# Quantitative study of structural distortions in the interface region of solar cells, using implanted positive muons

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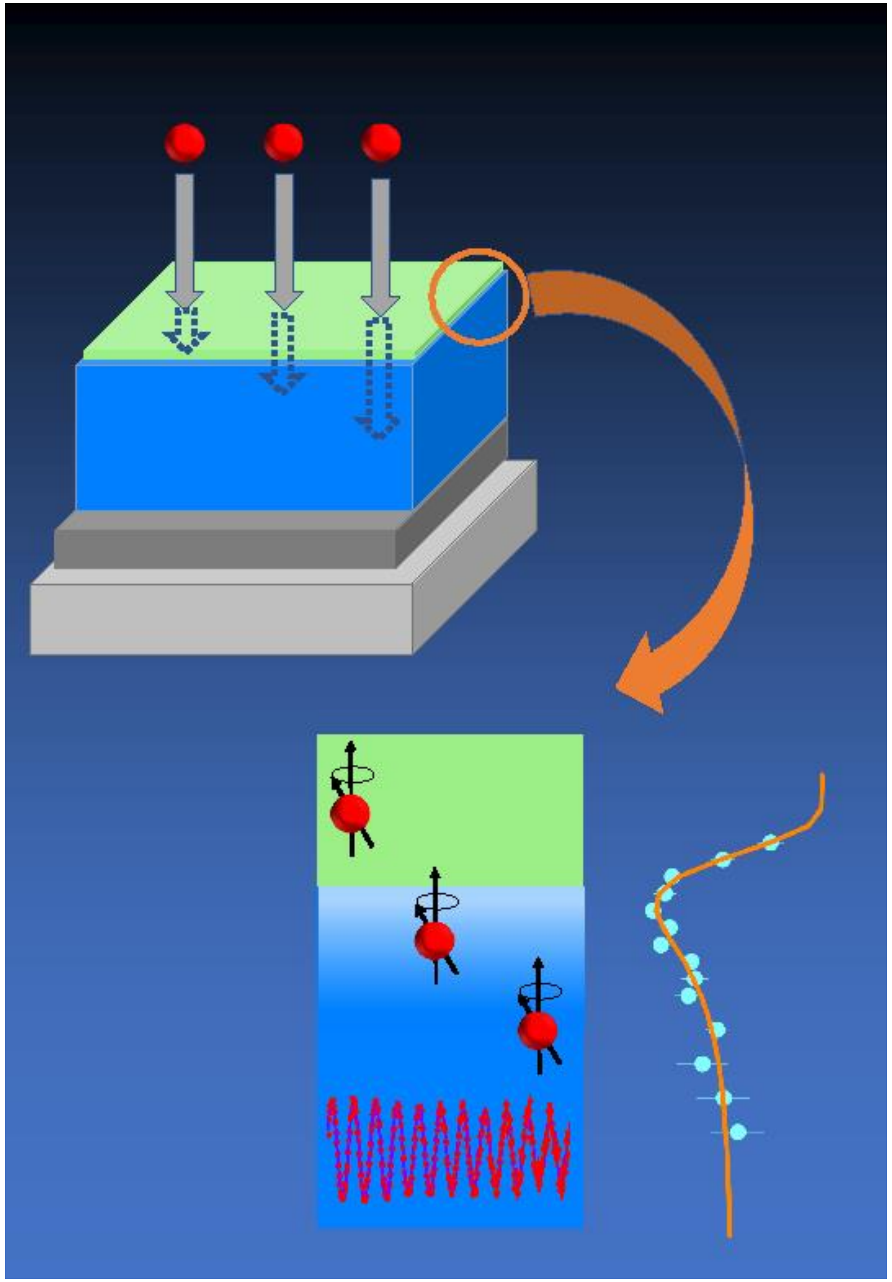
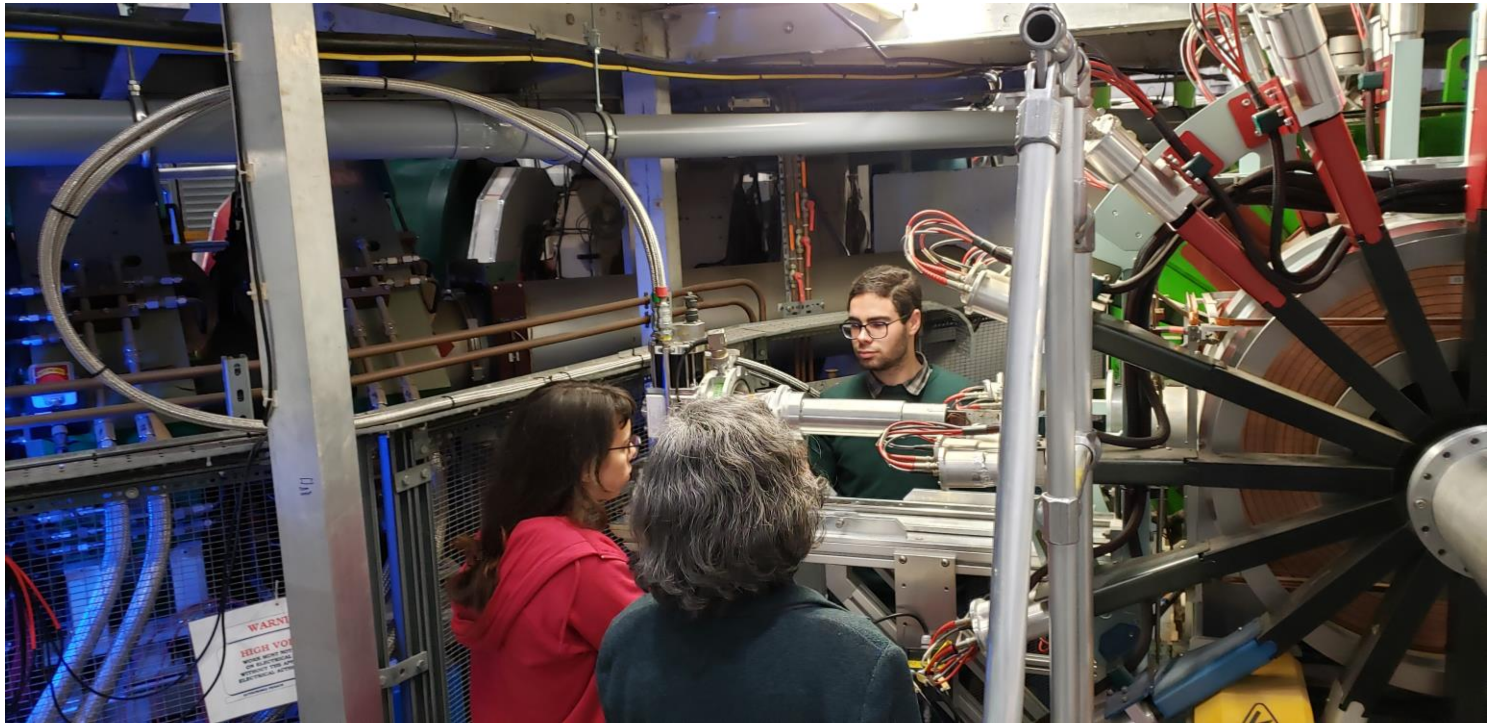
**Low Energy Muons team, PSI**: Maria Martins, Thomas Prokscha, Zaher Salman

