# *FENCES: Ferroelectric nanocomposites for enhanced solar energy efficiency*

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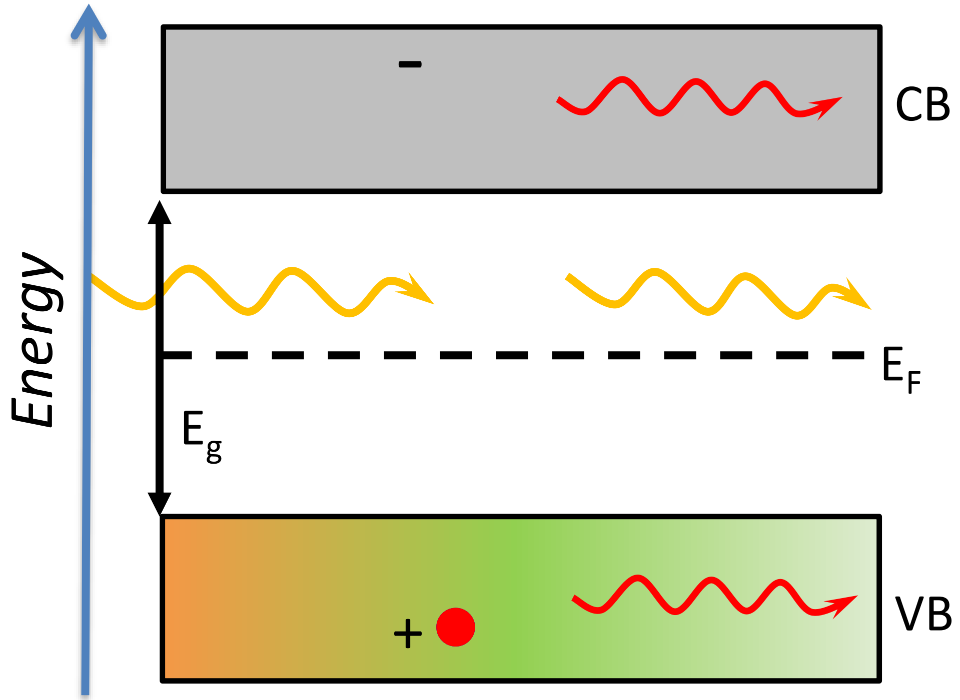
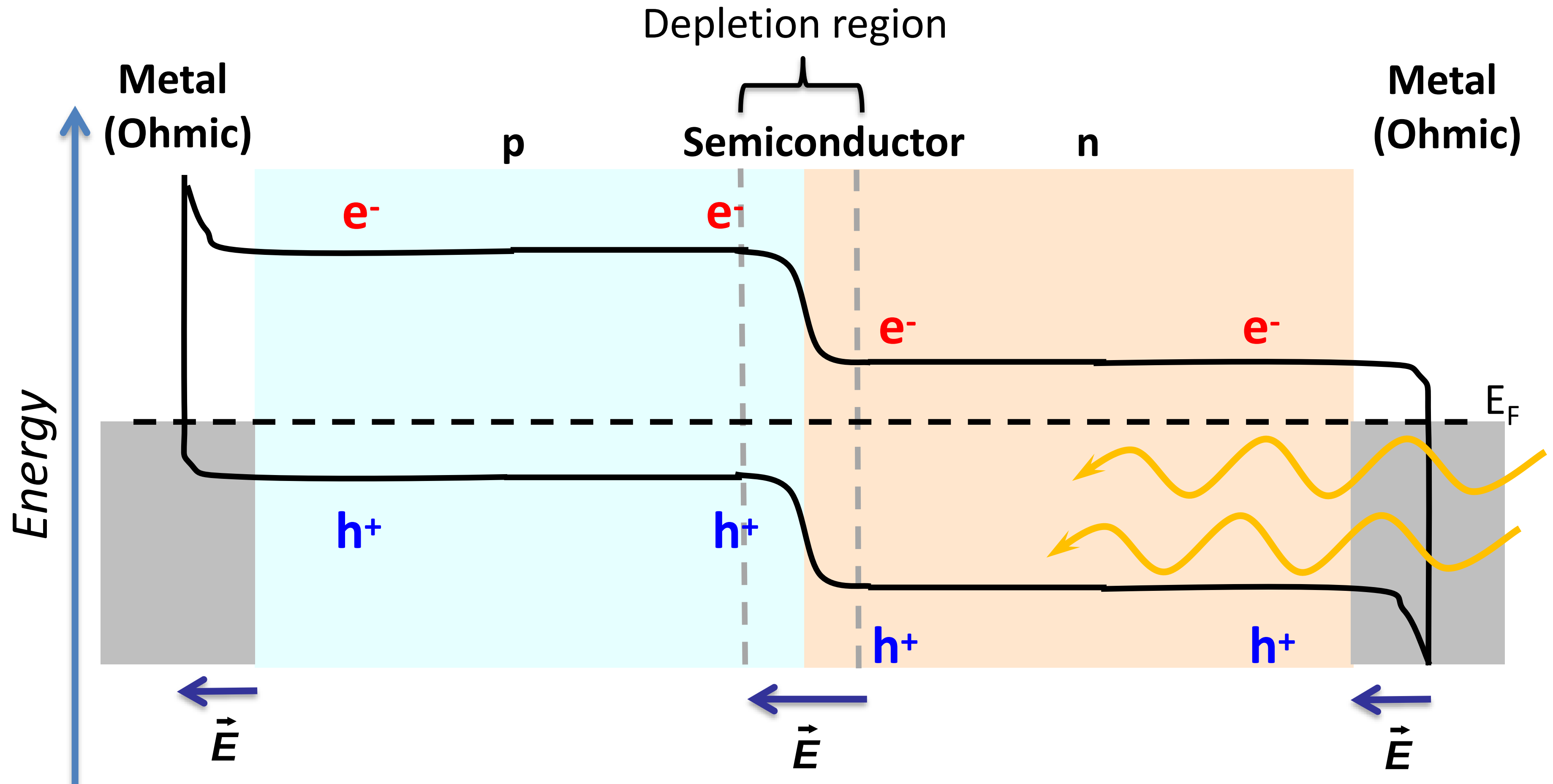
# How does a solar cell work?

