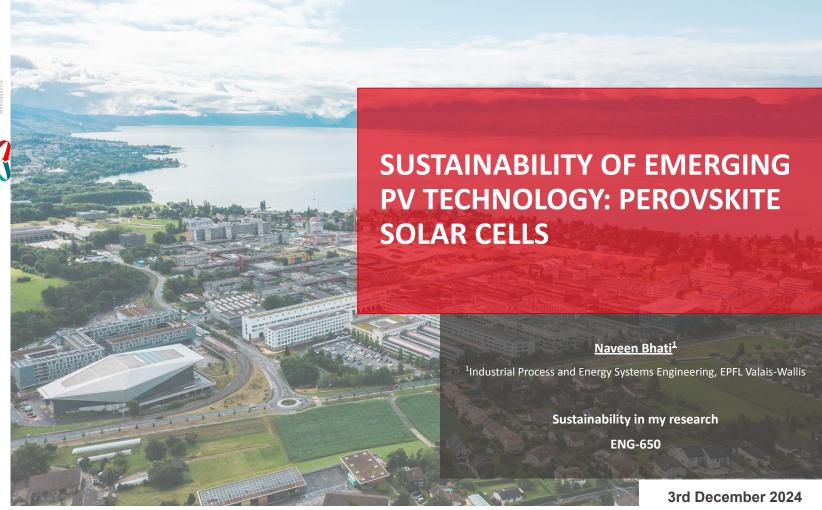
EPFL



I IPESE
Industrial Process
and Energy Systems
Engineering



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Photovoltaic (PV)

Technologies the electricity supply in future - Solar PV -> 50% of the tetal renewable production capacity to

meet the COP targets

PV technologies:

1st generation (thickness> 150um)

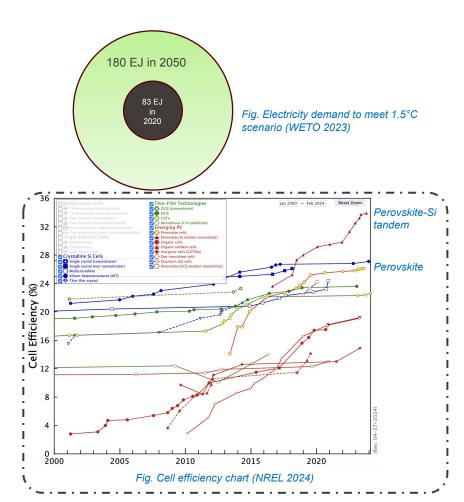
Monocrystalline-Si, polycrystalline-Si

2nd generation (thin-film PV, thickness< 10um)

CIGS, CdTe, CIS, a-Si, etc.

3rd generation (emerging PV, thickness < 10um)

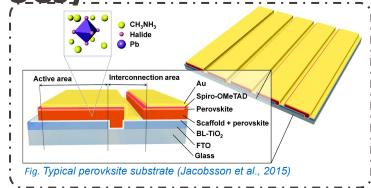
- Organic materials, perovskites, Dye-sensitized, Quantum dots,
- multi-junction, tandems
- PSCs reached >26% efficiency in single junction devices and 33.9% in tandem (Si) devices

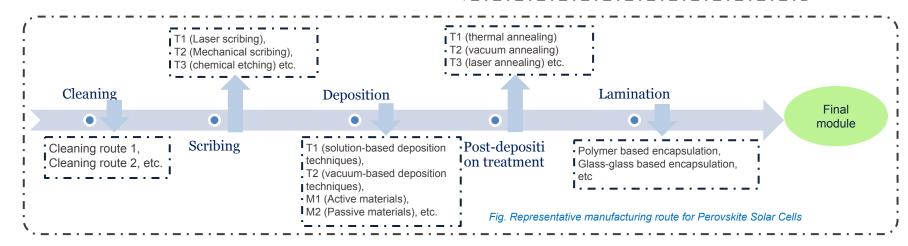




Perovskite solar cells (PSCs)

- Infinite space for the chemical composition (ABX₃) optimization
- Complex manufacturing process with a plethora of cell architecture options
- Range of materials and fabrication processes for all active layers



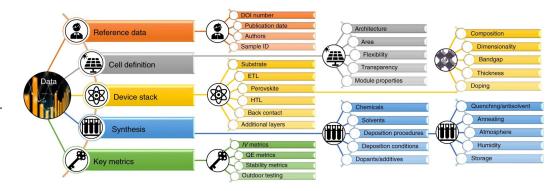




PSCs Recipes

FAIR database of perovskite solar cells recipes (Jacobsson et al. 2022)

