CENER
NATIONAL RENEWABLE ENERGY CENTRE
ADItech

VIPERLAB

VIPERLAB WORKSHOP-MODELAB
8th February 2022

GOBIERNO DE ESPAÑA
VICEPRESIDENCIA CUARTA DEL GOBIERNO
MINISTERIO PARA LA TRANSICIÓN ECOLÓGICA Y EL RETO DEMOGRÁFICO
MINISTERIO DE CIENCIA E INNOVACIÓN
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WHAT IS CENER

CENER, the National Renewable Energy Centre of Spain, develops applied research in renewable energies, and provides technological support to companies and energy institutions.

OUR MISSION

To generate knowledge in the renewable energy field and to transfer it to the industry in order to boost sustainable energy development.

OUR VISION

To be a research centre of excellence in the renewable energies field with international outreach.

CENER AT A GLANCE

ACTIVITY
Research,
Development
and Promotion of
Renewable Energies

RESEARCH AREAS
Wind Energy
Solar Photovoltaic Energy
Solar Thermal & Thermal Energy Storage
Biomass
Energy in Buildings
Renewable Energy Grid Integration

BOARD OF TRUSTEES
Spanish Ministry of Science & Innovation
Ciemat
Ministry for the Ecological Transition & Demographic Challenge
Regional Government of Navarre

OFFICES
Headquarters at Sarriguren (Spain)
Sangüesa (Spain)
Aoiz (Spain)
Seville (Spain)
Mexico

CENER MAIN FIGURES

100 M€

Infrastructures investment

> 1000

Clients around the world
5 continents

200

Staff employed

19 M€

2020 Annual Budget

RESEARCH AREAS

SOLAR ENERGY TECHNOLOGIES AND STORAGE

- WIND ENERGY
- PHOTOVOLTAIC SOLAR ENERGY
- SOLAR THERMAL & THERMAL ENERGY STORAGE
- BIOMASS
- ENERGY IN BUILDINGS
- RENEWABLE ENERGY GRID INTEGRATION

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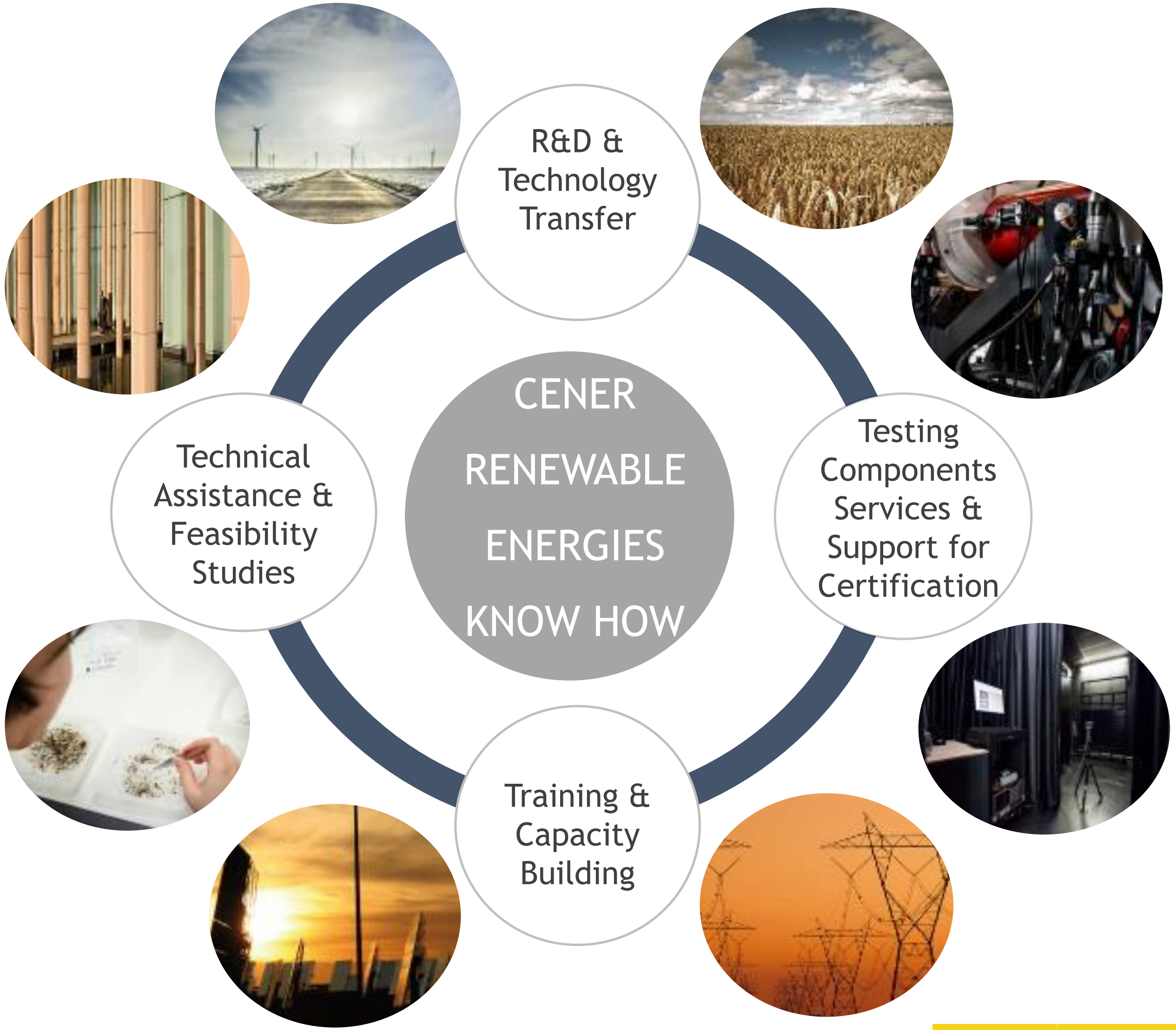
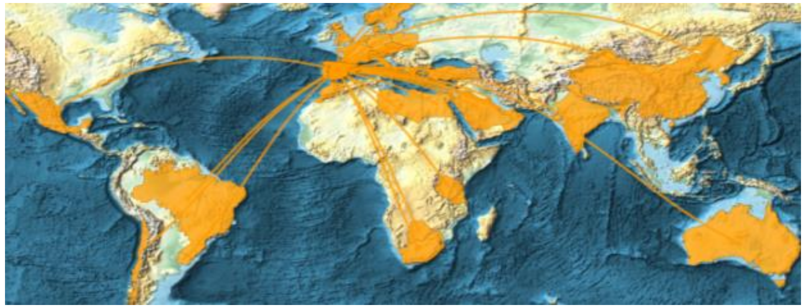
SERVICES


