ESRF Coherence Workshop, September 10th 2019

3D ptychography of 3rd generation solar cells

Jens Wenzel Andreasen

Technical University of Denmark

Department of Energy Conversion and Storage

jewa@dtu.dk

Photovoltaics

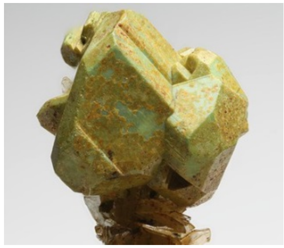
Wafer-based	Tandem/hybrid	Thin film	
Crystalline silicium 1st generation	tandem, hetero-, and multijuntion technologies	Established thin Film, amorphous Si, CIGS, CdTe 2nd generation	Emerging thin Film 3rd generation
Durable, low-cost	High efficiency ”space PV”	Relatively cheap and relatively high efficiency	Earth abundant and non toxic materials, flexibility
Long energy pay-back time	Expensive manufacturing of complex architectures	Scarcity and toxicity	Low efficiency, stability

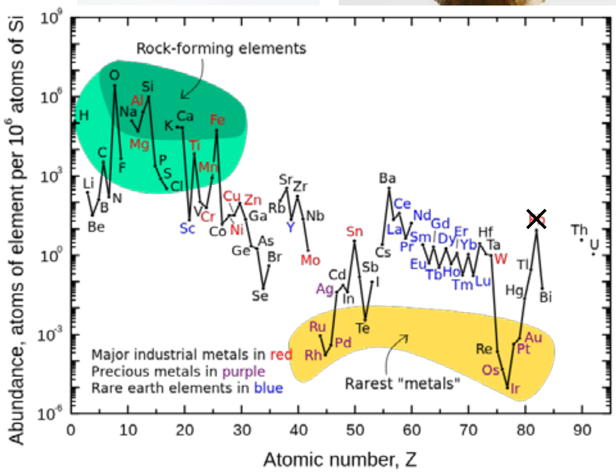
Motivations for research in 3rd generation solar cells

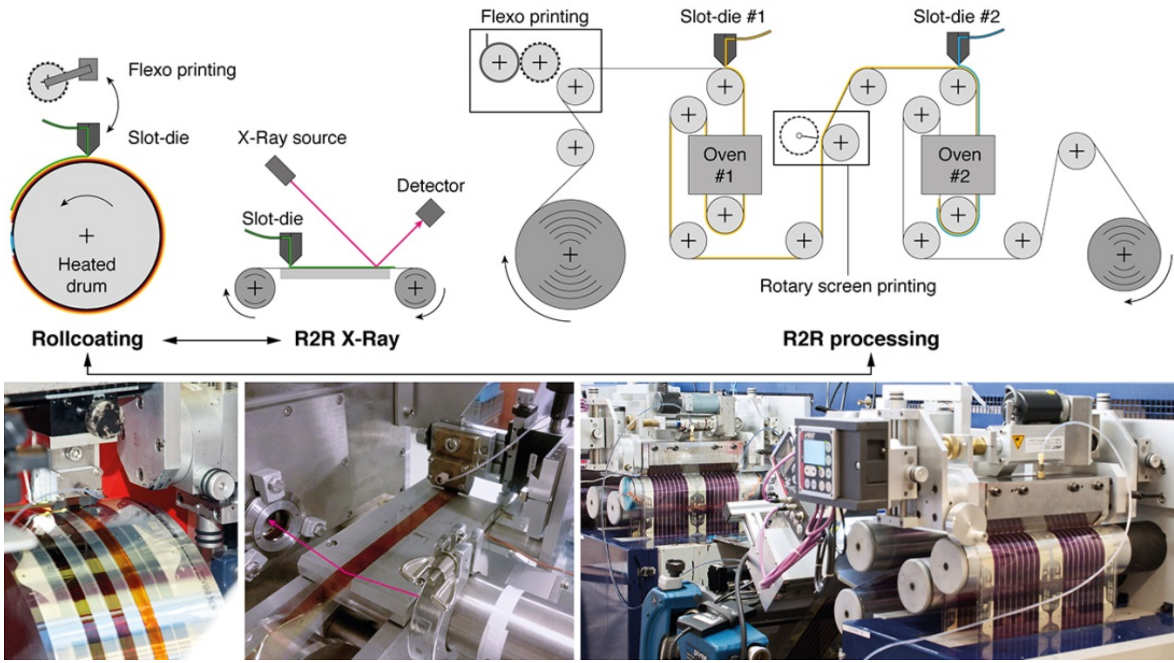
- Materials that are abundant, to avoid resource depletion as part of a global shift to sustainable energy solutions, including solar energy.
- Non-toxic materials to avoid an ecological disaster, especially in areas where safe end-of-life routines are not established, e.g. recycling.
- Low energy consumption of manufacturing to avoid long energy pay-back time, prohibiting a large scale, global boot-strapping transition to a sustainable energy society.
- Cheap manufacture to attract global and local investment in production to ensure a fast and pervasive introduction

