Rapid optimisation techniques

for thin-film materials and devices

Robert Treharne

Functional Thin Films

16th October, Coventry

@robtreharne

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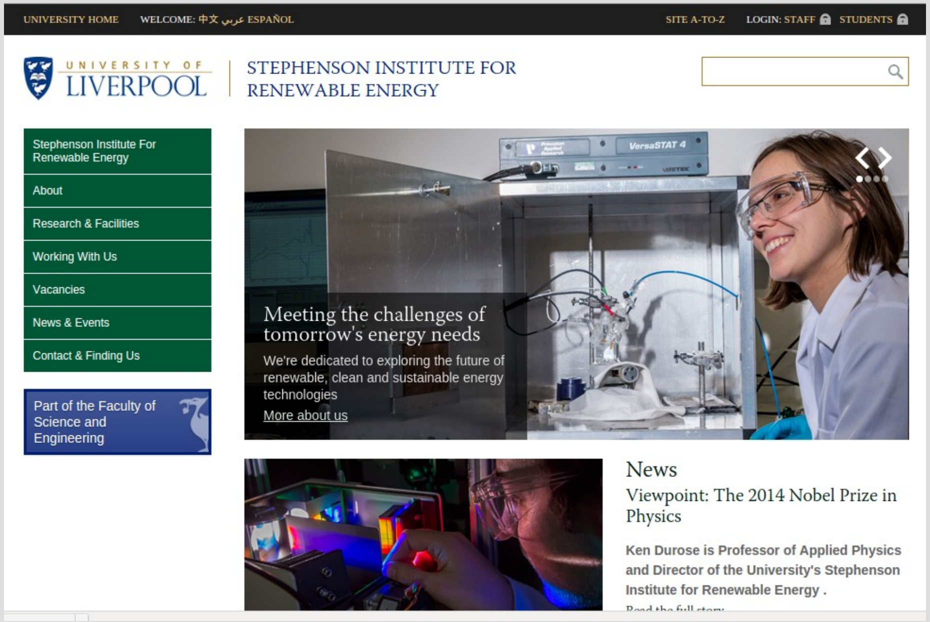

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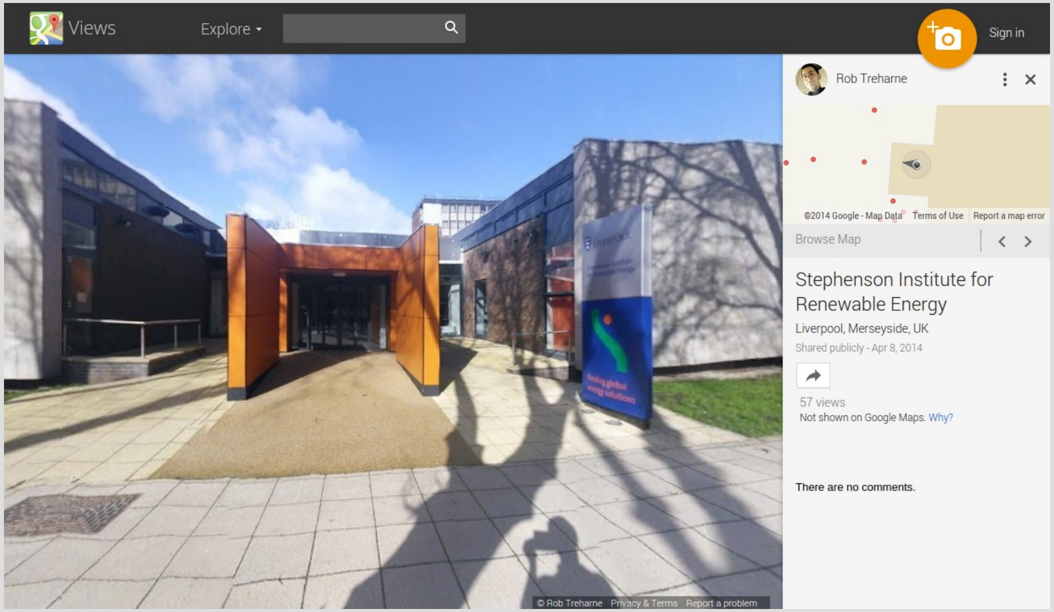
Ken Durose is Professor of Applied Physics and Director of the University's Stephenson Institute for Renewable Energy .



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Outline

1) Capabilities

2) What I mean by "Combinatorial"

3) **Case Study**: Transparent Conductors

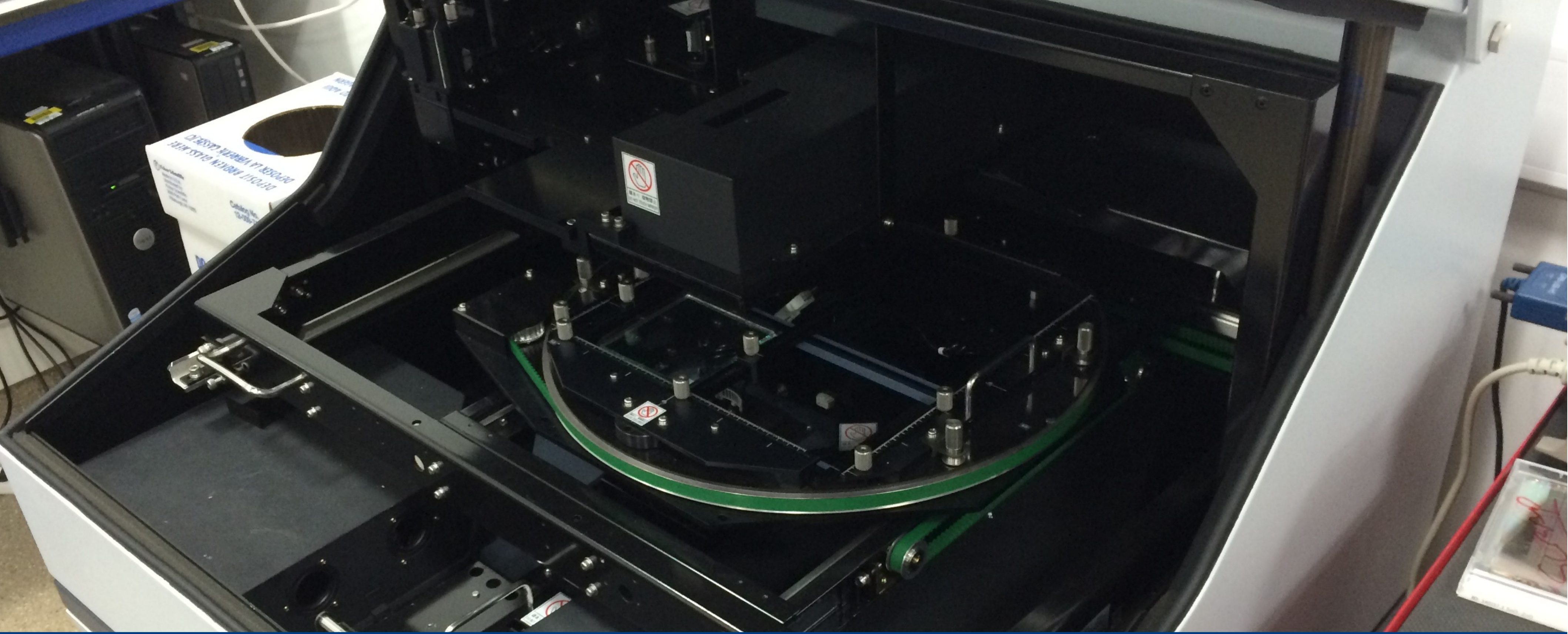
4) Other Applications

5) Other cool stuff

AJA Phase II-J

Multi-source RF sputtering system

ZnO	Ta2O5	MgO	ZnS	CdS	Ge	Ag
SnO2	Nb2O5		CdTe	Sb2Te3	Zn	Ti
TiO2	V2O5		ZnTe	As2Te3	Nb	Al
SiO2	V2O3		CdSe		Te	Cu
Al2O3	ZrO2		ZnSe		Sn	Bi



Optical Characterisation

- UV-VIS-IR (250 – 2000 nm): Shimadzu
- Variable Angle Ellipsometry: Woollam
- Both units have **scanning** capabilities

