Antimony Selenide (Sb_2Se_3)

✓ Absorption of sunlight
- Direct band gap of 1.2 eV
- High optical absorption coeff. [1]

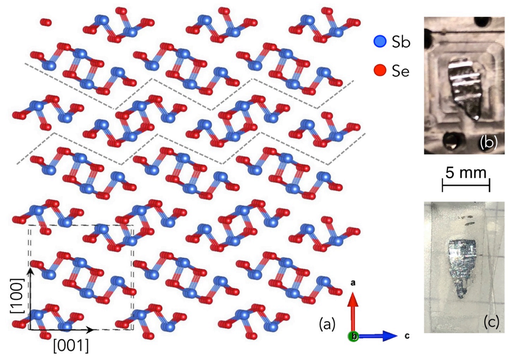
✓ Efficient charge separation
- 1D ribbons occupied by saturated
- atoms → low recombination losses [2]

✓ High stability against photocorrosion [3]

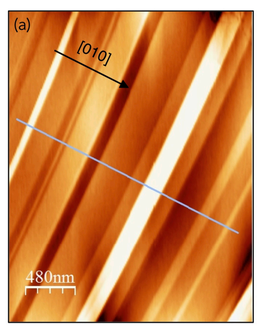
Model system for a cathode

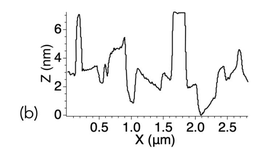
Water reduction catalyst (e.g. MoS_2)

