Imperial College London

Morphological and Photochemical Stability of PCBM in Organic Solar Cells

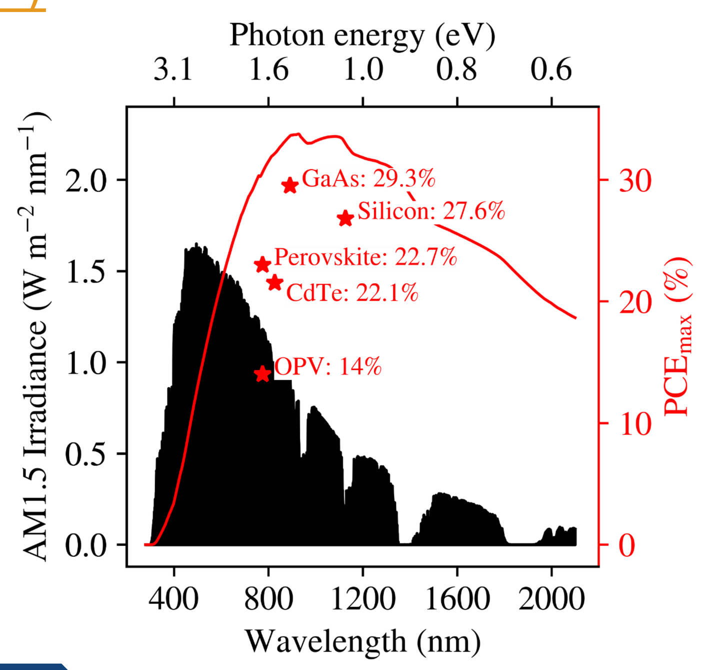
Sebastian Pont,[ab] Fabrizia Foglia,[c†] Anthony Higgins,[d] James R. Durrant,[abd] and João T. Cabral[ac]

s.pont14@ic.ac.uk

Introduction

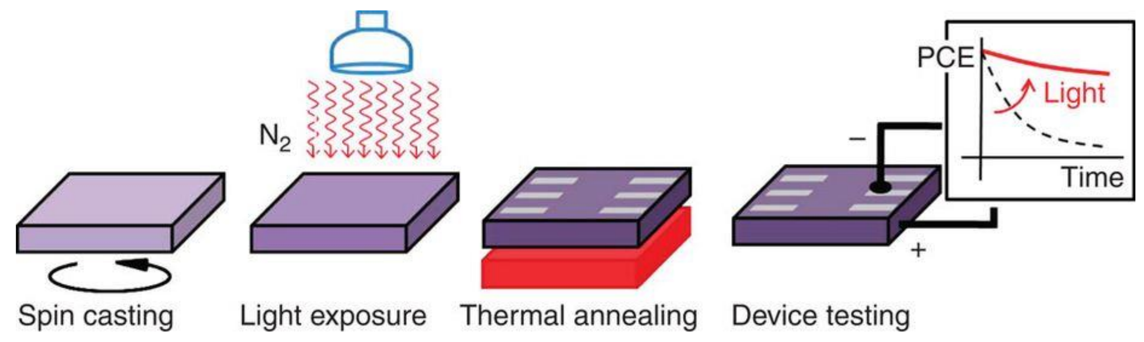
Organic photovoltaics (OPV)

- Efficiency continues to increase for **OPV reaching nearly 14%.**
- Potentially **low cost** to produce due to solution processing with roll-to-roll systems.
- Active layer commonly consists of electron donating polymer and electron accepting small molecule, e.g. PCBM.

