Abstract Submitted
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Development of $(MnO)_{1-x}(ZnO)_x$ Alloys for Water Splitting Applications[1] PAUL NDIONE, EMILY WARREN, HAOWEI PENG, STEPHAN LANY, DAVID GINLEY, ANDRIY ZAKUTAYEV, National Renewable Energy Lab — Using high throughput combinatorial synthesis, measurement and analysis methodologies, we rapidly investigate the composition related structural, optical, and electrical properties of $(MnO)_{1-x}(ZnO)_x$ alloys and identify candidates materials for a more detailed study in PEC applications. The $(MnO)_{1-x}(ZnO)_x$ thin films are synthesized using combinatorial pulsed laser deposition with continuous orthogonal gradients in both chemical composition and substrate temperature. The solubility limit of ZnO into MnO is determined using the disappearing phase method and found to decrease with increasing temperature. For example, $(MnO)_{1-x}(ZnO)_x$ deposited at 300 C exhibit only the tetrahedral wurzite (WZ) structure instead of the rocksalt (RS) one at x>0.4. Optical measurements indicate the strong reduction of the optical band gap associated with the RS to WZ transition, and are consistent with the first-principles theory prediction of E_{gap} =2.1 eV at a x=0.5 alloy composition. The values of the electrical conductivity for the Ga-doped $(MnO)_{1-x}(ZnO)_x$ samples deposited at 300 C from a 4% Ga-doped ZnO target are determined to be <2 S/cm and 100 S/cm for the RS and WZ structure respectively per atom of Ga. These results suggest that Ga-doped MnO-ZnO alloys present a promising materials system for water oxidation in a PEC cell.

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