HASPIDE Spectroscopic Characterization

Hydrogenated Amorphous Silicon PIxel DEtectors for ionizing radiation

M. Pedio WP1

HASPIDE STATUS: WP1

1) Spectroscopic characterization: Goals

→ Understanding the microscopic properties of the deposited films

→ Study of the interfaces
  - → Kapton/Metal, Metal/a-Si:H, Kapton/a-Si:H a-Si:H/contact layers in the devices

→ Provide feedbacks to simulation and production, to enlighten the link of microscopic properties with electrical measurements

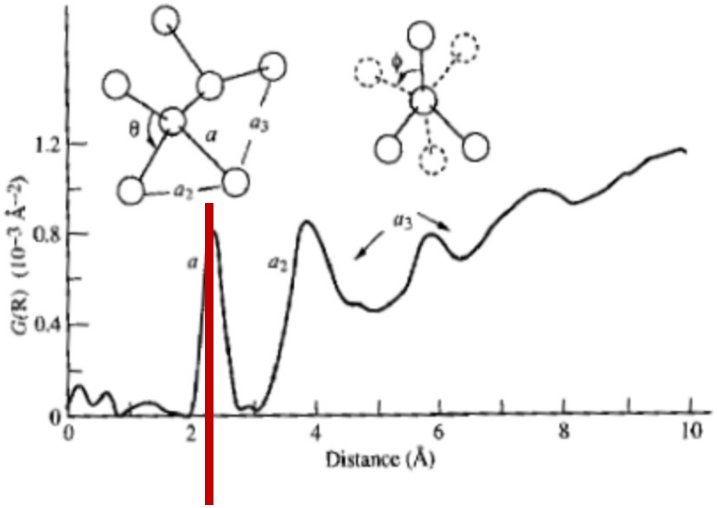
2) Spectroscopic characterization: Means

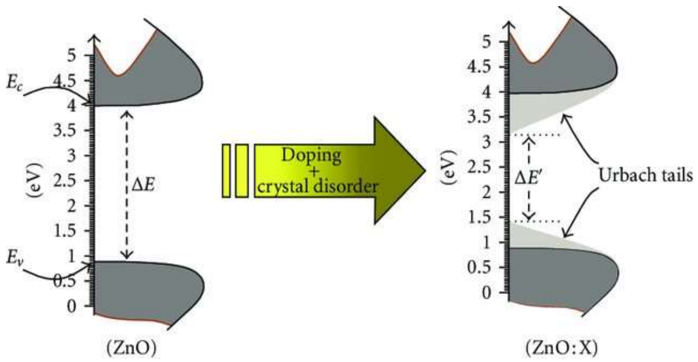
→ *Setup of a measuring station in Perugia for photon energies few eV (goal: commissioned in May)*

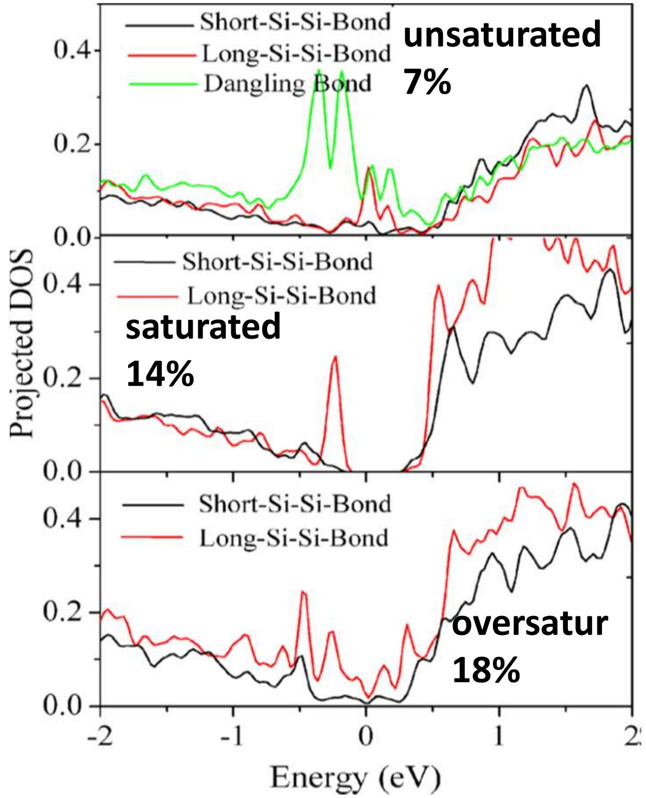
→ *Measurements at the soft-X, higher photon energies (Synchrotrons). Previous run at ELETTRA (TS) in 2022 In 2023 ELETTRA will not be available*

→ *We have found a possible alternative: Laboratory of Quantum Optics (LKO) Nova Gorica (summer 2023)*

a-Si:H properties





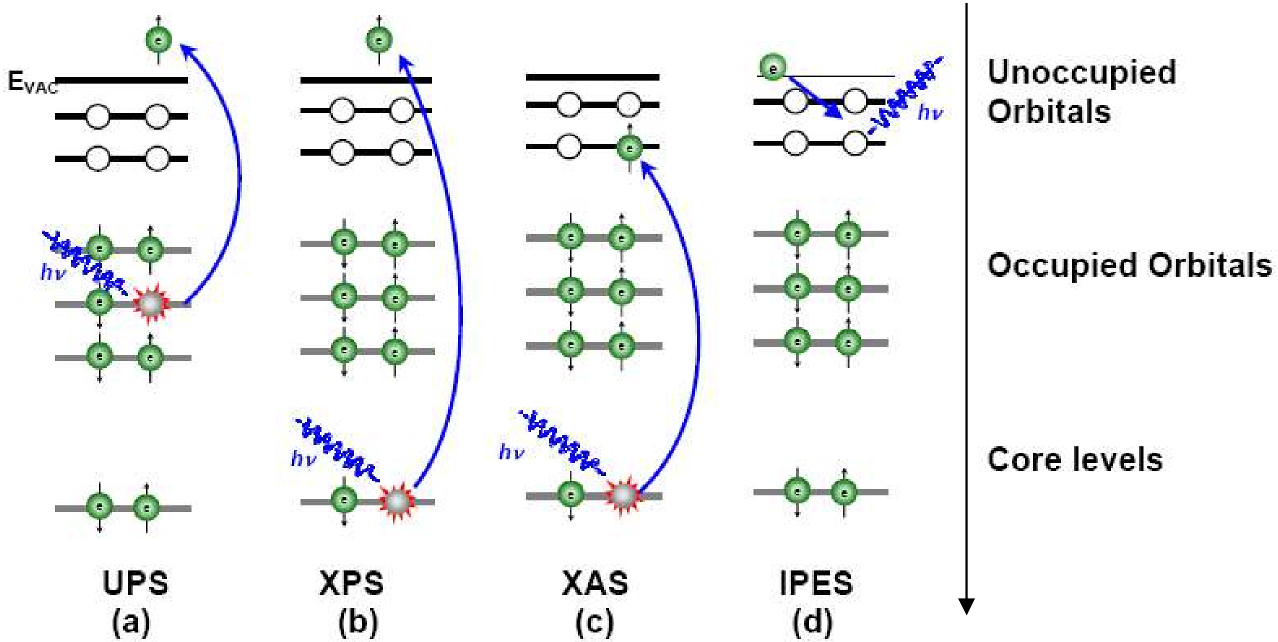


Density Functional Theory DFT calculations DOS vs Si-H bonds Legesse et al 2014

The specific band gap structure depends on the deposition conditions and film treatments (contacts, irradiation etc)

