**Scientific Achievement**

We predicted and synthesized new mixed-metal nitride alloys with improved optoelectronic properties. Specifically, we synthesized metastable \((\text{Sn,Ti})_3\text{N}_4\) spinels using non-equilibrium synthesis [1]. These \((\text{Sn,Ti})_3\text{N}_4\) alloys have lower hole effective masses and better transport than \(\text{Sn}_3\text{N}_4\) [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 (<3m₀) at 20% Ti
- Electron mass low (0.3m₀) for all studied Ti compositions
- Band gap favorable for optoelectronics (1–2 eV) for up to 30%–35% Ti
- Alloys challenging to synthesize (\(\Delta h_{\text{mix}} = 0.4 \text{ eV/at}, \Delta \mu_N = +1 \text{ eV}\))

**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 (\(10^{17}–10^{18} \text{ cm}^{-3}\)) up to 40%–50% Ti
- PEC photocurrent increases by 5x with addition of Ti