polymer

kesterite

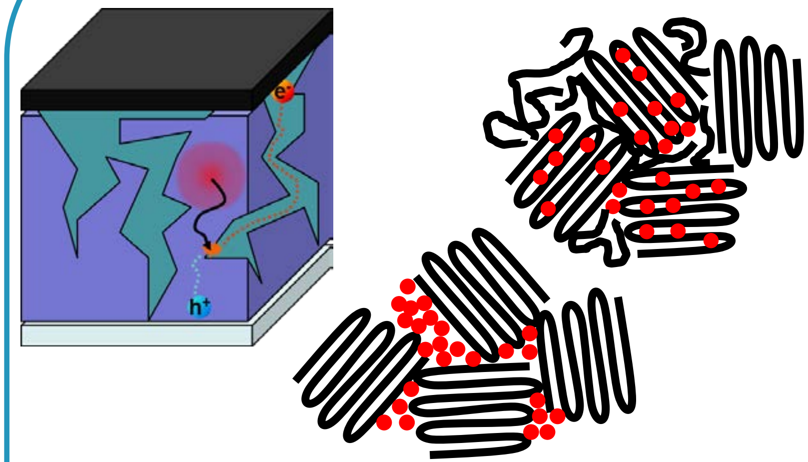




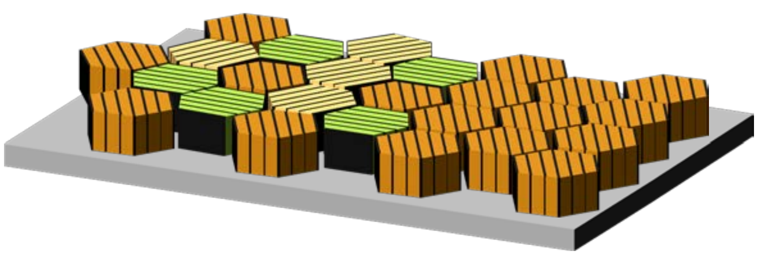


Nanostructure is key to performance for 3rd generation solar cells

Organic/polymer solar cells



Improved experimental probes of the physical structure of interfacial regions are needed



Inorganic, Cu_2ZnSnS_4 (CZTS) kesterite

Ultrahigh resolution in 3D is required to resolve donor-acceptor nanostructure

Materials of low atomic number, and of similar electron density

= low contrast for imaging

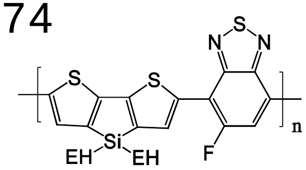
A zoo of secondary phases with very similar crystalline structures

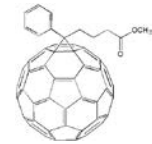
We need access to distribution of **phases**, orientations, defects and **stoichiometry**

Grain boundaries and other texture may be important

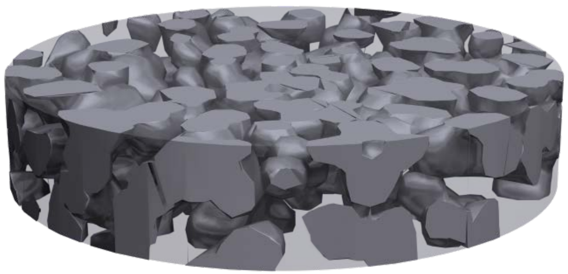
Improving organic tandem solar cells based on water-processed nanoparticles by quantitative 3D nanoimaging