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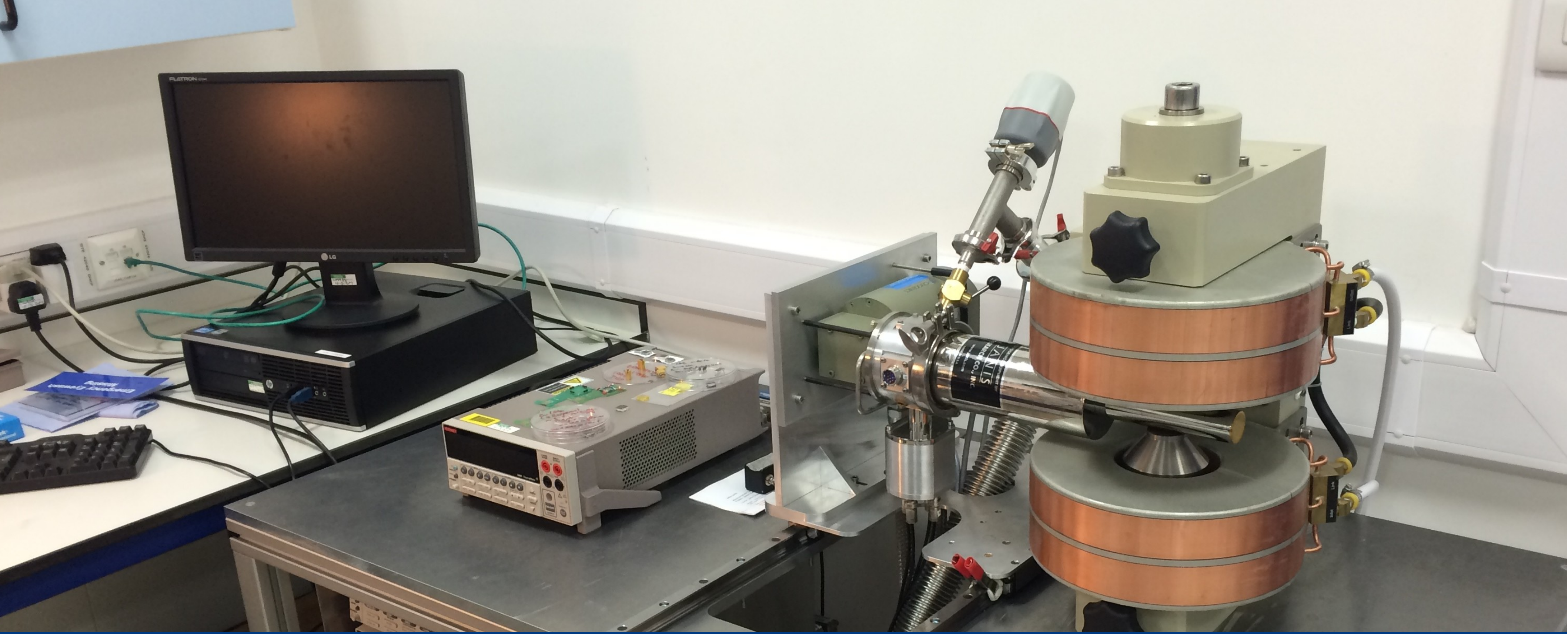

Electrical Characterisation

- Hall Effect – carrier conc & mobility
- 4PP – Sheet resistance – Scanning!

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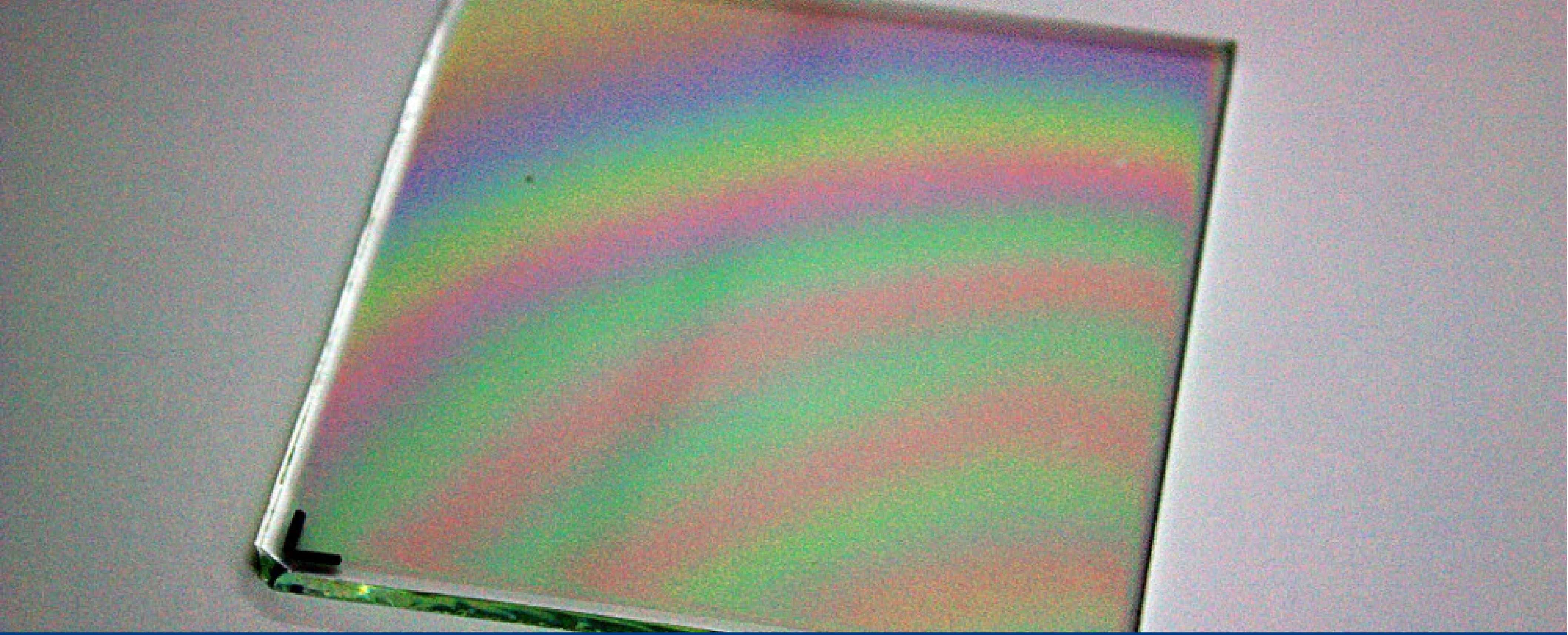

Shhh! Don't say the C-word

"Combinatorial" is sometimes a code term used to describe uncontrolled non-uniform deposition.

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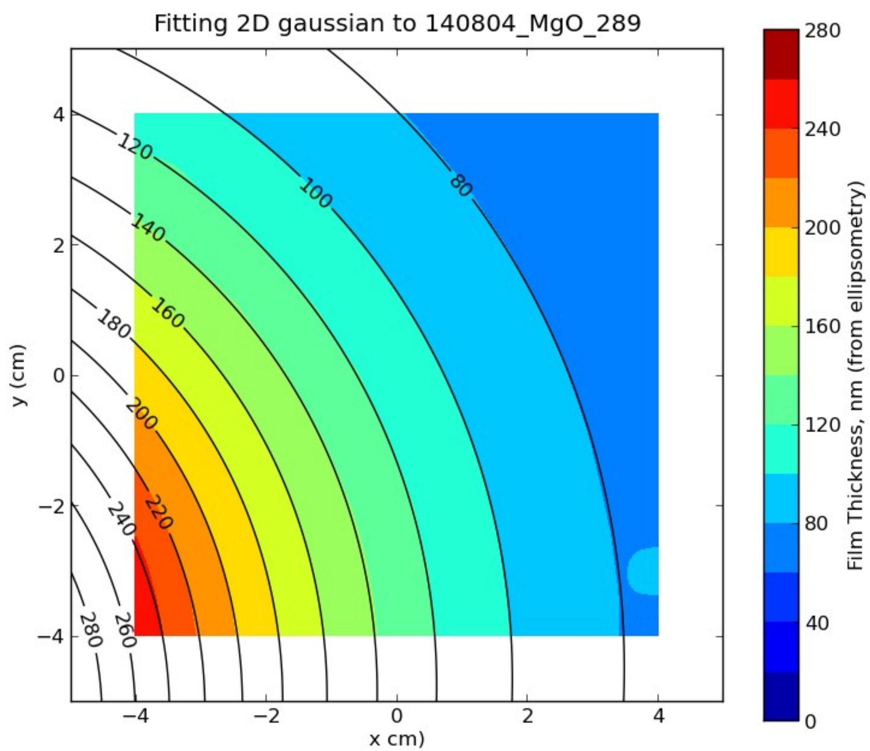