Sb_2Se_3 as photoabsorber

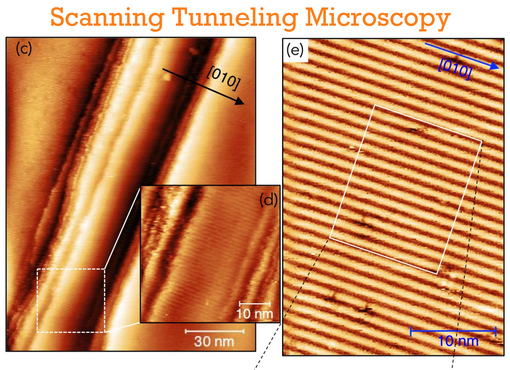


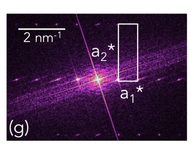
AFM
Atomic Force Microscopy

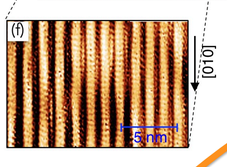




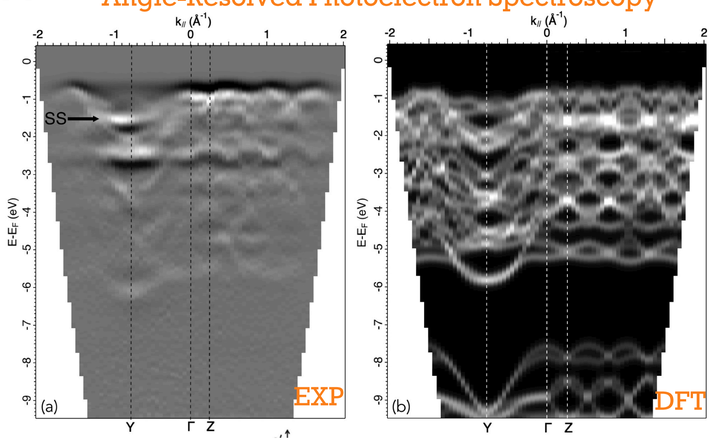
STM
Scanning Tunneling Microscopy

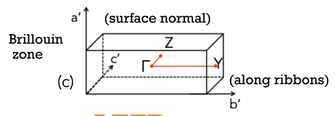




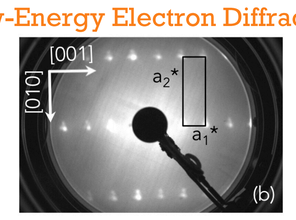


ARPES
Angle-Resolved Photoelectron Spectroscopy



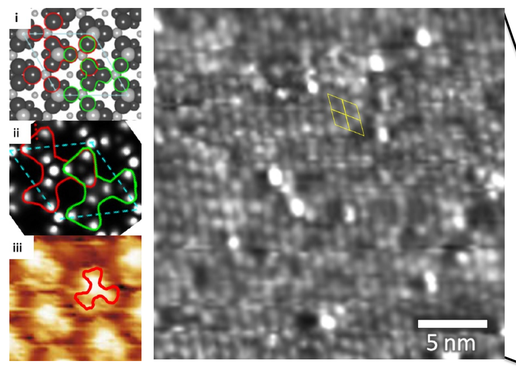


LEED
Low-Energy Electron Diffraction



Highly anisotropic surface [4]

Gallium Oxide (Ga_2O_3)/Cuprous Oxide (Cu_2O)



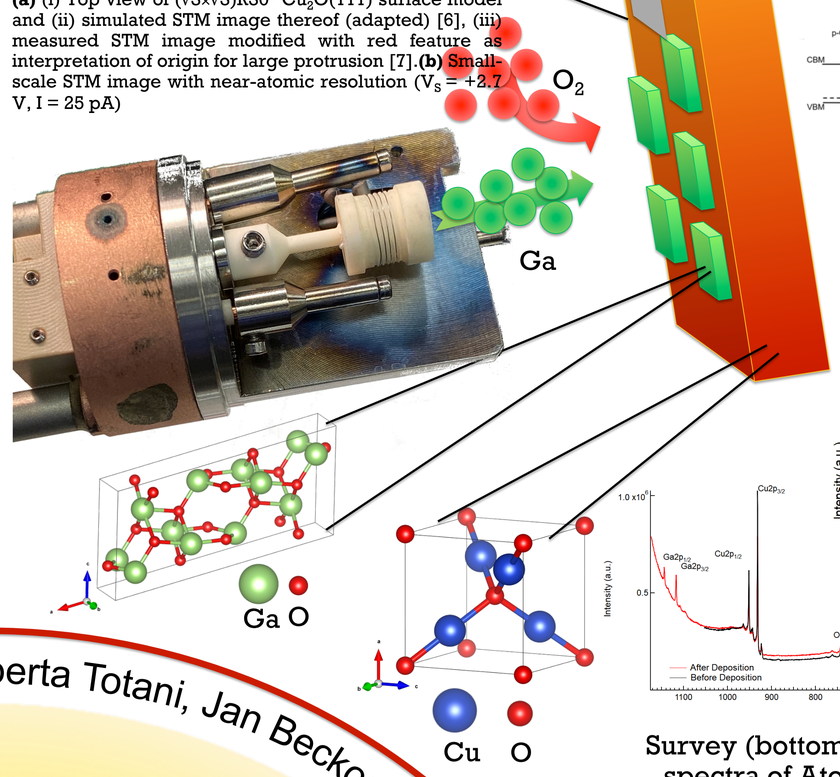
(a) (i) Top view of (√3×√3)R30° Cu_2O(111) surface model and (ii) simulated STM image thereof (adapted) [6], (iii) measured STM image modified with red feature as interpretation of origin for large protrusion [7].**(b)** Small-scale STM image with near-atomic resolution (V_s = +2.7 V, I = 25 pA)

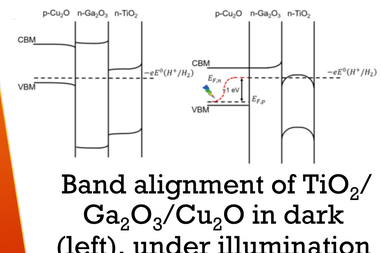
Surfaces/interfaces investigation on photocathode model systems for efficient and stable water reduction

