

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Trends of semiconductivity in 3d oxides¹ STEPHAN LANY, NREL
— Open shell transition metal oxides are usually described as Mott insulators, which are often viewed as being disparate from semiconductors. Based on the premise that the presence of a Mott gap and semiconductivity are not mutually exclusive, this work reviews electronic structure calculations on the binary 3d oxides, so to distill trends and design principles for semiconducting transition metal oxides. This class of materials possesses the potential for discovery, design, and development of novel functional semiconducting compounds, e.g., for energy applications. This presentation gives an overview for the band-structure trends of 3d oxides with special attention on the hybridization between the 3d crystal field symmetries with the sp bands, and on how this interactions affect the effective masses and the likelihood of self-trapping of electrons or holes.

¹Supported by DOE-SC-BES as part on an Energy Frontier Research Center.

Stephan Lany
NREL

Date submitted: 14 Nov 2014

Electronic form version 1.4