Impact on the device performance

Absorption and Electron spectroscopies



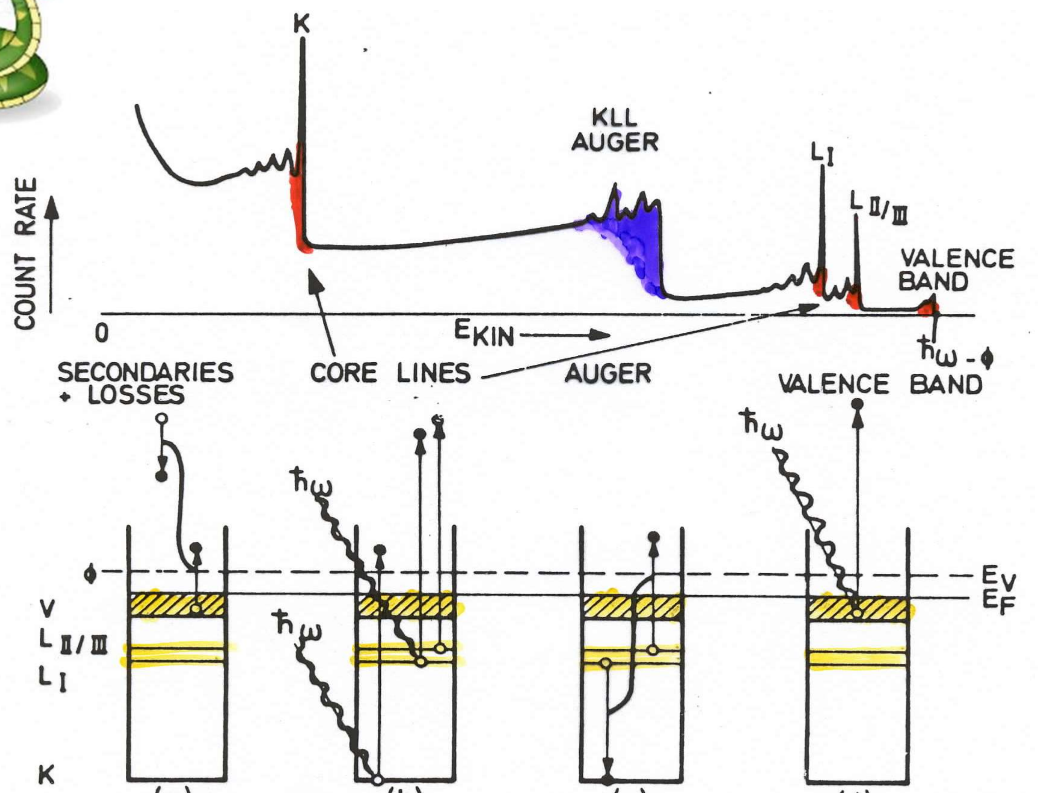
N-1

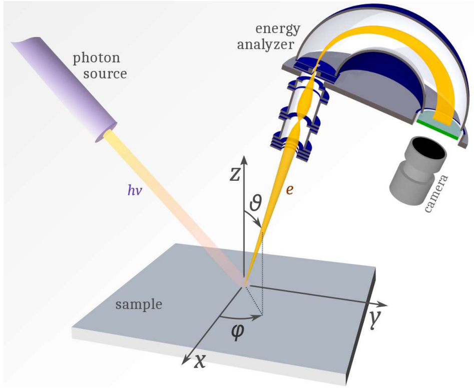
N+1

Linear response theory models the spectrum

Final state differs from the ground state

Photoelectric effect →Photoemission Spectroscopy



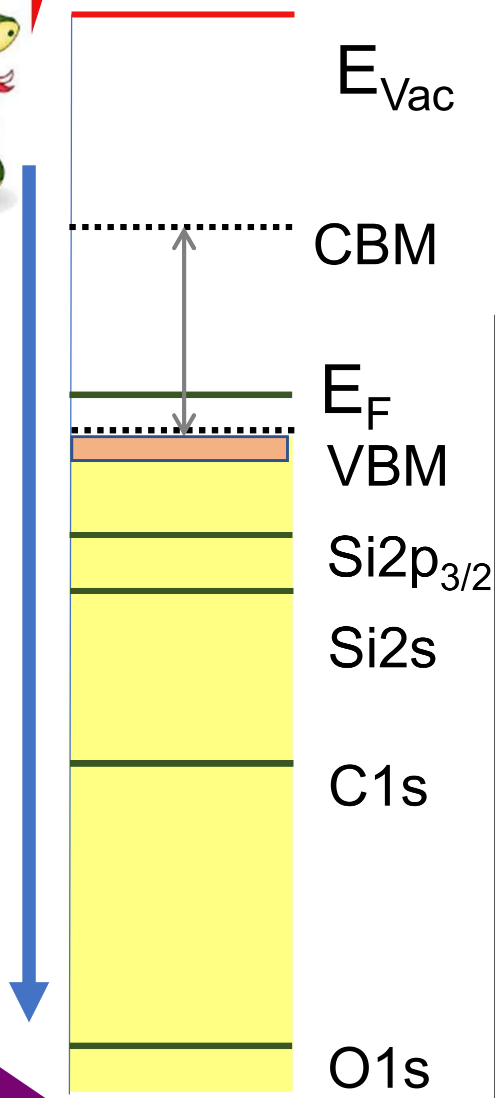


photon in-electron out

$$E_{kin} = \hbar\omega - E_b{}^F - \Phi$$

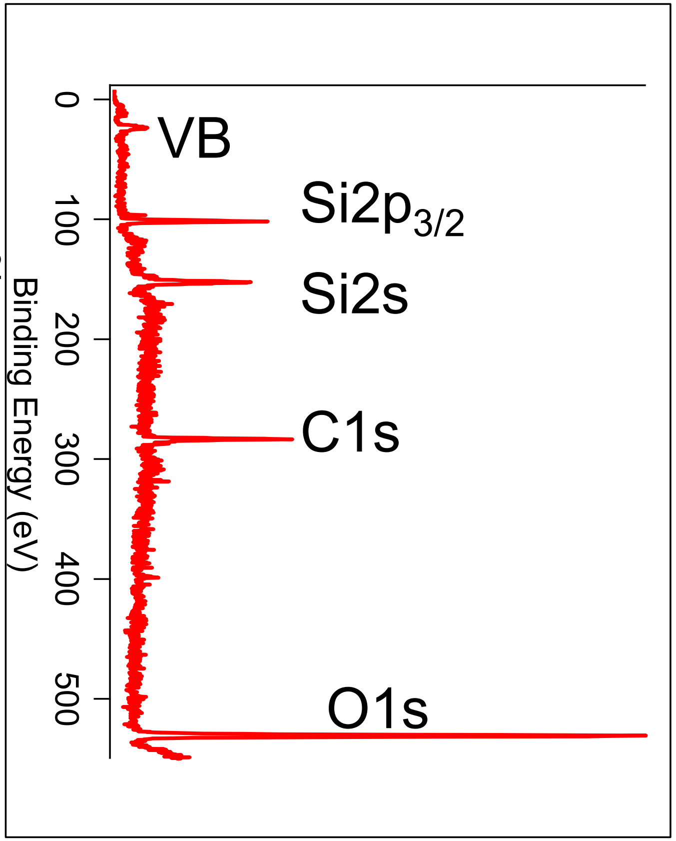
E_{kin} = Final State Kinetic Energy
Φ = Work Function
$E_b{}^F(k)$ = Binding Energy of the k-th Initial State

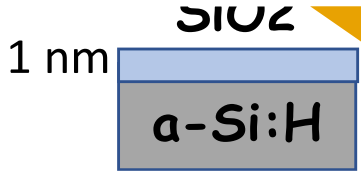
photoemission spectrum
Counts vs Kinetic Energy→ Binding Energy