R&D & Technology Transfer
Testing Components Services & Support for Certification
Training & Capacity Building
Technical Assistance & Feasibility Studies
CENER
RENEWABLE
ENERGIES
KNOW HOW

TEAM AND TRACK RECORD

Team photo(s)



International presence

HIGHLY SKILLED MULTIDISCIPLINARY TEAM OF PROFESSIONALS

The team:

- **45 researchers and engineers**
- Physicists, Chemists, Mathematicians, Industrial, Mechanical, Telecommunication and Computer Engineers.
- **Large experience in Solar Photovoltaic, Solar Thermal and Energy Storage technologies**.

Team's expertise:

- **Optical, Electrical and Thermo-fluid-dynamic simulation**
- Applied **optics, image and data processing**
- **Semiconductors, coatings** and functional materials
- **Meteorology, resource assessment** and forecasting
- **Quality Assessment,** inspection and testing

LARGE EXPERIENCE IN SOLAR AND STORAGE TECHNOLOGIES AND COMERCIAL PROJECTS

Commercial projects:

- **2.000+ projects**
- **1.000+ clients**
- **40+ countries**.
- Involved in **30+ PV plant projects** and **50+ STE plant projects**.

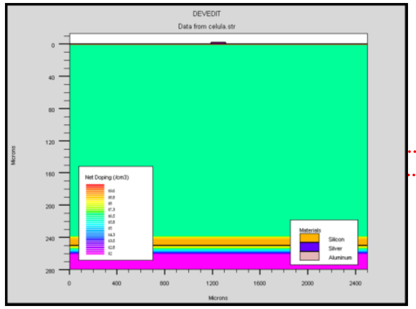
R&D Activity:

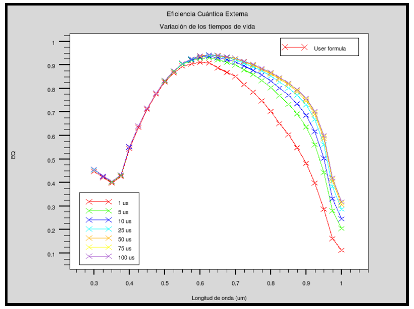
- **60+ public financed R&D projects**
- **230+ scientific publications**.
- **9 patents**
- **30+ alliances**
- **Main international forum and expert groups**.

INFRASTRUCTURES

MODELAB:

TCAD simulation tools – Silvaco software, with its different modules, is used for modelling the electro-optical behaviour of solar cells.

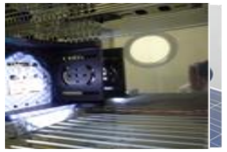


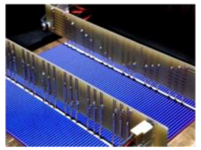


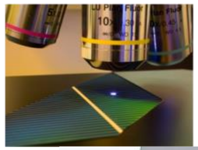
INFRASTRUCTURES IN VIPERLAB

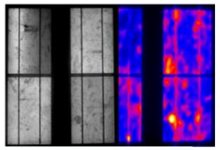
SOLPVLAB:

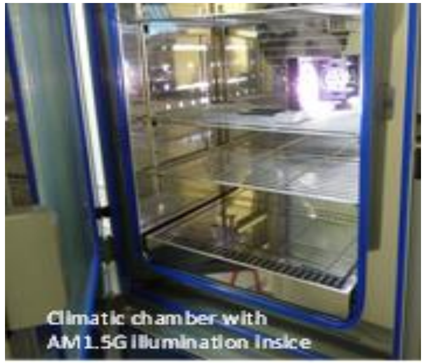
IEC Accredited PV Module testing Lab - development and application of specific protocols for characterization (electrical, optical, mechanical, duration, aging…) of photovoltaic devices based on organic or perovskites materials.











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Modelling and design of solar cells using TCAD Silvaco software, with its different modules.

Rational

- The ability to accurately simulate a solar cell prior to its fabrication is a key factor to drastically reduce experimentation time. In this way, **fabrication efforts are only dedicated to potentially well-performing devices**.

