# Using synchrotron radiation to gain atomic level insight into materials for solar cells

Ute Cappel

WISE fellow

Department of Physics and Astronomy, Uppsala University

Wallenberg Initiative Materials Science for Sustainability

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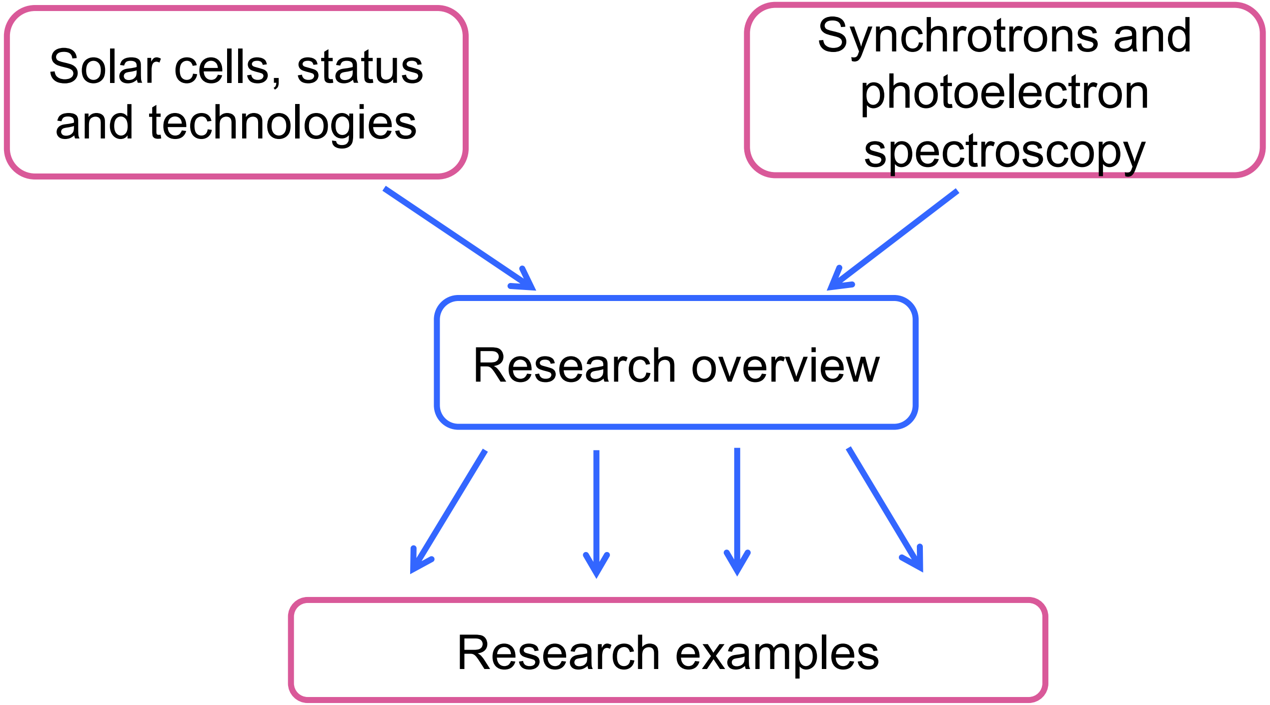
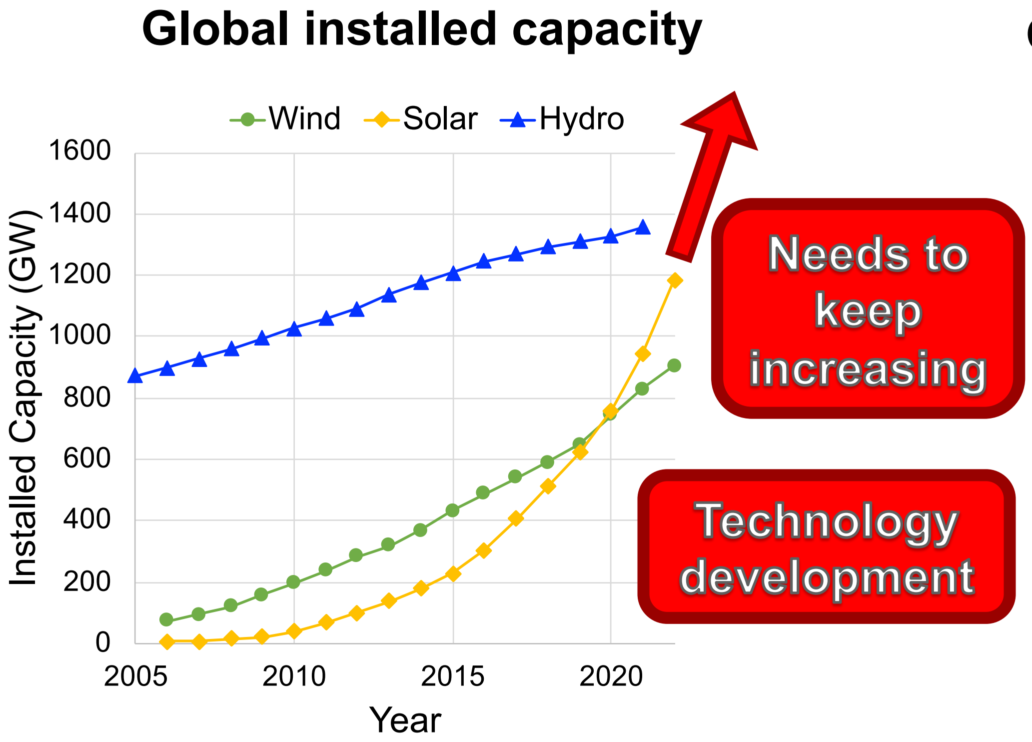
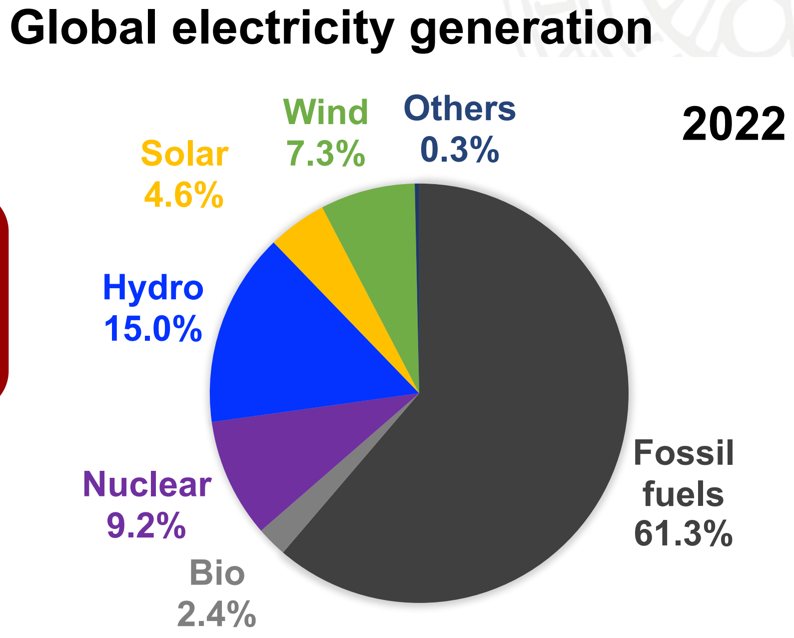
# Outline