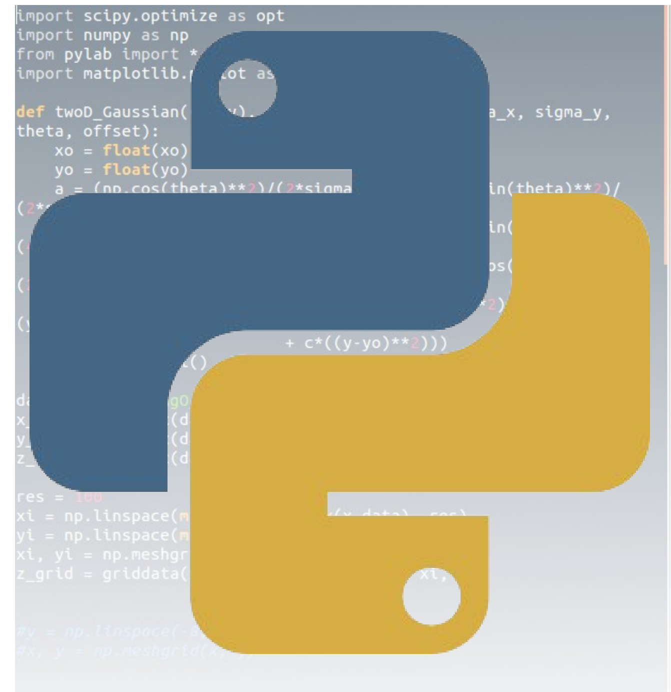

Controlled Non-Uniformity

- Profile from each gun described by 2D gaussian
- Excellent control over deposition parameters
- High run-to-run reproducibility
- Can predict multi-gun profiles

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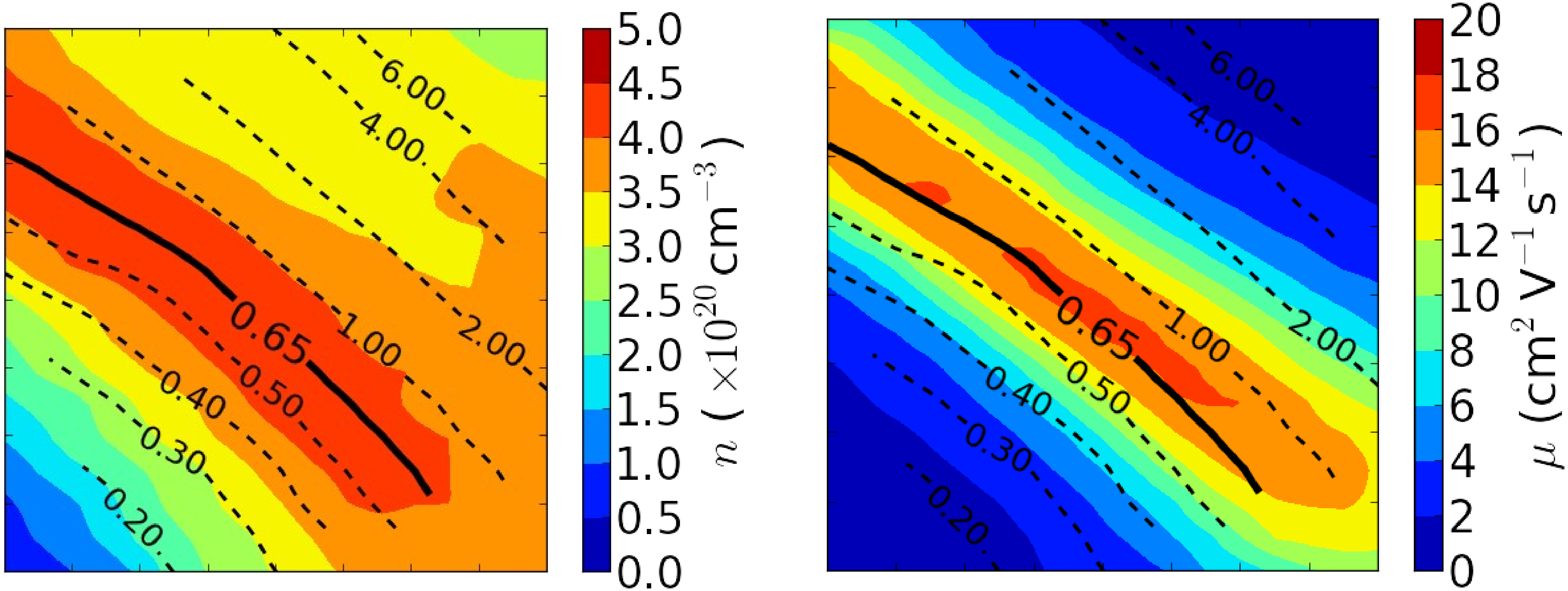
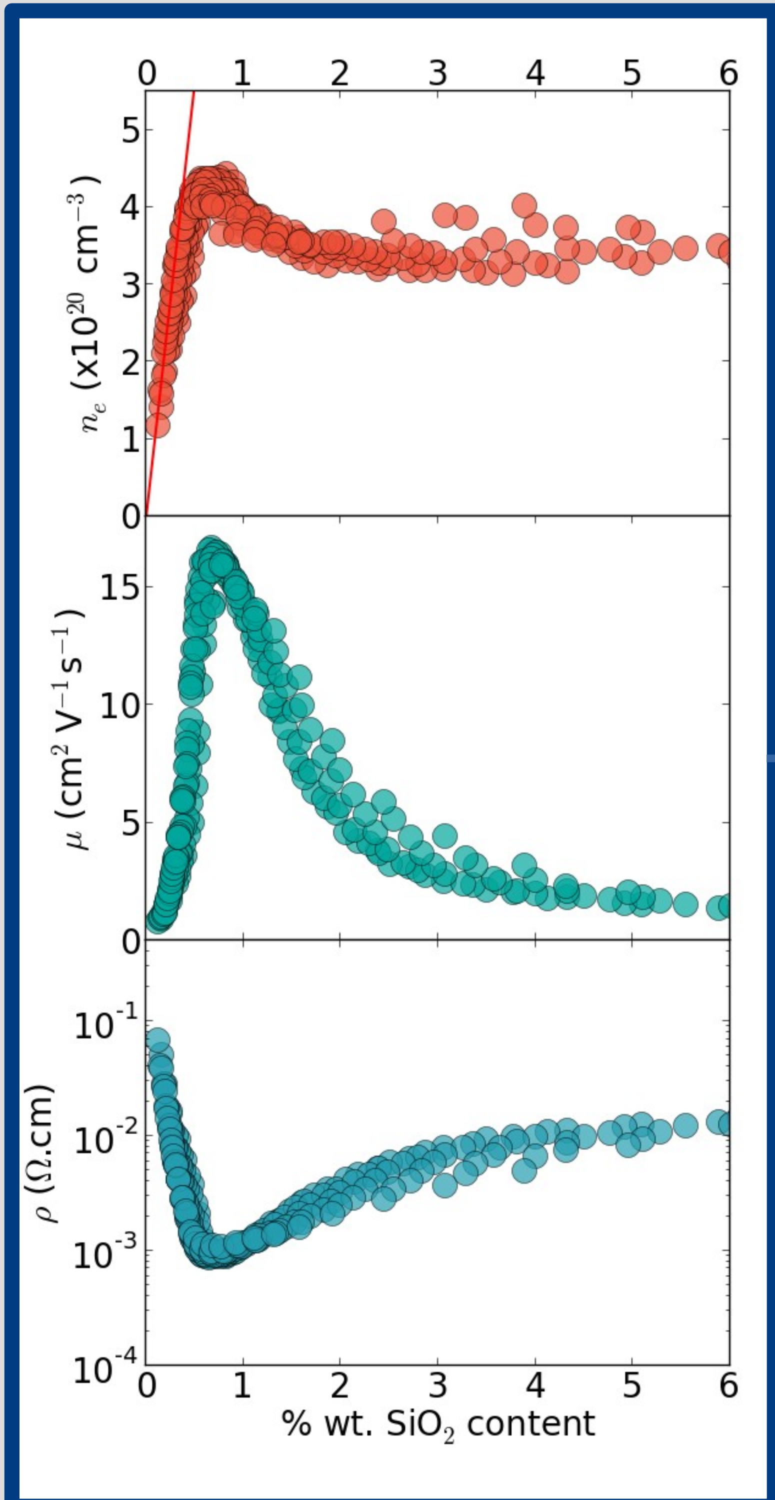