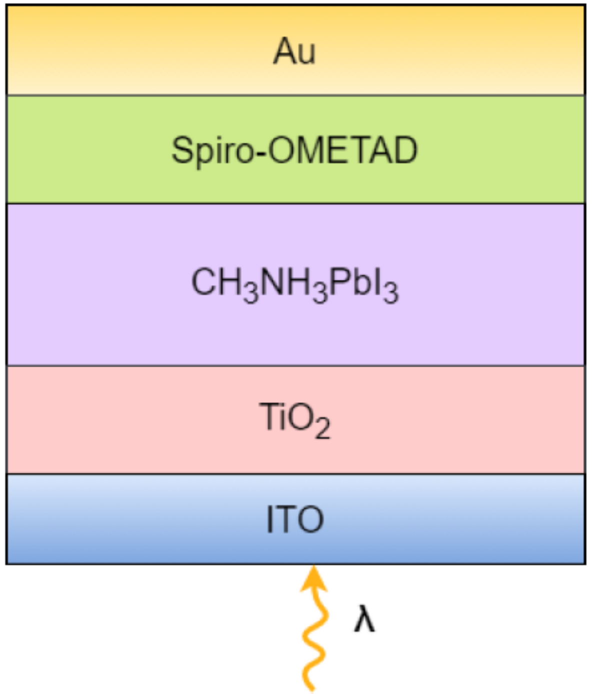
- The other way around, it allows the user to define their own materials, doping and designs for the solar cell according to the data extracted from the experimental results. This procedure **boosts the understanding of the physical mechanisms** influencing in the final result.

Device and Process simulation of perovskite devices:

- Athena (Suprem4) for individual process simulation
- Atlas device simulation with different toolkits
  - S-Pisces: for Si based technologies,
  - Blaze2D and Blaze3D for advanced materials,
  - Luminous and Luminous3D to model light absorption and photogeneration in non-planar semiconductor devices,
  - LED for light emitting diodes,
  - TFT and TFT3D for amorphous or polysilicon devices and
  - OLED and OTFT for organic devices.

- Other simulation tools available in CENER:
  - Performance of PV installations based on PVSYST
  - Reflectance and transmittance of micro and nano-structures based on MATLAB
  - Transient thermal behavior of PV devices based on MODELICA
  - **Tonatiuh**, an open-source computer program that, combining ray-tracing technologies and the statistical method of Monte Carlo, enables the simulation of the opto-energetic behavior of different devices

INPUT DATA



To define the model, the following steps are followed:

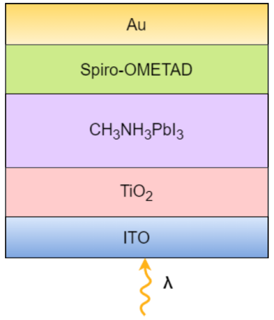
1. **Definition of the physical structure to be simulated and materials properties**
2. Definition of the physical models to be taken into account
3. Definition of the light and polarization conditions in which the electrical characteristics are going to be simulated.

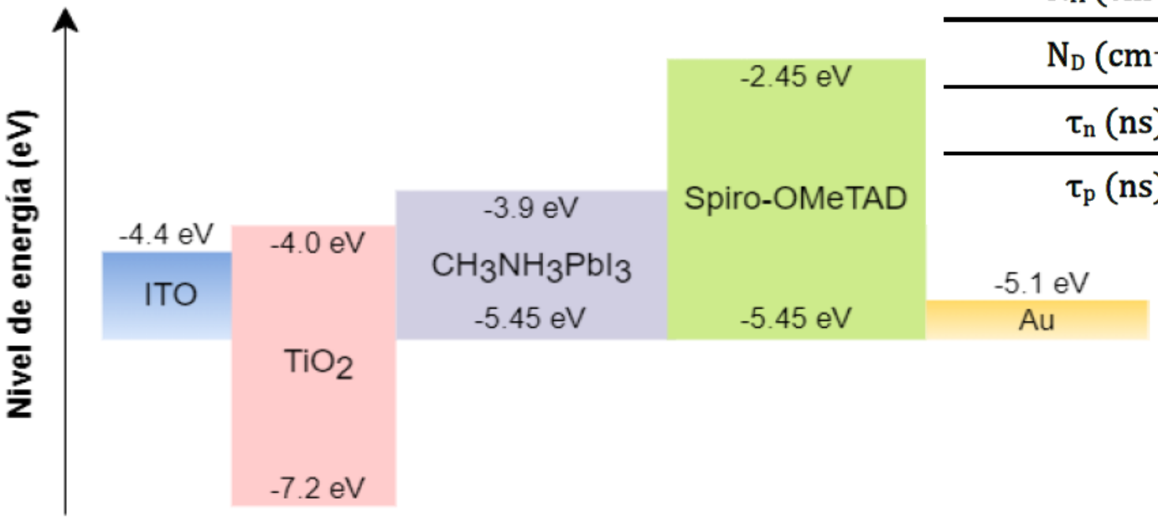
Hybrid planar perovskite cell, since it mixes inorganic materials, such as TiO2 and the electrodes, and organic materials such as perovskite and Spiro-OMeTAD

USE EXAMPLE MODELAB

INPUT DATA: Materials properties

	TiO_2	$CH_3NH_3PbI_3$	Spiro-OMeTAD
ε_r	19	100	3
E_g(eV)	3.20	1.55	3.00
χ (eV)	4.00	3.90	2.45
N_C (cm^{-3})	2.0×10^{18}	2.0×10^{18}	2.2×10^{18}
N_V (cm^{-3})	2.0×10^{19}	2.0×10^{19}	1.9×10^{19}
μ_n ($cm^2V^{-1}s^{-1}$)	0.2	1.0	2.0×10^{-4}
μ_p ($cm^2V^{-1}s^{-1}$)	0.1	1.0	2.0×10^{-4}
N_A (cm^{-3})	-	-	1.0×10^{18}
N_D (cm^{-3})	3.0×10^{19}	1.0×10^{13}	-
τ_n (ns)	100	1000	100
τ_p (ns)	100	1000	100





A. Hima, N. Lakhdar, B. Benhaoua, A. Saadoune, I. Kemerchou, and F. Rogti, "An optimized perovskite solar cell designs for high conversion efficiency," Superlattices Microstruct., vol. 129, no. February, pp. 240–246, 2019, doi: 10.1016/j.spmi.2019.04.007.