- >42400 cell recipes
- >100 deposition process sequence for each layer
- > 1000 stack sequence for each of the active layers (i.e., Electron transport layer (ETL), Perovskite, Hole transport layer (HTL))



ETL Deposition techniques



ETL STACKS

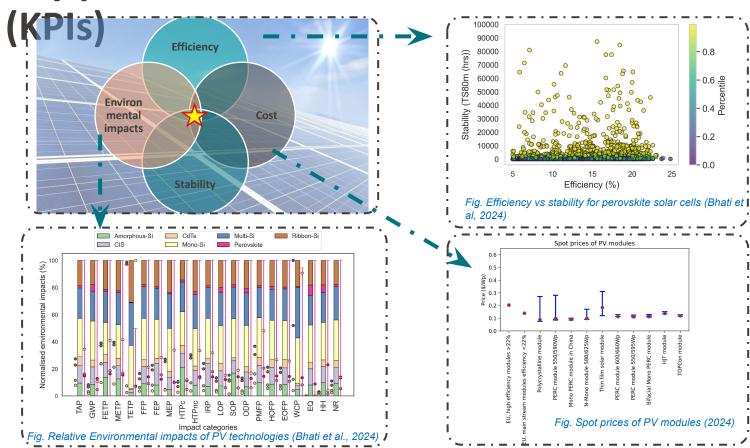




TiO2-c | TiO2-mp TiO2-c PCBM-60 PCBM-60 | BCP SnO2-np C60 | BCP SnO2-c TiO2-c | TiO2-mp | 7002-mp



Key performance indicators





CO₂ budget and Environmental impacts of PV Technologies

- Cumulative CO2
 emissions of PV
 production to meet the
 energy demand by 2050
 at 20% growth rate till 1.2
 TW/annum production
 level will significantly
 consume the overall CO2
 budget
- However, with significant research, this footprint can be reduced to 1.5% by 2050
- Further, a carbon-neutral PV production by transforming the energy infrastructure will keep impact below 1% of the cumulative budget

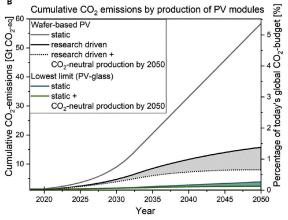


Fig. Carbon emissions scenarios for PV industry: cumulative CO2 emissions from the PV sector (Wagner et al. 2020)

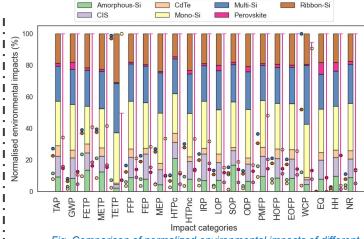


Fig. Comparison of normalized environmental impacts of different classes of PV technologies based on Recipe method (Bhati et al. 2024)

- On a median values basis (shown as bar) perovskite solar cells are having relatively less impact in all categories except HH and EQ
- On average (shown as scattered plots with error bars), PSCs are not significantly better moreover can be worse than si cells in categories like HH, EQ and NR



Hotspots in PSCs manufacturing

Hotsopts in the fabrication process:

- Based on hotspot analysis, on average, the etching stage contributes minimum to the overall fabrication process except in FETP, METP, HTPnc, EQ, and HH indicators
- Substrate+TCO selection and preparation stage has maximum impact in human health category
- Cleaning stage has maximum impacts in almost all categories
- Among active layers, perovskite layers have slightly higher values than ETL and HTL which are comparable to each other

Strategies to reduce impacts:

- Recycling of solvents used in the cleaning process (acetone has the maximum impact)
- Electricity consumption during ultrasonication also have high impact in certain cases
- Gold and gold-based electrodes should be avoided
- Certain ETLs like PCBM and perovskite layers like CsPbBr should be avoided to reduce the impacts in HH category

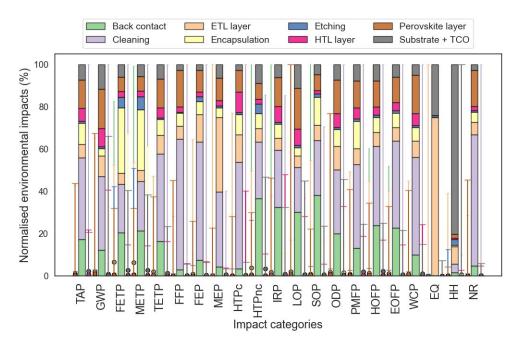


Fig. Relative environmental impacts of different fabrication steps for perovskite modules based on Recipe method (Bhati et al. 2024)