- Light absorbed, exciting electron to conduction band (CB) leaving hole in valence band (VB)
- Relaxation within band giving out heat (phonon)
- Relaxation between bands → recombination
- Gives out light again

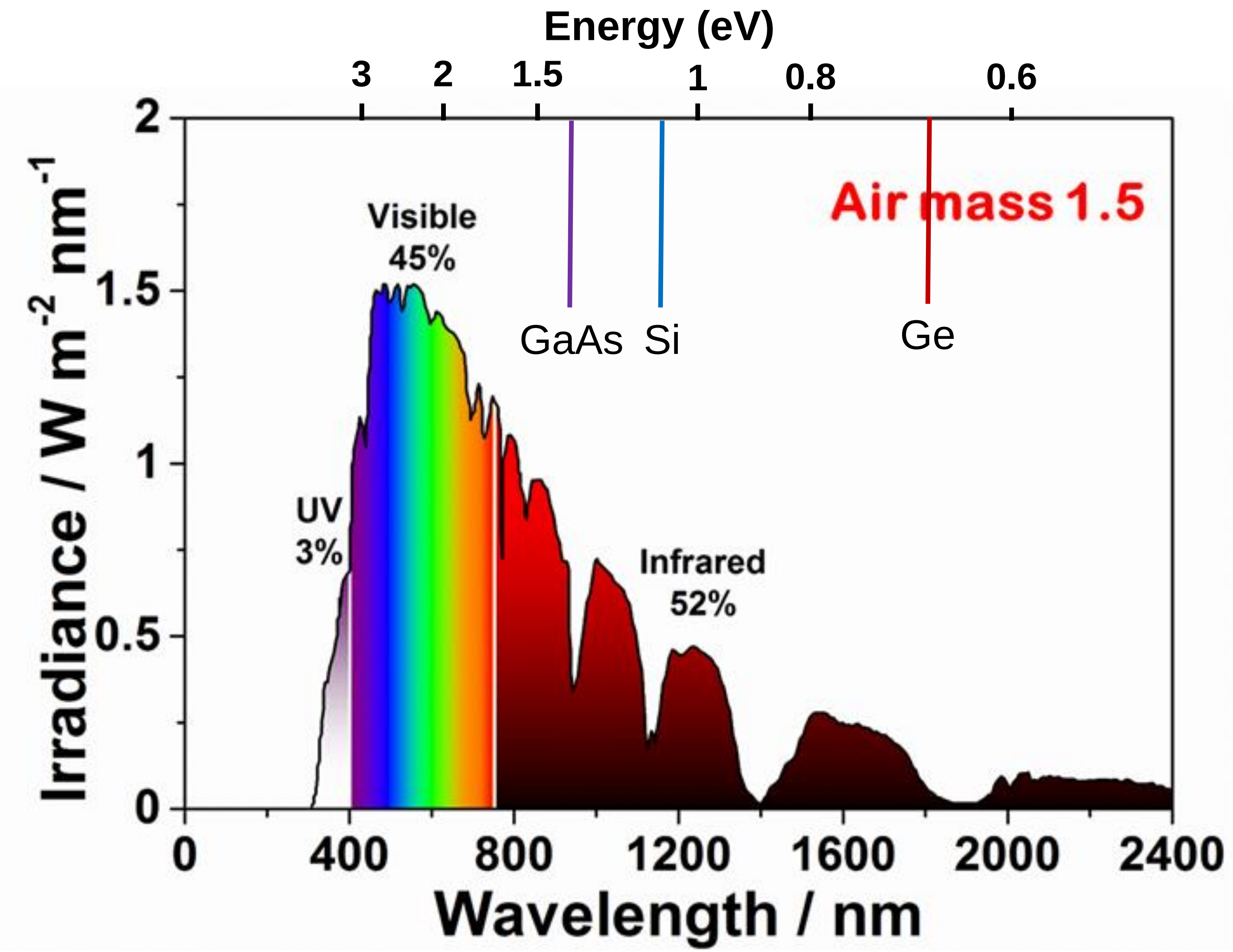


# How does a solar cell work?

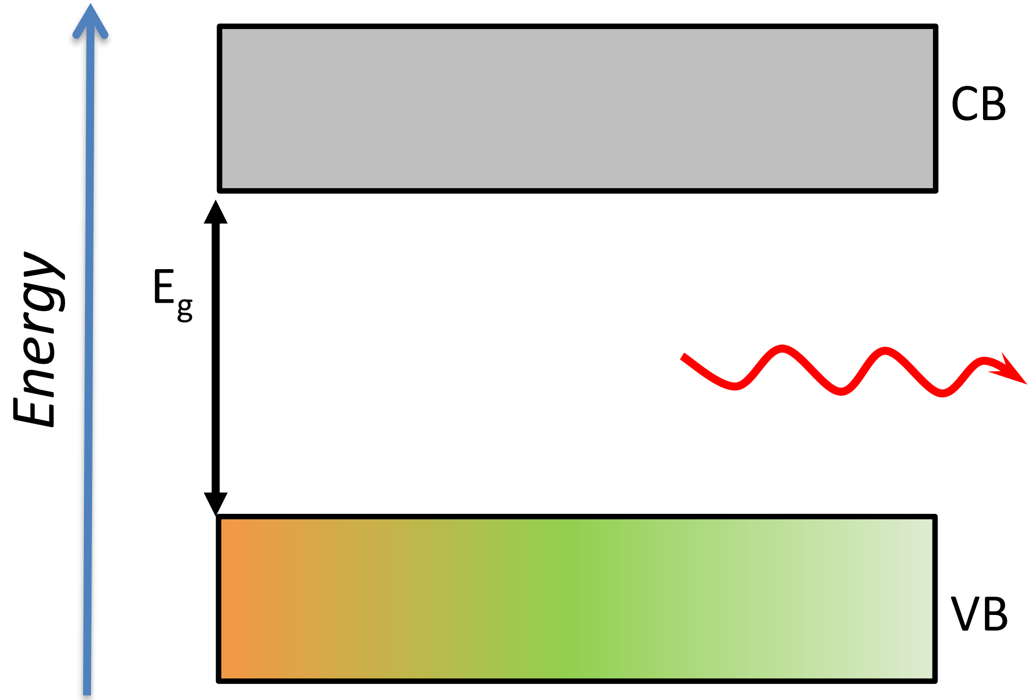



*Drift current:* results from electric field