M. Dadashbeik, D. Fathi, and M. Eskandari, "Design and simulation of perovskite solar cells based on graphene and TiO2.pdf," Sol. Energy, vol. 207, pp. 917–924, 220AD.

S. Van Reenen, M. Kemerink, and H. J. Snaith, "Modeling Anomalous Hysteresis in Perovskite Solar Cells," J. Phys. Chem. Lett., vol. 6, no. 19, pp. 3808–3814, Oct. 2015, doi: 10.1021/acs.jpclett.5b01645.

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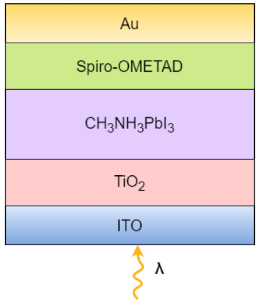
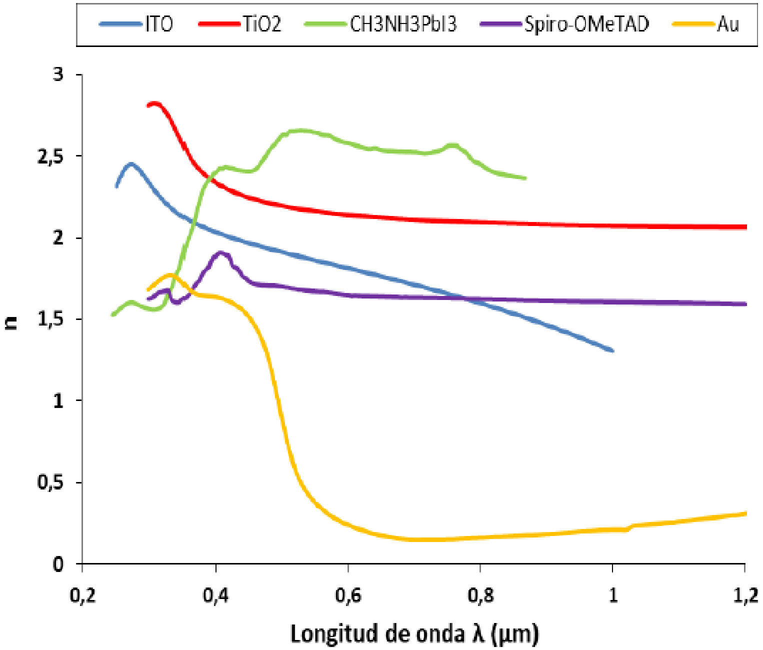
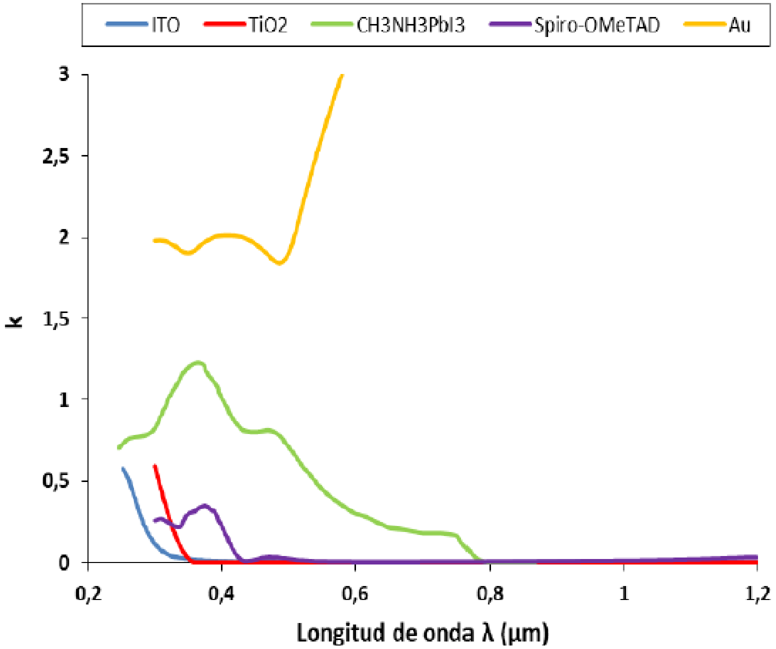
INPUT DATA: Materials properties



Transfer matrix method for the propagation of light rays. This matrix directly relates the amplitude of the electric fields of the transmitted and reflected waves with the amplitudes of the incident waves. Use the characteristic matrix that relates the tangential components of the electric fields E(z) and magnetic fields H(z) at the junctions of each of the layers.





J. A. Guerra *et al.*, "Determination of the complex refractive index and optical bandgap of CH 3 NH 3 PbI 3 thin films."