1 **Cu_2O**
- Photoabsorber
- Low cost
- Earth abundant
- Facile preparation

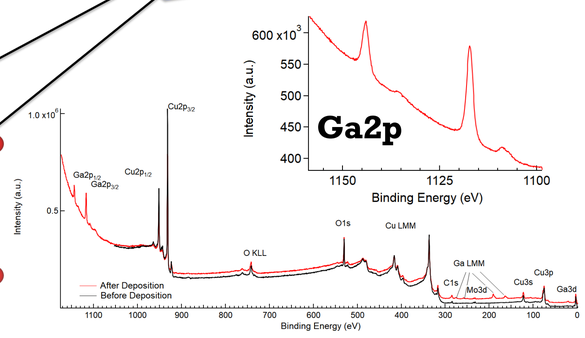
2 **Ga_2O_3/Cu_2O**
- Good CBM alignment
- Enhances photovoltage

3 **$TiO_2/Ga_2O_3/Cu_2O$**
- Augments stability
- Reduces photocorrosion





Band alignment of $TiO_2/Ga_2O_3/Cu_2O$ in dark (left), under illumination (right) [8].



Survey (bottom) and Ga2p (inset) XPS spectra of Atomic Layer Deposition (ALD) grown Ga_2O_3/Cu_2O.

Lisa Grad, Mert Taşkın, Roberta Totani, Jan Beckord

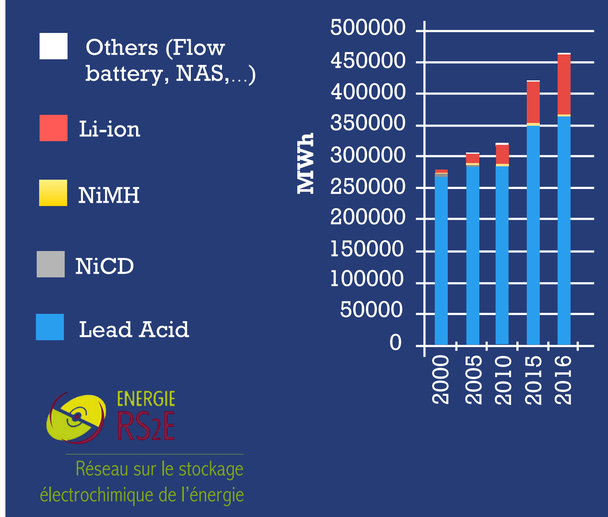
World Energy Issue: A help from Surface Science

URPP LightChEC

University of Zurich[UZH]

About energy storage

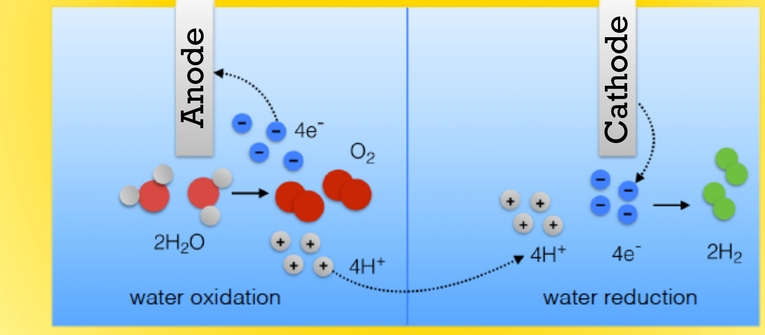
All batteries in the world (2016):



ENERGIE RS2E
Réseau sur le stockage électrochimique de l'énergie

Electricity consumption 2016
58000 GWh*

*Source: Swiss federal office of energy



Photocathalytic Water Splitting

✓ Storage of solar energy into chemical energy
✓ Non-polluting, cheap, and abundant materials
✓ Oxygen as only side product

