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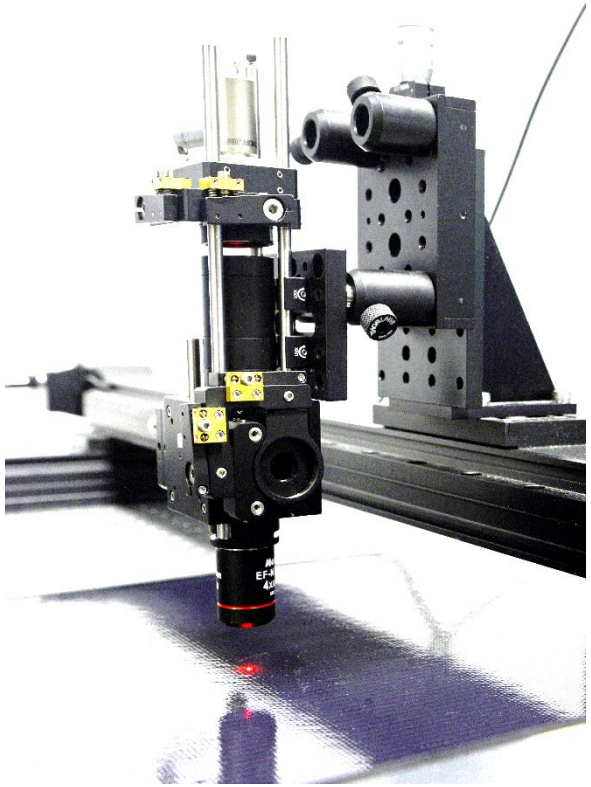

Accelerating the development of thin film photovoltaic technologies: an Artificial Intelligence assisted methodology using spectroscopic and optoelectronic techniques.

Robert Fonoll[1], Jon Garí[1], Enric Grau-Luque[1], Jacob Andrade[1], Ignacio Becerril-Romero[1], Pedro Vidal-Fuentes[1], Alejandro Perez-Rodriguez[1,2], Maxim Guc[1]

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Motivation: Complex fabrication of thin film PV devices fabrication (Kesterite case)

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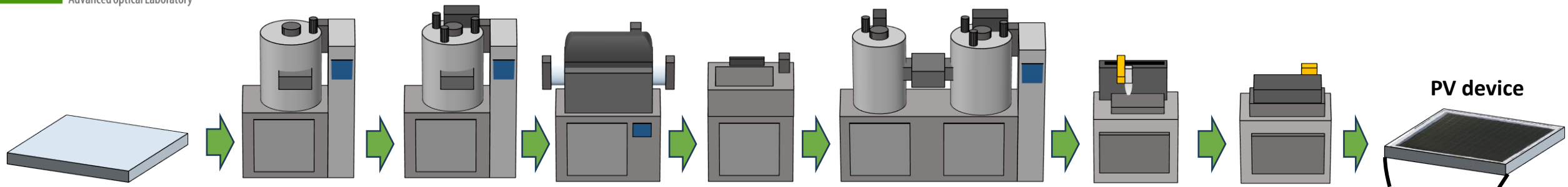


Glass Substrate

Sputtering: Metallic Back contact

Sputtering: Absorber precursor

Annealing: Light Absorber synthesis

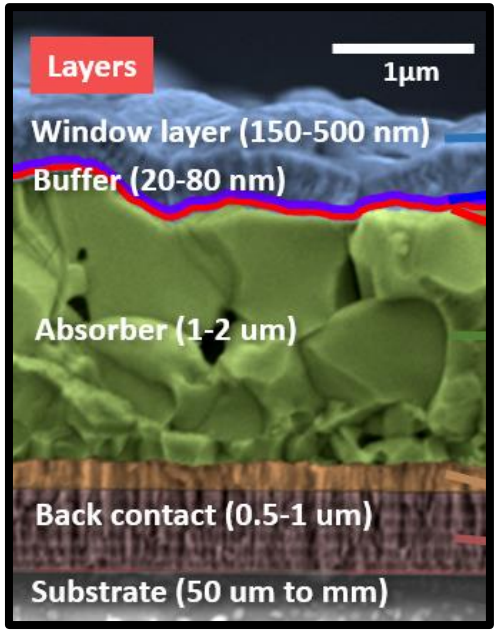
CBD: Carriers separation stack

Sputtering: Front Transparent contact stack

Annealing: System stabilization

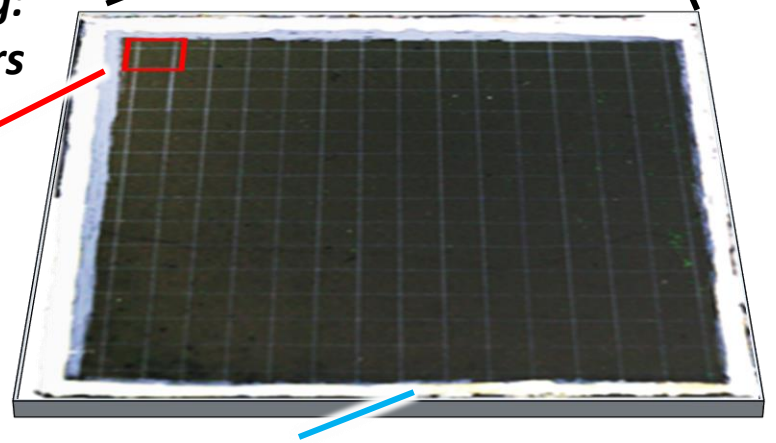
Scribing: Devices discretization

PV device



Complex fabrication process involving:
7 processes with >100 controllable parameters

