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
Drift current: results from electric field
Diffusion current: results from concentration gradient
→ Asymmetry
What are the limitations?
Semiconductors can only absorb photons with energy greater than the bandgap:

- $E_g = 2 \text{ eV}$
- 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
• 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
• $P = I \times V$
• *Compromise* → optimum bandgap of 1.34 eV, max PCE 33.7%

What are the limitations?

- Power out (efficiency)
- Absorption (current)
- Losses
  - Thermalisation (voltage) losses
  - Absorption (current) losses
  - Power out (efficiency)
Barium titanate is an oxide perovskite in tetragonal structure at room temperature

- Above 120°C $\text{BaTiO}_3$ is cubic
- Shifting of Ti$^{4+}$ causes a spontaneous polarisation
- There are two stable polarisation states
Ferroelectrics: bulk photovoltaic effect

- 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
**Ferroelectric bulk photovoltaic (BPV) effect**

- Poor light absorption & transport $\rightarrow$ Low current $\rightarrow$ Max. eff. $\sim$20%

- Voltage generation using UV only

- Charge separation via polarisation

- High voltage

**Ferroelectric photovoltage coupled to light absorber**

- High voltage

- Parallel arrangement

- Driving charge separation without charge transfer

- Visible light absorption $\rightarrow$ high current

**Semiconductor absorber**

- Light absorption & charge transport

- Voltage limited by built-in potential of junction (bandgap) $\rightarrow$ Max. eff. $\sim$34%

- Visible light absorption

- Charge separation via junction
FENCES: synthesis

- **Photoactive material**
- **BPV effect**
- **Ferroelectric**

**Solution-based**
- Inorganic precursor
- Hydrolysis/polycondensation reaction
- Organic/Inorganic Hybrid
- Spin-coating
- 750°C, 10 min
- Porous thin film
- Surfactant agent: triblock copolymer Pluronic-P123
- Inorganic precursor: Barium acetate + titanium butoxide in glacial acetic acid

**Pulsed Laser Deposition**
FENCES: synthesis

Photoactive material

BPV effect

Ferroelectric

PVs

p-type

n-type

Ferroelectric

PEC

Electrolyte

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

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1 µm
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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