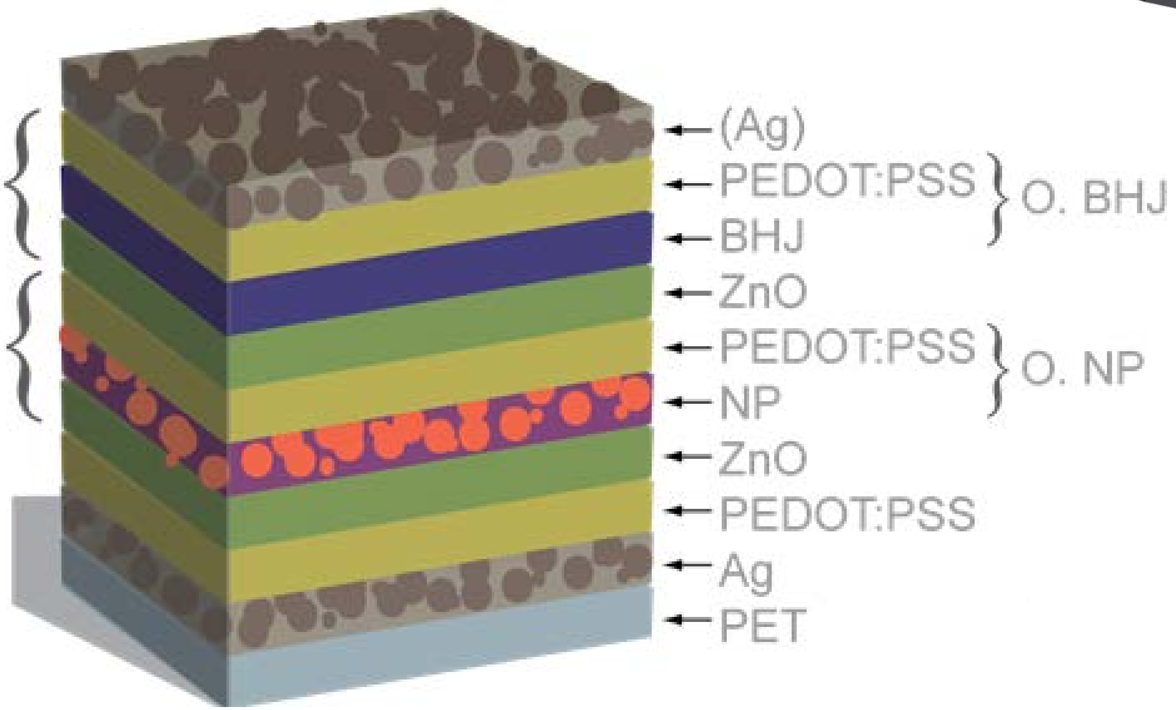
Nanoscale, 2015,7, 13765-13774
DOI: 10.1039/C5NR02824H