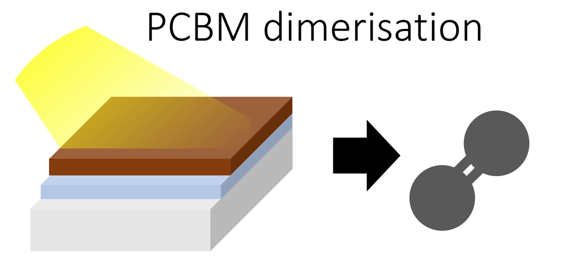


OPV Stability and PCBM Dimerisation

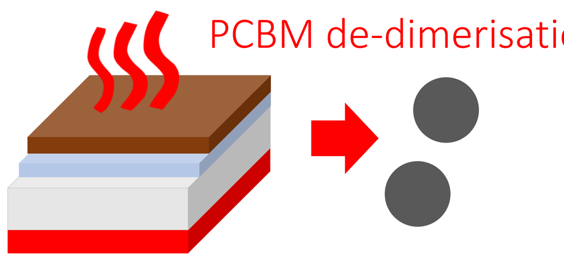
- **Stability is critical** for viable commercialisation of OPV.
- Dimerisation shown to improve stability of thermal stress (shown below[1]) but also suggested as a potential mechanism of 'burn-in'.
- Here, we probe the competition between **both light and temperature**, and the concentration dependence of this mechanism.