Energy level diagram

Spectrum





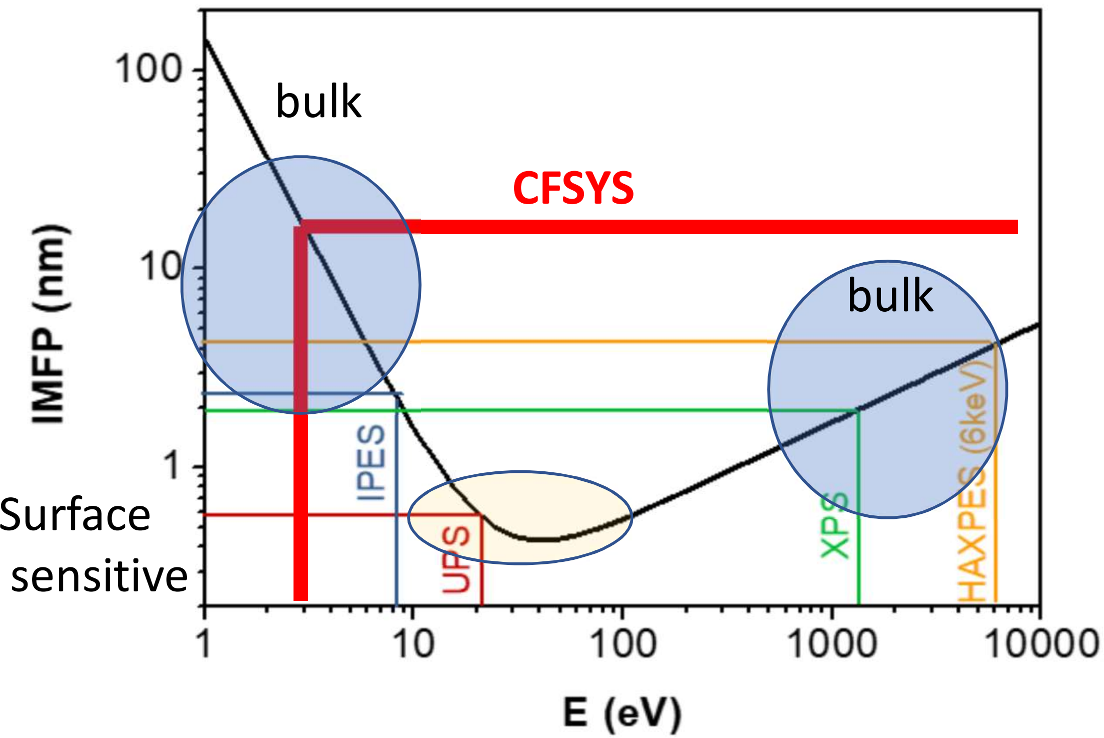
Monocromatic Photons from lamps or monochromatic Synchrotron radiation

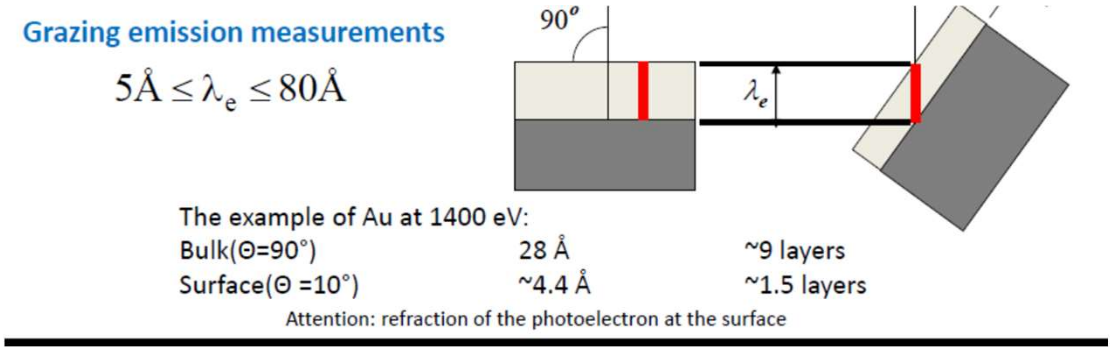
Electrons Counts at defined Kinetic energy detected by an Electron Analyser

Filled electronic States

M. Pedio

Sampling depth and maximum information depth





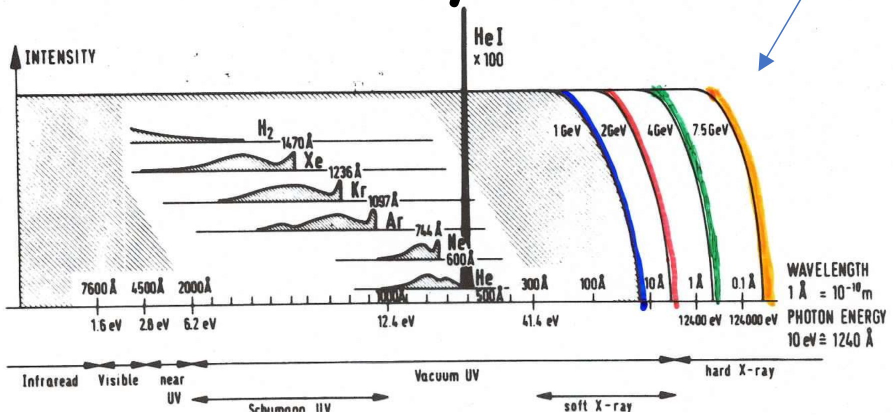
Since in photoemitted electrons are detected by the analyser, the possibility of their detection, in solids, is related to the inelastic mean free path **IMFP**

$$E_{kin} = \hbar\omega - E_b{}^F - \Phi$$

Sampling depth depends on the photoelectron Kinetic Energy ←→ photon energy

The maximum information depth is 3 times the IMFP

Spectral Intensity Distributions for a Variety of Standard Photon Sources and Synchrotron Radiation Sources



Photoemission energy resolution ΔE includes the photon source AND the electron analyser contributions

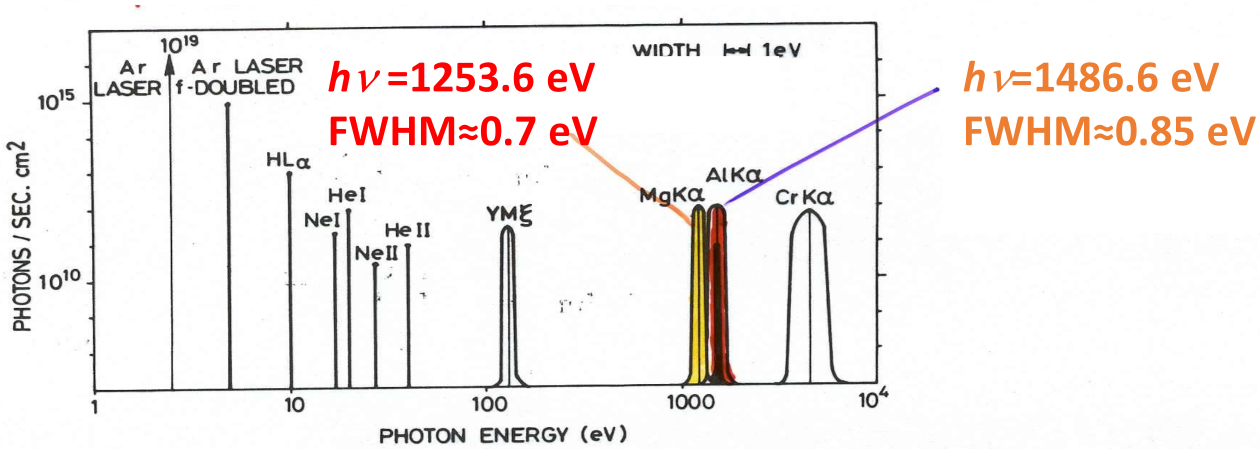
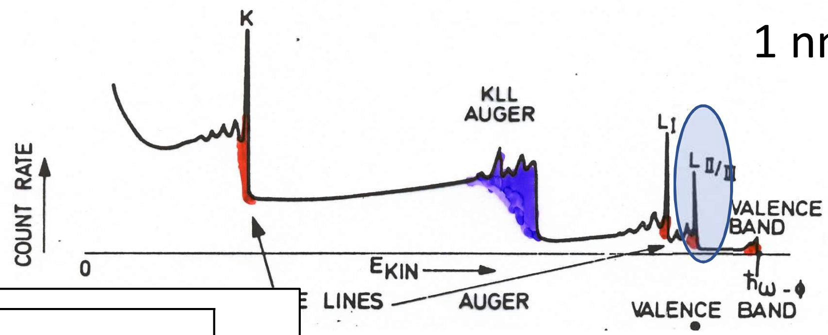


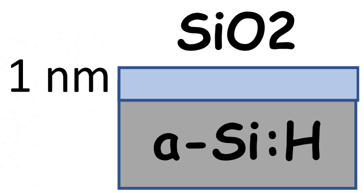
Fig. 5.5 Photon energies and intensities for line sources commonly used in photoemission experiments. Intensities are given for a 10 x 10 mm illuminated area at the sample position. Line widths are indicated on an expanded scale as shown in the top right corner. The AlK_α line is also shown after monochromatization (full peak)