*Diffusion current*: results from concentration gradient
→ ***Asymmetry***

# What are the limitations?



# What are the limitations?



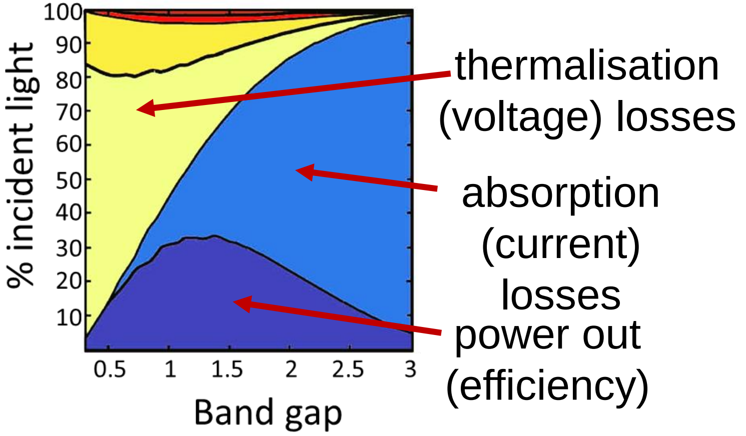

- Semiconductors can only absorb photons with energy greater than the bandgap
    - $E_g$ = 2 eV
    - Blue light (2.6 eV) illumination
    - Photon absorbed
    - Excess energy given out as heat