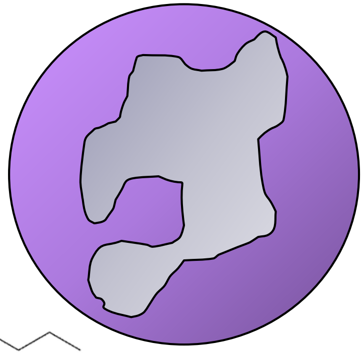


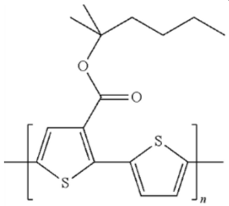


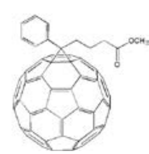
PDTSBT-F : PCBM









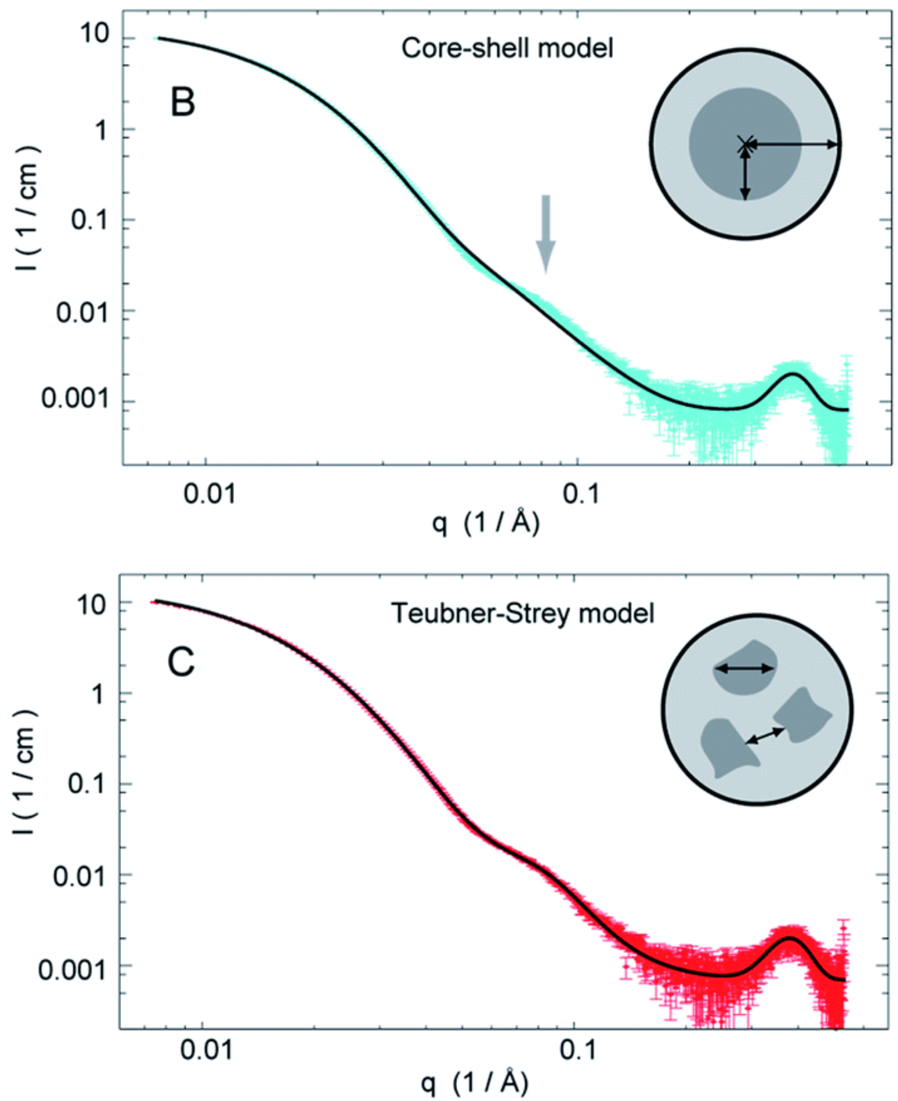


P3MHOCT : PCBM

Structure and crystallinity of water dispersible photoactive nanoparticles for organic solar cells

J. Mater. Chem. A, 2015, **3**, 17022-17031
DOI: 10.1039/C5TA04980F

The scattering contrast is there, at least for combinations of donor polymers with fullerene acceptors



Improving organic tandem solar cells based on water-processed nanoparticles by quantitative 3D nanoimaging

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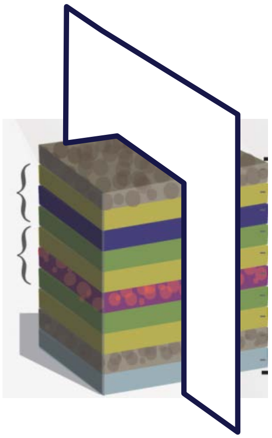