Complex device (6 layers)
with strong interaction between them



5x5 cm^2 sample
#196 3x3mm^2 Test-cell

Back Contact terminal

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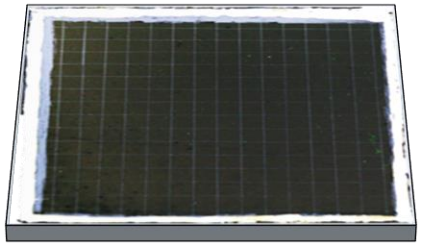
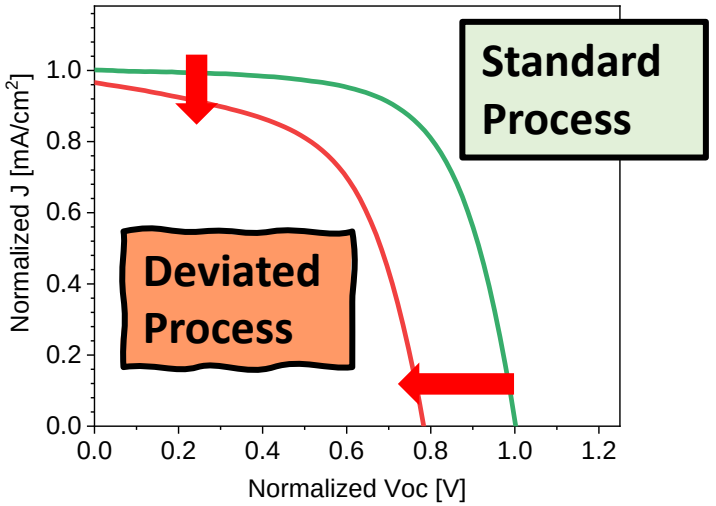
The performance of PV devices is defined as…

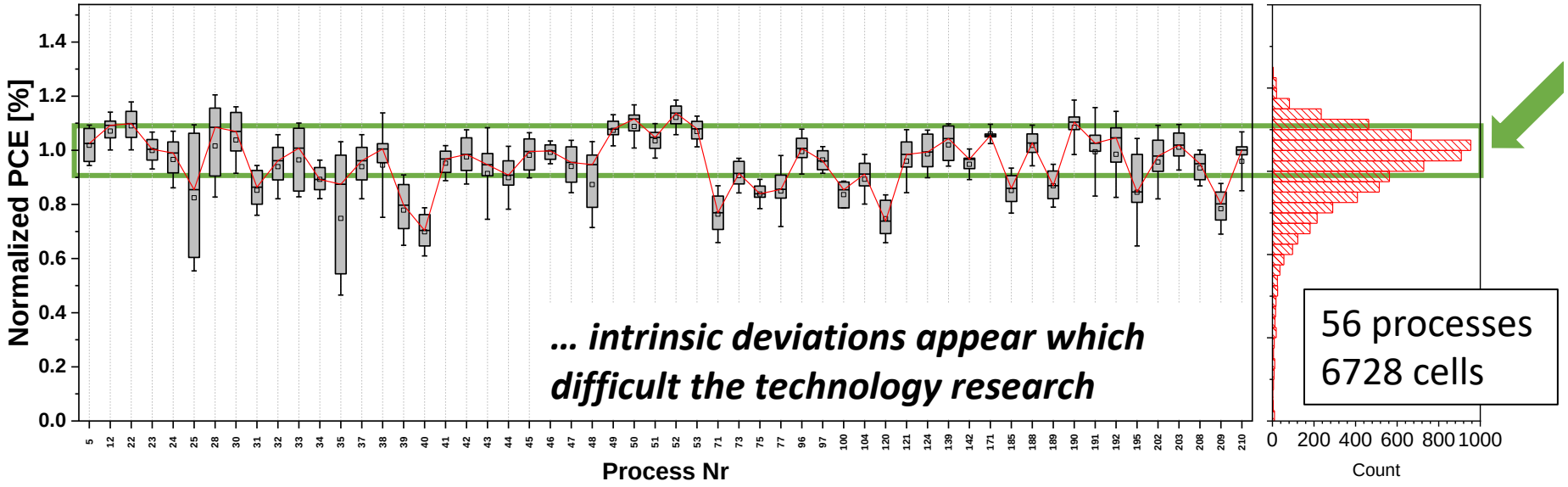


$$PCE = \frac{Photogenerated\ power}{Irradiated\ power}$$

$$PCE = \frac{J_{sc} \cdot Voc \cdot FF}{Light\ irradiation}$$



When reproducing the fabrication process…..



… intrinsic deviations appear which difficult the technology research

56 processes
6728 cells

PCE: 0.9-1.1 ➔48%
(10% deviation)

QUESTION:

Which is the origin of the fluctuations?
Can we do something?

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Methodology: workflow for the application of AI-assisted research

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Descriptors (data signal)

Characterization techniques → Data acquisition Automatization

Structured database

Data conditioning → Data fusion → Database splitting

Labels (Target)

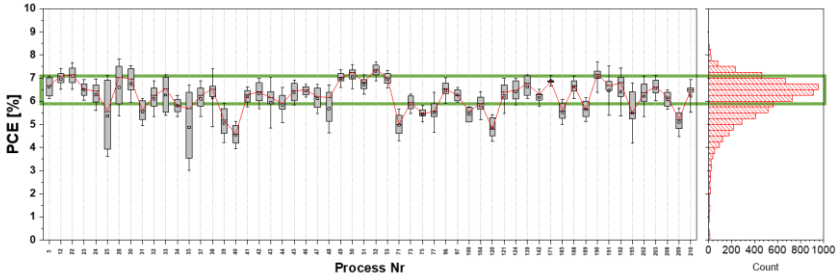
Relevant device parameters → Creation of classification criterion

ML Training data 70%

ML Model Testing data 30%

Which is the technological limitation?

Enric Grau-Luque, et al
Accelerating the Development of Thin Film Photovoltaic Technologies: An Artificial Intelligence Assisted Methodology Using Spectroscopic and Optoelectronic Techniques, Small Methods (2024) 2301573/17.



AI semi-supervised classification algorithm

PCA Algorithm
Unsupervised dimension reduction

LDA Algorithm
Supervised dimension reduction

≈10000D → 20D → 2D

Research and knowledge generation

descriptors validation → Identification of significant features → research in relevant properties / process steps

Technology Optimization strategies

PV Technology limitation

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Labeling (classification criteria)