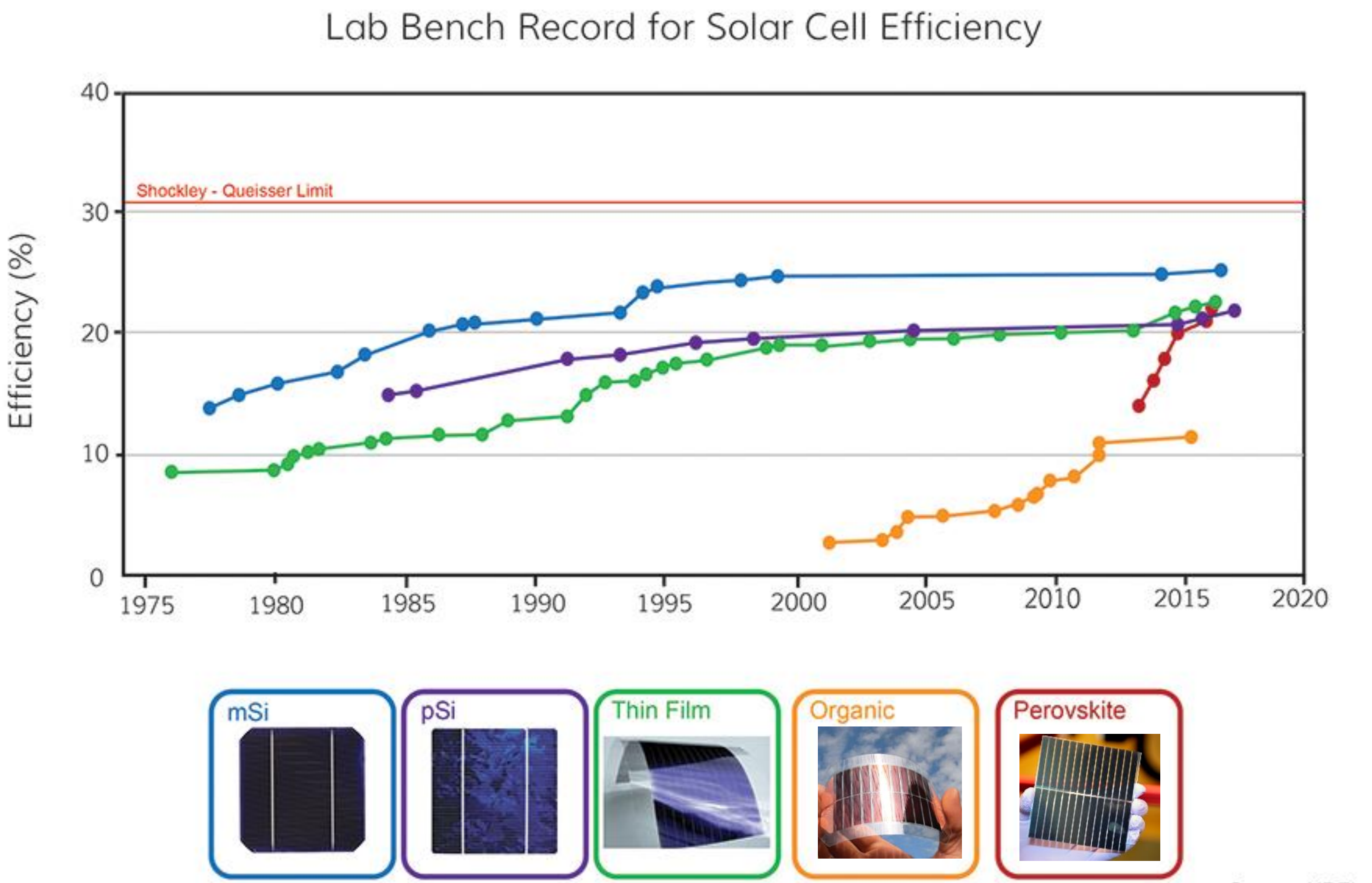
    - Orange light (2 eV) illumination
    - Photon absorbed
    - No excess energy