Solar cells, status and technologies
Synchrotrons and photoelectron spectroscopy
Research overview
Research examples

# Solar cells and electricity generation




Data from www.ren21.net, from www.iea.org and from https://ourworldindata.org

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# Solar cells – market today, new technologies

## Monocrystalline silicon

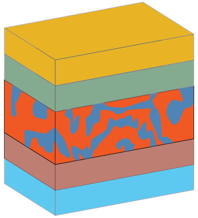
<20 US cent production cost per Watt

~20% module efficiency

26% record efficiency

~30% thermodynamic limit

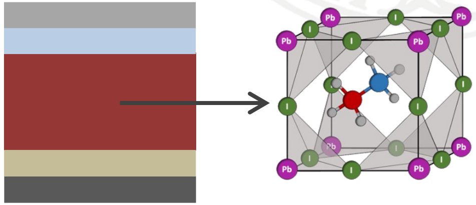
CIGS
23% record efficiency



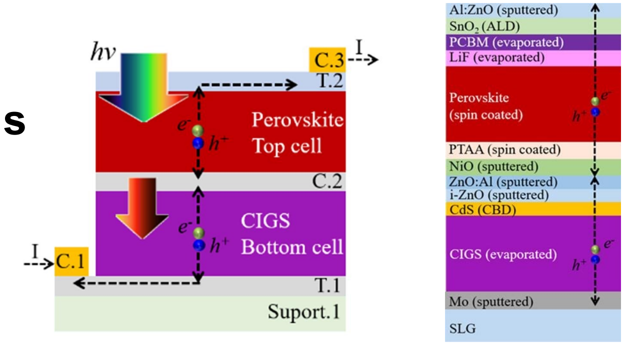
Organic solar cells
19% record efficiency

## Thin film solar cells

Perovskite ($ABX_3$)
26% record efficiency




## Tandem solar cells
**>30% record efficiency**

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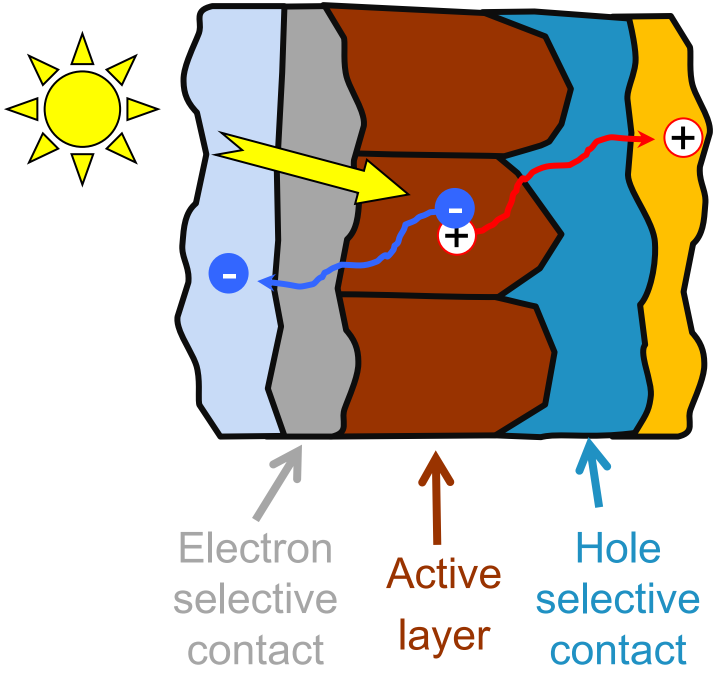
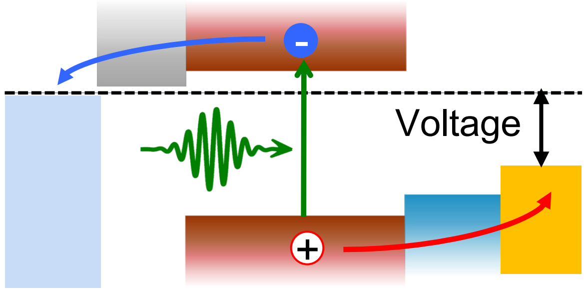
# Light-to-electricity conversion process