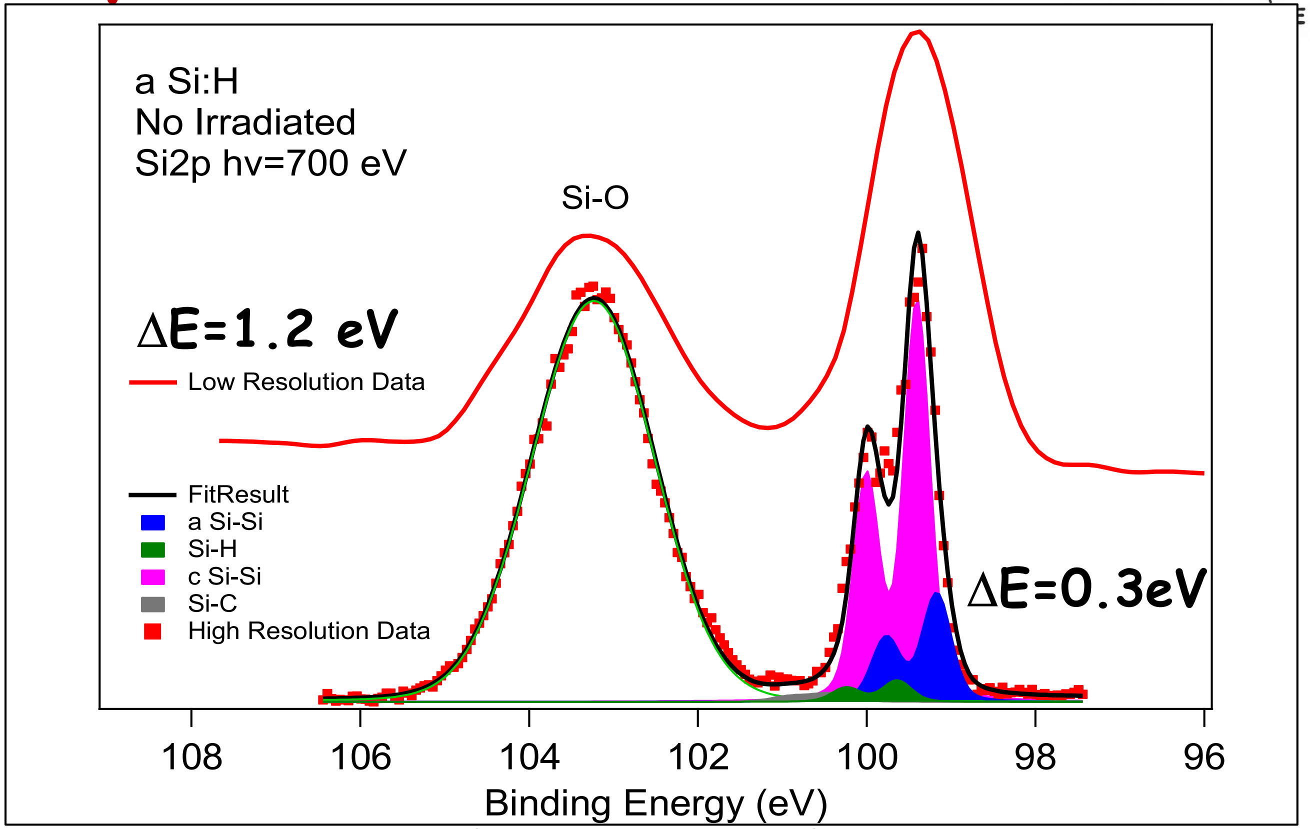
Standard laboratory XPS measurements have **ΔE=1-1.5 eV**

Synchrotron or monochromatic XPS **hundreds of meV**

Core level photoemission
Why
High Energy Resolution?
Synchrotron source result







Peverini et al. 2022 : a-Si:H on Silicon

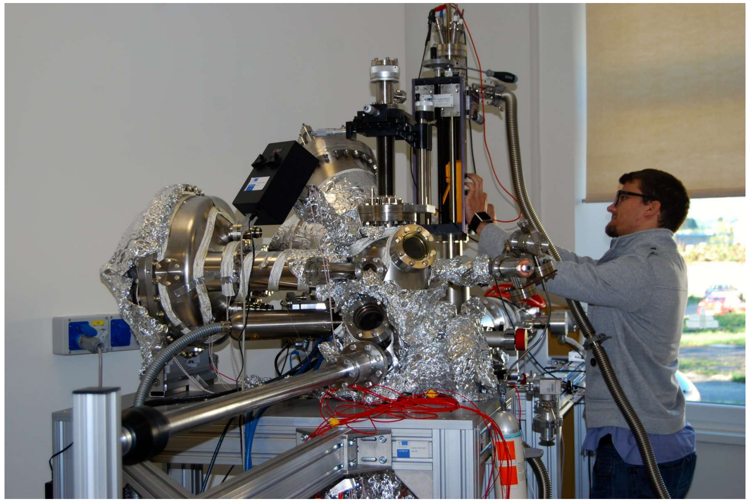
- Element sensitive
- Chemical shifts

High resolution Si 2p spectra allow to single out the different surrounding of Si in the a-Si:H at variance to standard lab photon source or low resolution spectra

a-Si:H on Kapton future tests at ELETTRA (**postponed**) and LKO (SLO)

The ELETTRA source in 2023 has drastically reduces the users access. Long shutdowns are foreseen for 2023.

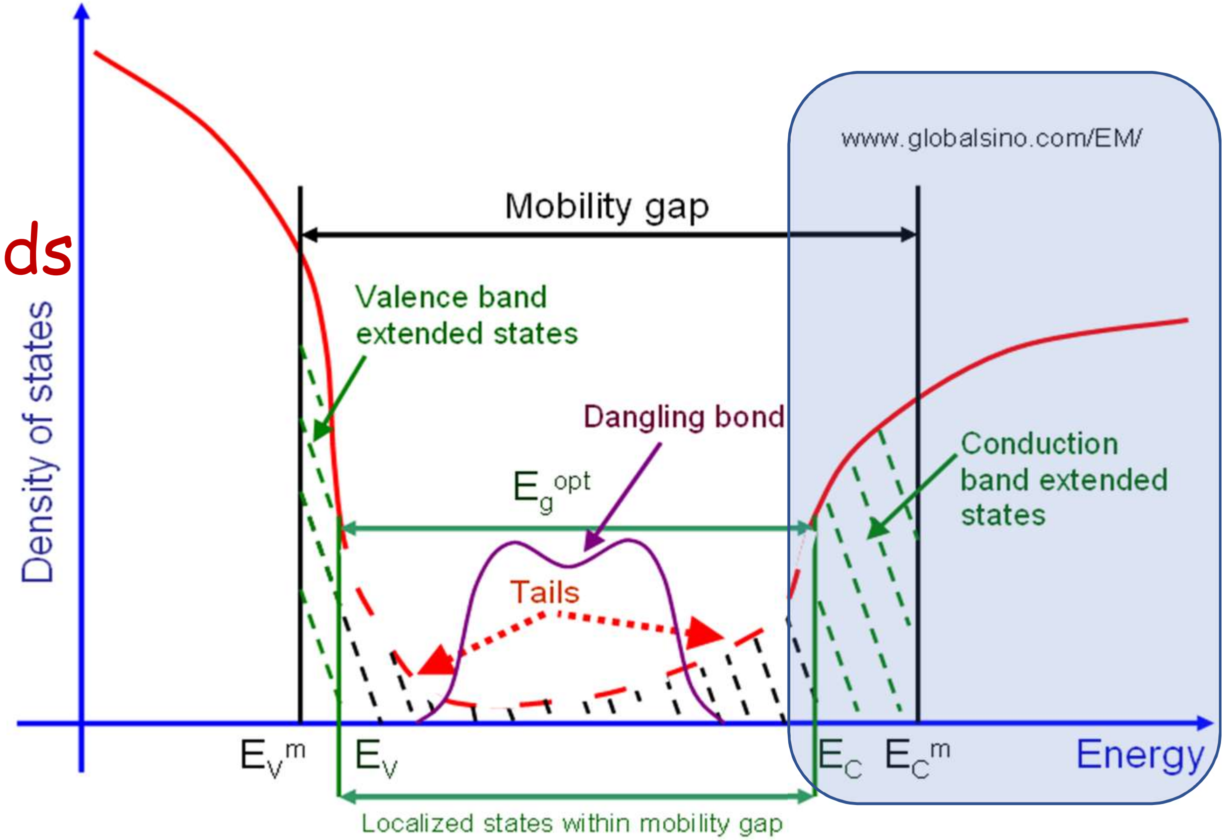
In alternative high resolution XPS measurements will be performed at the **laboratory of Quantum Optics (LKO) Nova Gorica Physics department** within the summer 2023. PhD student (F. Peverini) 3 months at LKO under supervision Prof. Barbara Ressel
https://www.ung.si/en/research/laboratory-of-quantum-optics/about/