    - Red light (1.6 eV) illumination
    - No absorption
    - Light passes through

# What are the limitations?

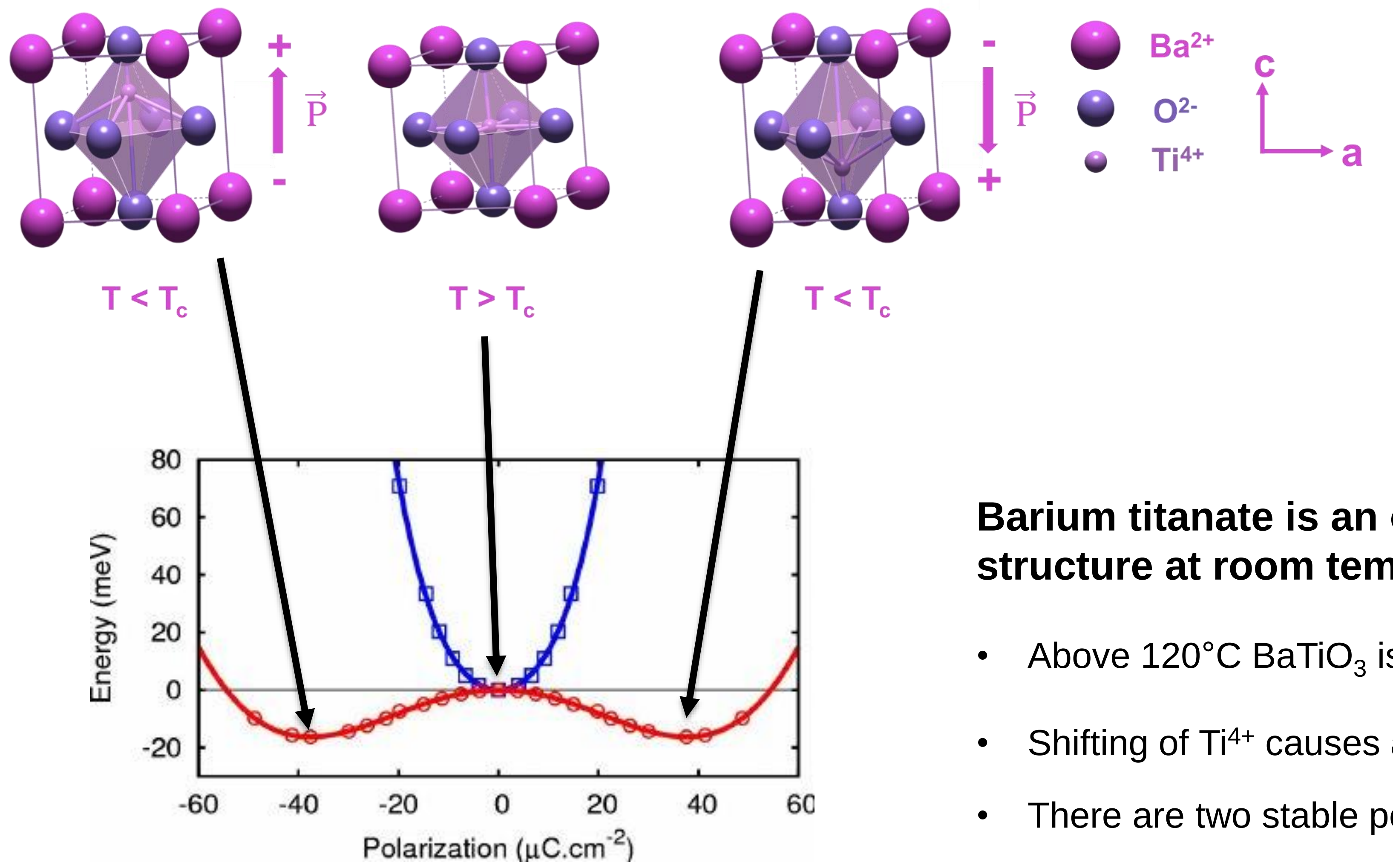
- Low energy light (below bandgap) not absorbed => narrow bandgap better
- Energy above bandgap lost through heat => larger bandgap better
- More photons = more current
- More energy = more voltage
- P = I x V
- *Compromise* → optimum bandgap of 1.34 eV, **max PCE 33.7%**




Source: NREL

# Ferroelectrics

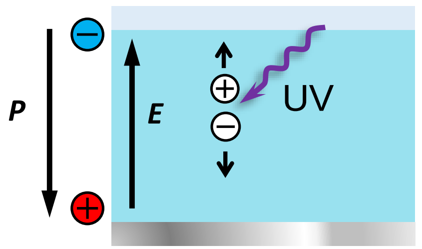



**Ferroelectric** materials possess *spontaneous polarisation* that can be switched between 2 or more stable states upon application of electric field

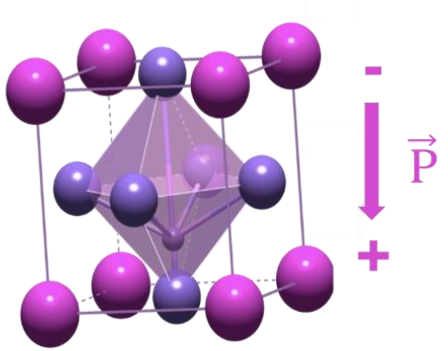
**Barium titanate is an oxide perovskite in tetragonal structure at room temperature**

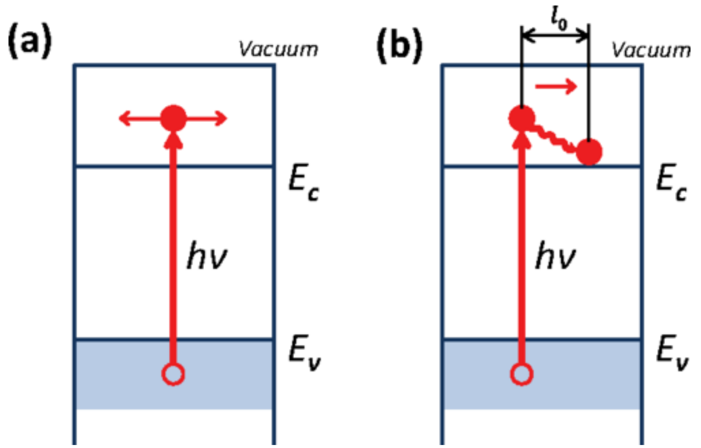
- Above 120°C $BaTiO_3$ is cubic
- Shifting of $Ti^{4+}$ causes a spontaneous polarisation
- There are two stable polarisation states

# Ferroelectrics: bulk photovoltaic effect




Charge separation
via polarisation




Symmetric
material

Non-symmetric
material

- Light absorbed by ferroelectric
- Asymmetry in ferroelectrics leads to charge separation
- Can produce very high voltage