1. Light absorption

2a. Electron transport / collection

2b. Hole transport / collection

- Layer-by-layer design (active layer + selective contacts)
- Different materials combinations

Fundamental understanding of energy conversion process at an atomic level

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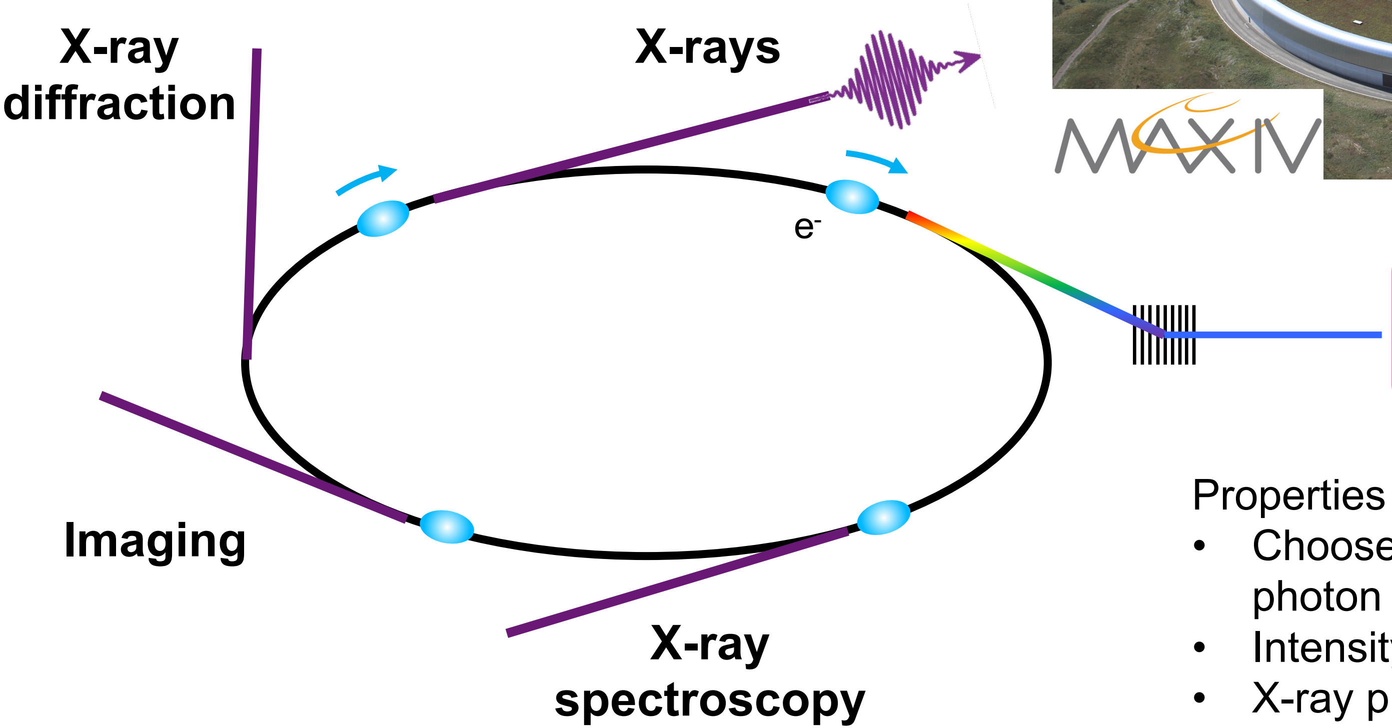
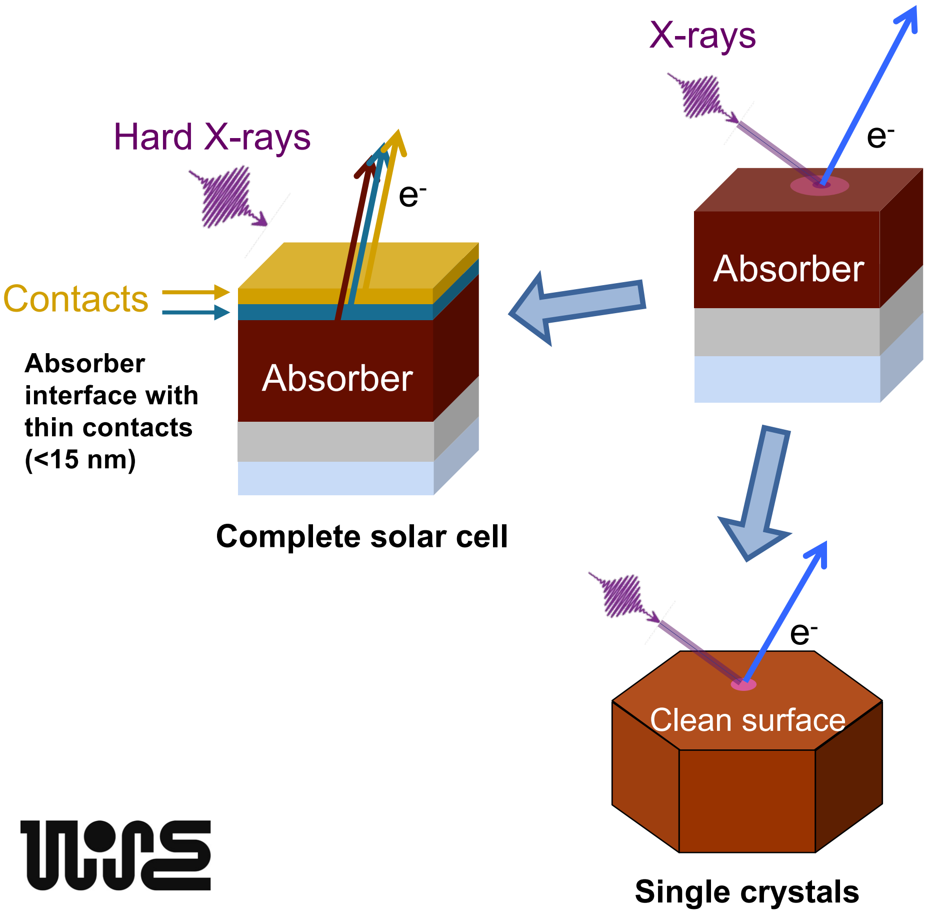
# Synchtrotron facilities