Light soaking (without O_2): PCBM dimerisation



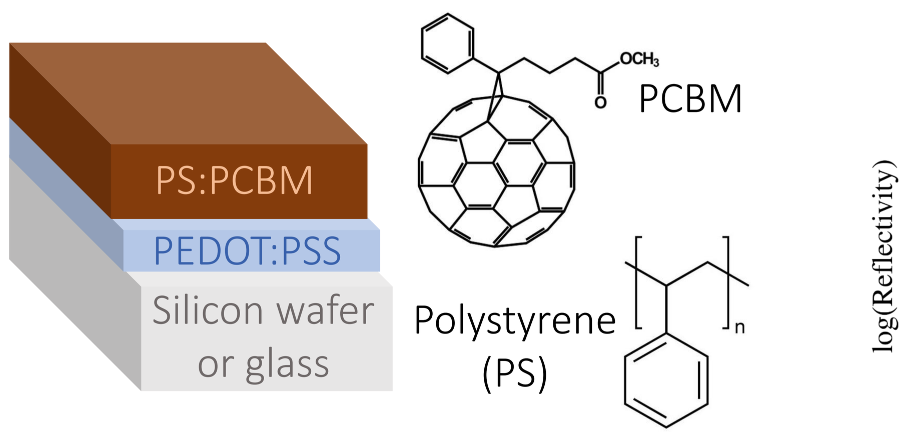
Thermal stress: PCBM de-dimerisation



Experimental Methods

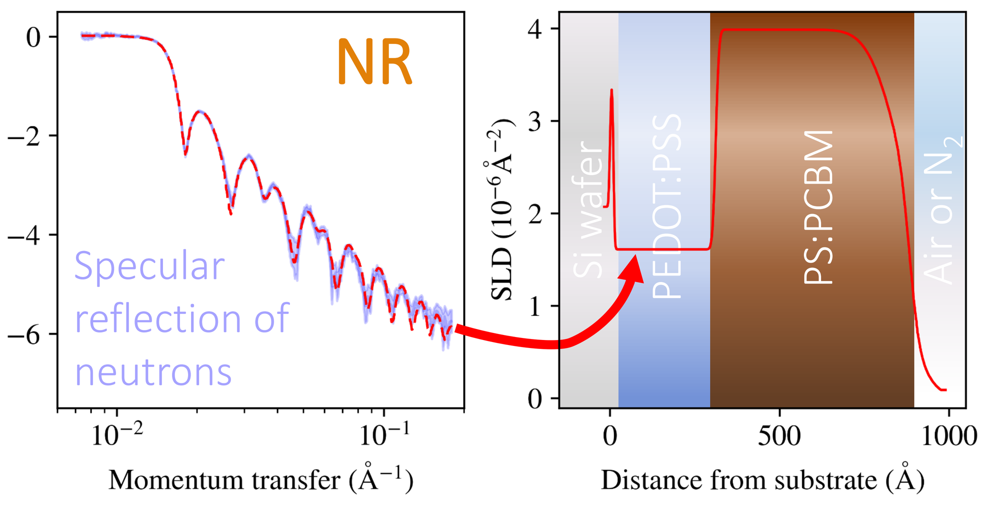
Materials

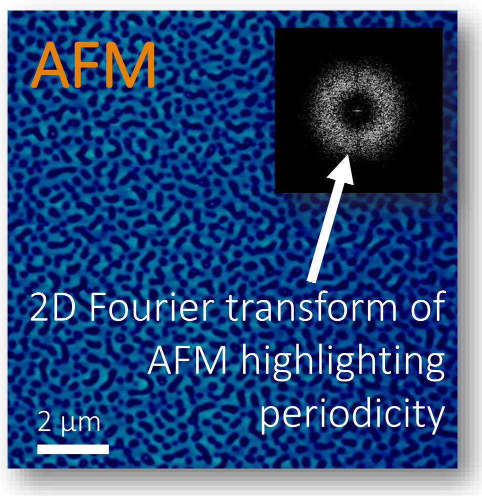
A model system of PS:PCBM with device representative substrate of PEDOT:PSS. This enabled focusing on PCBM stability.



Morphological studies

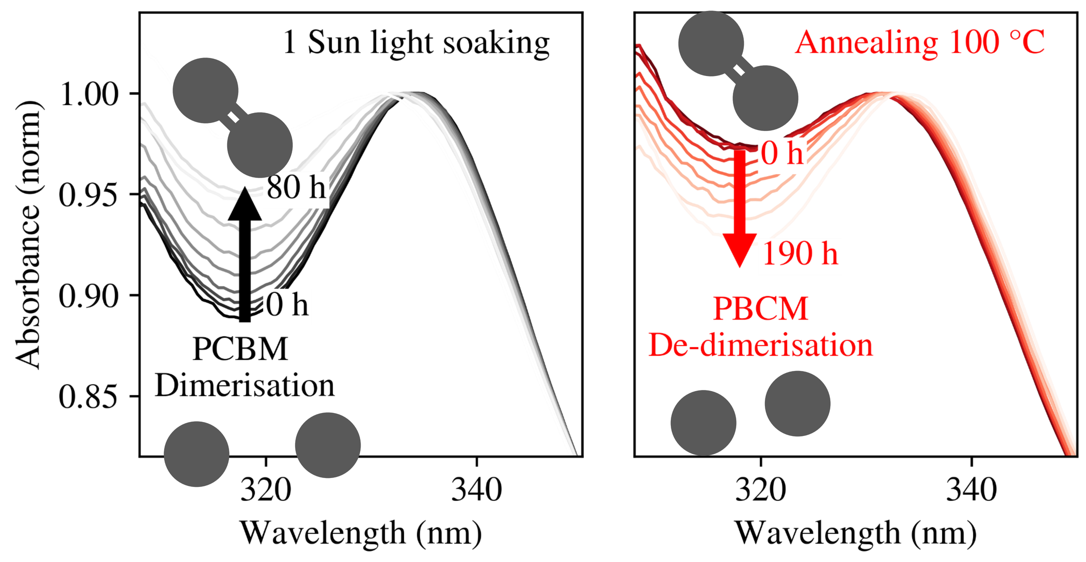
- *Neutron reflectivity* (NR) probes the **stratification** of the film to angstrom resolution, normal to the substrate. (below left)
- *Atomic for microscopy (AFM)* probes the **surface** stability. This gives roughness and surface periodicity from Fourier transform. (below right)





Photochemical studies

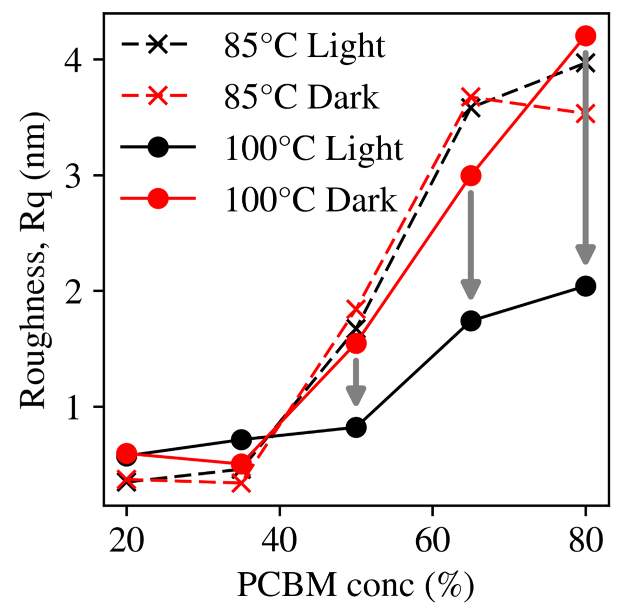
Absorption spectroscopy (UV-vis) can monitor PCBM **dimerisation** and **de-dimerisation** due to a feature change at ~320 nm. (below)