Mapping effects on absolute scale

- Based on the results of LCA, PSCs have the potential to reduce the impacts of PV technologies significantly
- However, the results are still relative and cannot be taken as guiding measures for designing or fabricating PSC
- For the same, the Environmental footprint method can be used to estimate the impacts under different categories
- Finally, these impacts can be translated into contribution to different planetary boundary (PBs) budgets
- However, there is still a need to allocate the budget for this technology against different PBs so the transgression can be measured specific to these technologies

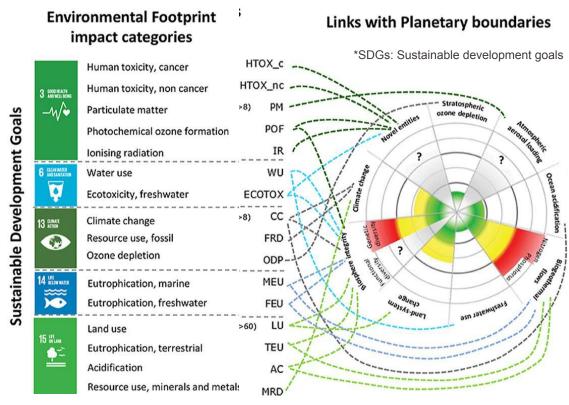


Fig. Connection between the LCIA impact categories of Environmental Footprint (EF) method, PBs and SDGs (Sala et al. 2020)



Trade-offs between various objectives

- Multiple criteria for designing these cells (like different PBs) and hence we need a mathematical framework to design the optimal recipes
- For the same, we can use multi-objective optimization to generate the optimal recipes by balancing the weights of different recipes
- Finally, with the generated recipes we can do a screening and evaluate the most potential candidates in the experimental setting to reduce the time in finding the optimal solutions

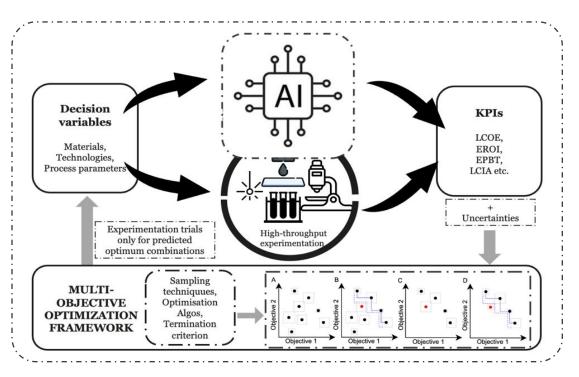
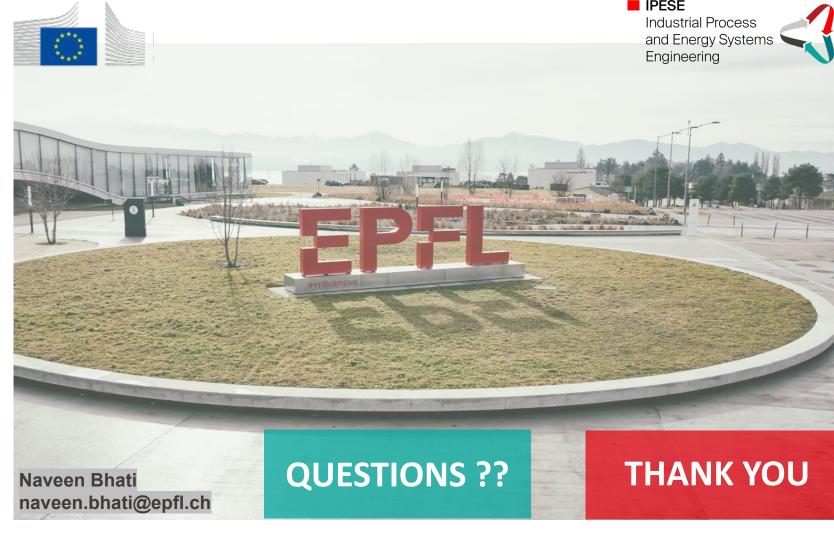


Fig. Framework for optimizing PSCs based on multiple objective functions





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Decision variables and design

space

Decision variables affecting the Key performance indicators of perovskite solar cells/modules include:

- Perovskite absorber layer composition
- Charge transport layer materials (ETL, HTL)
- Manufacturing techniques
- Post-deposition treatment technique
- Solvent composition
- Overall cell architecture

Manufacturing Cost : $MC = Cost_{materials} + Cost_{ener} + Cost_{equip} + Cost_{build} + Cost_{labour} + Cost_{util} + Cost_{automate} + Cost_{waste}$