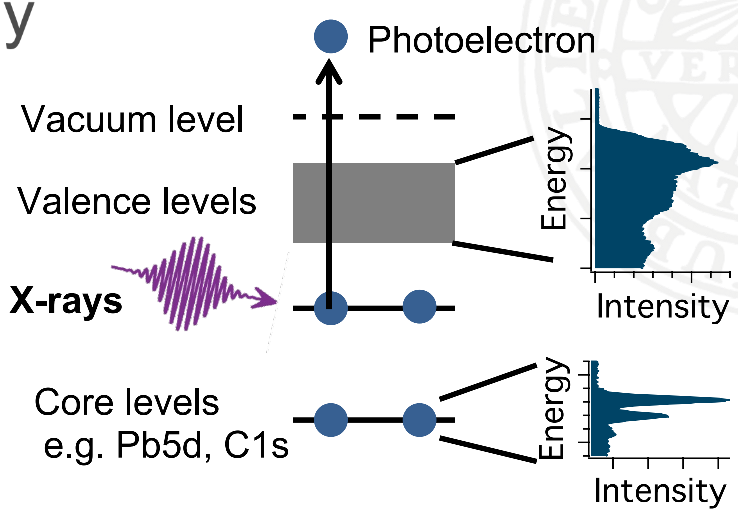




Properties of X-rays

- Choose and vary photon energy
- Intensity
- X-ray pulses

# Photoelectron spectroscopy




X-rays in – electrons out

Binding energy of electrons:

- Core levels (element and chemistry specific)
- Valence levels

Surface sensitive – escape depth of electrons

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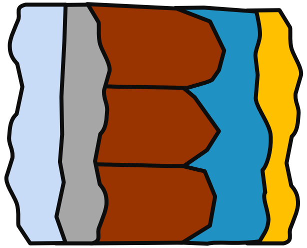
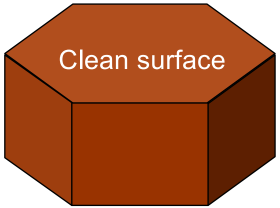
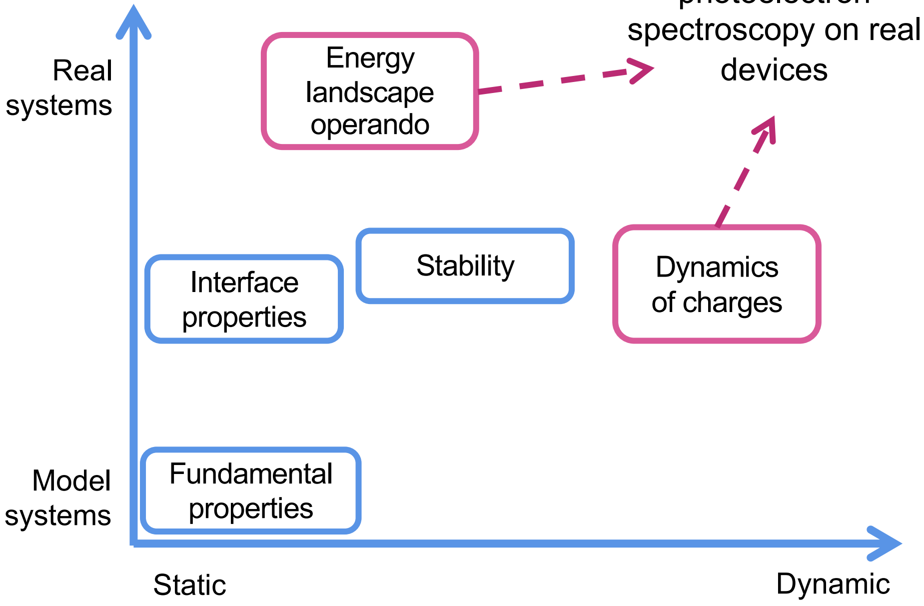
# Research overview



**Complete solar cell**




**Single crystal**




What are the fundamental properties of new materials?

