PROJECTS 2026: SOLAR PHOTOVOLTAIC MODELING

Topic: The Thermal Resilience of Emerging Tandem Technologies

Course: PHY_54401-EP Thin Film Photovoltaics – Modelling of Solar Cells

Timeline: January 14th – March 11th, 2026

Tools: SCAPS-1D, Python (Google Colab), NGSPICE, Generative AI

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1. Scientific Context & Rationale

Standard photovoltaic characterization occurs at **25°C (STC)**, but real-world operation in high-irradiance climates drives module temperatures above **65°C**.

For emerging **2-Terminal (2T) Tandem Solar Cells**, temperature is a critical disruptor. As temperature rises:

1. **Bandgaps narrow** (Varshni effect), altering absorption profiles.
2. **Charge carrier mobilities change**, affecting collection efficiency.
3. **Recombination rates increase**, reducing voltage.

The Engineering Challenge:

A 2T-Tandem relies on perfect Current Matching. A device perfectly aligned at 25°C may suffer from severe current mismatch at 65°C due to uneven thermal drifts.

Project Objective:

Students act as R&D engineers to design, simulate, and stress-test a Thin-Film Tandem architecture. The goal is to prove robustness and stability under thermal stress and simulate the final energy yield.

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2. Methodology: The 4-Phase Workflow

Students will apply a rigorous "Cell-to-System" workflow using a hybrid toolchain:

Phase 1: Physics Simulation (SCAPS-1D)

- Simulation of the **Top Cell** and **Bottom Cell** separately
- **Tandem Assembly:** Numerical reconstruction of the Tandem I-V curve with SCAPS (script)
- **Thermal Sweep:** Generating I-V curves across a temperature range (300K to 350K)

Phase 2: Data Analysis & Fitting (Python / Google Colab)

- **Analyse Tandem Assembly:** Numerical reconstruction of the Tandem I-V curve to analyze **Current Matching dynamics** and quantify **Mismatch Drift** at high temperatures
- **Parameter Extraction:** Fitting the generated I-V curves to extract the **Equivalent Circuit Parameters** (Single Diode Model) for the next phase

Phase 3: Module & Yield Simulation (Python + NGSPICE)

- **Module Conception:** Designing a series-connected module (e.g., 60 cells) with Bypass Diodes in NGSPICE
- **Yield Simulation:** Simulating the module's energy production (kWh) under specific environmental conditions (Irradiance + Temperature profiles), incorporating the thermal losses identified in Phase 2

Phase 4: Optimization Loop

- **Iterative Design:** Returning to Phase 1 (SCAPS) to adjust material thicknesses or bandgaps to minimize thermal losses and maximize the Energy Yield calculated in Phase 3

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3. The 6 Design Teams (Technology Tracks)

The cohort is divided into 6 specialized groups, each investigating a specific material pairing.

Important: Students must research and justify material parameters from scientific literature.

Team 1: Perovskite / CIGS

Key Physics Challenge: Interface Stability – Managing the optical coupling between a planar Perovskite and a rough CIGS surface.

Guiding Questions: - What perovskite composition achieves optimal current matching with CIGS? - How does CIGS grading (Ga/In ratio) affect the thermal response? - What is the thermal coefficient mismatch between both sub-cells?

Expected Deliverables: - Optimal top cell thickness for current matching at 25°C and 65°C - Temperature coefficient of the tandem vs. single-junction

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Team 2: Perovskite / CdTe

Key Physics Challenge: Bandgap Rigidity – Managing the relatively high CdTe gap and designing a suitable Top Cell to maintain current matching.

Guiding Questions: - What perovskite composition is required to match CdTe photocurrent? - How do halide segregation effects impact performance at elevated temperatures? - What are the Voc losses mechanisms in this pairing?

Expected Deliverables: - Optimal perovskite composition (cation and anion engineering) - Thermal stability analysis of wide-gap perovskites

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Team 3: All-Perovskite Tandem (Pb / Pb-Sn)

Key Physics Challenge: Homogeneity – Investigating if two Perovskite materials drift synchronously under heat.

Guiding Questions: - Do Pb-only and Pb-Sn perovskites have similar thermal coefficients? - How does Sn oxidation affect bottom cell stability? - What defect mechanisms dominate at high temperature?

Expected Deliverables: - Current matching stability over 25-65°C range - Recommendations for encapsulation requirements

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Team 4: Inverted (p-i-n) Perovskite / CIGS

Key Physics Challenge: Organic Stability – Analyzing the impact of temperature on organic Transport Layers (PCBM, C60, NiOx, PTAA).

Guiding Questions: - What is the thermal stability limit of each organic transport layer? - How does carrier mobility evolve with temperature in these materials? - Are inorganic alternatives viable?

Expected Deliverables: - Maximum operating temperature for each organic layer - Alternative inorganic transport layer recommendations

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Team 5: Perovskite / CZTSe (Kesterite)

Key Physics Challenge: Voltage Deficit – Addressing the severe Voc loss characteristic of Kesterites at high temperatures.