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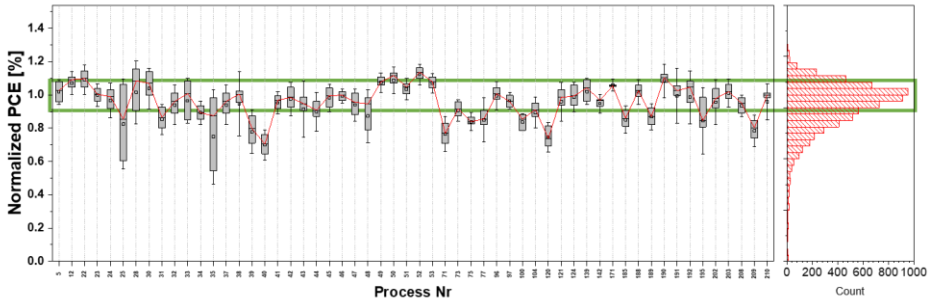
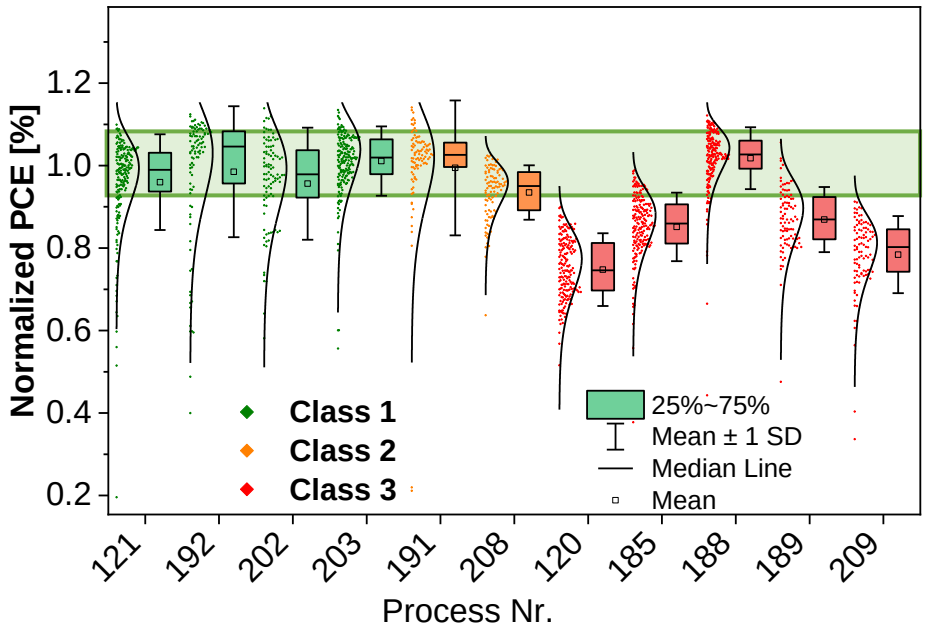
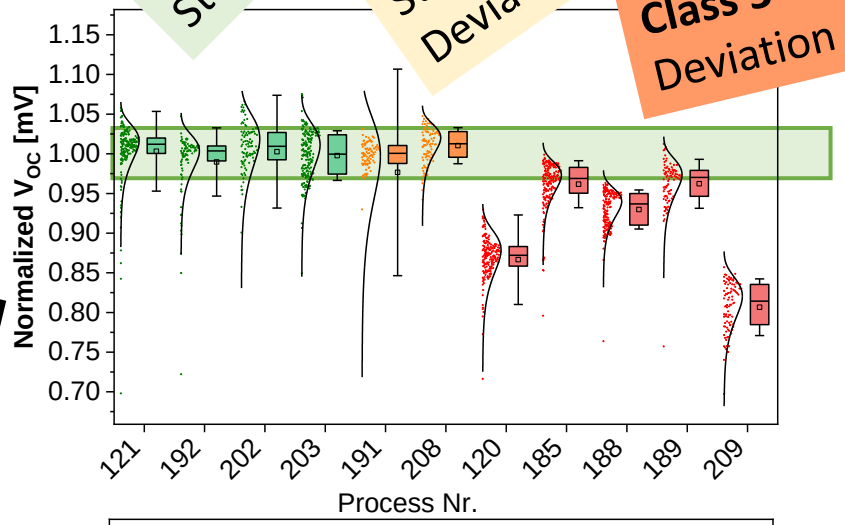


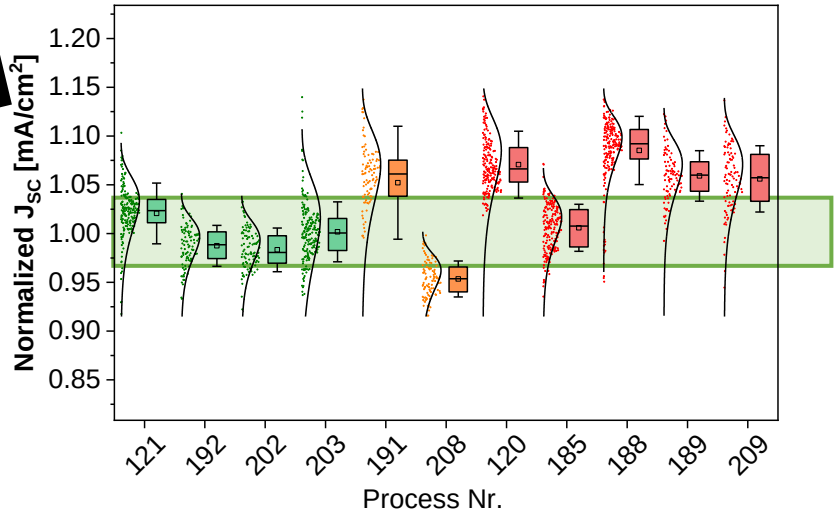


Class 1
Standard

Class 2
Standard Voc
Deviation on Jsc

Class 3
Deviation on Voc





Definition of classification criteria

11 samples (≈2000 cells) have been selected:

- ***4 with standard J_{sc} and V_{oc} values***
- ***7 with non-controlled process fluctuations***

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Creation of descriptors (relevant data set)

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Characterization restrictions:

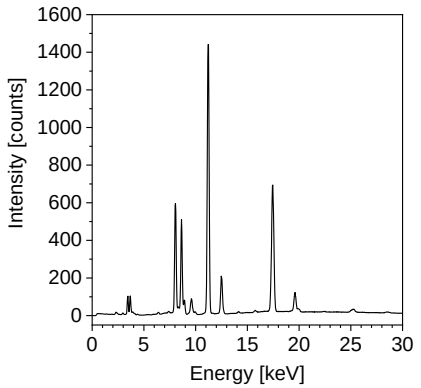
- Non-destructive
- No sample preparation required
- Fast acquisition (< 1min)
- Automatable (suitable for 'big data' acquisition)

Sensitive to changes on:

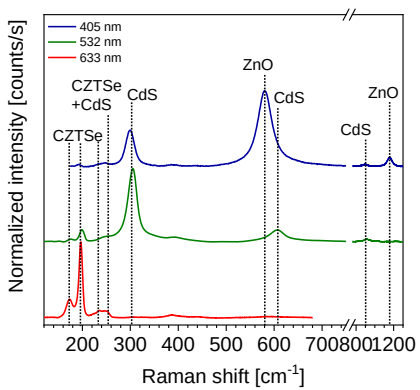
- Composition
- Thickness (nanoscale)
- Crystal structure and quality
- Secondary phases
- …

Do these descriptors provide information to describe the system?