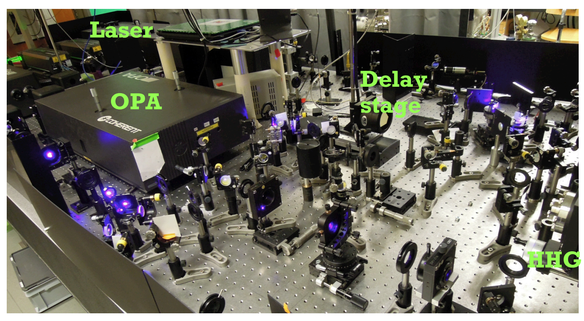
- What we do:
Fundamental research on innovative light absorber, catalyst and photosensitizers by means of Surface Science techniques.

- What we want to know:
Their electronic and morphological properties, how they interact with light and H_2O.

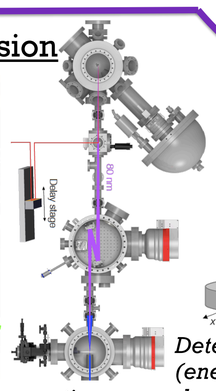
- And how:
- X-rays photoelectron spectroscopy and diffraction;
- Electron diffraction;
- Atomic force microscopy, scanning tunneling microscopy;
- Time-resolved X-rays photoelectron spectroscopy

Matthias Hengsberger, Jürg Osterwalder

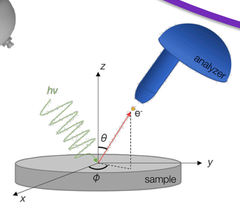
Time-resolved two-photon photoemission



Higher harmonics generation (HHG)

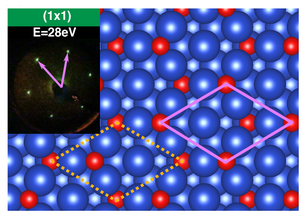


[5]

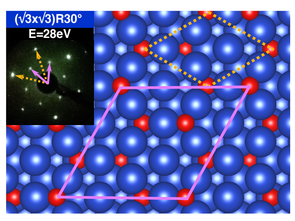


Detection of photoelectrons (energy- and angle-dependent)

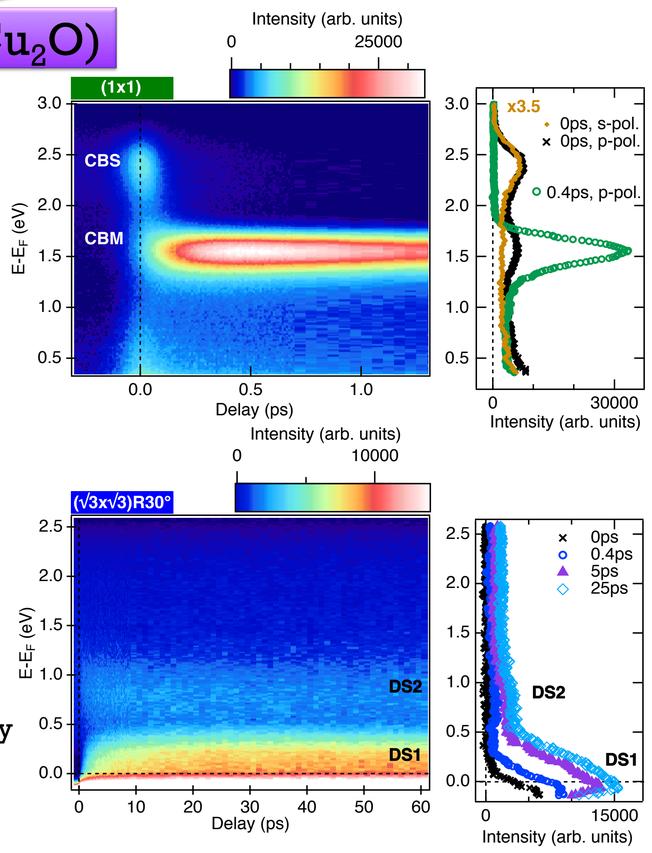
Cuprous Oxide (Cu_2O)