Guiding Questions: - What causes the large Voc deficit in Kesterites? - How does Cu/Zn disorder evolve with temperature? - Can bandgap grading (S/Se ratio) mitigate thermal losses?

Expected Deliverables: - Voc(T) curves and activation energy analysis - Strategies to minimize Kesterite Voc losses

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Team 6: Perovskite / Sb_2Se_3 (Antimony Selenide)

Key Physics Challenge: Exploratory – Characterizing the thermal behavior of the emerging quasi-1D Antimony Selenide material.

Context

Sb_2Se_3 is an emerging thin-film absorber with promising properties: earth-abundant, non-toxic, high absorption coefficient, and simple binary composition. However, it remains less mature than CIGS or CdTe, with current record efficiency around 10%.

Key Scientific Challenges

1. **Voc Deficit:** Why do Sb_2Se_3 cells show significantly lower Voc than theoretical limits?
2. **Anisotropic Transport:** How does the quasi-1D ribbon structure affect carrier collection?
3. **Defect Physics:** What are the dominant recombination centers?
4. **Interface Engineering:** What is the optimal buffer layer for Sb_2Se_3?

Guiding Questions

- How does the quasi-1D crystal structure affect thermal behavior?
- Is Sb_2Se_3 more or less thermally stable than CIGS/CdTe?
- What perovskite bandgap optimizes current matching?
- What are the dominant loss mechanisms at elevated temperature?
- Can Sb_2Se_3 compete with established bottom cell technologies?

Research Tasks

1. **Literature Review:** Find and justify all SCAPS parameters from peer-reviewed sources
2. **Absorption Spectrum:** Locate or extract optical constants (n, k, α) from literature
3. **Defect Analysis:** Identify the main defect types and their energy levels
4. **Interface Study:** Compare different buffer layers (CdS, ZnO, TiO_2)
5. **Thermal Modeling:** Extract temperature coefficients from simulations

Expected Deliverables

- Complete SCAPS model with justified parameters (referenced)
- Temperature coefficient comparison with other tandem configurations
- Identification of thermal bottlenecks specific to Sb_2Se_3
- Critical assessment: Is Sb_2Se_3 viable for tandem integration?

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4. Schedule & Milestones

The project runs for 8 weeks with a mix of autonomous work and coaching.

January 14th: KICK-OFF

- Introduction to the "Thermal Challenge"
- Distribution of Base SCAPS templates
- **Tutorial:** SCAPS Scripting & Google Colab Workflow

January 14th – March 11th: PROJECT EXECUTION

- **Mode:** Autonomous group work with **Remote Coaching**
- Students execute Phases 1 through 4
- Teams define their own internal milestones

Project Timeline

Date	Week	Phase	Milestone	Deliverable
Jan 14	1	Kick-off	Project launch	Team formation
Jan 21	2	Literature	Parameter research	Parameter table with references
Jan 28	3	Phase 1	Single-junction modeling	Top & Bottom cell .def files
Feb 4	4	Phase 1	Model validation	J-V curves vs. literature
Feb 11	5	Phase 2	Tandem assembly	Current matching analysis
Feb 18	6	Phase 2	Thermal sweep (300-350K)	Temperature coefficients
Feb 25	7	Phase 3	Module simulation	NGSPICE model + Yield
Mar 4	8	Phase 4	Optimization & Writing	Draft report
Mar 11	-	Defense	Final presentation	Report + Slides

March 11th: FINAL DEFENSE

- **Final Presentation:** Each group presents their findings (Thermal Stability analysis + Final Energy Yield)
- Submission of the Scientific Paper/Report

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5. Resources Provided

To ensure feasibility within the timeframe, students are provided with a **Digital Starter Kit**:

Templates

- Base SCAPS structure files (.def templates)
- Google Colab Notebook for I-V analysis and parameter extraction
- NGSPICE module templates

Documentation

- SCAPS-1D user manual
- Guide on temperature-dependent simulations
- AI usage guidelines (scripting and debugging only)

What Students Must Find Themselves

- **All material parameters** (bandgaps, mobilities, densities, etc.)
- **Absorption spectra** for their specific materials
- **Defect parameters** from literature
- **Justification** for every parameter used

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6. Evaluation Criteria

Criterion	Weight	Description
Literature Research	20%	Quality of parameter sourcing and justification
Technical Depth	25%	Quality of SCAPS simulations and physical understanding
Innovation	15%	Creative solutions to thermal challenges
Data Analysis	20%	Quality of parameter extraction and interpretation
Report & Presentation	20%	Scientific writing, clarity, and communication

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7. Expected Learning Outcomes

By the end of this project, students will have:

1. **Mastered literature research** for material parameters
2. **Understood SCAPS-1D** for multi-junction solar cell simulation
3. **Analyzed thermal effects** on photovoltaic performance
4. **Developed Python skills** for data analysis and circuit simulation
5. **Experienced R&D workflow** with iterative design methodology
6. **Produced publishable-quality** analysis of emerging technologies

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Good luck to all teams – and remember: justify every parameter!