Coffee with Physics
23 November,2022

*Coffee first, than physics*



# Coimbra Group

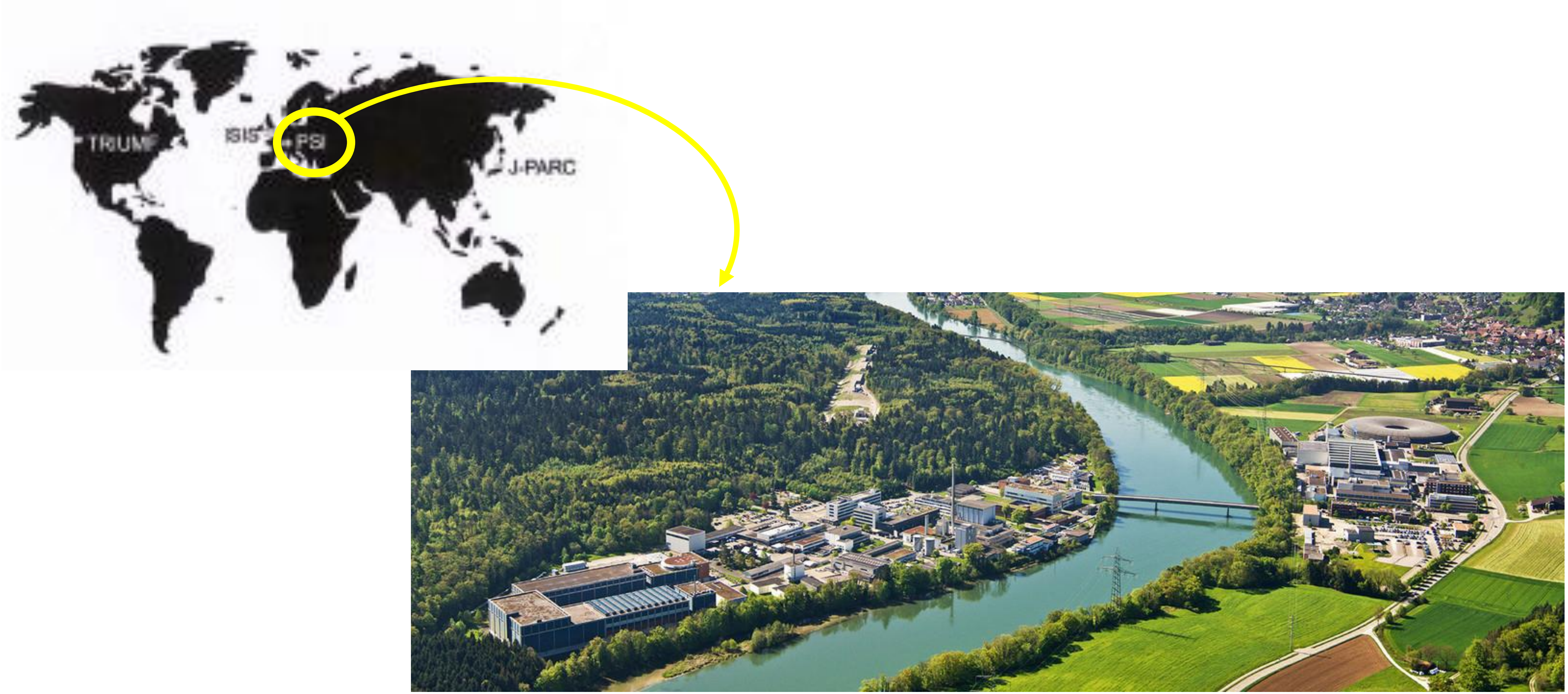


# INL : The Nanofabrication for Optoelectronics Application (NOA) group in Braga (leader: Pedro Salomé)


Marco

Xavier

# Paul Scherrer Institut – PSI - Switzerland



# Muon production

- Producing pions by colliding protons into a target of light elements (carbon or beryllium):