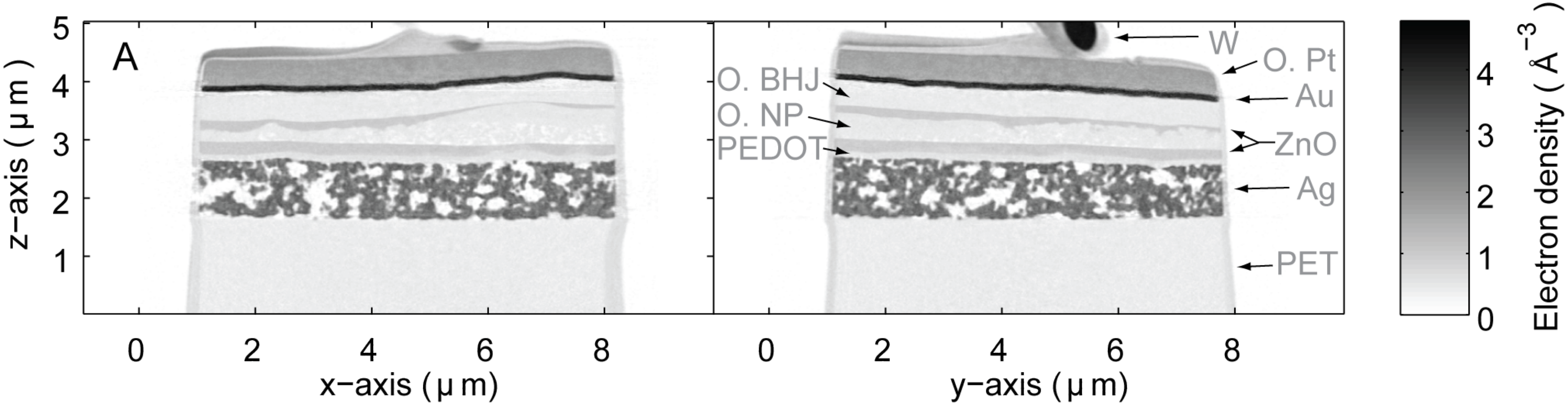

[cSAXS beamline at the Swiss Light Source, Paul Scherrer Institut]

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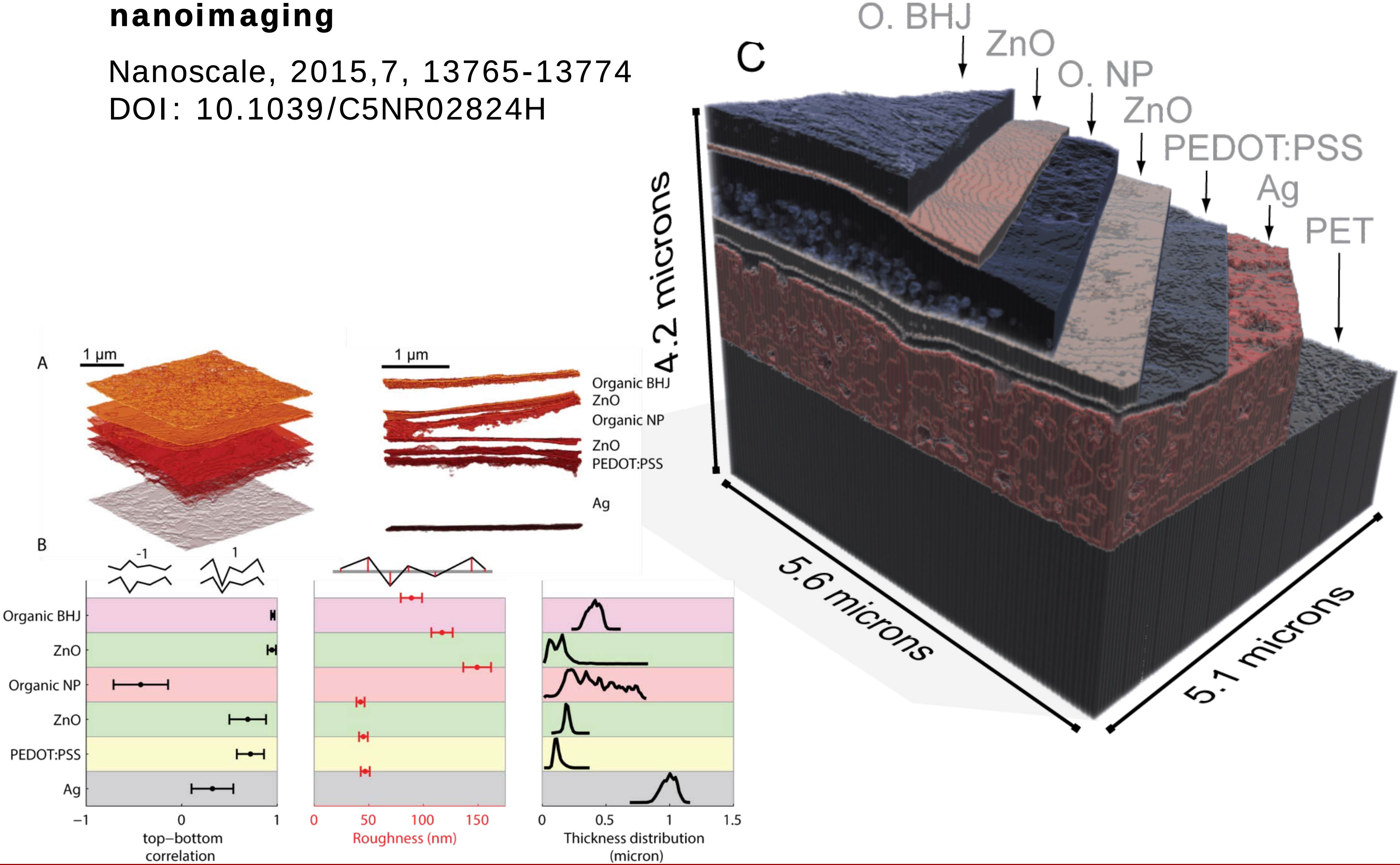