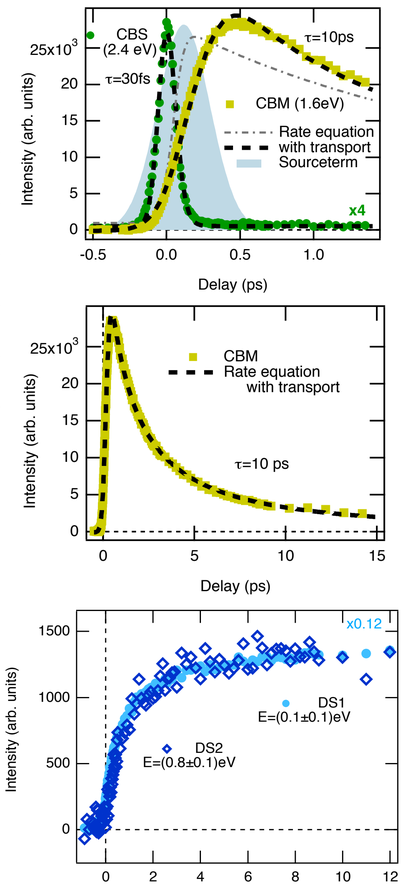


Bulk-terminated surface
⟶ Long-living conduction band population



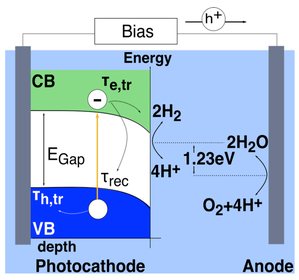
Surface with high density of ordered defects
⟶ Trapping in defect states



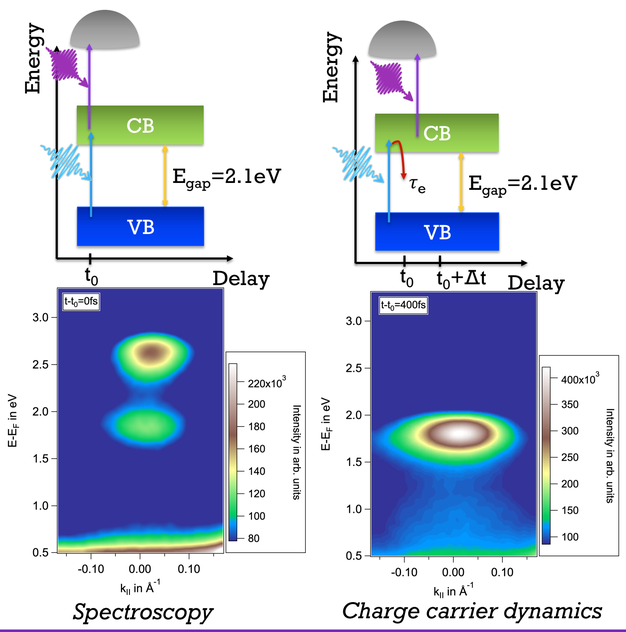


Cu_2O(111): Influence of surface defect density on the lifetime of photo-excited charge carriers in the conduction band

Cu_2O as photocathode for photocatalytic water splitting



- ✓ High absorbance due to small direct band gap (2.1eV)
- ✓ Downward band bending towards the surface supports charge separation
- ✓ Long lifetime of photo-excited charge carriers in the conduction band at the surface mandatory



Spectroscopy *Charge carrier dynamics*

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[1] Y. Zhou *et al.,* Adv. Energy Mater. 2014, 4, 1301846.
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[4] R. Totani *et al.*, Phys. Rev. Materials 2019, just accepted
[5] A. Schuler, Dissertation (2018)
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[7] Önsten *et al.,* Surf. Sci., 603, 2009
[8] Pan *et al.,* *Nat Catal.,* 1, 412–420 2018

Acknowledgments

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