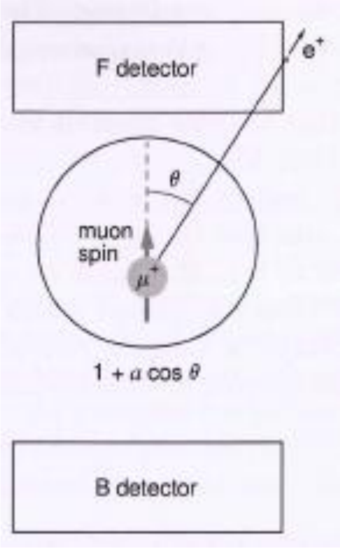
$$p + p \rightarrow p + n + \pi^+$$

- Pions decaying at rest produce 100% polarized muons

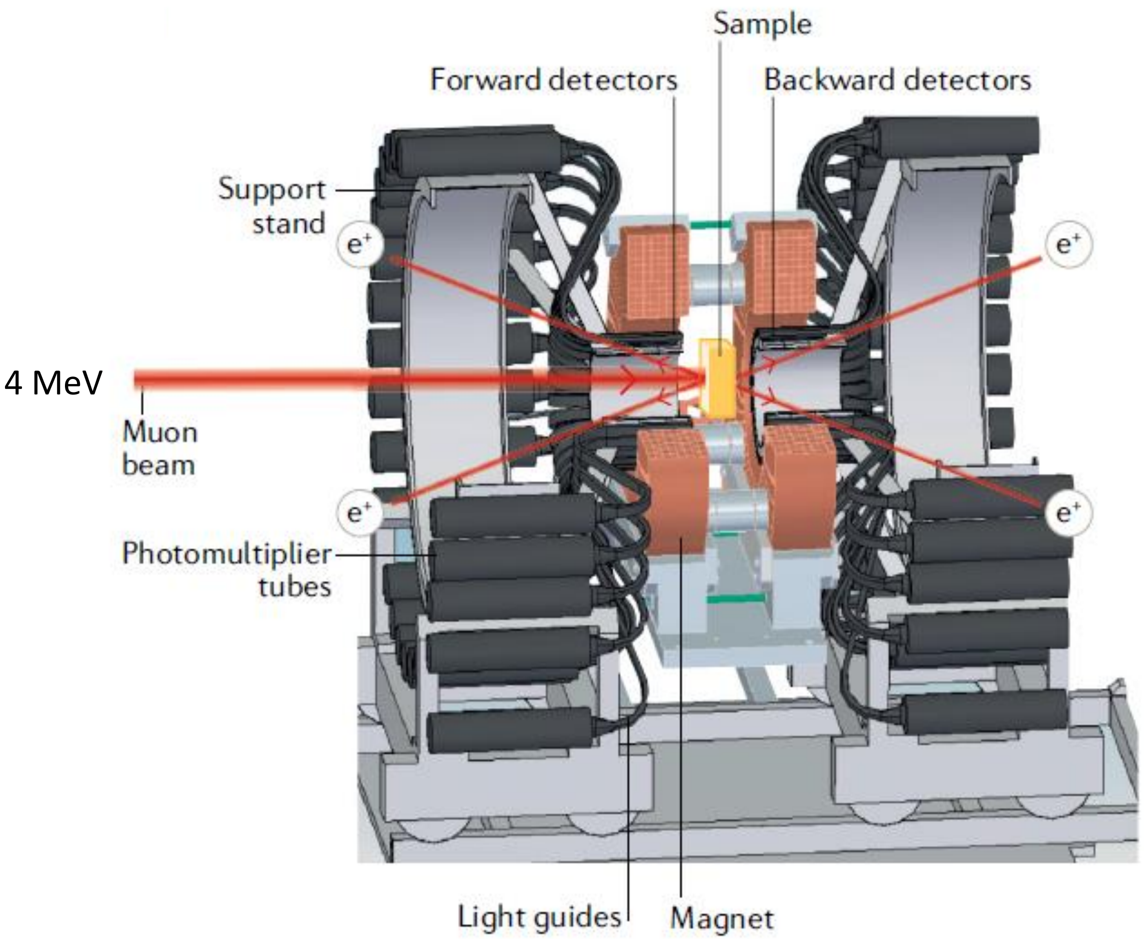
$$\pi^+ \rightarrow \mu^+ + \nu_\mu$$

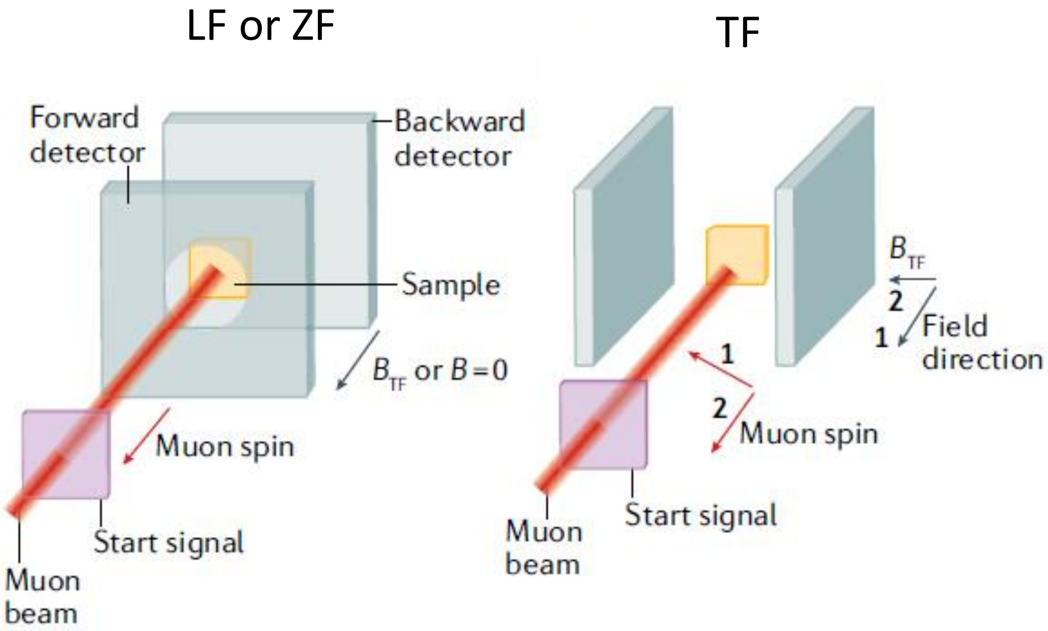
- Muons decay with an average lifetime of 2 $\mu$s ; the positron is emitted preferentially in the spin direction.
- The difference between counts in Forward and Backward detectors leads to experimental Asymmetry of the emitted positrons.
