, Indiana University Bloomington, CRISTIAN BATISTA, T-4, LANL — We study magneto-electric phenomena in multiferroic materials, which exhibit ferroelectricity due to the charge ordering. Using rare-earth iron oxides as an example, we derive an effective model, which takes into account the Coulomb interaction, magnetic superexchange and spin-orbit effects, and is consistent with the recent X-ray absorption spectroscopy measurements in multiferroic LuFe$_2$O$_4$. Then we demonstrate, how the interplay between quantum fluctuations and geometric frustration stabilizes the charge and ferrimagnetic spin orderings. The strong coupling, due to the double-exchange mechanism, between these orders, leads to a large magneto-electric response. Our results provide a complete physical description of the magneto-electric properties of charge-ordered multiferroics.