Scientific Achievement:
We computationally predicted lifetime-limiting point defects in SnS—the sulfur vacancy $V_S$ and impurity-related substitutionals $Fe_{Sn}$, $Co_{Sn}$, and $Mo_{Sn}$. We also optimized growth parameters to suppress these defects and achieved $>1$ ns lifetime in SnS crystal samples.

Significance and Impact:
Device modeling indicates that $>1$ ns lifetimes enable $>10\%$ SnS devices if we can translate this success to thin films. To our knowledge, this is the first-ever $>1$-ns lifetimes in SnS. Thus, 1-ns lifetime in SnS constitutes a major advance in the main limiting factor for SnS devices.

Research Details:
• Predicted defect impact on lifetime with DFT (collaboration with WUSTL through SERIIUS) and Shockley-Read-Hall recombination model.
• Crystal growth from 99.9999%-pure Sn and S.
• Control for sulfur content and metal impurity content.
• Improved minority-carrier lifetime to $>1$ ns in S-rich, high-purity crystals.
• Close-spaced sublimation furnace has been built to translate these learnings to thin films, with preliminary indications of lifetime improvements over previous thin films.


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