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Band-Gap Tuning in Perovskite-type Ferroelectric $ZnSnO_3$ by Doping and Core-Shell Approach for Solar Cell Applications CORISA KONS, ANUJA DATTA, Florida Cluster for Advanced Smart Sensor Technologies and Department of Physics, University of South Florida, PRITISH MUKHERJEE, Center for Integrated Functional Materials and Department of Physics, University of South Florida — Ferroelectric (FE) perovskite materials are an emerging class of potential absorbers in next generation solar cells due to their spontaneous polarization which facilitates electron-hole separation and drive charge carriers at opposite ends. With a large remnant polarization of $\approx 59\ \mu C/cm^2$, perovskite-type $LiNbO_3$ (LN)-$ZnSnO_3$, containing earth abundant elements is of much interest as a high performance solar absorber. However, the wide band-gap in $ZnSnO_3$ (~ 3.7 eV) is unsuitable to absorb the broad solar range, which can be overcome by band-gap engineering. Here, we discuss band-gap tuning through substitutional doping (Sb, Cu, Ca, Ba) in LN-type $ZnSnO_3$ nanorods, synthesized by a facile solvothermal process. A band-gap as low as 2.5 eV was obtained in 5 at.% Ca doped $ZnSnO_3$ nanorods showing superior FE properties. The current-voltage ($I - V$) measurements under light revealed multiple orders of enhancement as compared to the dark. The band-gap in $ZnSnO_3$ is also found to be a strong function of the lattice constant which is tuned by introducing a slight strain through lattice mismatching using a core shell approach. A detailed structural, optical, and FE analyses are provided to predict the future of this technologically important material in next generation FE photovoltaics.

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