LKO Monochromatic XPS source and Scienta electron analyser
$\Delta E = 0.4$ eV

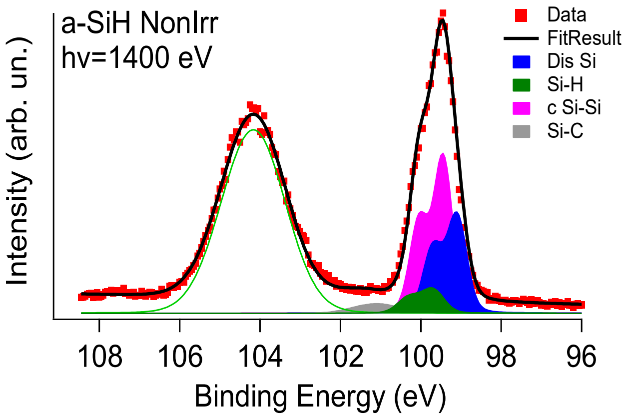
Density of electronic states (DOS) transport gap a-Si:H

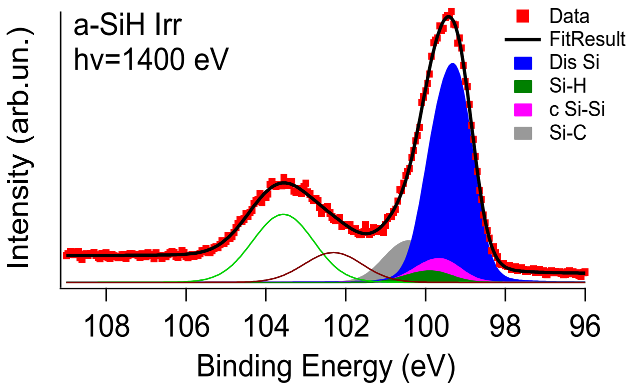
valence and
conduction bands
DOS

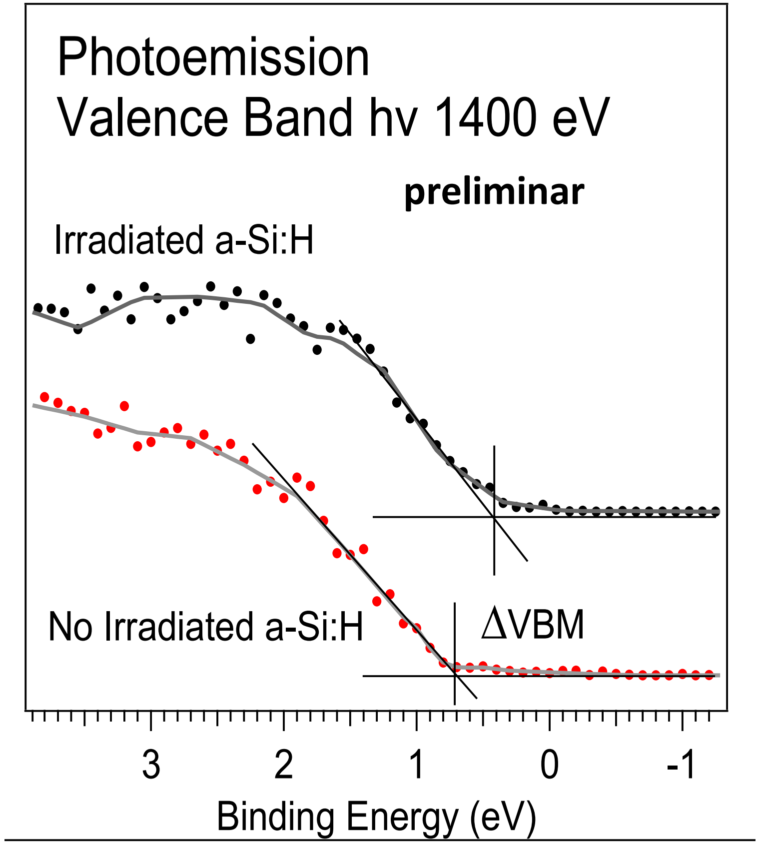


The band (Urbach) tail and **the localized states** exhibit modifications connected with the a-Si:H thin-films properties →the exact band gap structure depends on the specific microstructure of a-Si:H (deposition conditions etc) that can impact significantly the device performance.

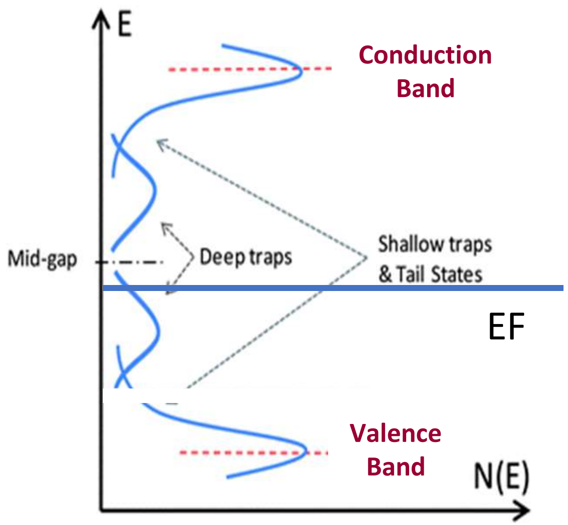
No Irradiated and Irradiated a-Si:H/Si Photoemission results







Valence Band Maximum differences in the two cases.

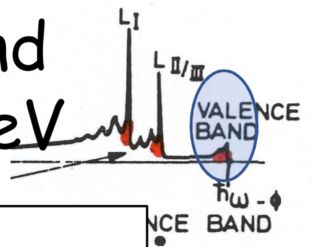


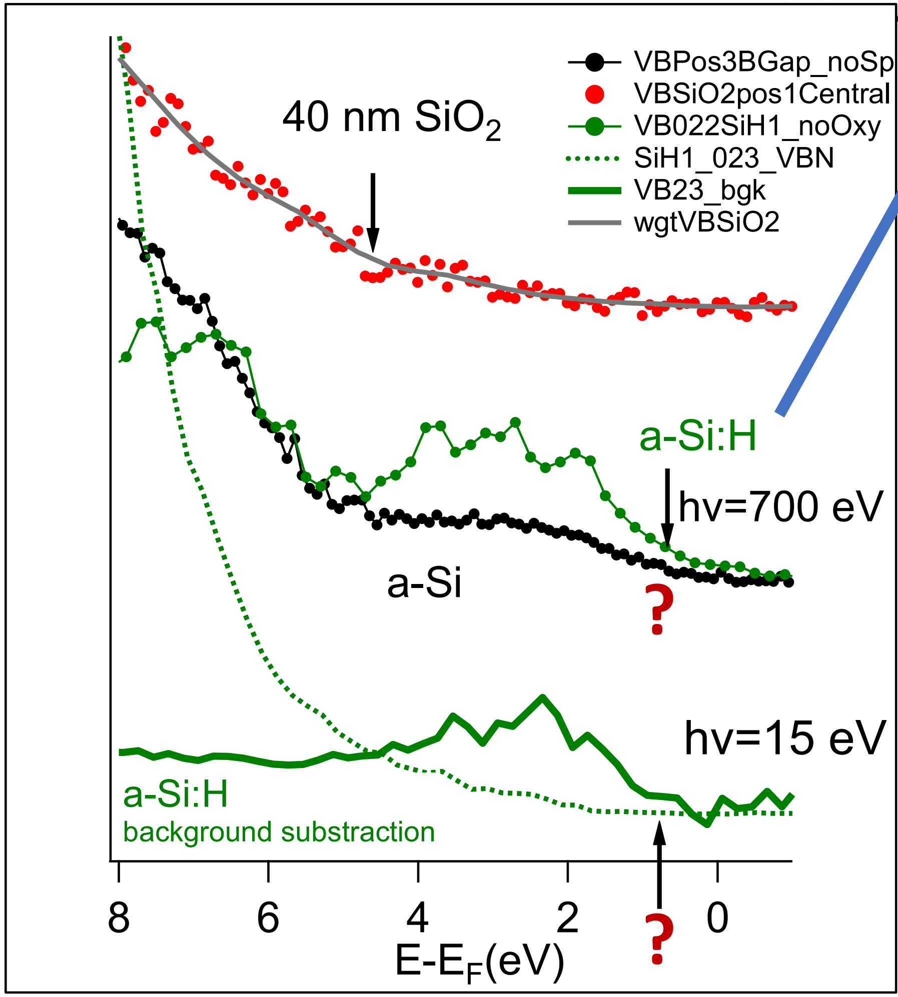
Irradiation increases the amorphous silicon

How are Urbach tail/Localized states?