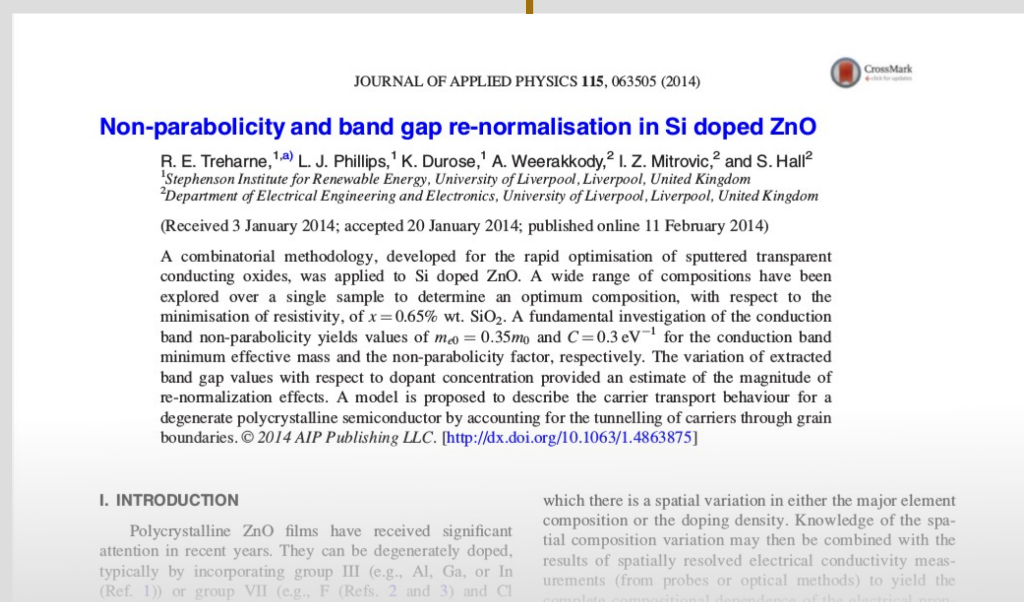
Case Study: **Transparent Conductors**

- Essential materials for PV and consumer electronics
- Combinatorial doping study: <u>Si doped ZnO</u>
- Sample **hundreds** of compositions in a single sample
  - Mapping opto-electronic properties vs dopant composition
- Extrapolation!



Can do this in 1 day
(that's a big deal)

Can also extract some fundamental physics



JOURNAL OF APPLIED PHYSICS **115**, 063505 (2014)

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Non-parabolicity and band gap re-normalisation in Si doped ZnO

R. E. Treharne,[1,a)] L. J. Phillips,[1] K. Durose,[1] A. Weerakkody,[2] I. Z. Mitrovic,[2] and S. Hall[2]
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[2]*Department of Electrical Engineering and Electronics, University of Liverpool, Liverpool, United Kingdom*

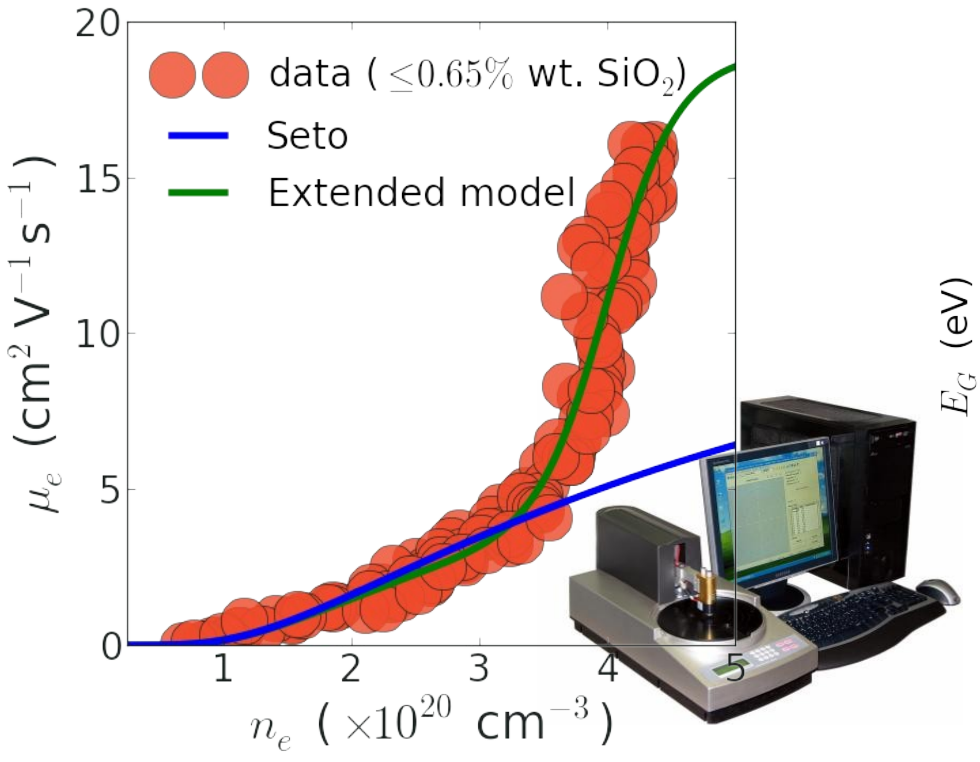
(Received 3 January 2014; accepted 20 January 2014; published online 11 February 2014)

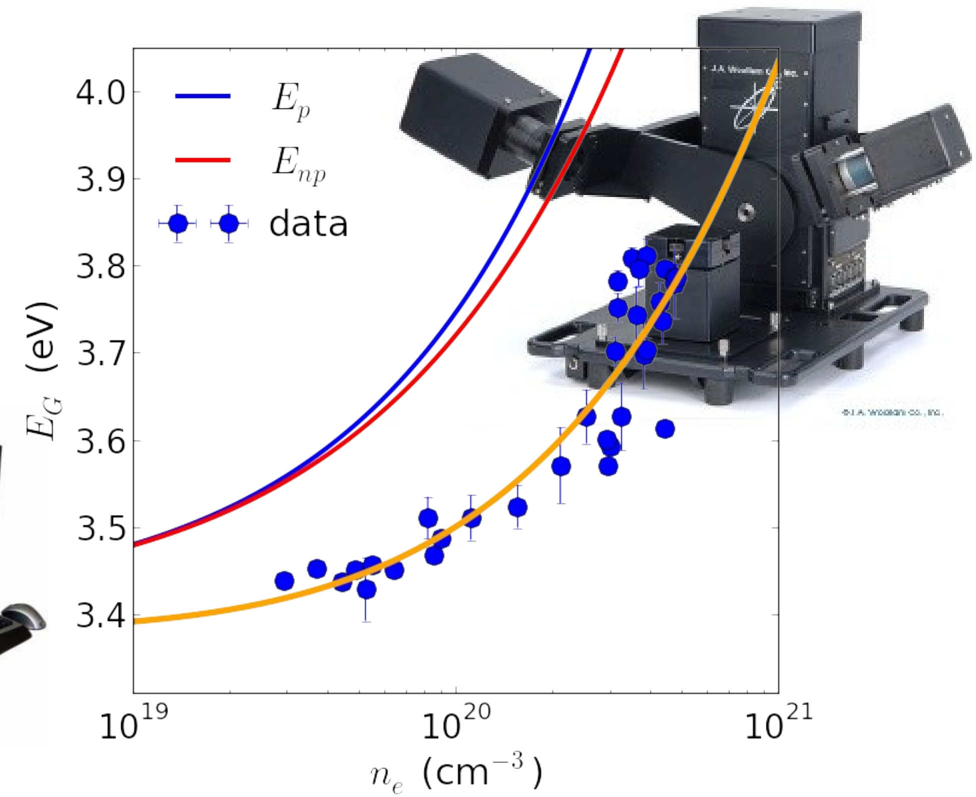
A combinatorial methodology, developed for the rapid optimisation of sputtered transparent conducting oxides, was applied to Si doped ZnO. A wide range of compositions have been explored over a single sample to determine an optimum composition, with respect to the minimisation of resistivity, of $x = 0.65\%$ wt. SiO_2. A fundamental investigation of the conduction band non-parabolicity yields values of $m_{e0} = 0.35m_0$ and $C = 0.3\ \mathrm{eV}^{-1}$ for the conduction band minimum effective mass and the non-parabolicity factor, respectively. The variation of extracted band gap values with respect to dopant concentration provided an estimate of the magnitude of re-normalization effects. A model is proposed to describe the carrier transport behaviour for a degenerate polycrystalline semiconductor by accounting for the tunnelling of carriers through grain boundaries. © *2014 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4863875]