Results and Discussions

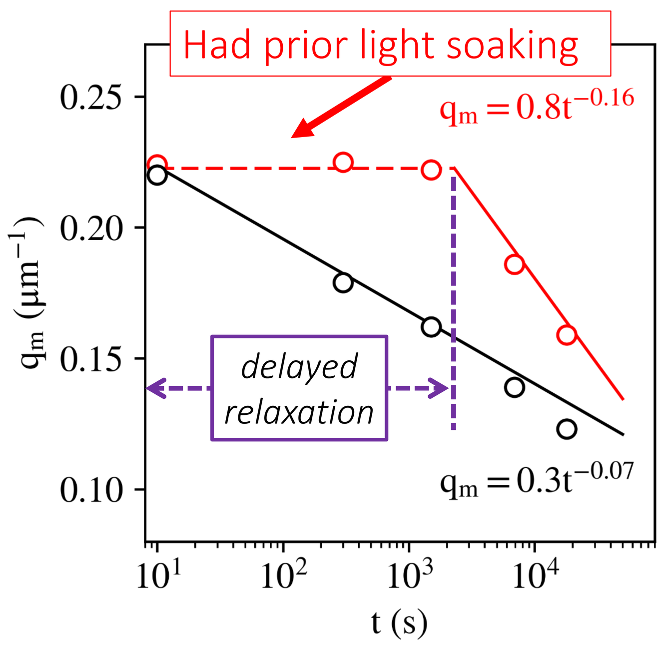
Morphological stability under illumination and thermal stress

AFM analysis:
After annealing at 85 °C and 100 °C, with and without light, topographical relaxation observed at 100 °C in the dark *only*. Light constrains reduction in surface roughness.



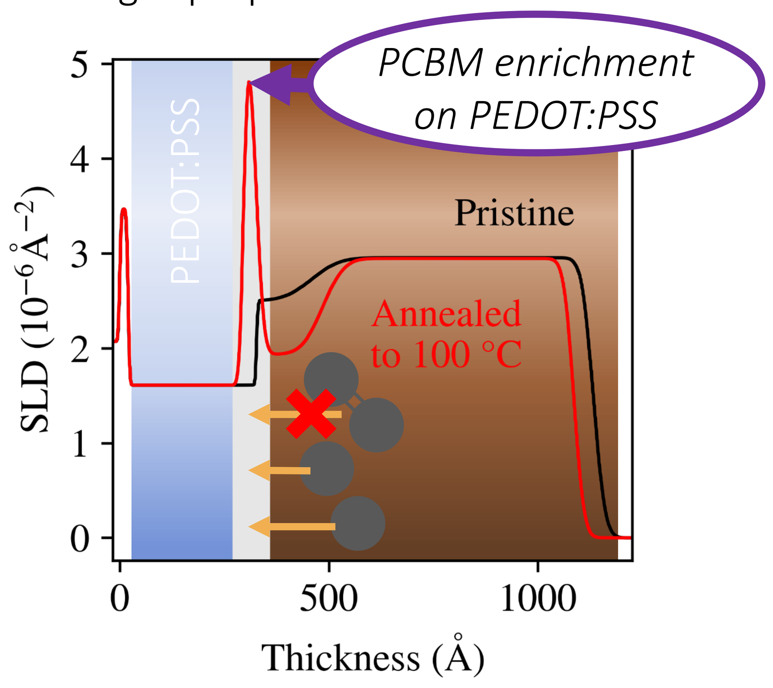
AFM Fourier transforms (FT) while annealing at 120 °C:
Annealing at 120 °C in the dark, with and without prior light soaking.