What are the properties of interfaces (e.g. energy alignment)?

What are the mechanisms behind degradation?

What are the interface properties under device operation?

How do charges move and how fast?

How do charges move in a real device?

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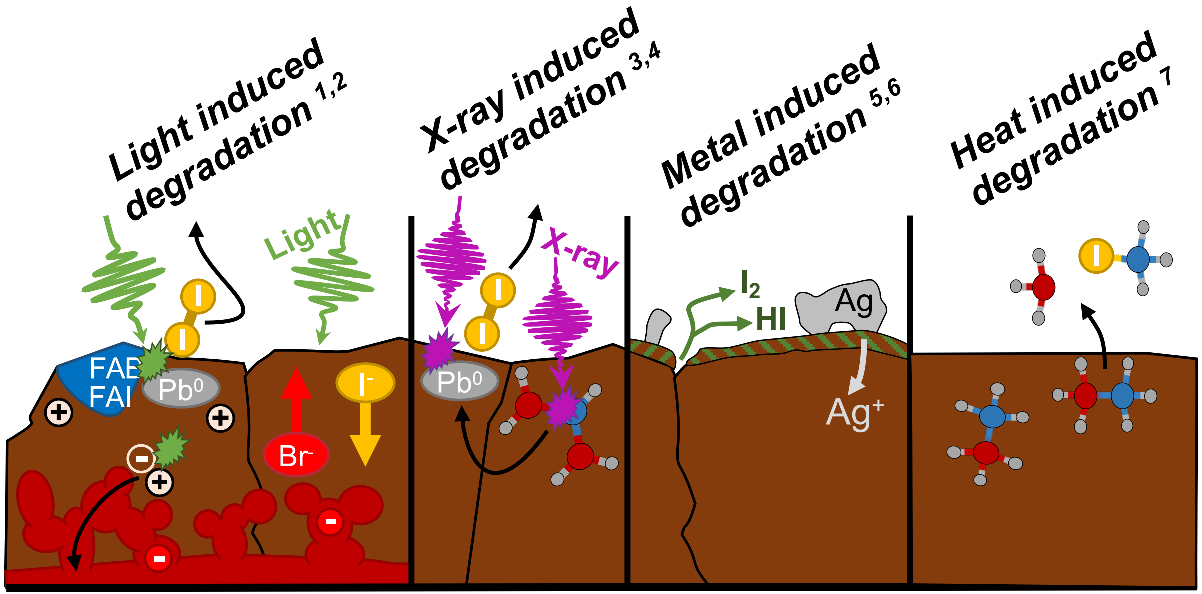
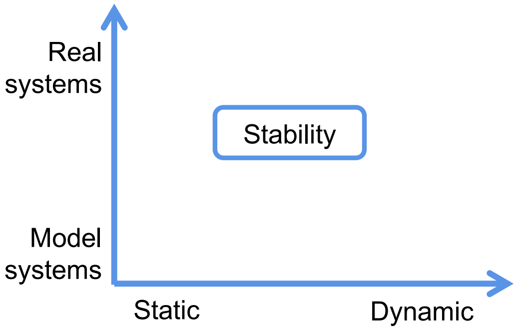
# Stability of lead halide perovskites





1. Cappel et al., *ACS Appl. Mater. Interfaces* **9**, 34970-34978 (2017).
2. Svanström et al., *J. Mat. Chem. A* **6**, 22134-22144 (2018).
3. Svanström et al., *Phys. Chem. Chem. Phys.*, 2021, **23**, 12479–12489.
4. García-Fernández et al. *Phys. Chem. Chem. Phys.*, 2024, **26**, 1000
5. Svanström et al., *ACS Appl. Mater. Interfaces* **12**, 7212-7221 (2020).
6. Svanström et al. *ACS Mater. Au*, **2**, 301-312 (2022).
7. Kammlander et al. *Chem. Comm.* **58**, 13523-13526 (2022).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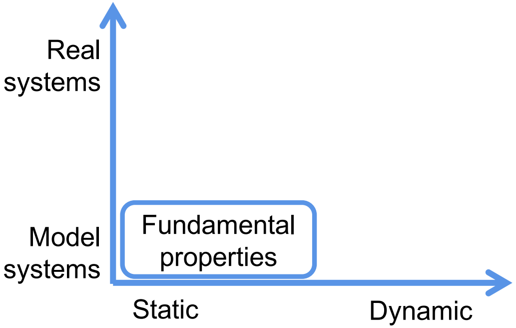
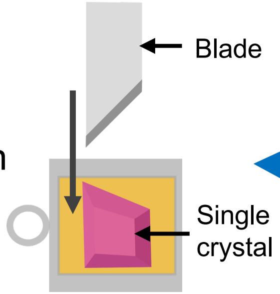
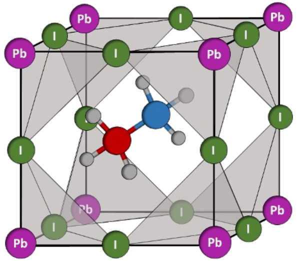
# Photoelectron spectroscopy of perovskite single crystals