I. INTRODUCTION

Polycrystalline ZnO films have received significant attention in recent years. They can be degenerately doped, typically by incorporating group III (e.g., Al, Ga, or In (Ref. 1)) or group VII (e.g., F (Refs. 2 and 3) and Cl

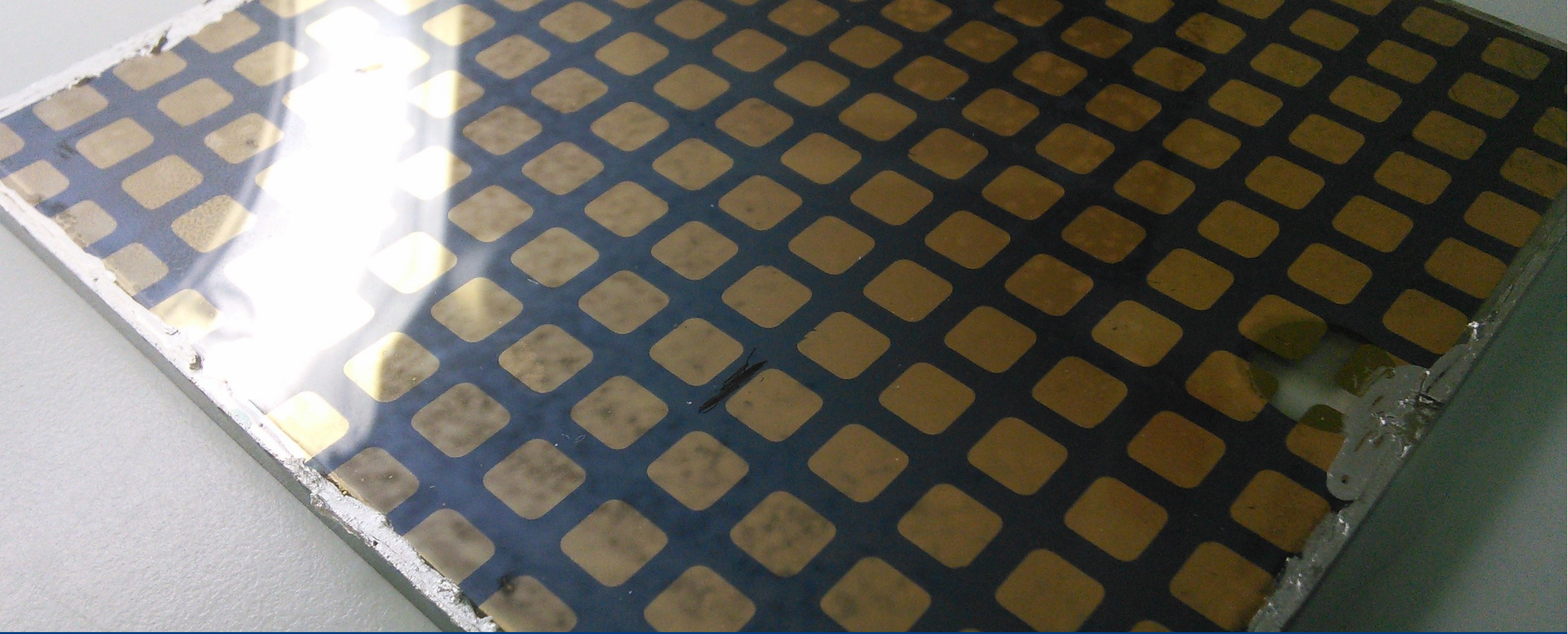
which there is a spatial variation in either the major element composition or the doping density. Knowledge of the spatial composition variation may then be combined with the results of spatially resolved electrical conductivity measurements (from probes or optical methods) to yield the





Going deep!

- Effective Mass – dependent on dopant conc.
- Transport mechanisms: Scattering – **new physical models!**
- Electronic structure: Shape of conduction band
- **ALL WITH ONE CONSISTENT SAMPLE!**



Further Applications

Optimising Thin-Film PV

CdTe, CZTS, perovskites

Transparent Electronics

ZnO TFTs

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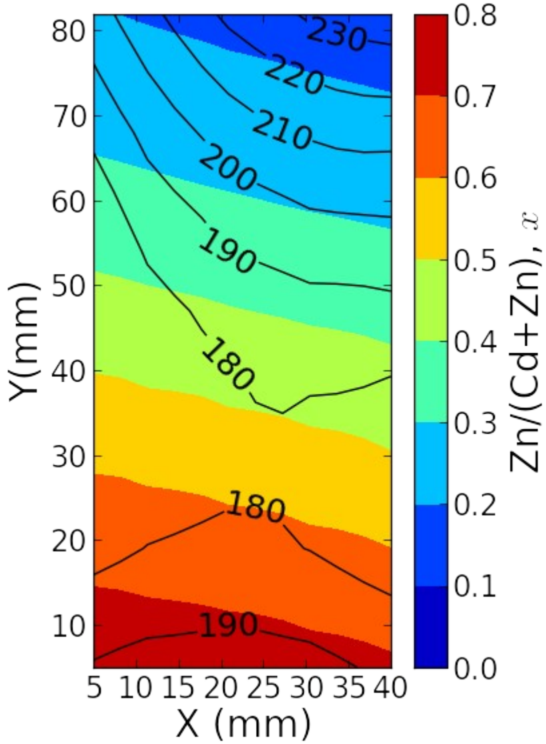