Peverini et al. 2022 : a-Si:H on Silicon

Standard Valence band photoemission hv>20 eV





Why CFSYS Valence band photoemission at low photon energy < 8eV

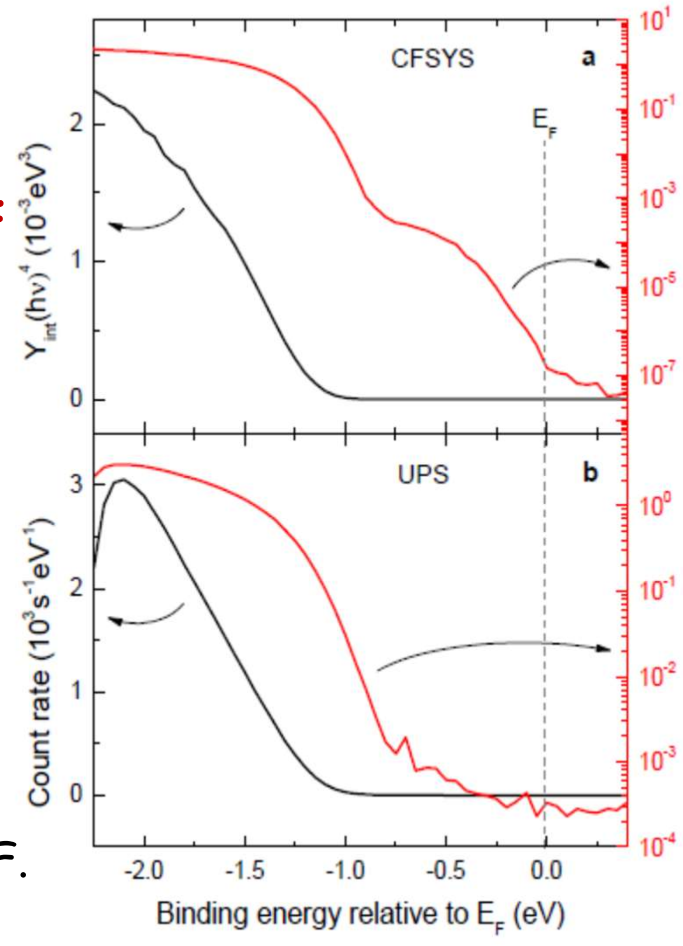
CFSYS measures and quantifies

-energy position of gap states

-density of active defect states in band gap

in a-Si:H down to 10^{15} states/cm^3

M. Sebastiani, L.D. Gaspare, G. Capellini, C. Bittencourt, F. Evangelisti, Phys. Rev. Lett.(1995)

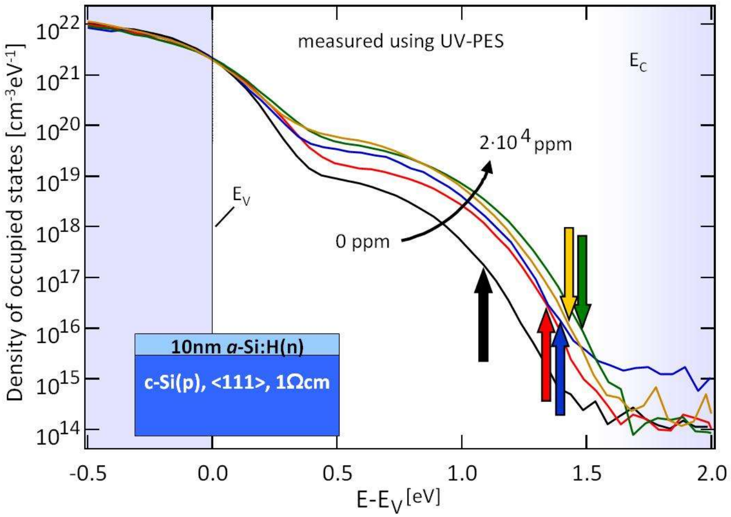


L. Korte group, Berlin

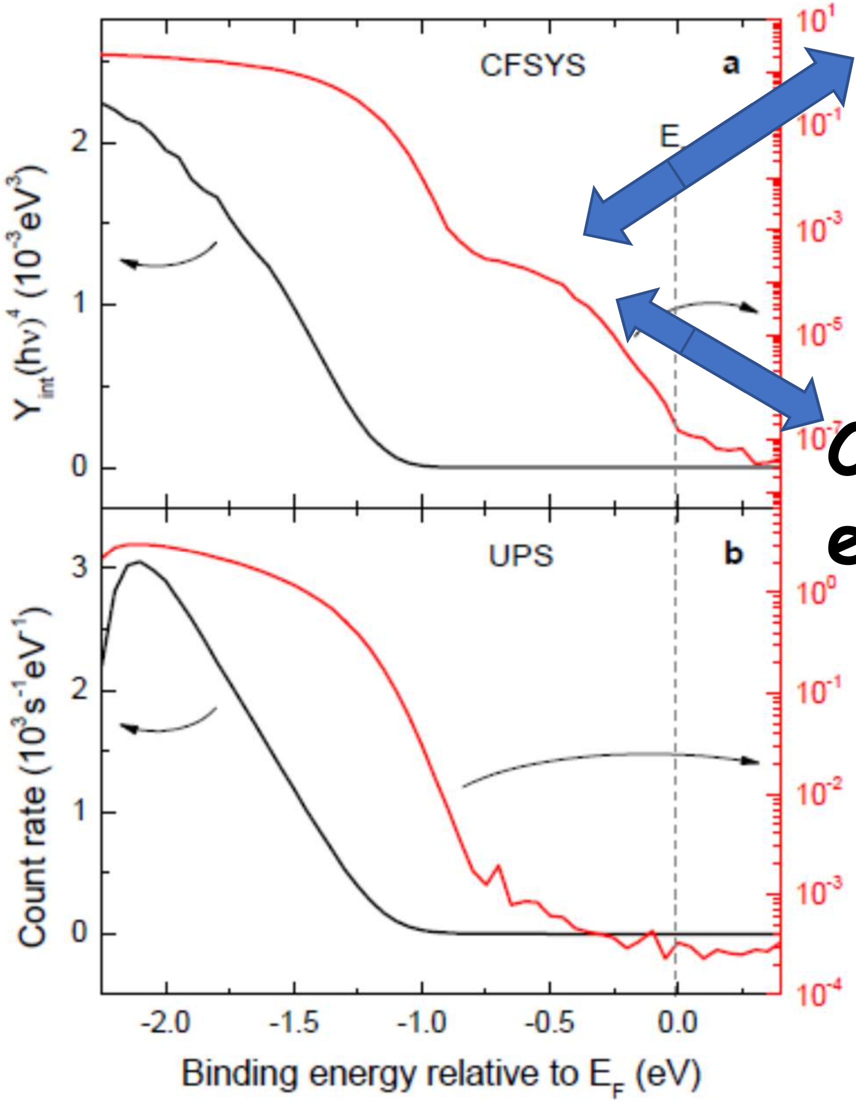
Control Defect Density in the gap

CFSYS distinguishes between **tail, shallow and deep gap states**

crucial for optimization of a-Si:H devices before and after irradiation



CFSYS example a Si:H Density of Defects in the gap
L. Korte group , Berlin



I_{leak}

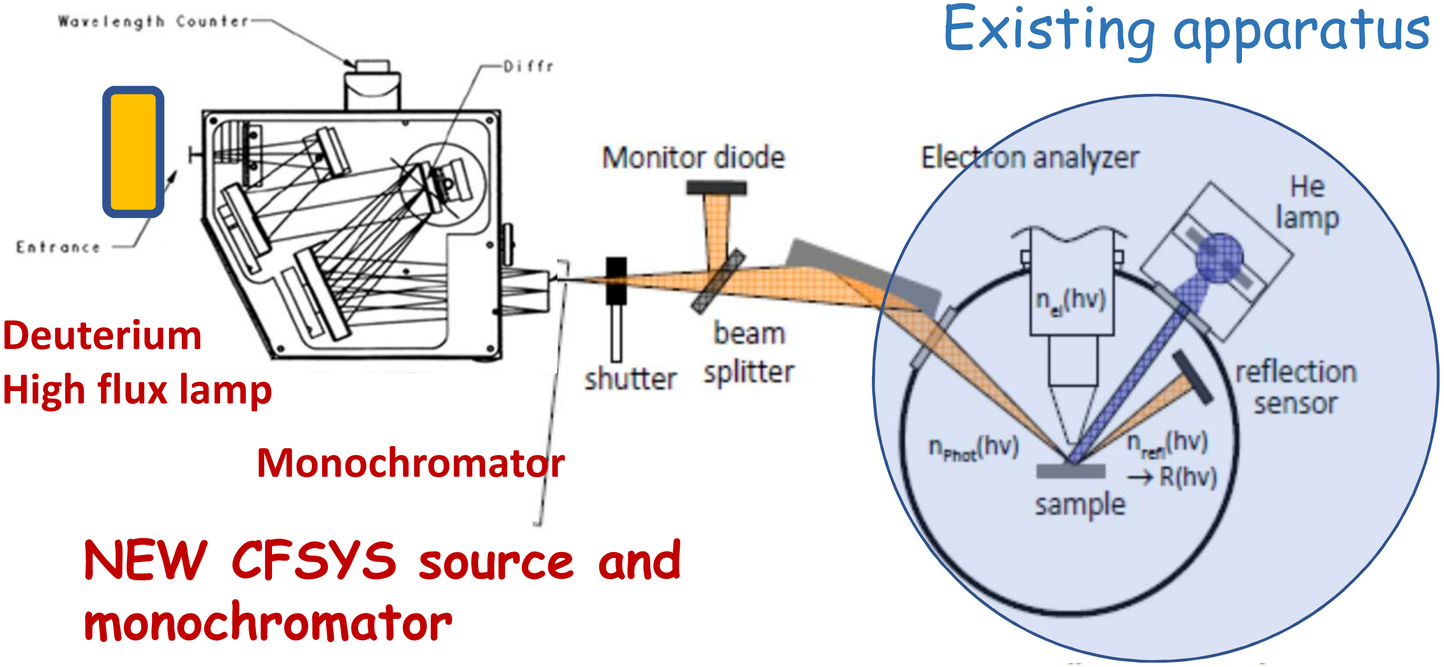
Charge Collection efficiency

Radiation Sensitivity [nA/cGy]

Implementation of the existing UHV photoemission system Perugia

- **CFSYS** constant final state yield spectroscopy: **Ek photoemitted electrons vs photon energy.**
- **System controlled by a dedicated computer and electronics**
- **New acquisition program for the remote control selection of the monochromator photon energy**

Existing apparatus



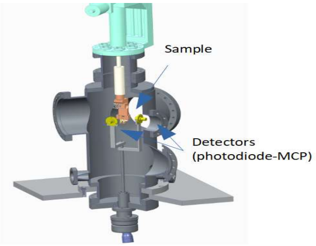
NEW CFSYS source and monochromator

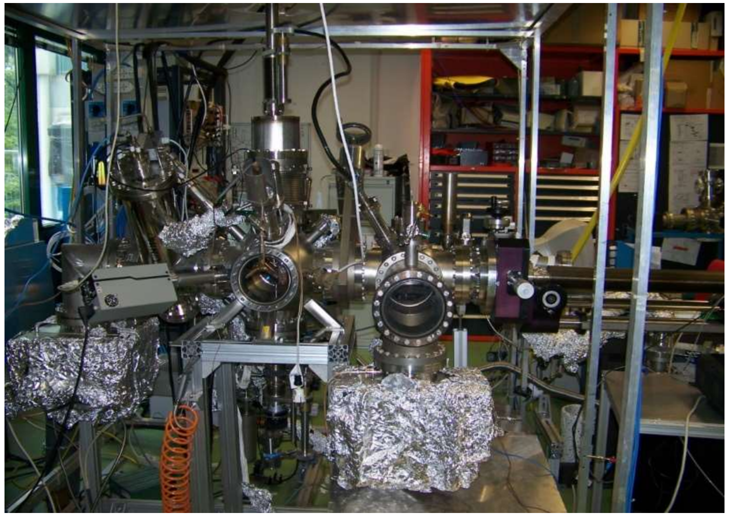