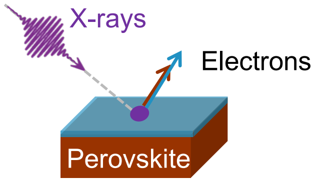



Cleave crystals to obtain clean surfaces

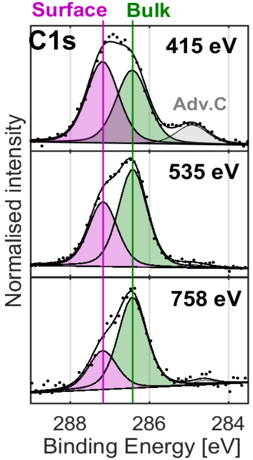


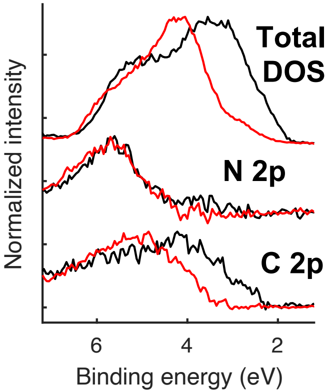



FlexPES@

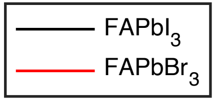



Surface structure from core level spectra

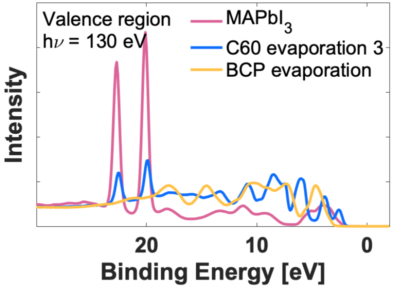



Valence band composition from resonant PES




Interfaces with selective contacts using in-situ evaporation




A. García-Fernández et al., *Small*, 2022, 2106450.

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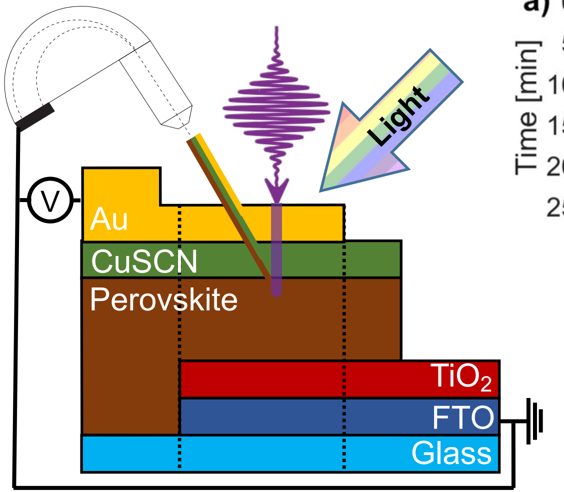
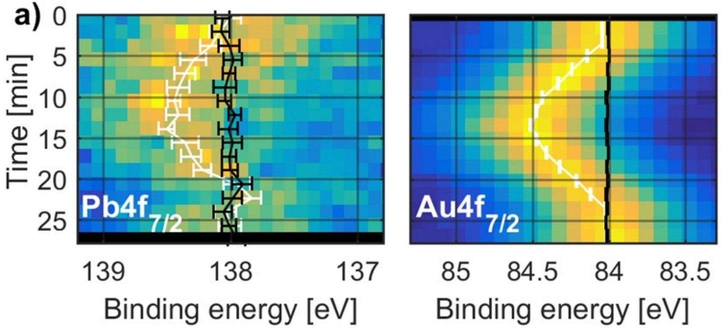
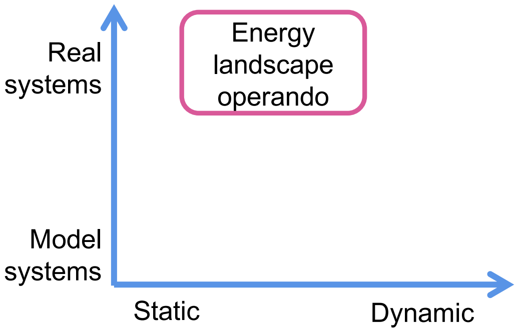
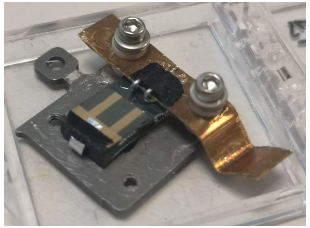
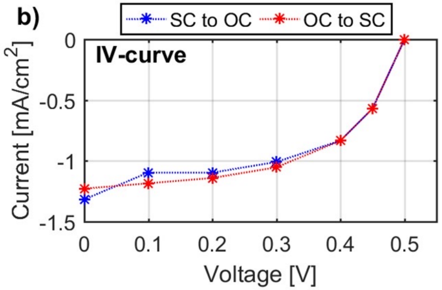
# Perovskite solar cell during operation

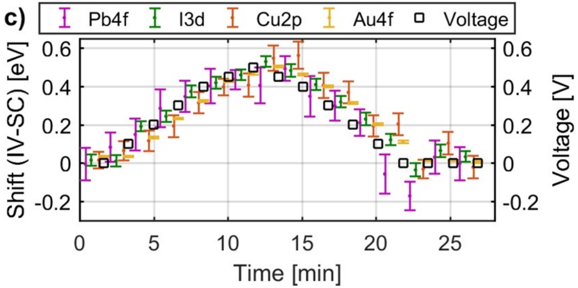





**Can use information to determine where photovoltage is generated and lost**

Svanström et al. *ACS Appl. Mater. Interfaces* **15**, 12485-12494 (2023).