- The experimental Asymmetry yields the muon polarization at the moment of decay.

$$\mu^+ \rightarrow e^+ + \bar{\nu}_\mu + \nu_e$$



# Schematic of a typical μSR spectrometer



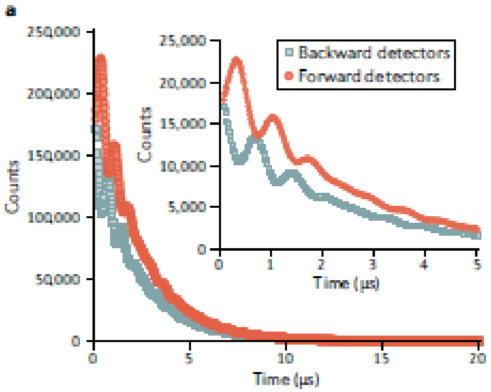


Positrons generated by decay of muons at rest in a sample are measured using counters placed in front of and behind the sample.

# TF µSR signal of $\mu^+$

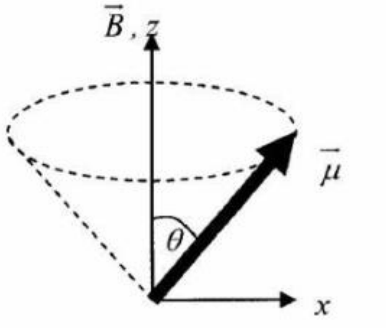
$$N(t) = N_0 \exp\left(-\frac{t}{\tau_\mu}\right)(1 + a_0 P_x(t))$$