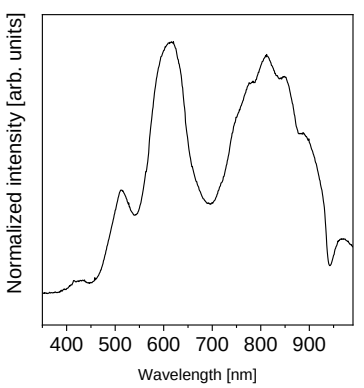
XRF



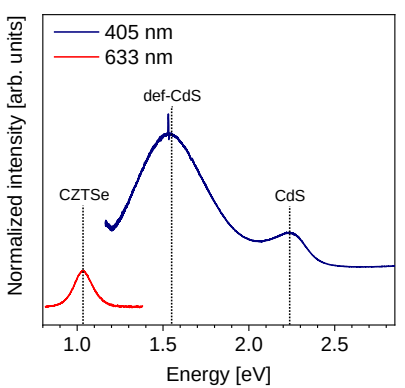
Raman



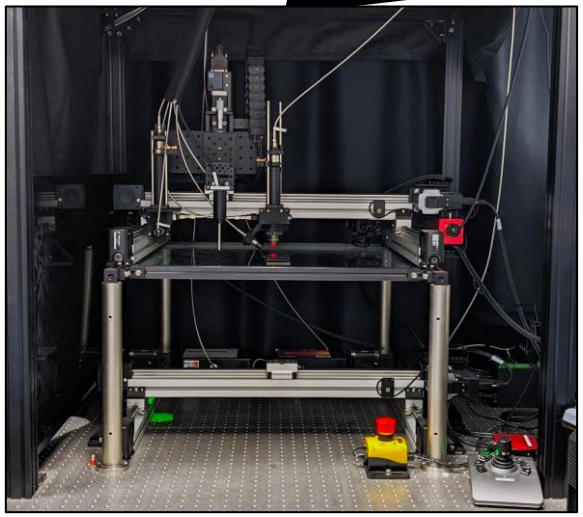
Reflectance

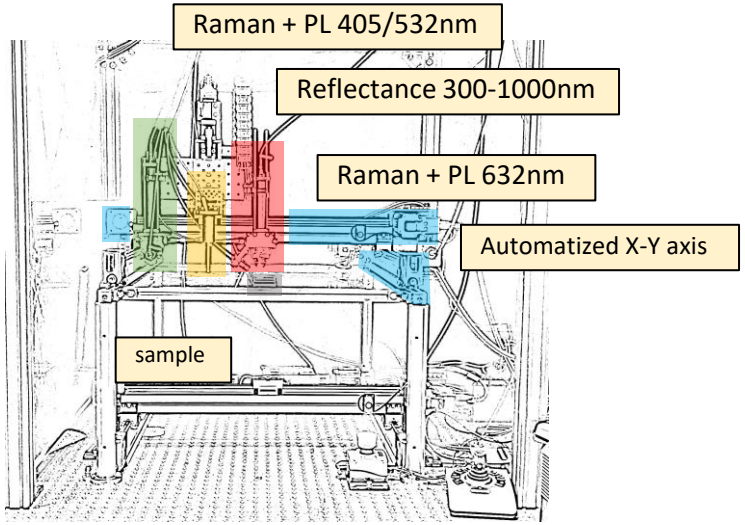


Photoluminescence



XRF





IREC developed combinational characterization platform

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Structured database

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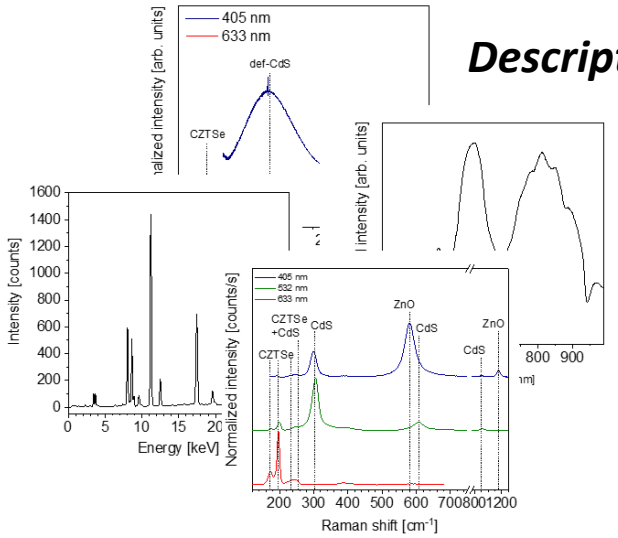
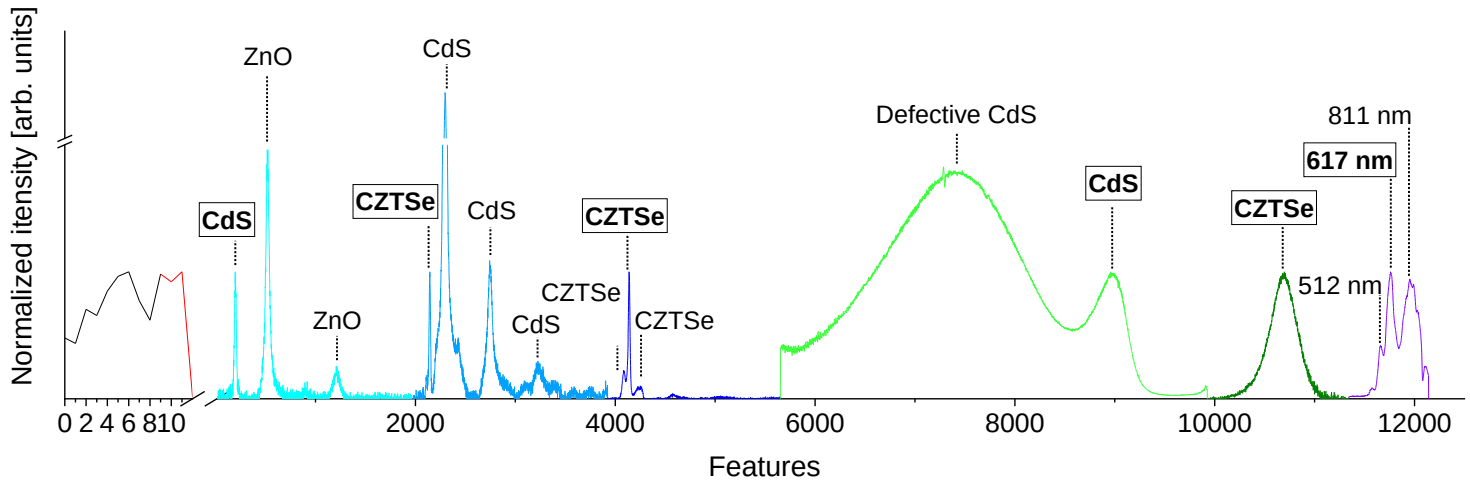


Descriptors…..



