

New Selection Metric for Design of Thin-Film Solar Cell Absorber Materials

Scientific Achievement

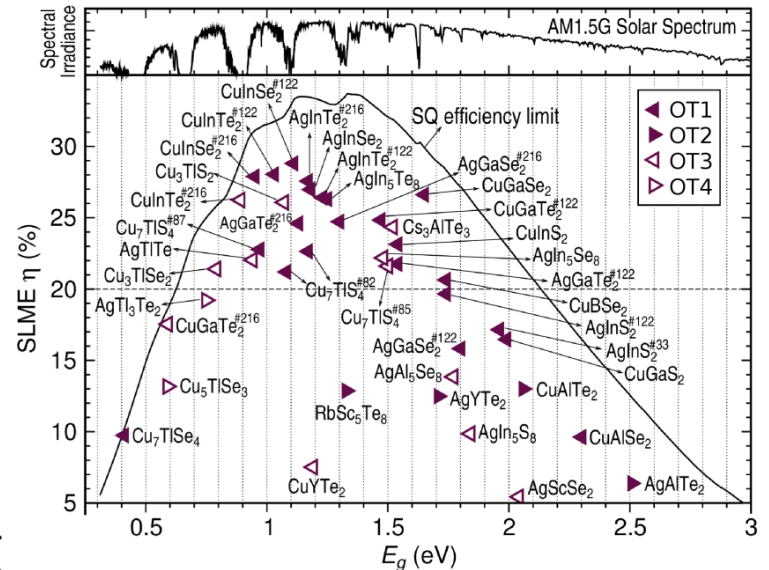
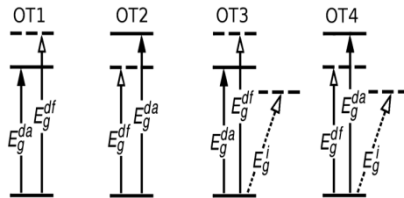
Spectroscopic Limited Maximum Efficiency (SLME) is a new and calculable selection metric to identify new and/or improved photovoltaic (PV) absorber candidate materials for thin-film solar cells.

Significance and Impact

SLME significantly narrows down the material search space (from thousands to tens of materials) for thin-film PV absorbers, and it provides more advanced guidance for the experimental synthesis.

Research Details

- SLME accounts for the physics of absorption, emission, and recombination by directly calculating absorptivity and considering the optical transition characteristics—not just the bandgap, which is the only quantity commonly considered previously.
- High-throughput, first-principles calculations of SLME—based on quasi-particle theory for ~300 materials comprising Group I, III, and VI elements—identified at least 24 materials that could show promise as highly efficient PV absorbers.
- SLME allows us to identify direct-gap materials (optical transition OT1 type) and indirect materials (OT3 type) that are equally promising for high SLME (>20%). We are now applying SLME to other materials.



24 identified materials (some novel, some already known) with an SLME > 20%, narrowed from an initial base of >1000 candidates. The optical types (OT) are defined to left.

L. Yu and A. Zunger, *Phys. Rev. Lett.* **108**, 068701 (2012).