AFM FT peak, q_m, decreases when annealed at 120 °C.
A delay for the light soaked sample: decrease initiates when sufficient de-dimerisation occurs.

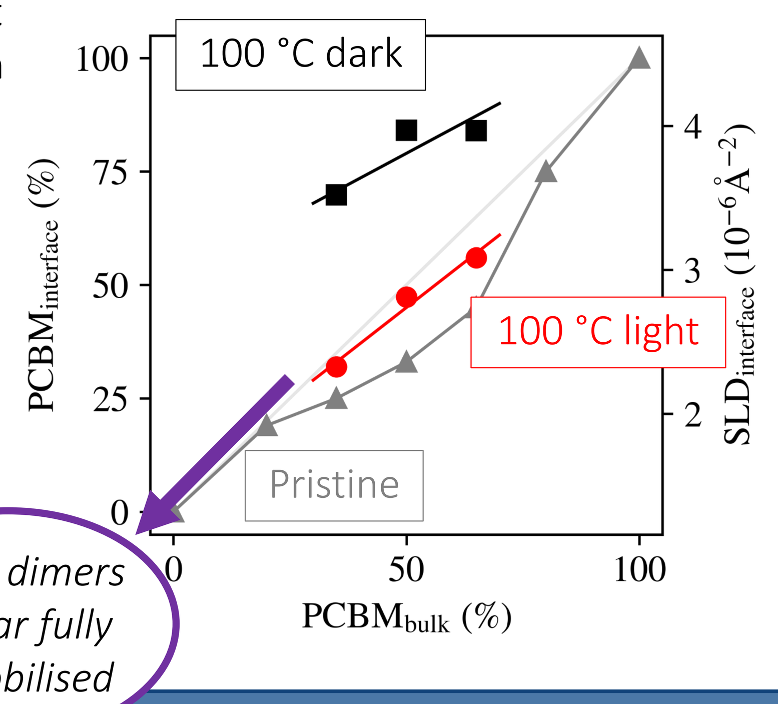


In-situ **NR from 20 – 100 °C , with and without light:**
Measurements of Si/PEDOT:PSS/PS:PCBM while annealing to monitor changes perpendicular to the substrate.

No significant changes were observed until 100°C, when enrichment of PCBM occurs on the PEDOT:PSS interface.

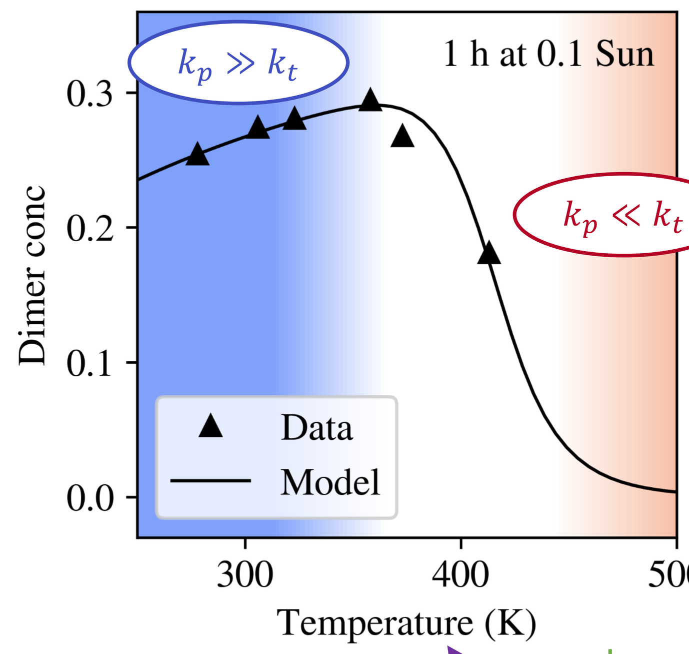


PCBM enrichment is supressed when annealing with light soaking. Further analysis shows rate of enrichment is independent of dimer concentration:



PCBM dimerisation reaction kinetics

Calculating the dimerisation rate of reaction (k_p):
Using UV-vis as an assay (above), k_p was found from the equation below, (with known de-dimerisation rate of reaction, k_T)[2] giving a dimerisation activation energy, $E_a \approx 0.024$ eV.