Labeling…..

Class	Voc	Jsc
Class 1	Ok	Ok
Class 2	Ok	deviation
Class 3	Deviation	

Generation of a coherent dataset :

- **>2000 data points**
- **>10000 descriptors from 4 characterization techniques per data point**

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AI semi-supervised classification algorithm

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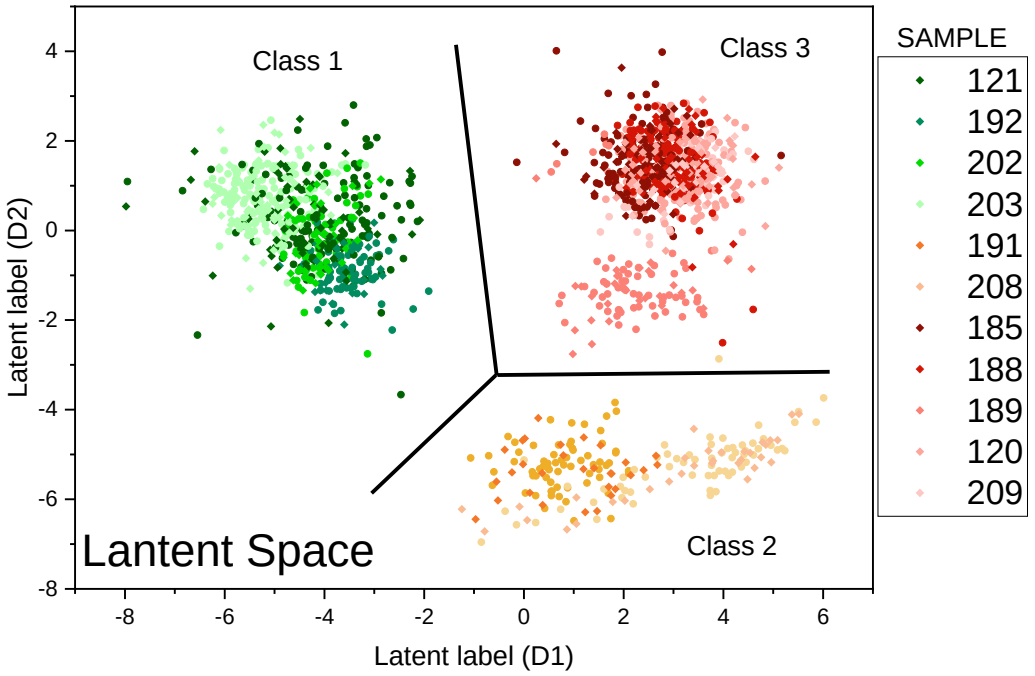
AI semi-supervised classification algorithm

PCA Algorithm
Unsupervised dimension reduction

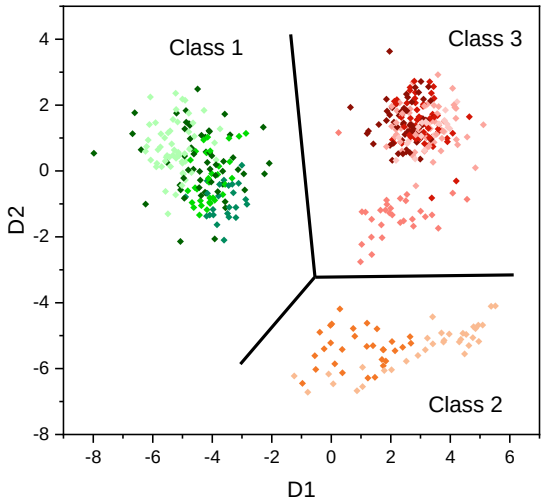
LDA Algorithm
Supervised dimension reduction

≈10000D
↓
20D
↓
2D

Training (70%) Score 99.82%



Test (30%) Score 98.93%



Latent space➔ good classification

- **Correlation between** the **descriptors** (characterization) and the **labeling** (optoelectronics)
- It's possible to **identify the origin of the deviations**

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Research and knowledge generation