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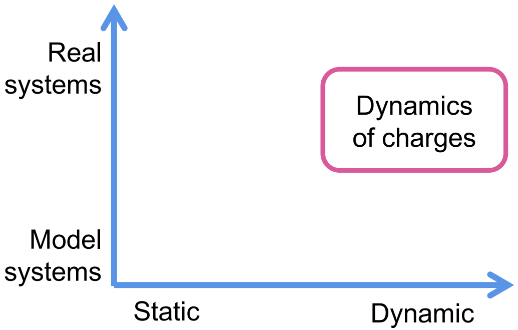
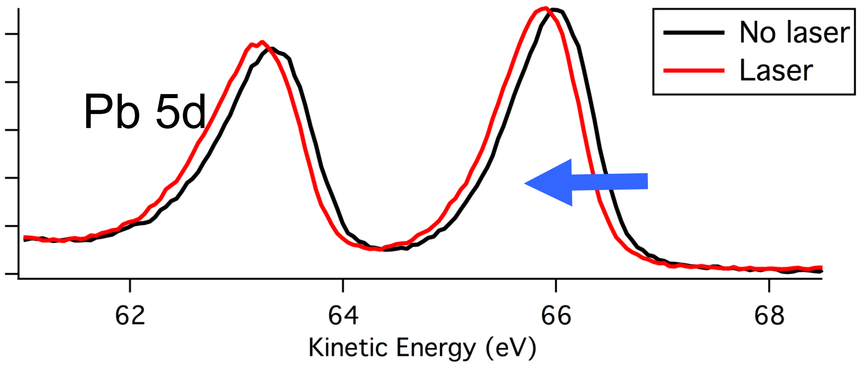
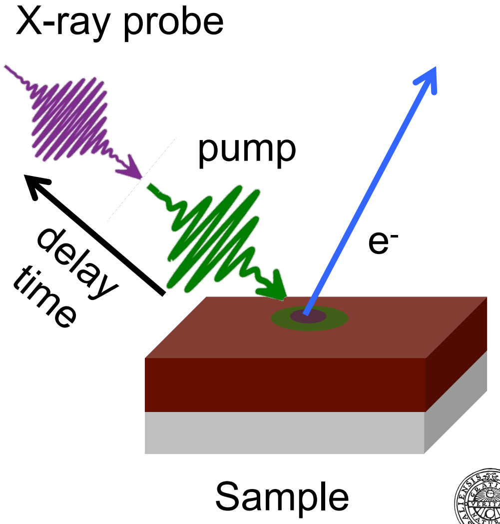
# Dynamics of charges: Time-resolved PES

**Laser pump pulse:** induce changes

- **X-ray probe pulse:** Follow these changes over time
- Time resolution depends on pulse length of X-rays and laser
- Follow photovoltage through core level shift




T. Sloboda et al. *Scientific Reports,* 10, 1-14 (2020).

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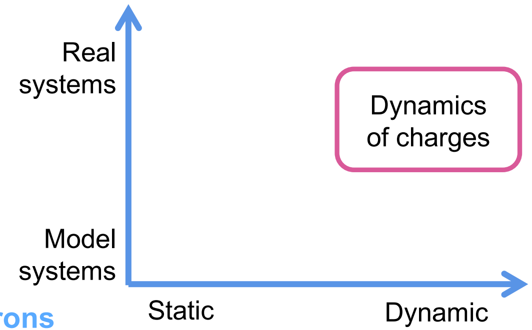
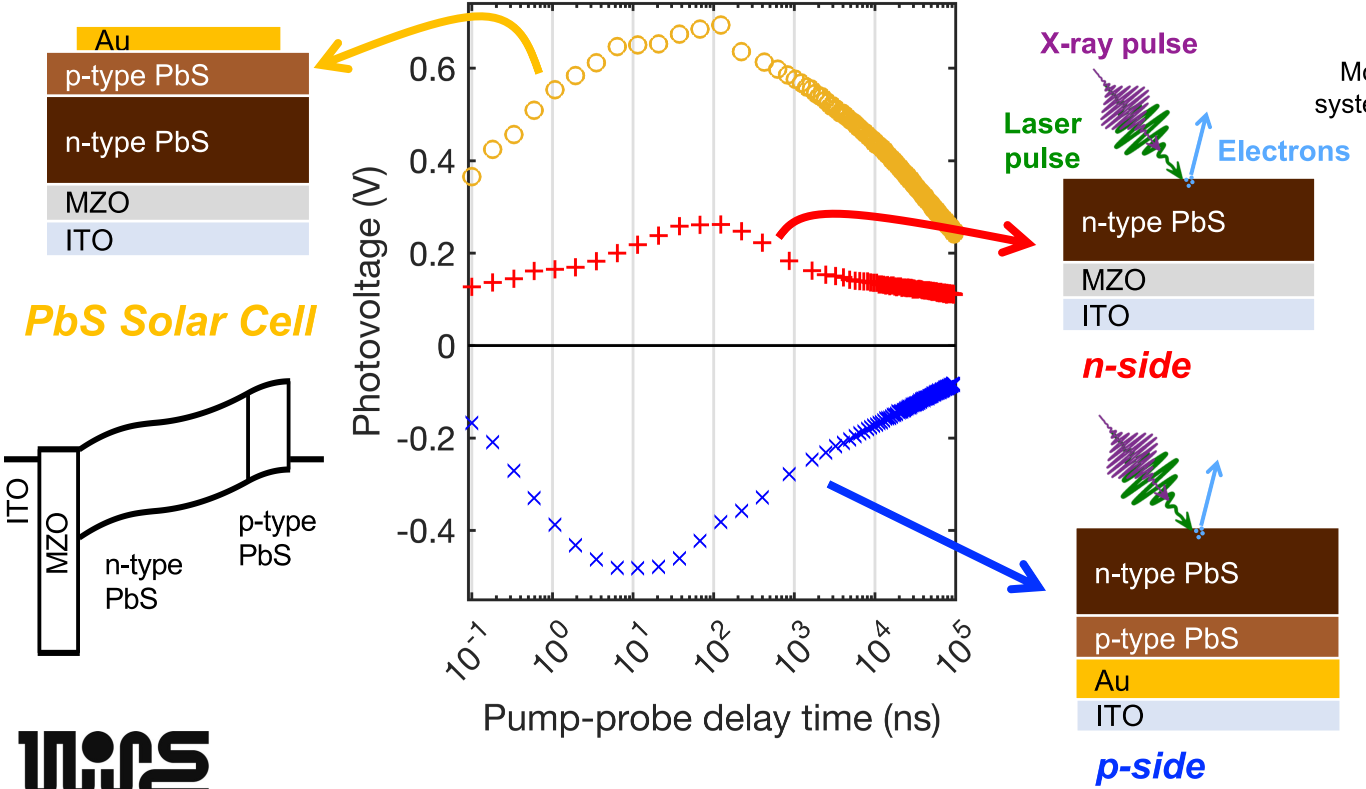
# Dynamics in PbS quantum dot solar cell