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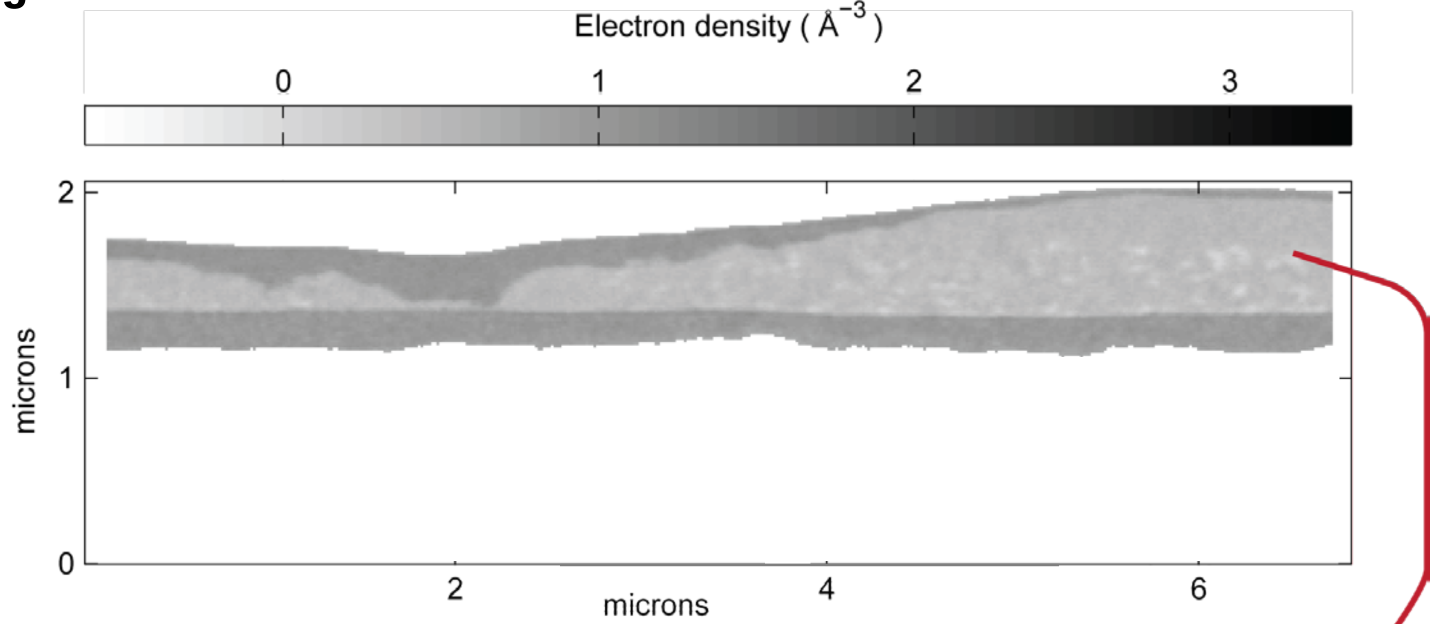