Ultra High Vacuum Chamber
P<3*10e-10 mbar

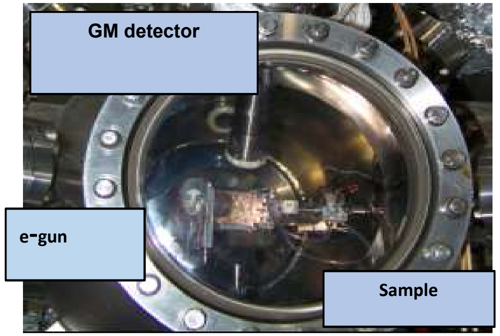
Sample on a UHV manipulator

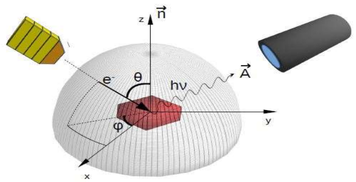
Laboratorio Spettroscopie Perugia

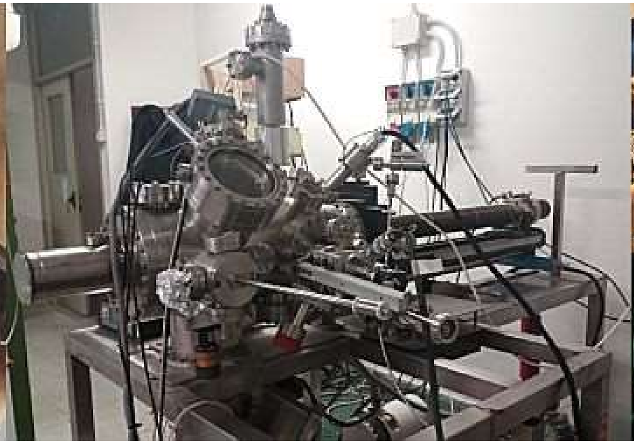
SIPE
nanoStructures
Inverse
Photoemission
and Excitation
dynamic

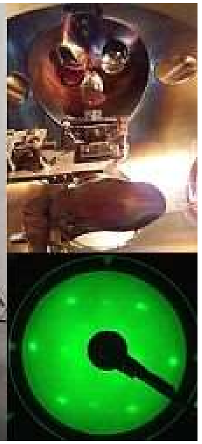












***ACROSS* -**
Advanced
ChambeR fOr
Surface Studies

CNR-IOM at the UniPG Physics Department.
2 Ultra High Vacuum UHV systems for photoemission and inverse photoemission spectroscopies.

Each UHV system equipped with a UHV 4-axis manipulator with a variable temperature sample holder (100-1000K), an electron energy analyser for UPS measurements and a standard surface science preparations tools (LEED, ion sputtering).

Time schedule CFSYS Perugia
Mounting and commissioning

Monochromator arrival,	January	
first tests	January	February
Support design		
Mounting at the UHV chamber	February	April
Optics and spot onto the sample test		
CMA commissioning	February-April	
Update Acquisition code	April	June
CFSYS Spectrum	May	August

4) Sensor characterization: Points to be addressed:

→ **sensitivity:**

- depends on contact type? How?
- depends on surface, volume, thickness, shape?
- depends on bias? And how S/N depends on bias?

→ **stability:**

- how much time to stabilize from biasing?
- priming will make better the device behaviour?