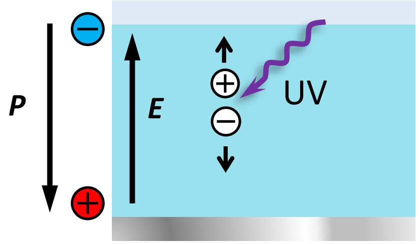
**BUT**

- Most ferroelectrics only absorb UV light

→ Low current
→ **Low efficiency**

# ERC: FENCES

**Ferroelectric bulk photovoltaic (BPV) effect**




Charge separation via polarisation

✓ High voltage

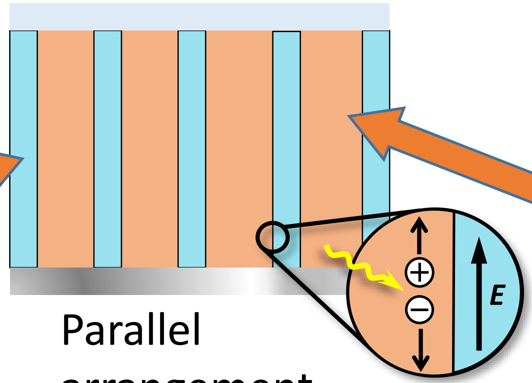
✗ Poor light absorption & transport

→ Low current

→ Max. eff. ~20%

Voltage generation using UV only

Ferroelectric photovoltage coupled to light absorber



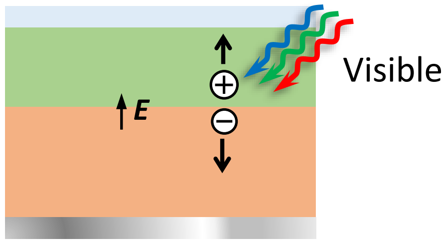

Parallel arrangement

Driving charge separation without charge transfer

Visible light absorption

→ high current

**Semiconductor absorber**



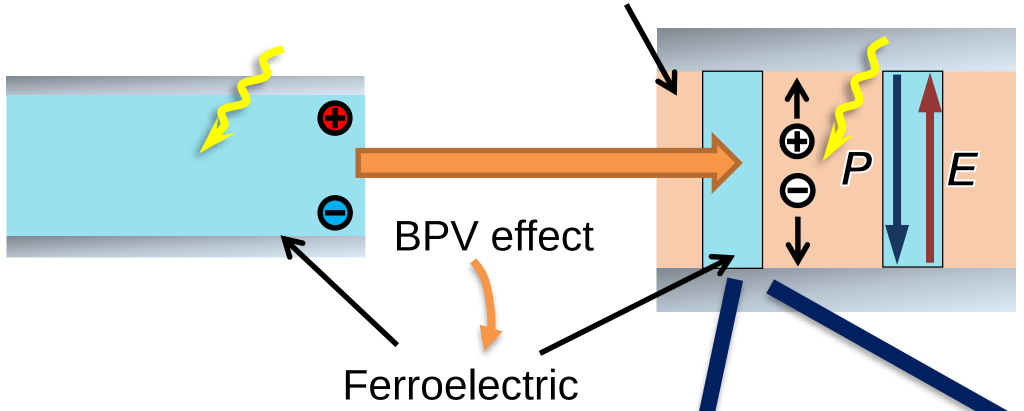

Charge separation via junction

✓ Light absorption & charge transport

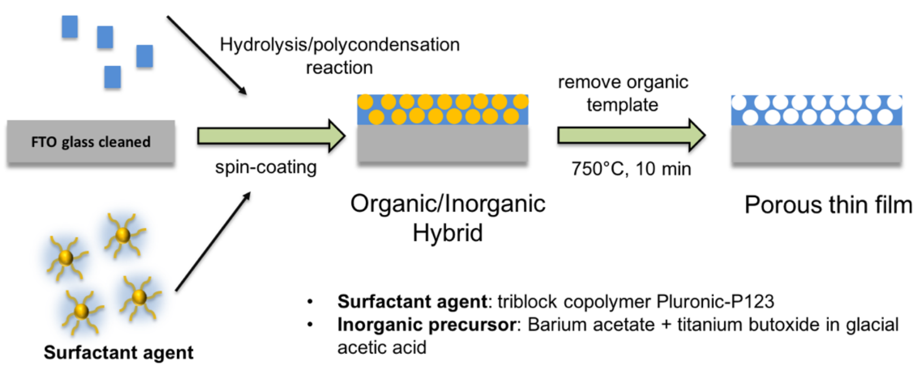
✗ Voltage limited by built-in potential of junction (bandgap)