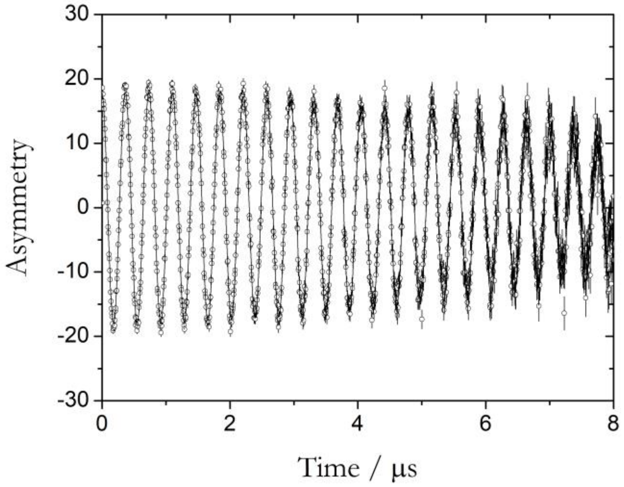
$a_0$ is the empirical maximum; B defines z direction



Muon polarization in x direction:

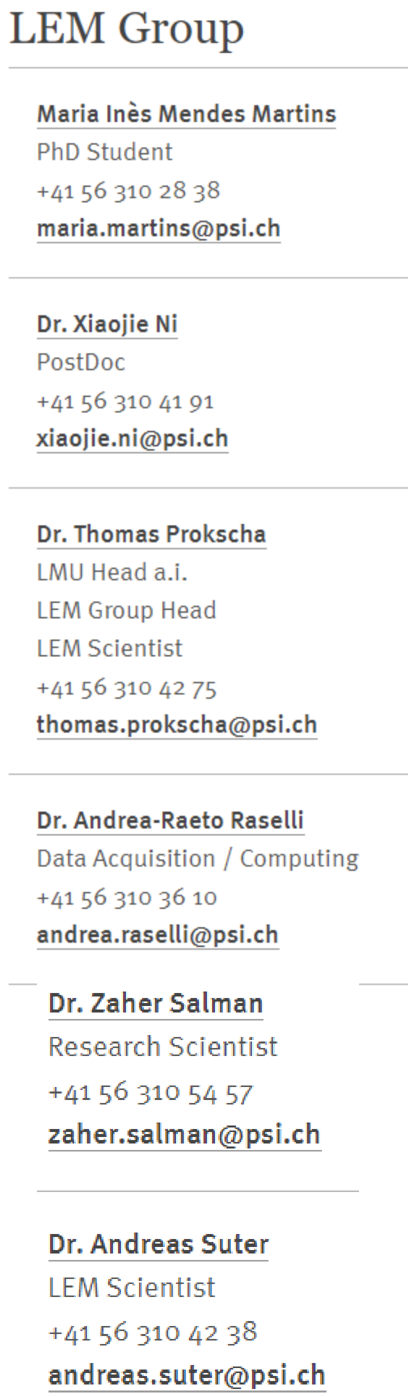
$$P_x(t) = G_x(t)\cos(\gamma_\mu B_{\mathrm{TF}} t)$$





TF µSR signal if the muon remains in a positively charged state (diamagnetic signal).