Samples

Samples	Goal	Principal Techniques	Not
100nm-1μm a-Si:H on c-Si	Check Density of States (DOS) in the gap, Energy level alignment and stoichiometry	CFSYS PG, HR XPS, XAS done μRaman	1 μm è ind
From 10nm, 20nm a 1μm a-Si:H on Kapton	Confronto con i layer depositati su silicio cristallino	CFSYS PG HR XPS μRaman	Minimum thickness
From 10nm, 20nm a 1μm a-Si:H on c-Si	Check Density of States (DOS) in the gap and at the interface (if possible), Energy level alignment and stoichiometry	CFSYS PG HR XPS μRaman	1 μm è indicativo
Nude Kapton and metal layer/kapton	Substrate characterization	AFM HR XPS μRaman	Roughness, Metal/Kapton interface

Selected devices even after irradiation will be measured after this schedule

HR XPS to be perfomed at LKO Nova Gorica

People involved

Perugia

- Francesca Peverini PhD student
- Maddalena Pedio associated INFN
- Nicola Zema associated INFN

Collaboration with

- Stefano Cristiani Technician CNR-IOM
- Alberto Verdini CNR-IOM
- Silvia Caponi CNR-IOM PG μRaman

Trieste/NG

- Roberto Gotter CNR-IOM
- Technical services CNR-IOM

Federica Bondino,
Igor Pis, Elena Magnano BACH beamline 2024

Barbara Ressel Nova Gorica (SLO)

Thanks you for your attention

HASPIDE 2023, WP1, spectroscopies applied to a-Si:H devices at Perugia

CFSYS is a variant of conventional photoelectron spectroscopy (source He lamp, 21.2 eV) with near-UV light excitation ‘constant final state yield spectroscopy’ CFSYS (source: Deuterium lamp coupled with monochromator, photons within 3-6eV) ref [1] applied to the valence band maximum region. Using this technique, the position of the surface Fermi level E_F is obtained and the density of recombination active defect states in the amorphous hydrogenated silicon (a-Si:H) band gap down to 10^{15} states/cm^3 can be detected and quantified, ref [2].

Low-energy photoelectron spectroscopy measurements can be used to obtain directly the energy position of gap states. This technique allows for distinguishing between tail, shallow, and deep gap states, a crucial information for the optimization of a-Si:H devices, before and after irradiation at high dose.

Part of the experimental set-up needed for CFSYS measurements has being bought and/or ordered by CNR. The Ultra High Vacuum experimental chamber mounts a Cylindrical Mirror Analyser in commissioning. Feasibility test by conventional photoemission on a-Si:H films and devices has been performed recently, in other CNR laboratories.

1 M. Sebastiani, L.D. Gaspare, G. Capellini, C. Bittencourt, F. Evangelisti, Phys. Rev. Lett. 75 (1995) 3352
2 L. Korte & M. Schmidt, J. Non-Cryst. Sol. **354** (2008) 2138-43

Xe/Deuterium lamp, monochromator, CFSYS

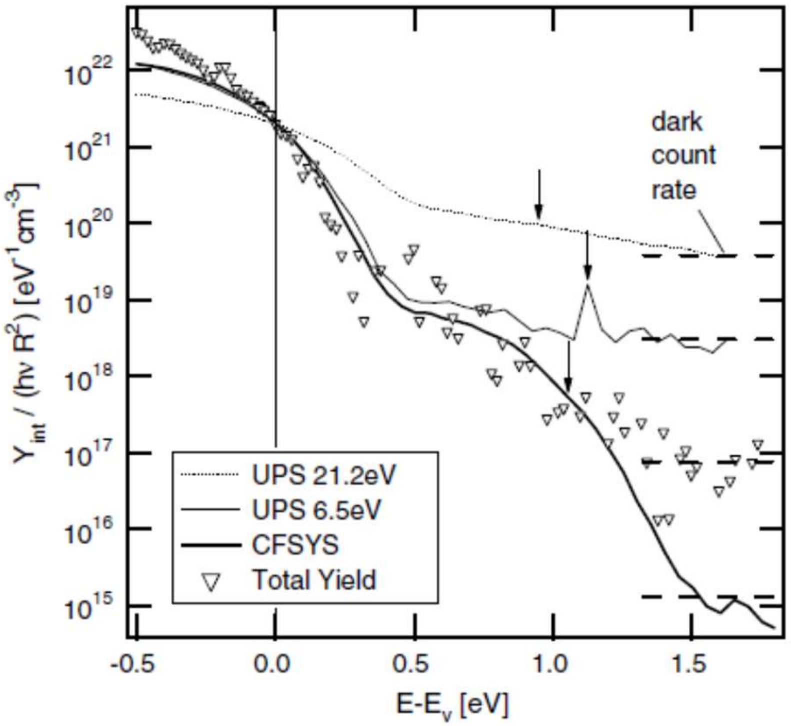
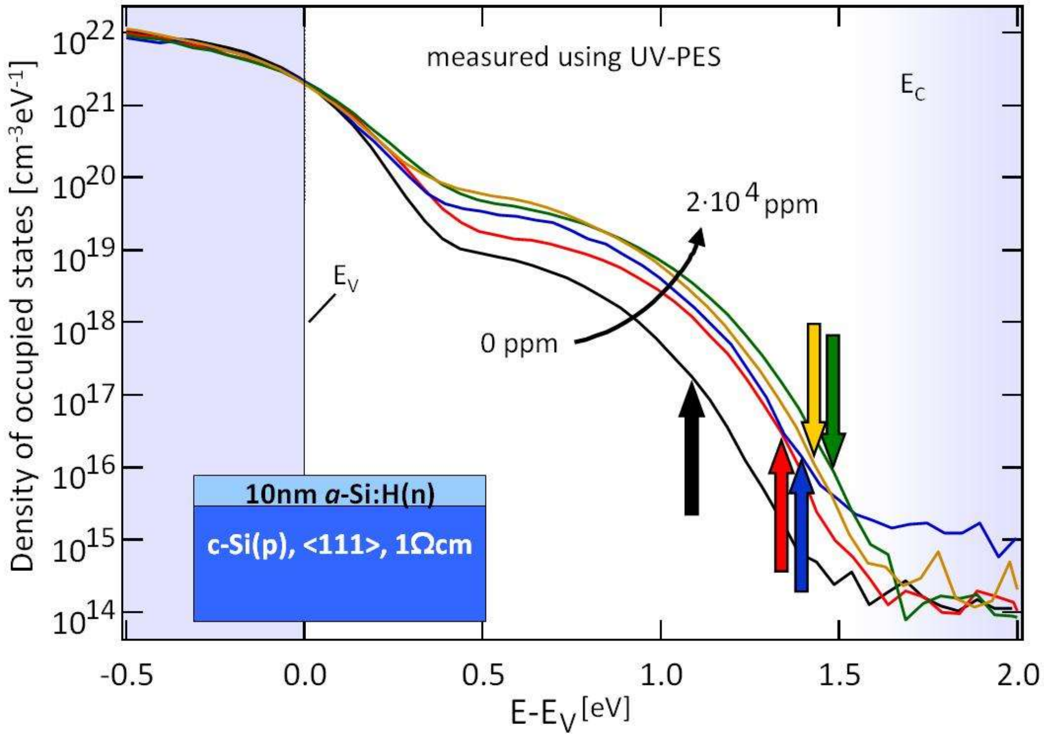


Fig. 1. Comparison of the sensitivity of CFSYS measurements with standard UPS ($h\nu = 21.2$ eV), with UPS measured at lower excitation energy (6.5 eV), and with total yield measurements. The abscissa has its origin at the valence band edge, arrows mark E_F, except for total yield. The dark count rates (noise levels) are also marked by the dashed lines. The sample is a 10 nm thin intrinsic a-Si:H layer.



L. Korte, M. Schmidt “Investigation of gap states in phosphorous-doped ultra-thin a-Si:H by near-UV photoelectron spectroscopy”
Journal of Non-Crystalline Solids 354 (2008) 2138–2143

CFSYS

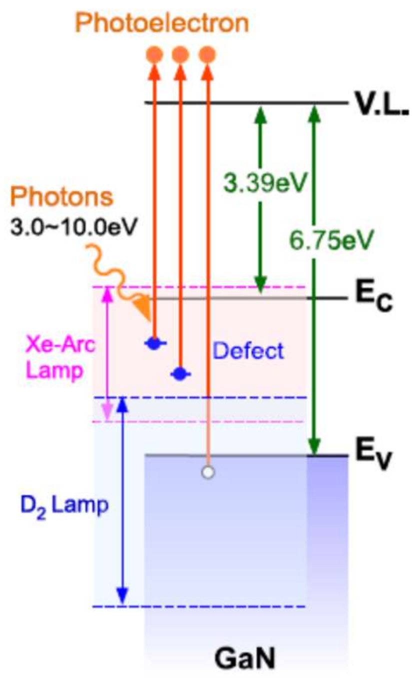


Fig. 5. (Color online) Energy band diagram of wet-cleaned epitaxial GaN. Energy region of PYS measurements shown in Fig. 6 is also shown in this energy band diagram.

Akio Ohta *et al* 2018 *Jpn. J. Appl. Phys.* **57** 06KA08