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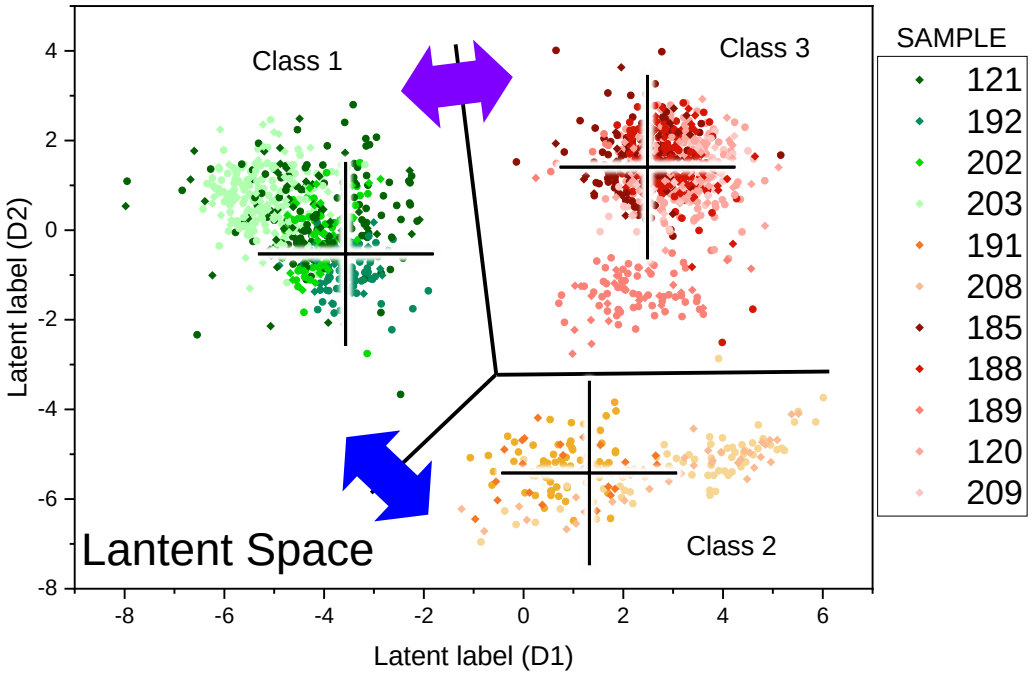
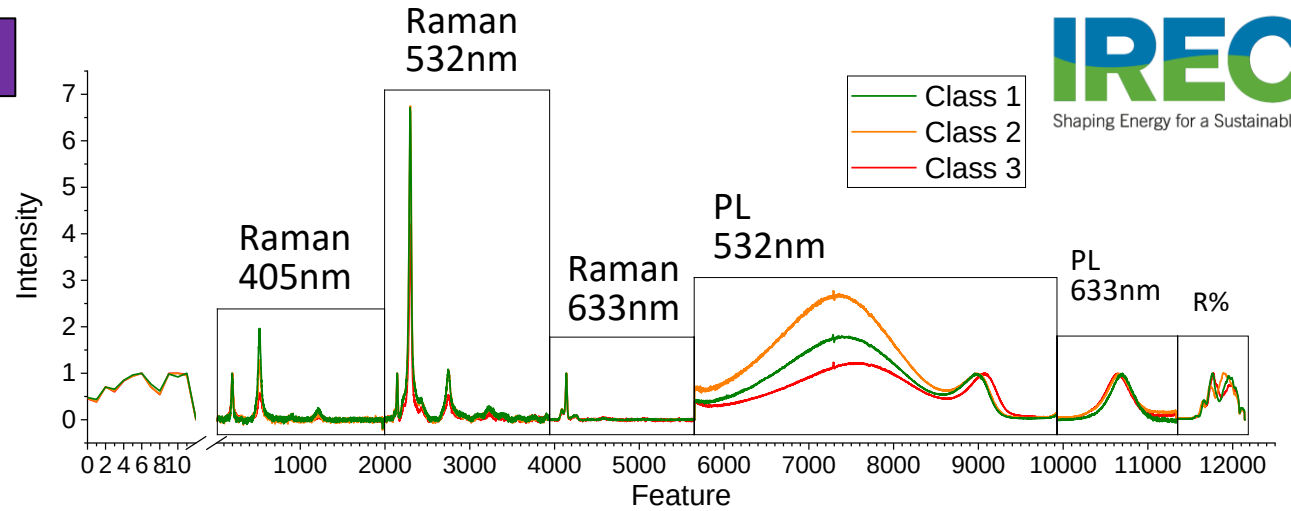
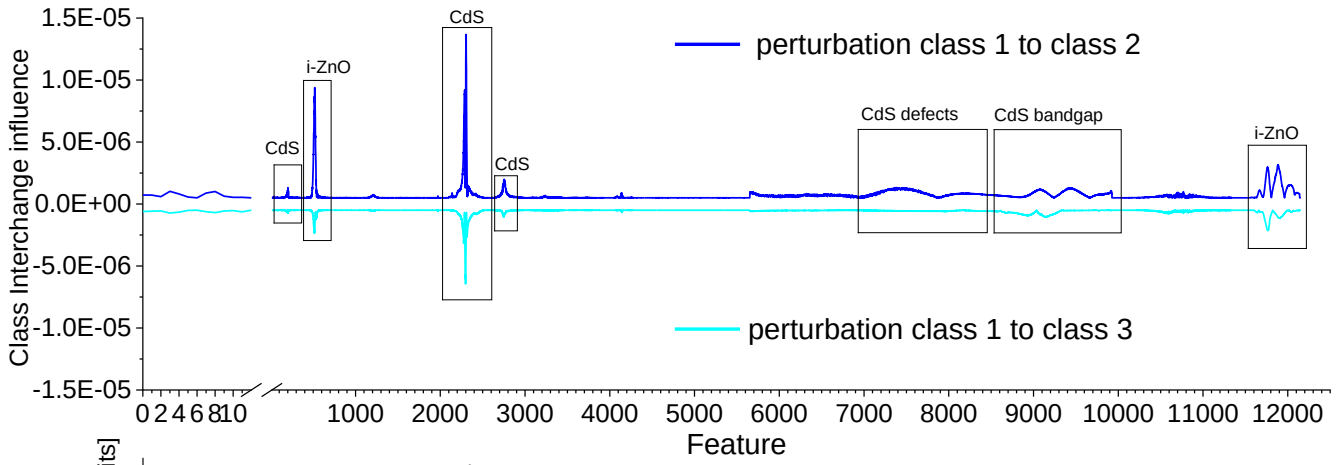
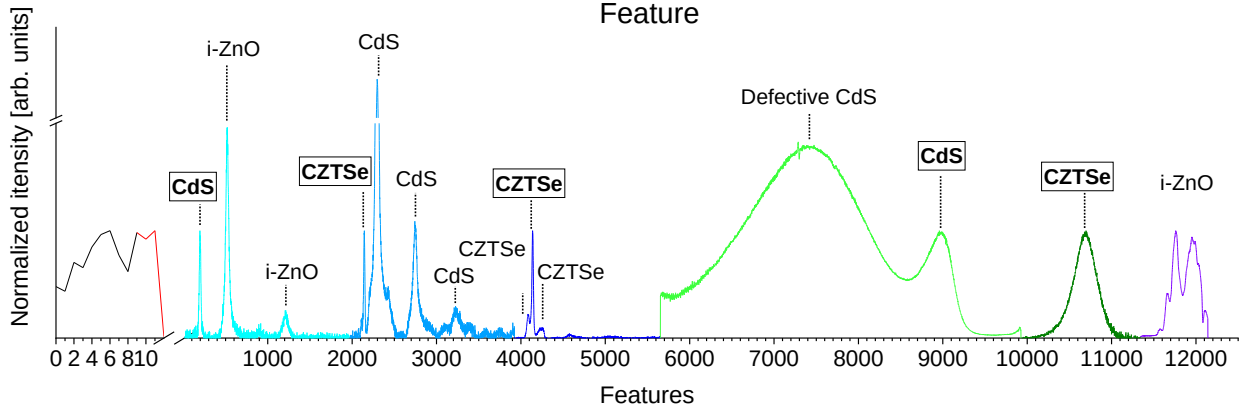