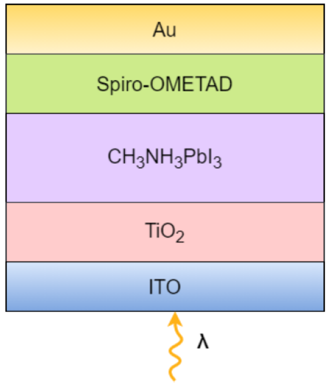
T. A. F. König *et al.*, "Electrically tunable plasmonic behavior of nanocube-polymer nanomaterials induced by a redox-active electrochromic polymer," *ACS Nano*, vol. 8, no. 6, pp. 6182–6192, Jun. 2014, doi: 10.1021/nn501601e.

S. Sarkar *et al.*, "Hybridized Guided-Mode Resonances via Colloidal Plasmonic Self-Assembled Grating," *ACS Appl. Mater. Interfaces*, vol. 11, no. 14, pp. 13752–13760, Apr. 2019, doi: 10.1021/acsami.8b20535.

J. Queisser ; 3, . A Richter, M. Hermle, and S. W. Glunz, "Achievement of More Than 25% Conversion Efficiency With Crystalline Silicon Heterojunction Solar Cell," *IEEE J. Photovoltaics*, vol. 32, no. 3, pp. 1433–1435, 1961, doi: 10.1364/OE.23.00A263.

D. I. Yakubovsky, A. V. Arsenin, Y. V. Stebunov, D. Y. Fedyanin, and V. S. Volkov, "Optical constants and structural properties of thin gold films," *Opt. Express*, vol. 25, no. 21, p. 25574, Oct. 2017, doi: 10.1364/oe.25.025574.

USE EXAMPLE MODELAB



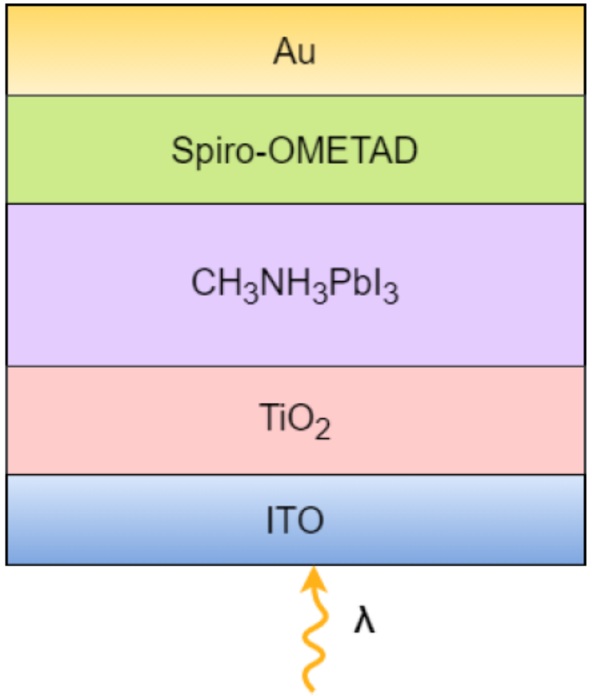
Definition of the physical models to be taken into account.

Through these models, the physical phenomena of recombination, mobility and the narrowing of the bandwidth of the semiconductor and the statistics of the charge carriers are introduced, among many other possibilities.

Material	Capa	Tipo	Modelo de recombinación	Modelo de movilidad
TiO_2	ETL	Inorgánico	Shockley Read-Hall	Concentración de los portadores
$CH_3NH_3PbI_3$	PSK	Orgánico	Langevin	Pool-Frenkel
Spiro-OMeTAD	HTL	Orgánico	Langevin Shockley Read-Hall	Pool-Frenkel

