# Design of Metastable Tin Titanium Nitride Semiconductor Alloys

## Scientific Achievement

We predicted and synthesized new mixed-metal nitride alloys with improved optoelectronic properties. Specifically, we synthesized metastable $(Sn,Ti)_3N_4$ spinels using non-equilibrium synthesis [1]. These $(Sn,Ti)_3N_4$ alloys have lower hole effectives masses and better transport than $Sn_3N_4$ [2].

## Significance and Impact

We demonstrated that theory-guided materials design in the space of metastable alloy materials coupled with thin-film synthesis techniques can yield real-world materials with improved properties for energy-conversion applications, including photoelectrical hydrogen production.

## Research Details

**Theoretical results (Fig. 1):**

- Hole effective mass decreases with Ti, becomes low ($<3m_0$) at 20% Ti
- Electron mass low ($0.3m_0$) for all studied Ti compositions
- Band gap favorable for optoelectronics (1–2 eV) for up to 30%–35% Ti
- Alloys challenging to synthesize ($\Delta h_{mix}$ = 0.4 eV/at, $\Delta \mu_N$ = +1 eV)

**Experimental results (Fig. 2):**

- Spinel alloy films synthesized at 280°C with up to 50%–60% Ti
- Band gap first increases to 2 eV, then decreases with increasing Ti
- Doping stays moderate ($10^{17}$–$10^{18}$ $cm^{-3}$ ) up to 40%–50% Ti
- PEC photocurrent increases by 5x with addition of Ti


[1] A. Bikowski, A. Zakutayev, et al., *Chem. Mater.* **29**, 6511 (2017).

[2] C.M. Caskey, A. Zakutayev, et al., *J. Mater. Chem. C* **3**, 1389 (2015).


**Theory:**

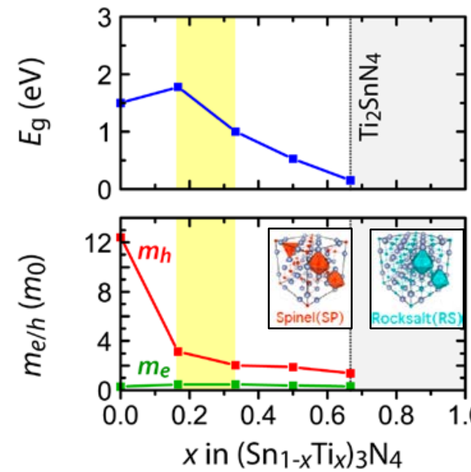


**Fig. 1.** Predicted properties

**Experiment:**

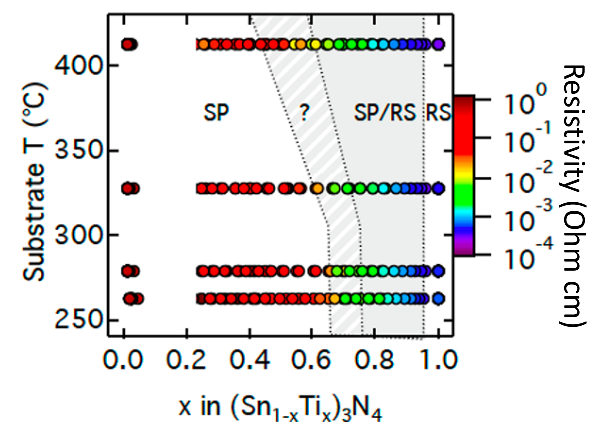


**Fig. 2.** Measured properties

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