Good classification

- *Permits the detection of relevant signatures for the classification*
- *Application of perturbations allow to discriminate relevant features*
- *Opens the possibility to understand the underlying physics*

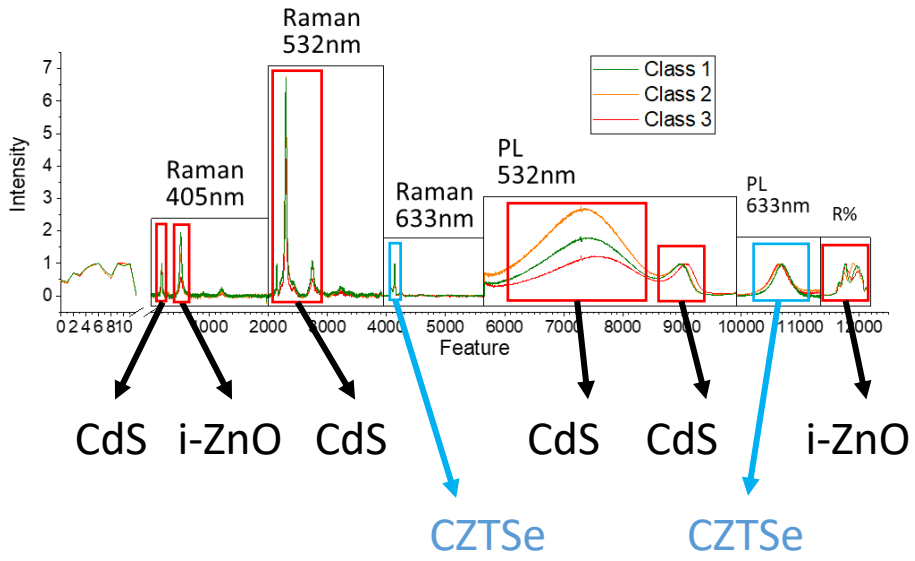






Research and knowledge generation

Merging the information



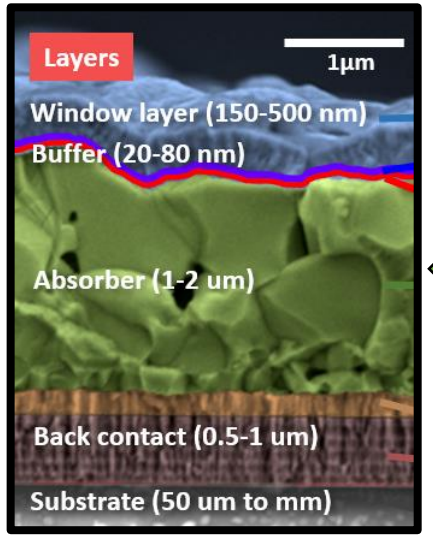
Automatic research:

Permits the identification of the fluctuation's origin

Classification	Voc	Jsc	Fluctuation origin
Class 1	Ok	Ok	
Class 2	Ok	Deviation	Deviations controlled by i-ZnO
Class 3	Deviation		Deviations controlled by CdS

i-ZnO Layer

CdS Layer



CZTSe fabrication process does not produce the fluctuations

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Research and knowledge generation