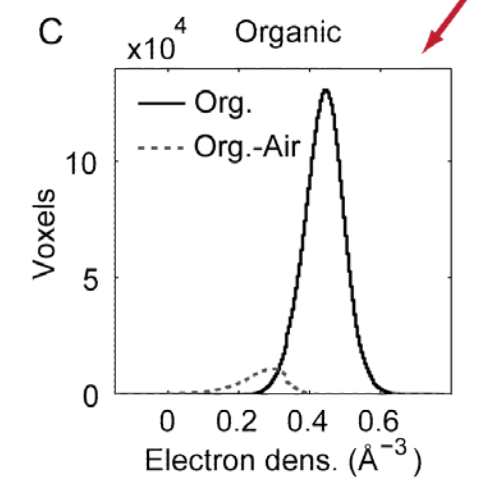

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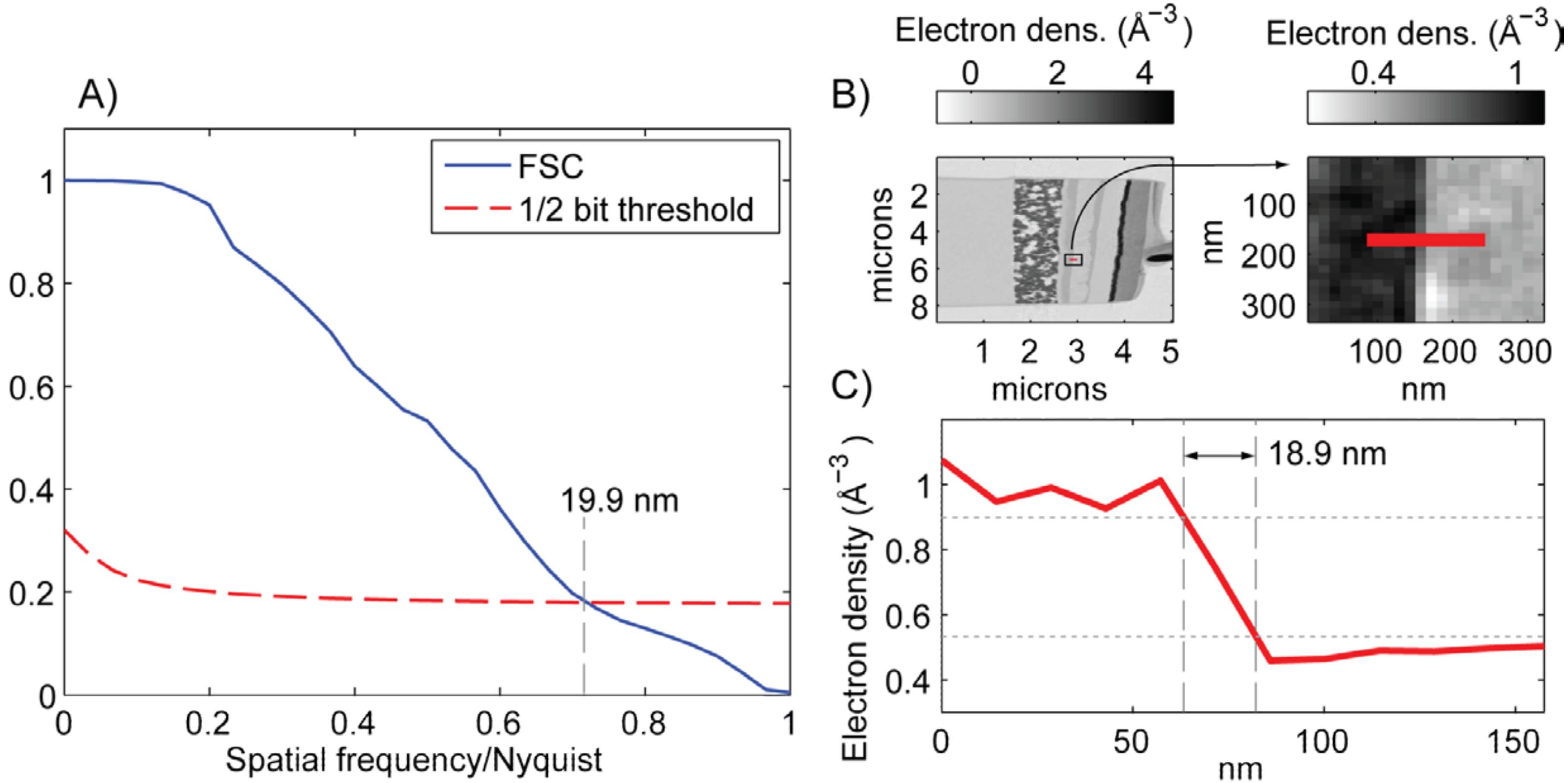
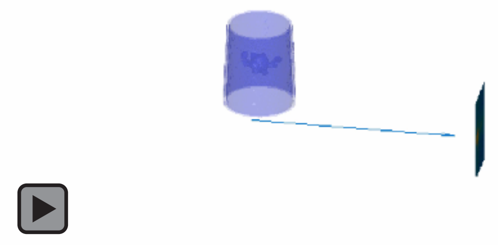


