MIP: PARADIM at Cornell University, DMR-1539918
Local User Project - 2020

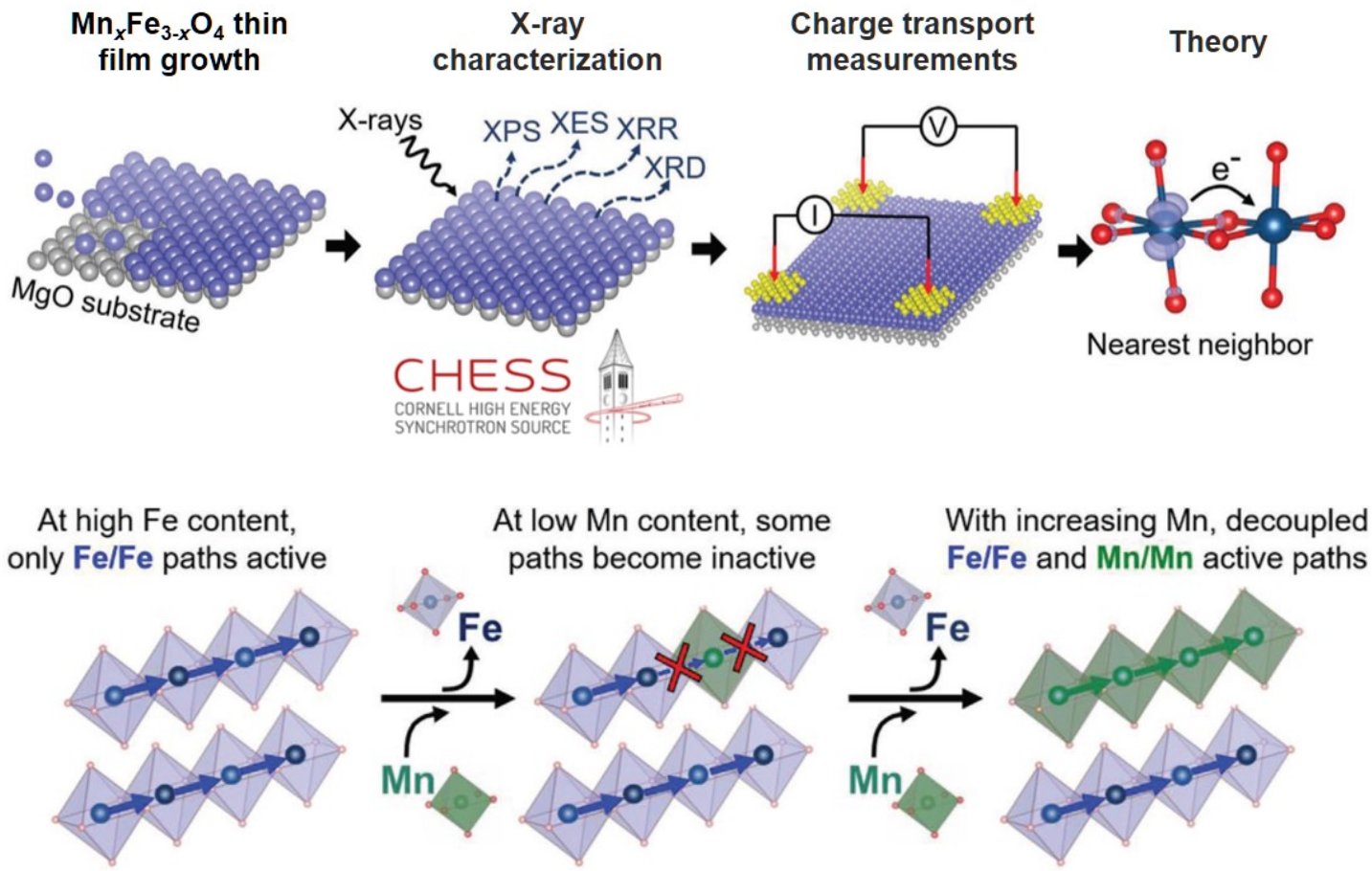
A Classic Model for Oxides gets a much-needed Update

R.D. Robinson, L.F. Kourkoutis, and D.G. Schlom, Cornell University
M. Caspary Toroker, Technion – Israel Institute of Technology

Metal oxides—also known as ceramics—are commonly used as insulators. Nonetheless, depending on their composition, they do transport electric currents. To model the electronic transport, scientists often rely on a sixty-year-old model, developed for oxides with only one cation type (binary oxides). Unfortunately, this model fails to correctly describe electronic transport for ternary or more complex oxides.

Users of PARADIM put the classic model to a rigorous test. They used PARADIM's unique synthesis capabilities to prepare single crystals starting from a well-studied binary oxide, Fe_3O_4. Additional $Mn_xFe_{3-x}O_4$ crystals, with higher amounts of Mn incorporated, were prepared without change of the crystal structure. The distribution of atoms within each crystal was determined at PARADIM's Electron Microscopy facility and CHESS, an NSF-funded research center. By studying the electronic transport in this series of $Mn_xFe_{3-x}O_4$ crystals, the classic model was shown to not accurately reproduce the measurements for the ternary oxide.

Advanced theoretical simulations and modeling revealed that electricity travels between alike sites—here along distinct Fe or Mn pathways. By revising the classic model to include such transport channels and the ability to jump between transport channels, a new model that accurately describes the transport measurements and is applicable to ternary oxides was born.



A. Bhargava *et al.*, *Adv. Mater.* (2020) doi.org/10.1002/adma.202004490.