Combining with characterization experience…

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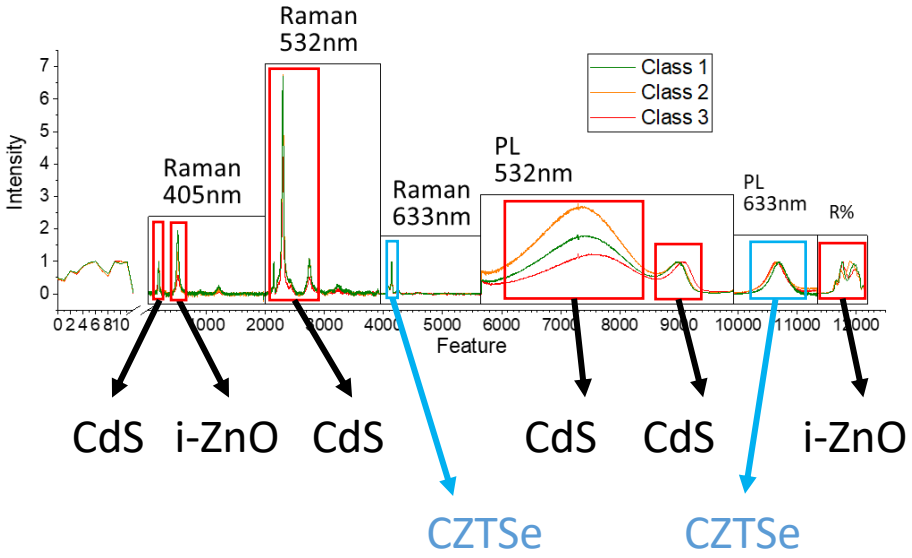
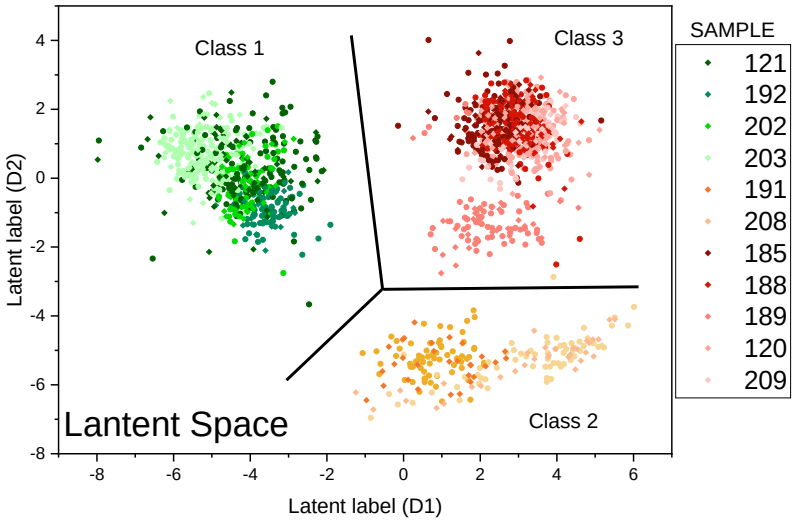
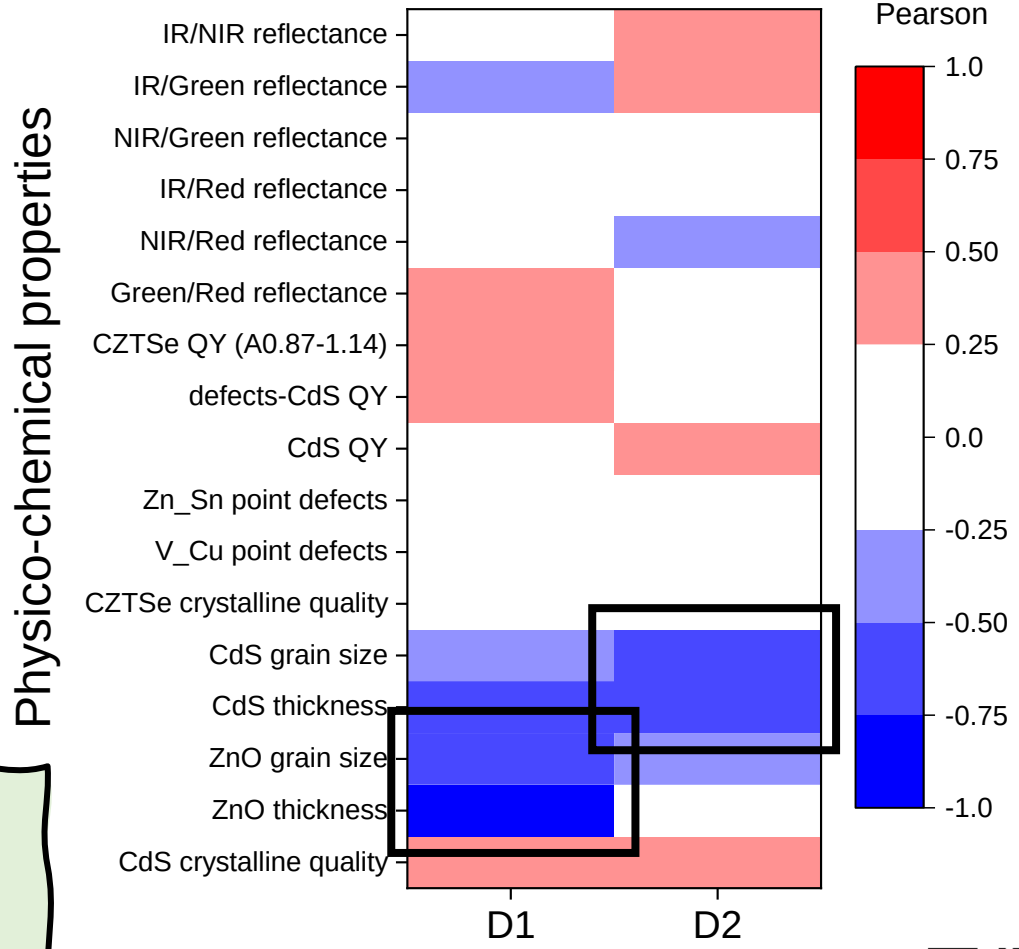




Permits understanding the origin and provide solutions



Robert Fonoll –Rubio, et al
Insights into the Effects of RbF-Post-Deposition Treatments on the Absorber Surface of High Efficiency Cu(In,Ga)Se2 Solar Cells and Development of Analytical and Machine Learning Process Monitoring Methodologies Based on Combinatorial Analysis
Adv. Energy Mater. 2022, 12, 2103163

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Conclusions

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This work has introduced:

- A robust methodology to accelerate the research on complex thin-film photovoltaic materials and devices.
- It demonstrates its validity using artificial methods in real research cases to identify the origins and causes of fluctuations during the manufacturing of a PV device.
- This universal methodology can be applied to a broad range of materials and devices, simplifying analysis in highly complex situations where conventional methods fail or are too time-consuming.
- The methodology not only speeds up the discovery process but also provides an explainable machine learning model, enhancing understanding of the technologies under study. Its ultimate goal is to equip the scientific community with a framework that promotes the integration of AI and combinatorial analysis in material and device R&D.

Enric Grau-Luque, et al
Accelerating the Development of Thin Film Photovoltaic Technologies: An Artificial Intelligence Assisted Methodology Using Spectroscopic and Optoelectronic Techniques,
Small Methods (2024) 2301573/17.

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Beyond this work

Thank you for your attention!!

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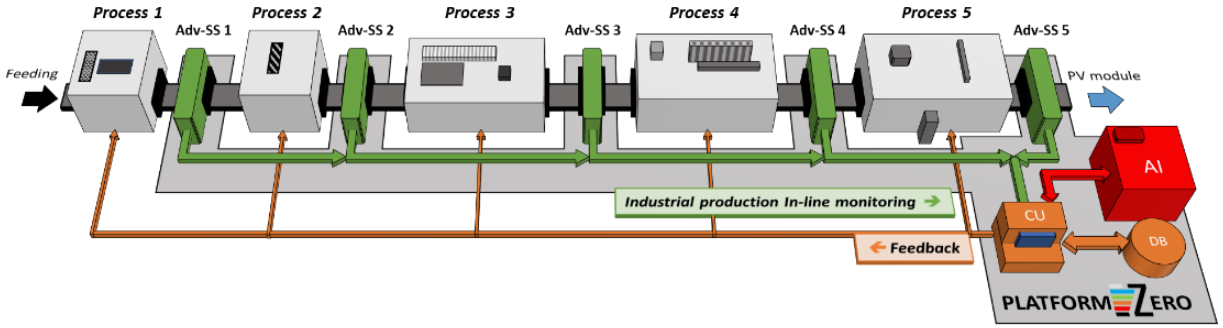
Technology validation on real production lines

Customizable AI-based in-line process monitoring platform for achieving zero-defect manufacturing in the PV industry (Platform-ZERO)
January 2023 – December 2026

"**The goal of this project** is to adapt, integrate, and validate this strategy as a tool for industrial process monitoring in 2 photovoltaic companies and 2 pilot lines, with the aim of improving the quality of photovoltaic devices and reducing their environmental impact."



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http://www.platform-zero-project.eu/

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