**Charge dynamics at different interfaces**

**Pump = 2.4 eV (515 nm)**
**Probe = 360 eV**
**Time resolution = 70 ps**

**PM4@ BESSY**

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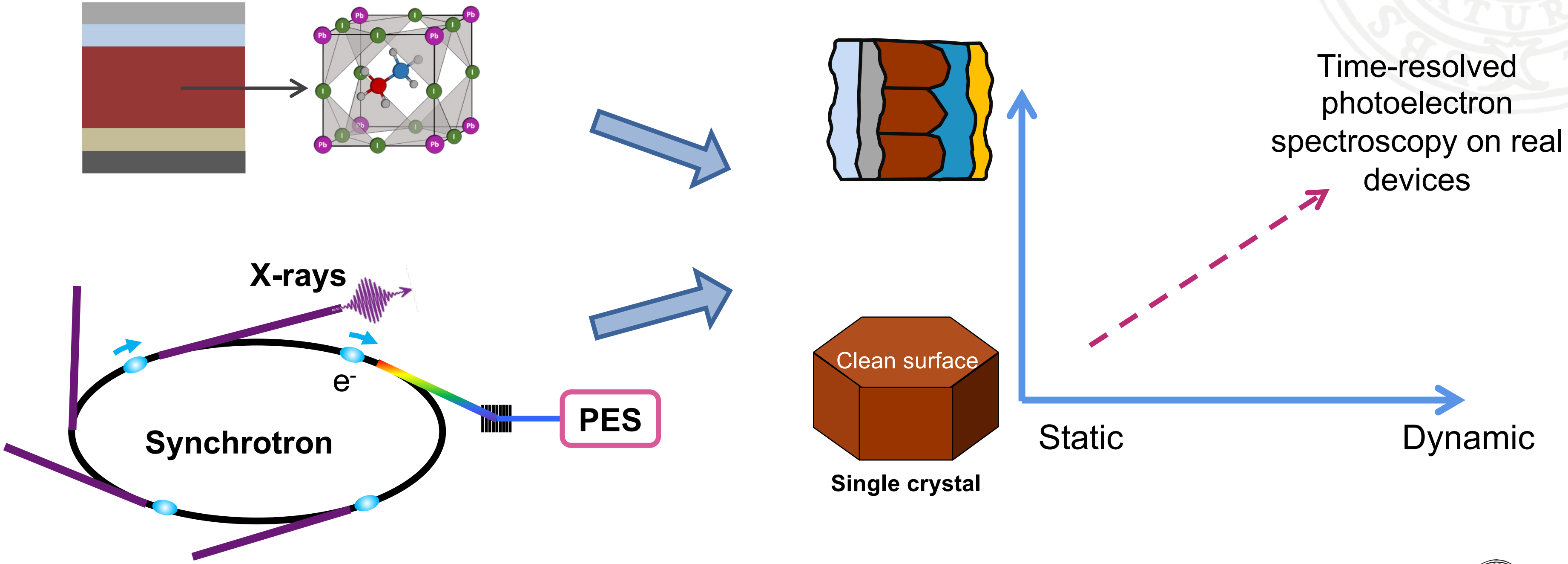
T. Sloboda et al. *Scientific Reports,* 10, 1-14 (2020).

# Summary

## Photoelectron spectroscopy to gain atomic level insight into energy conversion process in solar cells




- Use insights to develop materials and devices

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