→ Max. eff. ~34%

# FENCES: synthesis

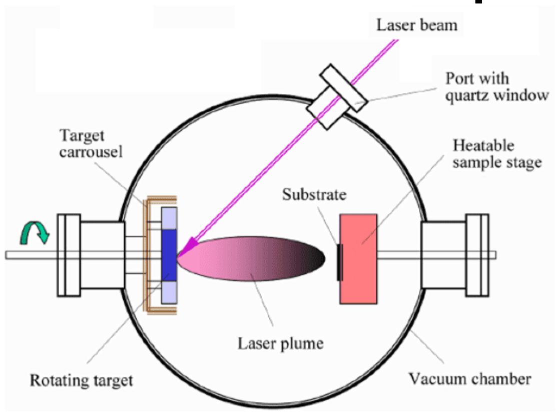


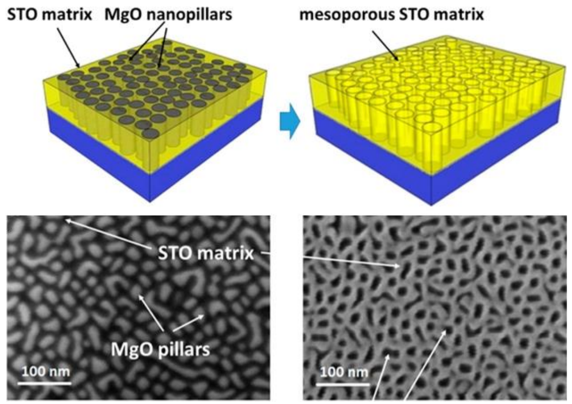

## Solution-based




- **Surfactant agent**: triblock copolymer Pluronic-P123
- **Inorganic precursor**: Barium acetate + titanium butoxide in glacial acetic acid

## Pulsed Laser Deposition



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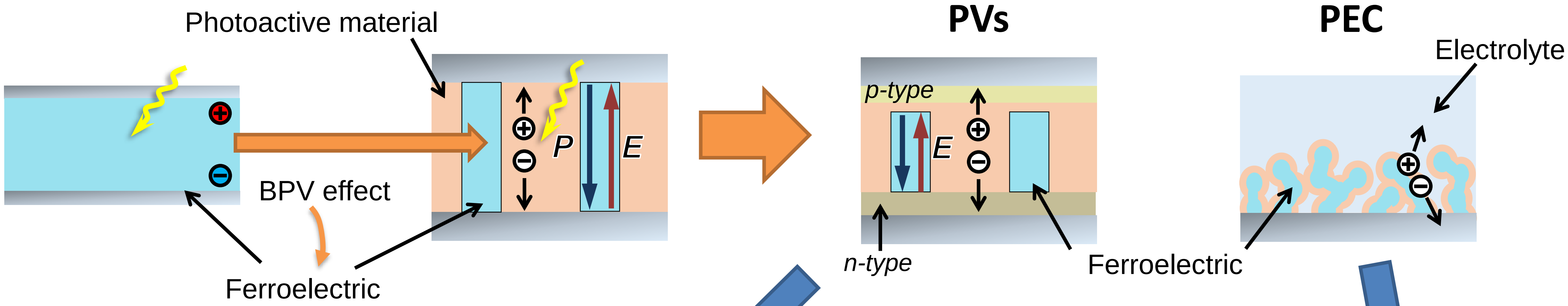
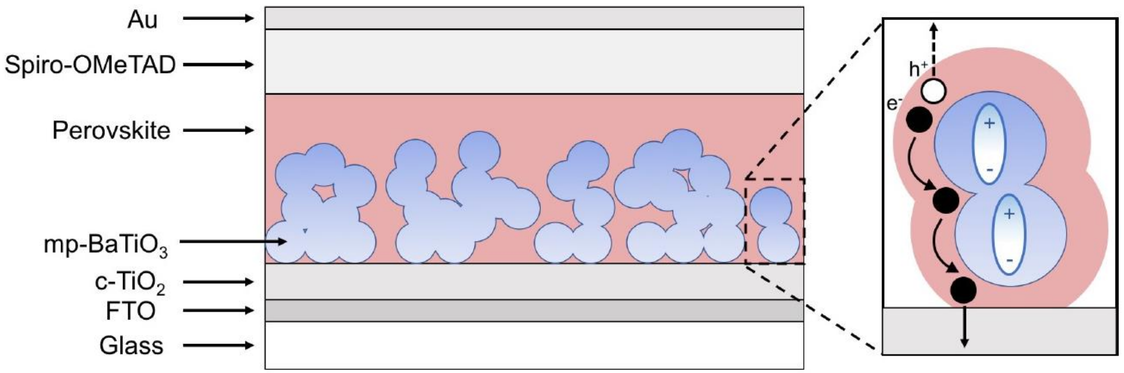
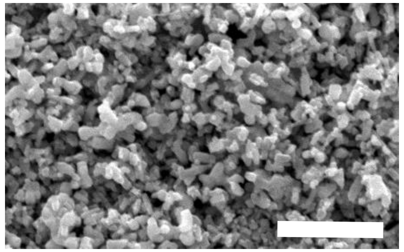