+ Surface recombination

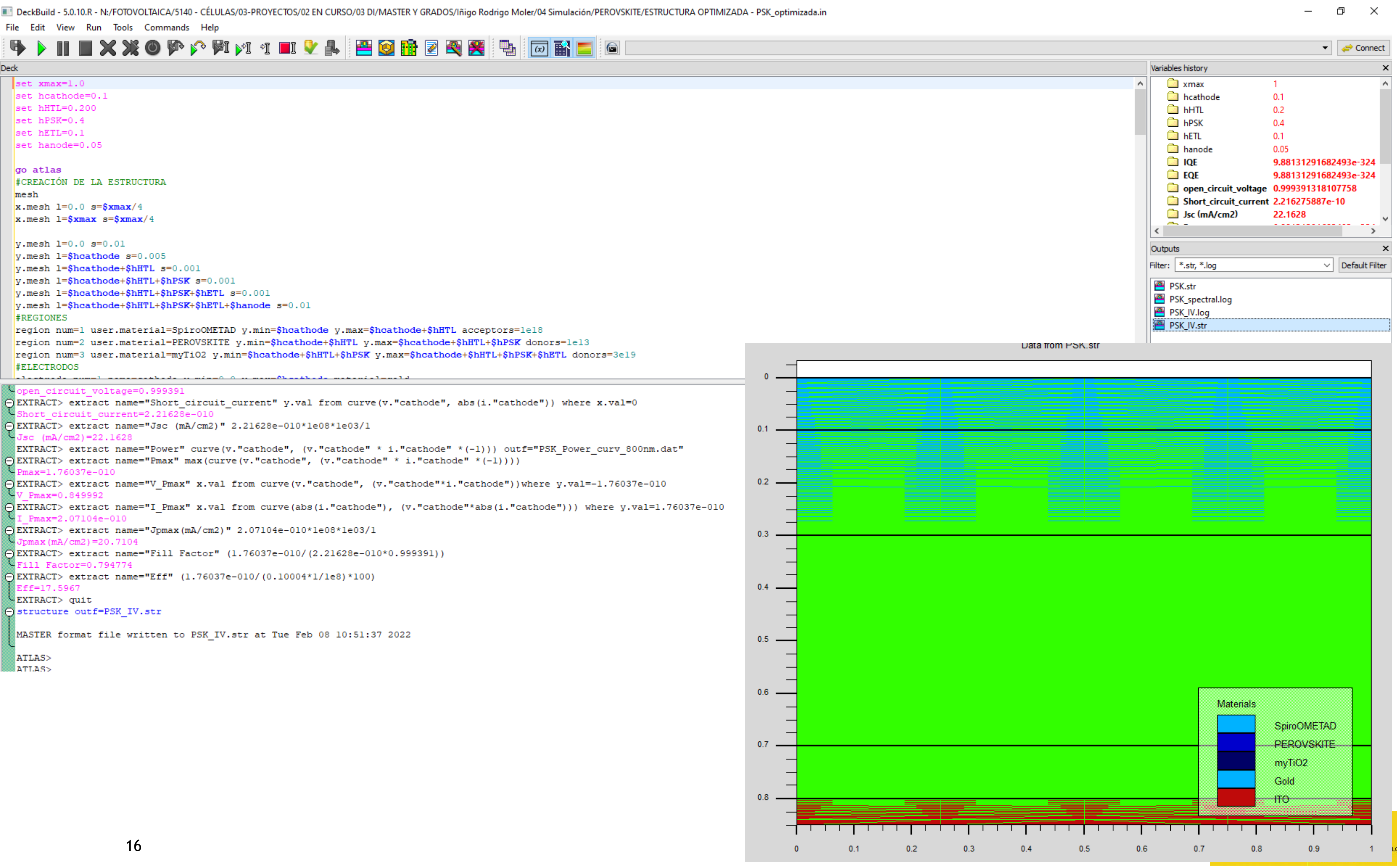
INPUT DATA



Definition of the light and polarization conditions in which the electrical characteristics are going to be simulated.

- IV curve
- light spectrum AM 1.5G
- etc

USE EXAMPLE MODELAB

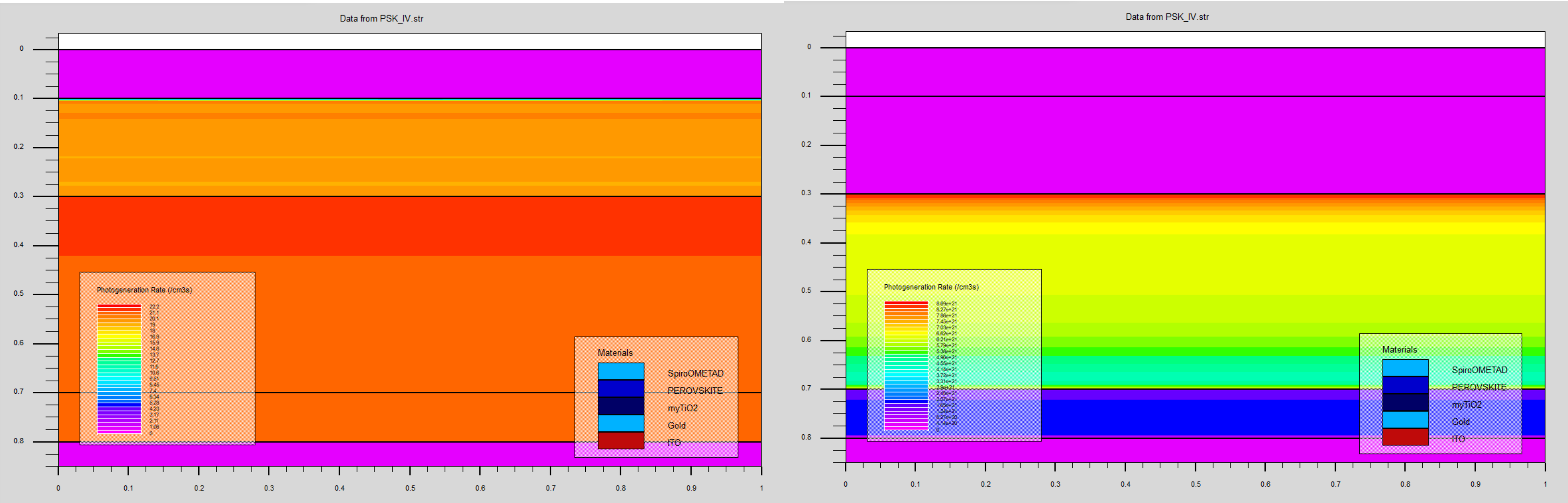


The simulator uses **finite element analysis**. To do this, the device must be approximated by a 2D or 3D mesh, which will be composed of a certain number of nodes.

The movement of the carriers within the structure can be modeled by applying to each of the nodes a set of **differential equations derived from Maxwell's equations**, basically:

Poisson's equation, continuity equations and drift-diffusion equations

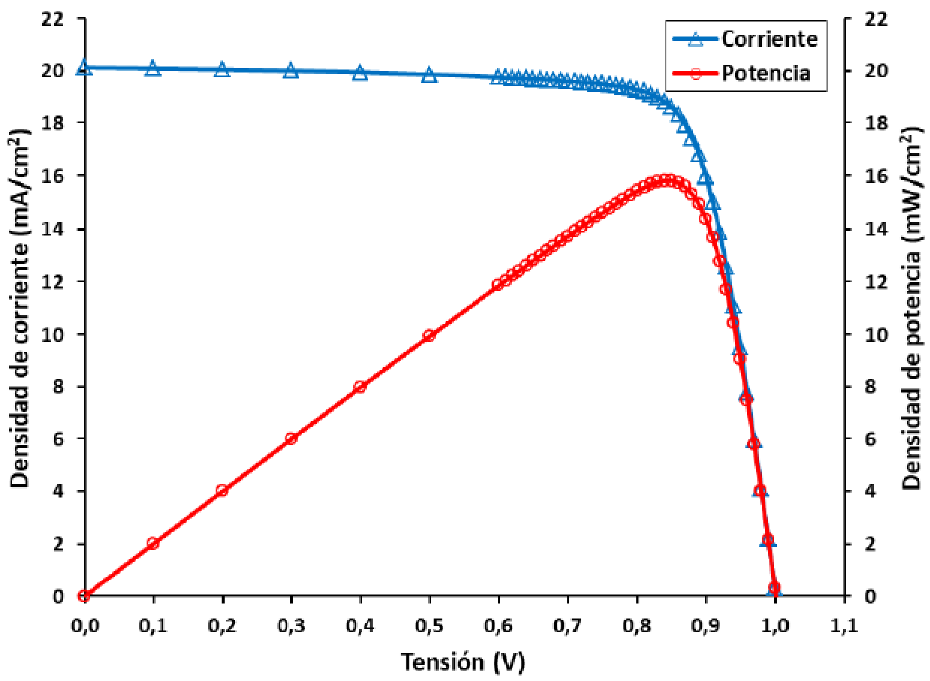
USE EXAMPLE MODELAB



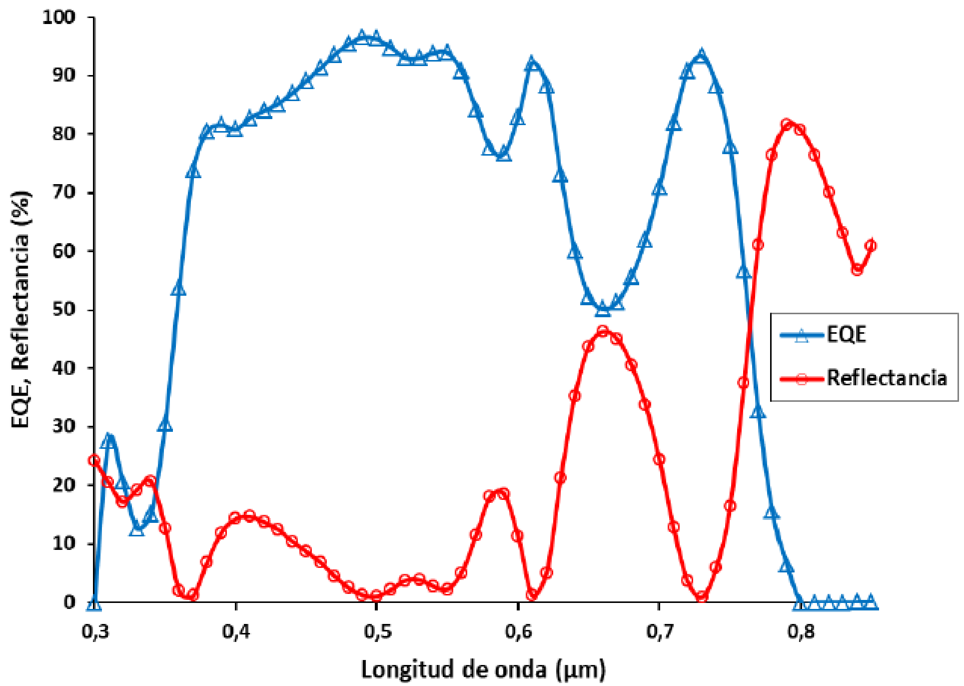
It is possible to show spatially resolved: photogeneration rate, recombination rate, photon absorption, potential, current density, optical intensity, electric field, electron and hole concentration, etcetera

