Design of Semiconducting Tetrahedral $Mn_{1-x}Zn_xO$ Alloys

Scientific Objective

Design a novel semiconducting transition metal oxide alloy with absorption in the visible and with favorable electron and hole transport properties.

Potential Significance and Impact

Realization of a new semiconductor material with potential application for solar water-splitting and demonstration of the potential of materials design beyond equilibrium.

Details

- Background: Good semiconducting properties are desirable but rare to find among transition metal oxides.
- Methods: Electronic structure theory and combinatorial thin-film synthesis and characterization using pulsed laser deposition (PLD).
- Results: Structure transition from rock salt (RS) to wurtzite (WZ) above x = 0.3, non-equilibrium phase diagram, band gaps, carrier transport mechanism, n-type doping, and band lineup.

H. Peng, P. Ndione, D.S. Ginley, A. Zakutayev, S. Lany, (submitted). Work was performed at the National Renewable Energy Laboratory and supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Energy Frontier Research Centers, under Contract No. DE-AC36-08GO28308 to NREL.

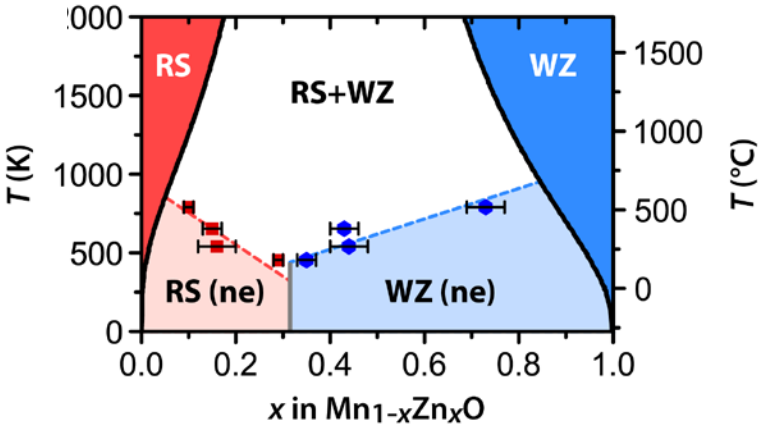

Fig. 1: Calculated equilibrium (solid lines and dark colors) and experimental non-equilibrium phase diagram (data points and light colors) for PLD growth.

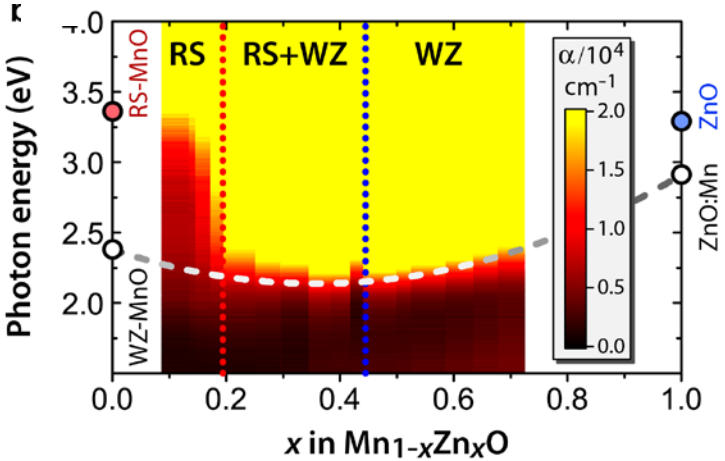

Fig. 2: Measured absorption coefficient α (contour plot) and calculated band gaps (circles and dashed line).