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Engineering the bandgap of ferroelectric $ZnSnO_3$ via sulfur substitution BRIAN KOLB, ALEXIE KOLPAK, MIT — Since its recent discovery, ferroelectric $ZnSnO_3$ has been investigated for utility in a number of applications. Its strong remnant polarization and good conductivity, for example, make it attractive as a photovoltaic material, but its relatively large 3 eV bandgap limits its potential usefulness. We find that the bandgap of $ZnSnO_3$ is highly sensitive to changes in lattice volume, which can be effected either with application of external strain or by substituting sulfur for oxygen. Upon forming the fully-substituted $ZnSnS_3$, the bandgap reduces to a near-optimal 1.3 eV while retaining many of the important properties of the oxide, including a strong polarization. In this talk we describe the physics governing the tunable electronic structure of $ZnSnO_3$, discuss the stability of the $ZnSnS_3$ analogue, and propose a route to its use in a photovoltaic cell by growth on a GaN substrate.

Brian Kolb
MIT

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