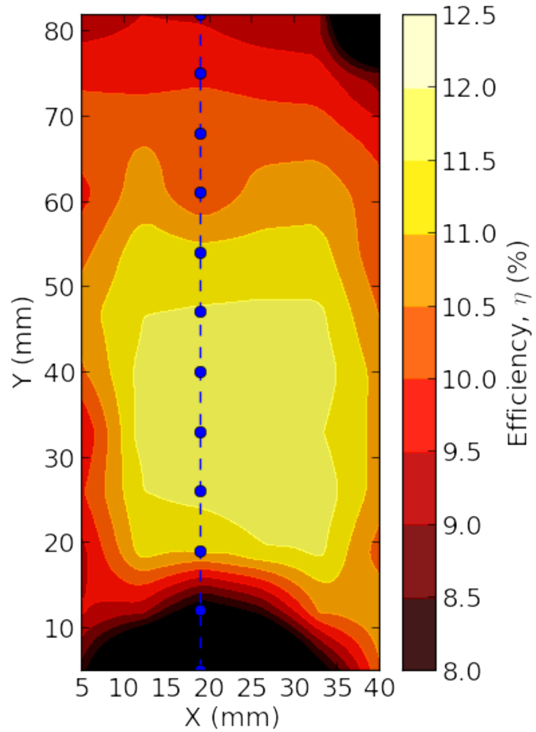

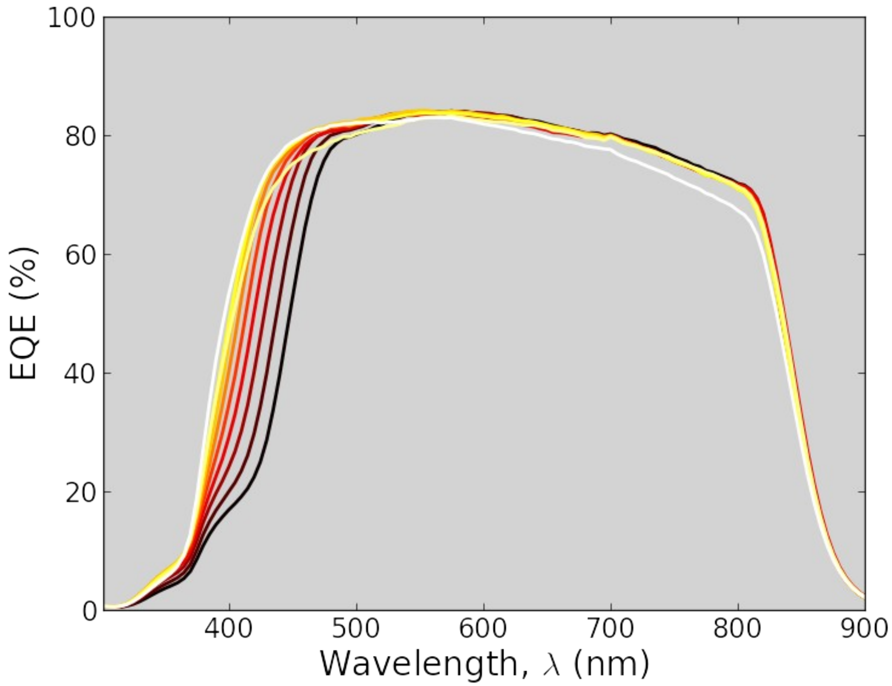

Example: $Cd_{(1-x)}Zn_xS$ layers for CdTe TFPV

- Can investigate x = 0.1 – 0.7 in one device
- Mapping performance with respect to x
- Optimum x~0.6 identified
- Improvement in V_{oc} identified
- Highly consistent data sets

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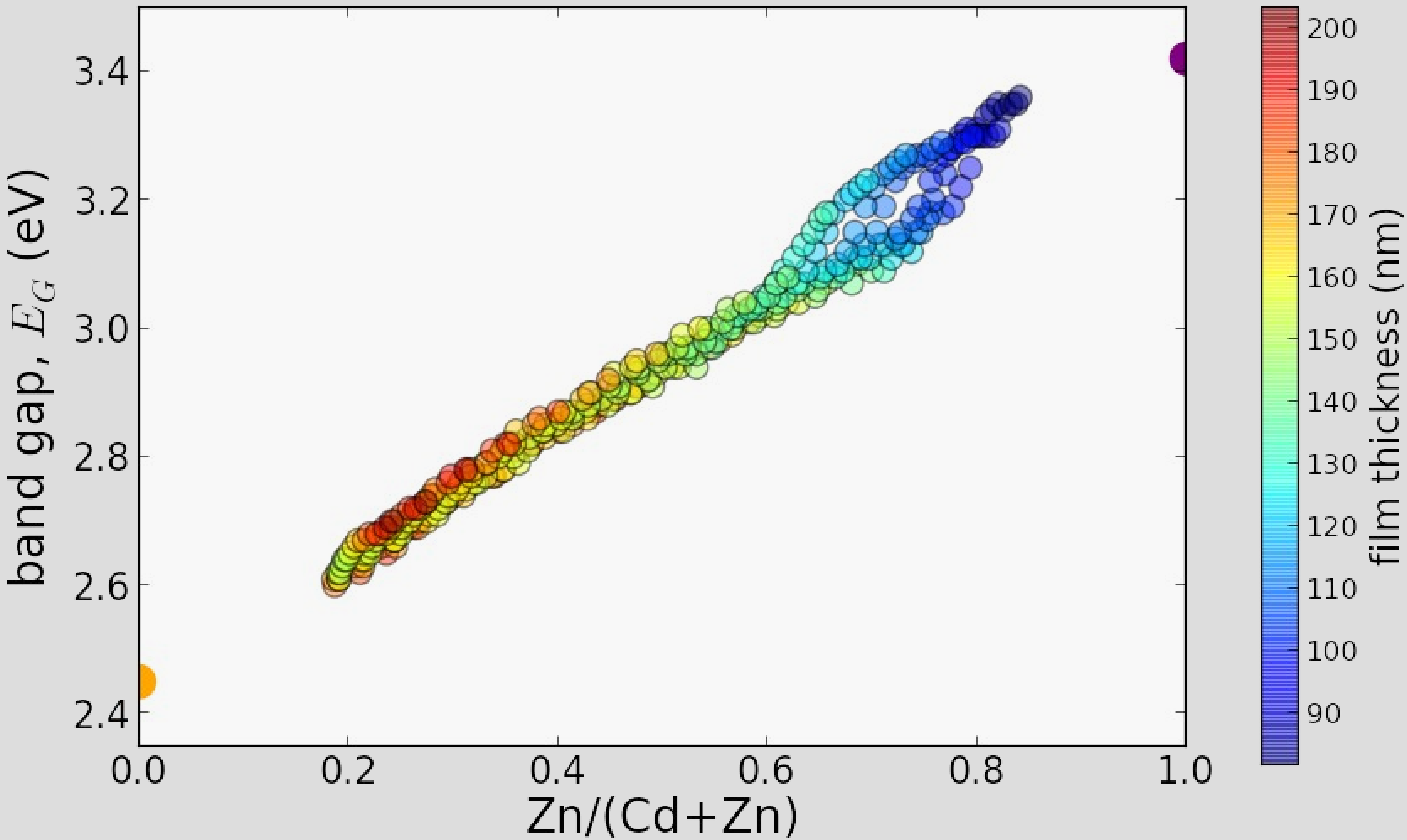
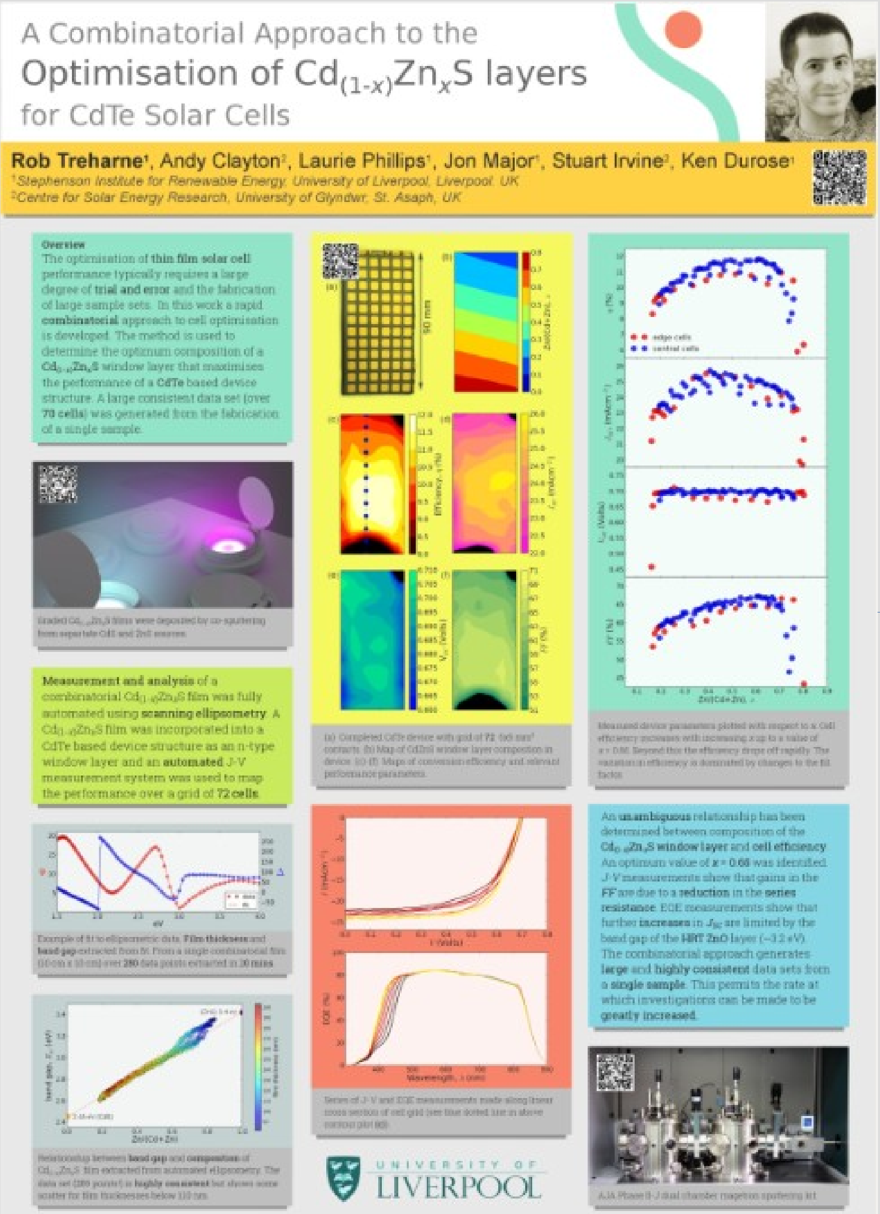
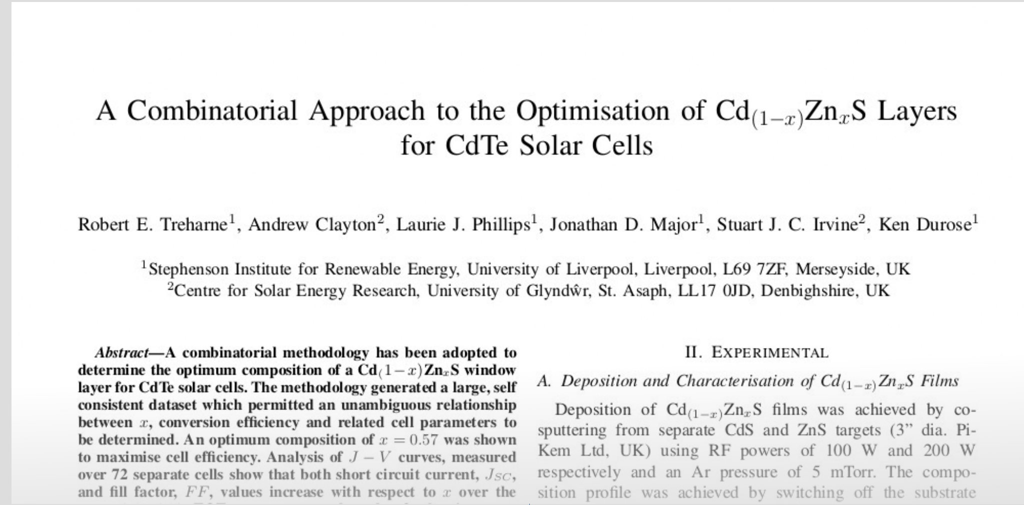