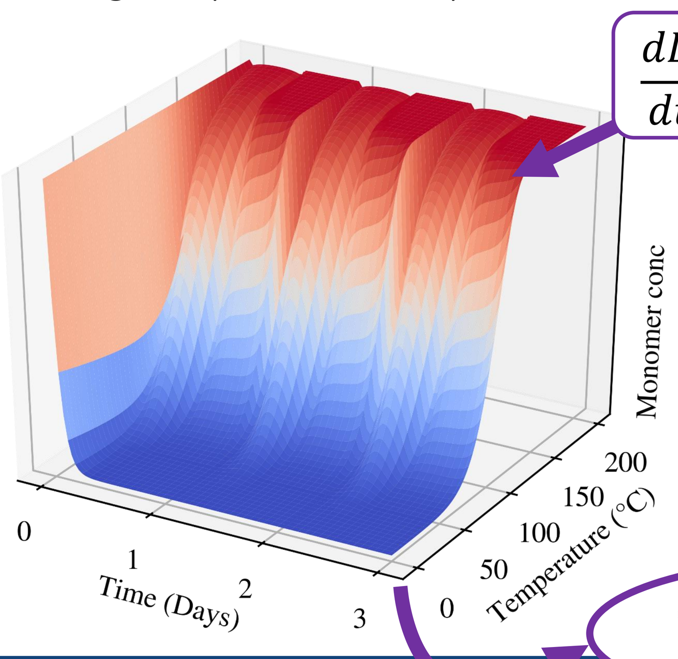
In-operando **conditions:**
Solving the reaction kinetics for monomer (M), and dimer (D), with cyclic temperature (±30) and light reproduces *in-operando* conditions.

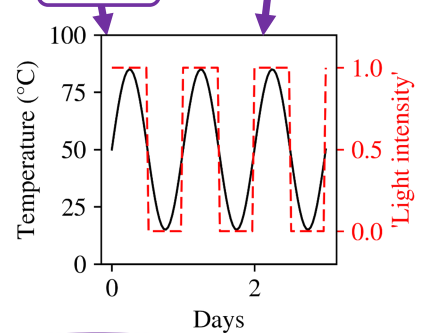
known / unknown

$$k_p = Ae^{-E_a/k_B T}$$

$$\frac{dD}{dt} = 0.5k_p M(t) - k_T D(t)$$

$\propto T, L$ $\quad$ $\propto T$





Conclusions

1. The first detailed study examining competitive effects of light and thermal stress, simultaneously.
2. Significant morphological instability observed at 100 °C with PCBM concentrations from 20-65%.
3. Topographical relaxation of the top interface and PCBM enrichment on the bottom PEDOT:PSS interface observed for non-light soaked samples.
4. Modelling of the PCBM enrichment suggests PCBM dimers are fully immobilised, significantly inhibiting both surface relaxation and PCBM stratification of the film.
5. PCBM dimerisation activation energy found with in-operando modelling of monomer concentration.

References & Affiliations

1. Li Z, Wong HC, Huang Z, Zhong H, Tan CH, Tsoi WC, et al. Performance enhancement of fullerene-based solar cells by light processing. Nat Commun. 2013;4(2227):1–7.
2. Wong HC, Li Z, Tan CH, Zhong H, Huang Z, Bronstein H, et al. Morphological Stability and Performance of Polymer–Fullerene Solar Cells under Thermal Stress: The Impact of Photoinduced PC 60 BM Oligomerization. ACS Nano. 2014 25;8(2):1297–308.
3. Pont S, Foglia F, Higgins A, Durrant J, and Cabral J, *Adv Func Mat, under revisions.*

Affiliations: [a] Centre for Plastic Electronics, Imperial College London, London, SW7 2AZ. [b] Department of Chemistry, Imperial College London, London, SW7 2AZ. [c] Department of Chemical Engineering, Imperial College London, London, SW7 2AZ. [d] College of Engineering, Swansea University, Bay Campus, SA1 8EN. [†] Present address: Institute of Pharmaceutical Science, King's College London, London, SE19NH.

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