Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Zinc stannate as a solar cell material BRIAN KOLB, ALEXIE KOLPAK, Massachusetts Inst of Tech-MIT — Semiconducting ferroelectric materials are attractive as solar absorbers because they have a built in polarization that facilitates electron-hole separation and can drive carriers to opposite ends of the device. $ZnSnO_3$ is an exciting material that has recently been shown to be ferroelectric with a relatively large (50 $\mu C/cm^2$) remnant polarization. It holds potential as a solar absorber because it is a direct gap material composed of relatively cheap, abundant, and non-toxic elements. The bandgap of ideal $ZnSnO_3$ is too large to make it an efficient solar absorber. However, like many semiconducting oxides containing tin, the bulk bandgap is an extremely strong function of the lattice constant. In fact, just a few percent change in the lattice constant of $ZnSnO3_3$ can alter its bandgap by as much as a factor of 2-4. This opens the possibility of tuning the bandgap by applying a slight epitaxial strain, which can be accomplished by affixing a $ZnSnO_3$ film to a substrate with a modest lattice mismatch. In this work we use sophisticated methods (DFT and GW) to identify materials that can be affixed to a $ZnSnO_3$ film, modifying its bandgap to a near optimal value. Attention will be paid to the bandgap, band alignments, and the thermodynamics of the interfaces.

Brian Kolb
Massachusetts Inst of Tech-MIT

Date submitted: 15 Nov 2013 Electronic form version 1.4