band gap, E_G (eV)
3.4
3.2
3.0
2.8
2.6
2.4
0.0
0.2
0.4
0.6
0.8
1.0
Zn/(Cd+Zn)
film thickness (nm)
200
190
180
170
160
150
140
130
120
110
100
90





A Combinatorial Approach to the Optimisation of $Cd_{(1-x)}Zn_xS$ Layers for CdTe Solar Cells

Robert E. Treharne[1], Andrew Clayton[2], Laurie J. Phillips[1], Jonathan D. Major[1], Stuart J. C. Irvine[2], Ken Durose[1]

[1]Stephenson Institute for Renewable Energy, University of Liverpool, Liverpool, L69 7ZF, Merseyside, UK
[2]Centre for Solar Energy Research, University of Glyndŵr, St. Asaph, LL17 0JD, Denbighshire, UK

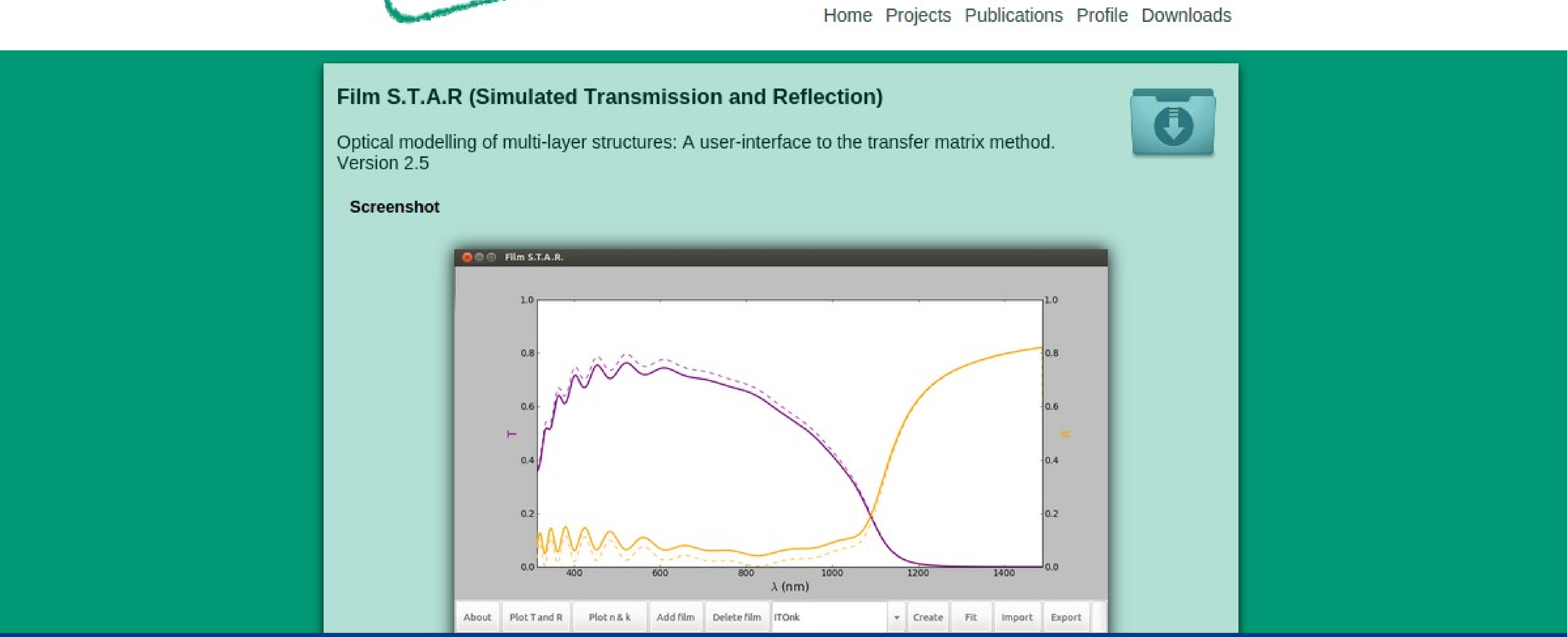
***Abstract*—A combinatorial methodology has been adopted to determine the optimum composition of a $Cd(1-x)Zn_xS$ window layer for CdTe solar cells. The methodology generated a large, self consistent dataset which permitted an unambiguous relationship between x, conversion efficiency and related cell parameters to be determined. An optimum composition of $x = 0.57$ was shown to maximise cell efficiency. Analysis of $J-V$ curves, measured over 72 separate cells show that both short circuit current, J_{SC}, and fill factor, FF, values increase with respect to x over the**

II. EXPERIMENTAL

A. Deposition and Characterisation of $Cd_{(1-x)}Zn_xS$ Films

Deposition of $Cd_{(1-x)}Zn_xS$ films was achieved by co-sputtering from separate CdS and ZnS targets (3" dia. Pi-Kem Ltd, UK) using RF powers of 100 W and 200 W respectively and an Ar pressure of 5 mTorr. The composition profile was achieved by switching off the substrate

Recently presented at
40th IEEE PVSC Colorado



Other Stuff

Film S.T.A.R

- Thin-film optical database
- Multi-layer modelling
- Currently developing public webapp