Direct three-dimensional tomographic reconstruction and phase retrieval of far-field coherent diffraction patterns

Phys. Rev. A, 2019, **99**, 023801



Mitigate Radiation Damage by Optimizing Dose Distribution (Dose fractionation theorem)

Simultaneous Phase-retrieval and Tomographic Reconstruction of Far-field Coherent Diffraction Patterns

Requirements:

Parallel coherent illumination

Exact knowledge of scanning positions

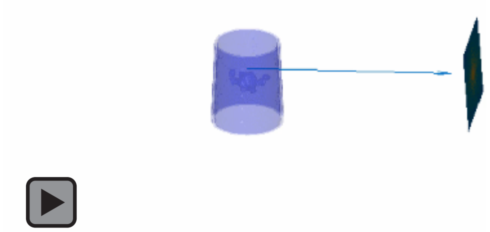
Illumination function (currently)

Sufficient overlap between illuminations in 3D

Returns:

Tomographic reconstruction of complex refractive indices

(Illumination function)



How can we benefit from the much higher brilliance of the EBS?

Better signal to noise ratio could be what we need to resolve nanostructures in organic solar cells, if we can control radiation damage.

In situ ptychographic tomography is currently very limited in scope. EBS could lead to much faster experiments, for proper *in situ* studies.

Much faster experiments would allow a finer energy resolution of resonant studies giving access to full details of chemical speciation.

Hyperspectral ptychography could be a very interesting approach in this respect.

Probably, better detectors will be required to realize this. Smaller pixel size, better energy resolution.

DTU

DTU Energy - Imaging and structural analysis

- Tiago Ramos
- Giovanni Fevola
- Azat Slyamov
- Emil Bøje Lind Pedersen
- Karl Thydén
- Peter Stanley Jørgensen

DTU Informatics and Mathematical Modeling

- Per Christian Hansen
- Jakob Sauer Jørgensen

cSAXS, Swiss Light Source

- Mariana Verezhak
- Ana Diaz
- Manuel Guizar-Sicairos
- Mirko Holler

DTU Photonics Engineering

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- Andrea Crovetto

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MUMMERING

MUltiscale, Multimodal and Multidimensional imaging for EngineeRING

SEEWHI

European Research Council
Established by the European Commission

Solar Energy Enabled for the World by High resolution Imaging

CINEMA

the allianCe for ImagiNg and Modelling of Energy Applications

Danmarks Grundforskningsfond
Danish National Research Foundation

Sino-Danish Centre of Excellence "Danish-Chinese Center for Organic-based Photovoltaics with Morphological Control"

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