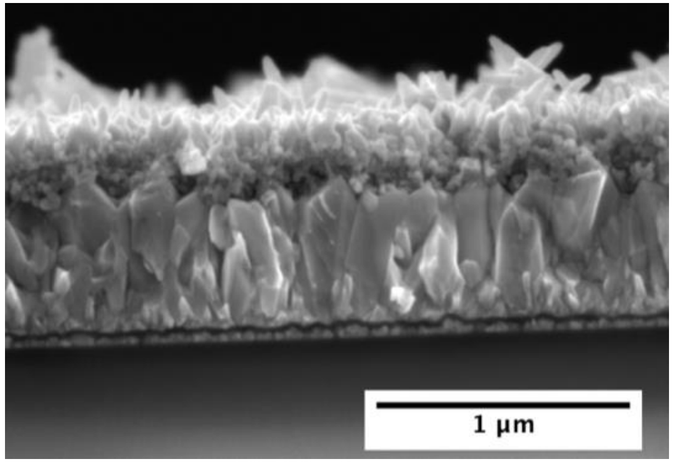




Chloe Forrester



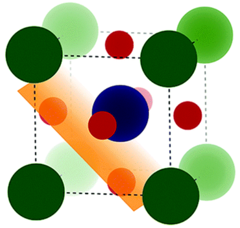
Adriana Augurio

BaTiO$_3$/Fe$_2$O$_3$

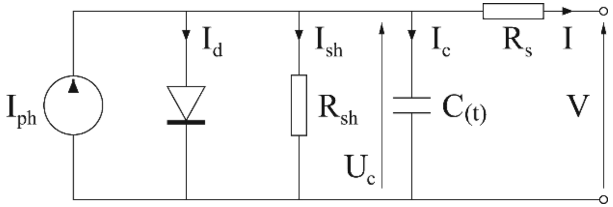


# FENCES: modelling & measurement

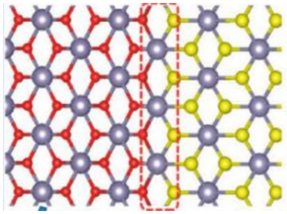
## **Modelling** (collaboration with Dr Keith Butler)



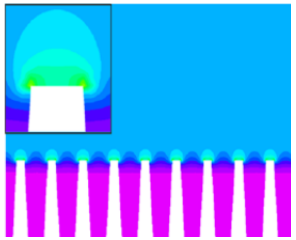
Computational screening




Equivalent circuits



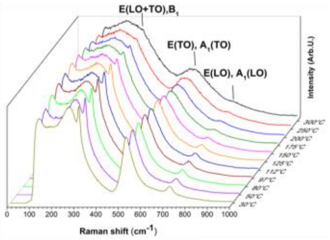
DFT: polarization & interfaces

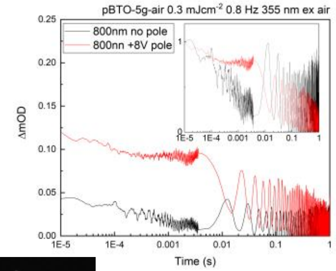


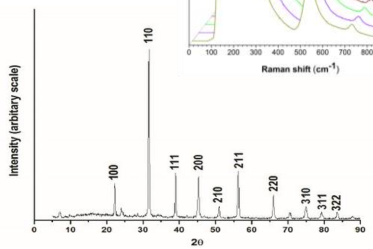
Finite Element

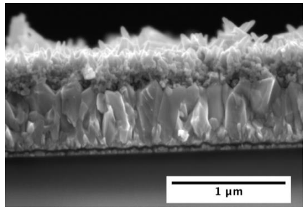
## **Characterisation**

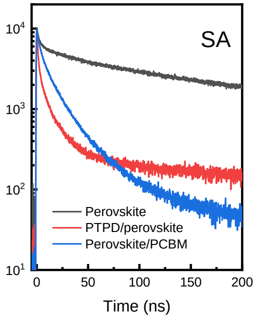
XRD, Raman, SEM, PL, tr-PL, TAS etc…



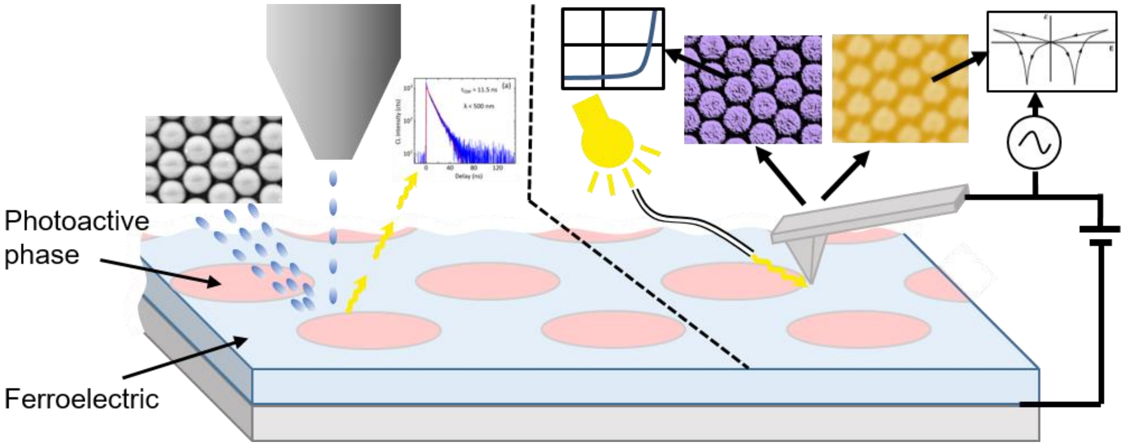




Coupled AFM, pc-AFM, PFM with tr-CL-SEM mapping



# Thank You

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