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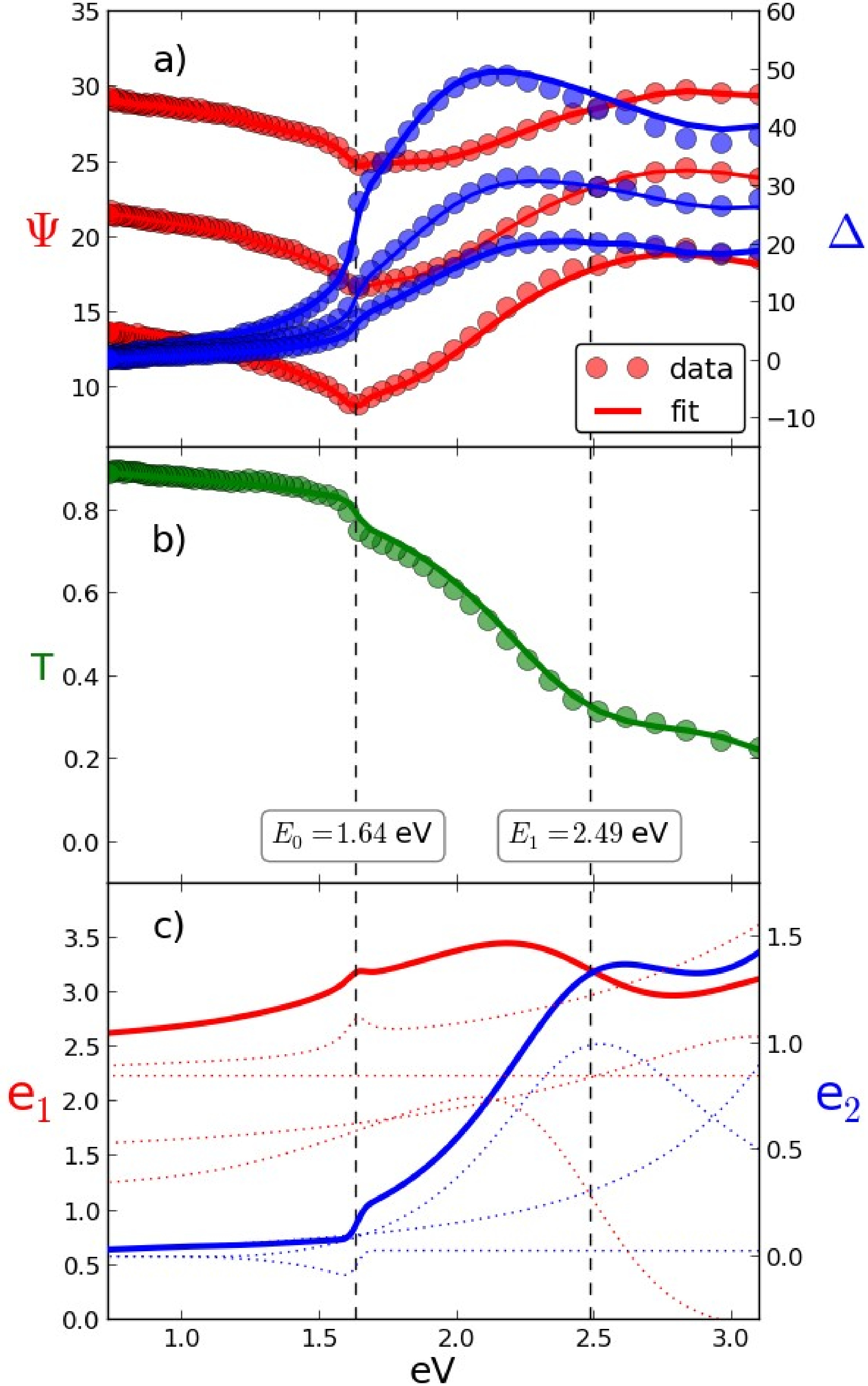
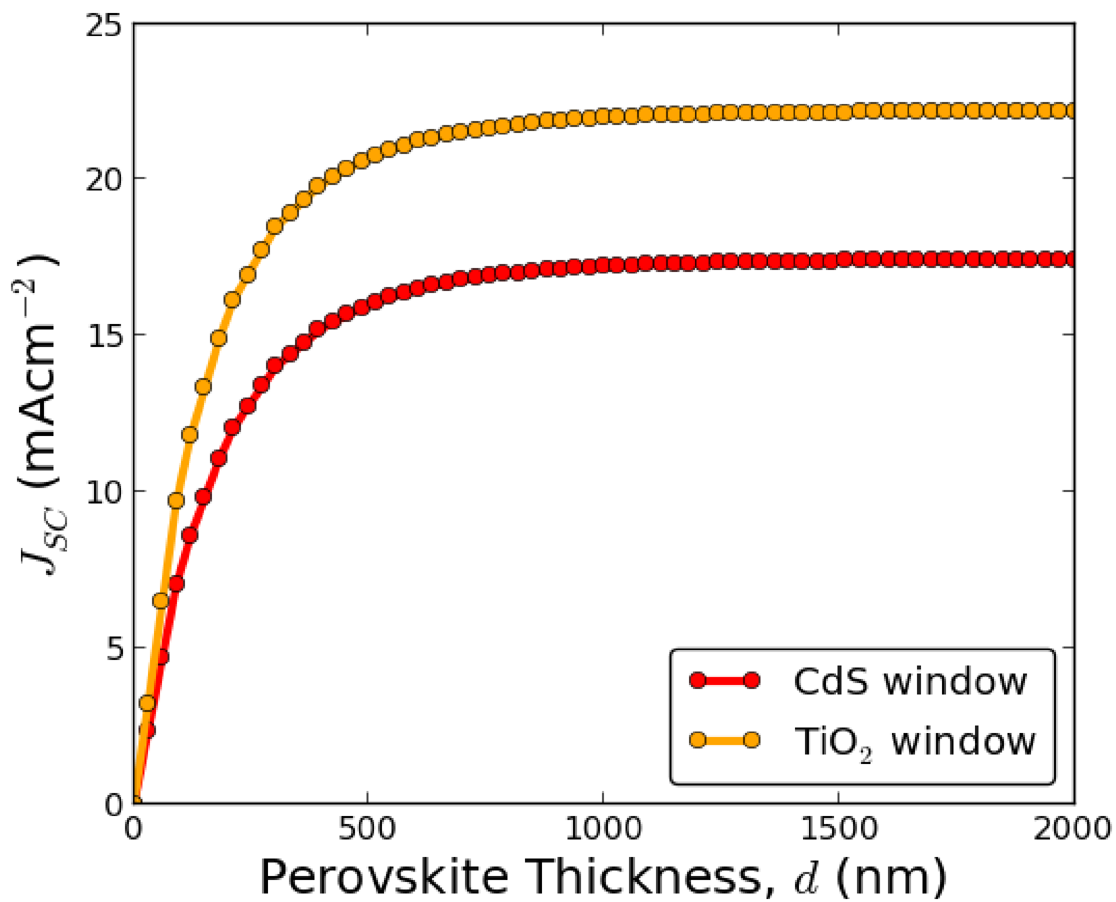


Perovskite!

- Ellipsometry of perovskite film
- n and k extracted
- Multi-layer model to determine optimum thickness for device



Other Stuff

Recent breakthroughs

- $MgCl_2$ activation of CdTe solar cells
- No need for toxic $CdCl_2$
- CdTe: Old dog, new tricks!

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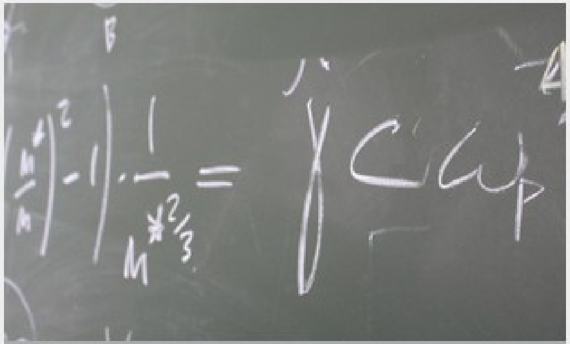

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