Solve the equations

IV curve



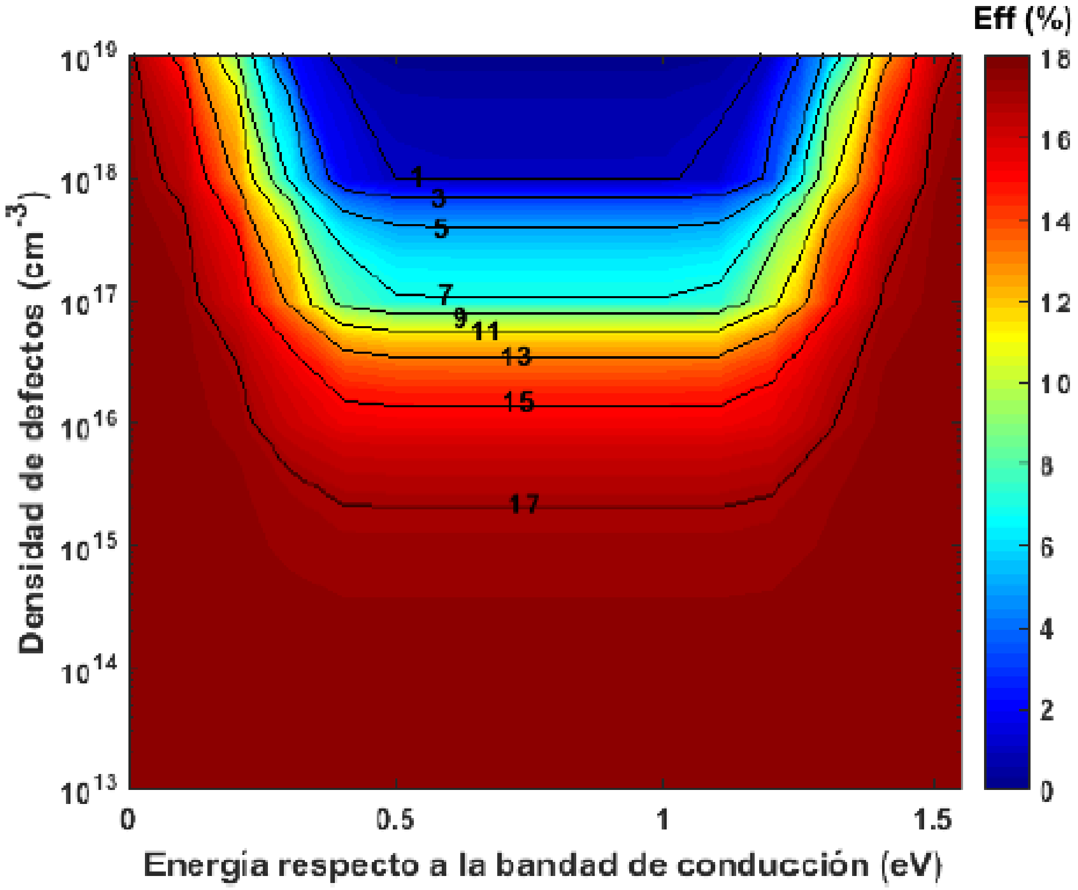
Spectral response + reflectance



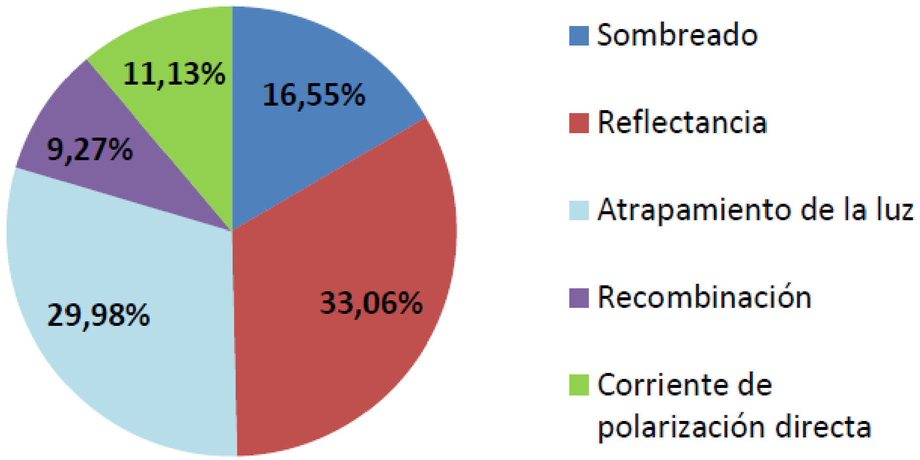
V_{OC} (V)	J_{SC} (mA/cm^2)	V_{mpp} (V)	J_{mpp} (mA/cm^2)	P_{max} (mW/cm^2)	FF $(\%)$	Eff $(\%)$
1.00	20.12	0.84	18.81	18.80	78.40	15.80

Other results:

Efficiency, Voc, Jsc, FF as a function of density of defects



Analysis of power losses



Capacities summary: ***simulate electrical and optical performance of realistic PV solar devices***

- The extraction of the electrical characteristics, photogeneration mapping, and spectral response of the solar cell based on its physical structure.
- Models can not only simulate **simple solar cells but also more advanced solar cell designs** including doping gradients, optical properties, recombination and contact grid shading.
- In addition, it is possible to study the details of photo generation of carriers in **multi-junction solar cells** of different technologies (Si, CIGS, Perovskites, Kesterites, other) by modelling the behaviour of different structures to match the cells involved in the junction. Therefore, heterojunction structures in the shape of tandem of different technologies can be simulated.
- Furthermore, **complex light spectra and different irradiation levels** can be modelled in order to replicate indoor or outdoor conditions for PV devices that are installed in specific locations.
- Optical modelling of **light management** in tandem configurations, addressing the directional and spectral composition of solar radiation can be performed using Luminous 2D and Luminous 3D modules of Silvaco TCAD. Those modules are designed to model light management, absorption and photogeneration, **in planar and non-planar**; i. e. with periodical or random structures, solar cells using methods like ray tracing, transfer matrix, beam propagation and finite difference time domain. The result takes into account internal and external reflection, refraction and dispersion as well as different light incident angles. That information allows optimizing the **matching between the absorption spectra of two cells involved in a tandem**.
- Last, apart from 2D PV devices, we can perform 3D models.

Modality of access

- Details on access: **Online**
- Number of days spent typically for an experiment: **5 days**
- Unit of access (how many user visits are expected): **9 user visits**;
- Scheduling will be done to avoid conflicts with CENER needs.
- During the number of days for the experiment: the system to be used will be fully dedicated to user.

Support offered by CENER personnel:

- Preparatory work will be done based on a form to be filled with the description of project and telco.
- Quality of scientific environment and user access: Technicians and researchers dedicated to R&D who could assist users on the definition of the simulations.
- Realization of the simulation and shipment of the results to the user (other modalities could be discusses particularly with each user)

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What is our objective

- To provide **easy and effective access** to our Virtual and Physical infrastructures

- To **exchange knowledge** and to **establish useful links** with the perovskite community

- To support the positioning of **Europe as leader** in the tandem c-Si/perovskite technology

TELL US ABOUT YOUR NEEDS!!

Thank You Very Much!

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