Introduction: How does a solar cell work?
Photovoltaic (PV) materials in solar cells convert solar (sunlight) energy into electrical energy. PV’s crystalline properties result in two energy bands: a low-energy valence band (VB) and a high-energy conduction band (CB). In a solar cell, electrons in the VB absorb light energy (photons) from the sun and are "kicked up" into the CB, leaving behind a hole in the VB. High-energy CB electrons are collected through a contact, which results in an electrical current.

Commercial silicon solar cells harvest a small portion of available solar energy and have efficiency under 30%. An ongoing engineering challenge is to develop high-efficiency PV materials at low cost.

Design guideline 1: Use more of the sun’s energy spectrum
Design guideline 2: Avoid energy loss through electron-hole recombination.

Two Theoretical Models for Up-conversion
Up-conversion increases solar-energy conversion efficiency. It works by stacking together materials with different band gaps to harvest a wider range of solar energies.

1. Colloidal Device: Materials synthesized in solution
   - Cost effective: Easy to mass produce

2. Epitaxial Device: Up-conversion materials are deposited layer by layer artificially
   - Theoretical max solar-energy conversion efficiency > 50%
   - Enables two-photon process to harvest both high and low energy photons.
   - Tweaking the composition of InAlGaBiAs creates a favorable slope to reduce recombination.

Method
We model the behavior of electrons and holes in material-specific potential profiles by solving the time-independent Schrödinger equation:

\[ -\Psi''(x) + V(x)\Psi(x) = E\Psi(x) \]

\( \Psi \): Wave function of particle (predicts where particle will be located)
\( V \): Potential (determined by band gaps of the materials)
\( E \): Energy states available to electrons and holes
Boundary condition: zero on each side
Solve to get \( \Psi \) and energies (E)
\( \Psi \): Probability that an electron or hole will be found at a given location.

Tools: MATLAB with Chebfun package
Chebfun is open-source software for MATLAB that solves differential equations numerically.

Motivation
Making physical prototypes of nano-structured materials is time consuming and expensive. By developing computational models, researchers can predict the behavior of materials and adjust model parameters to choose the most promising materials to work with in the lab.

Conclusion
Preliminary results show that the code holds promise for delivering useful predictions for material performance. Computational models suggest that both devices may slow recombination from low energy states.

Path Forward
1. Complete analysis of preliminary results to compare against experimental data.
2. Refine the algorithms for up-conversion models.
3. Tweak parameters to optimize device performance.
4. Apply methods to other new device architectures.

Results
2. Epitaxial Device: Multilayer device
   - Theoretical max solar-energy conversion efficiency
   - Enables two-photon process to harvest both high and low energy photons.
   - Tweaking the composition of InAlGaBiAs creates a favorable slope to reduce recombination.

Colloidal Device
- Dashed lines: hole states
- Solid lines: electron states
- Orange arrow: area of electron loss
- Energy levels (E)
- Photoluminescence (PL)
- PL data courtesy of Dr. Diane Sellers, UD Materials Science and Engineering

Epitaxial Device
- Dashed lines: hole states
- Solid lines: electron states
- Orange arrow: area of electron loss
- Energy levels (E)
- PL data courtesy of Dr. Diane Sellers, UD Materials Science and Engineering

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