# Low-Energy Muons Group (LEM)



## LEM Group

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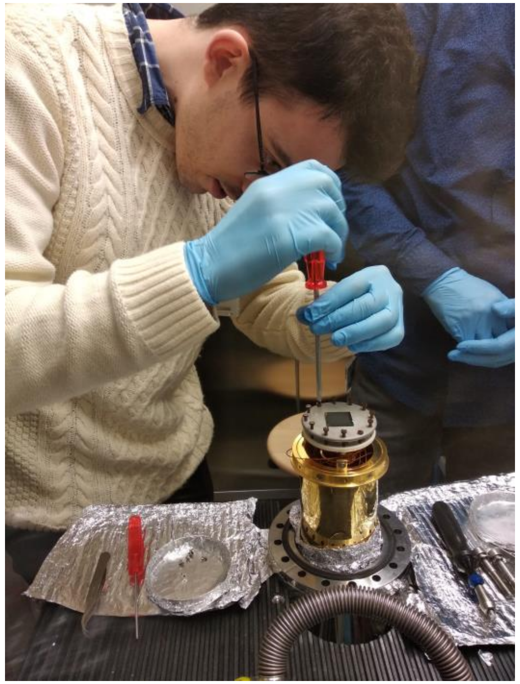
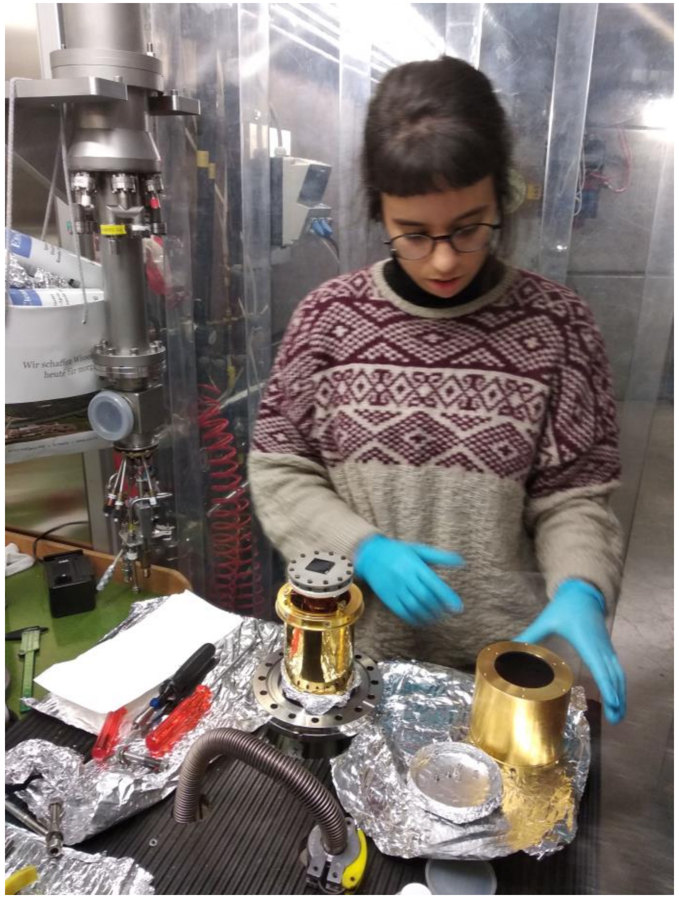
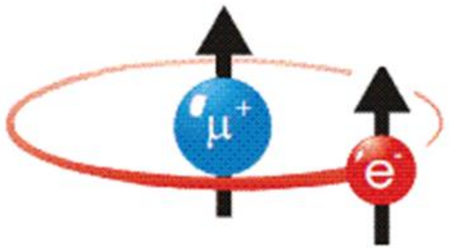
Low energy muons (LE-μ +) with tunable energy between ~0.5 and 30 keV penetrate only to a depth between a few and few hundreds of nm, depending on their energy. Hence they provide the desired non-destructive, non-invasive and microscopic probe for local investigations of properties near surfaces and in thin samples.

# Coimbra and INL at LEM,PSI, Switzerland



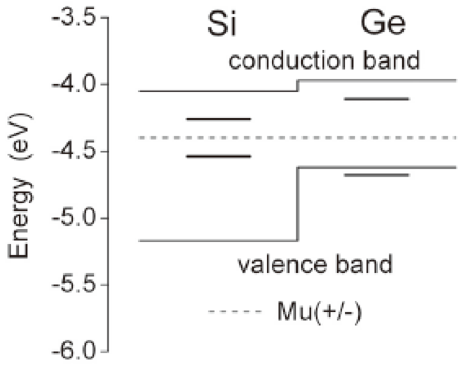


# Muonium as a model for isolated hydrogen in semiconductors and insulators

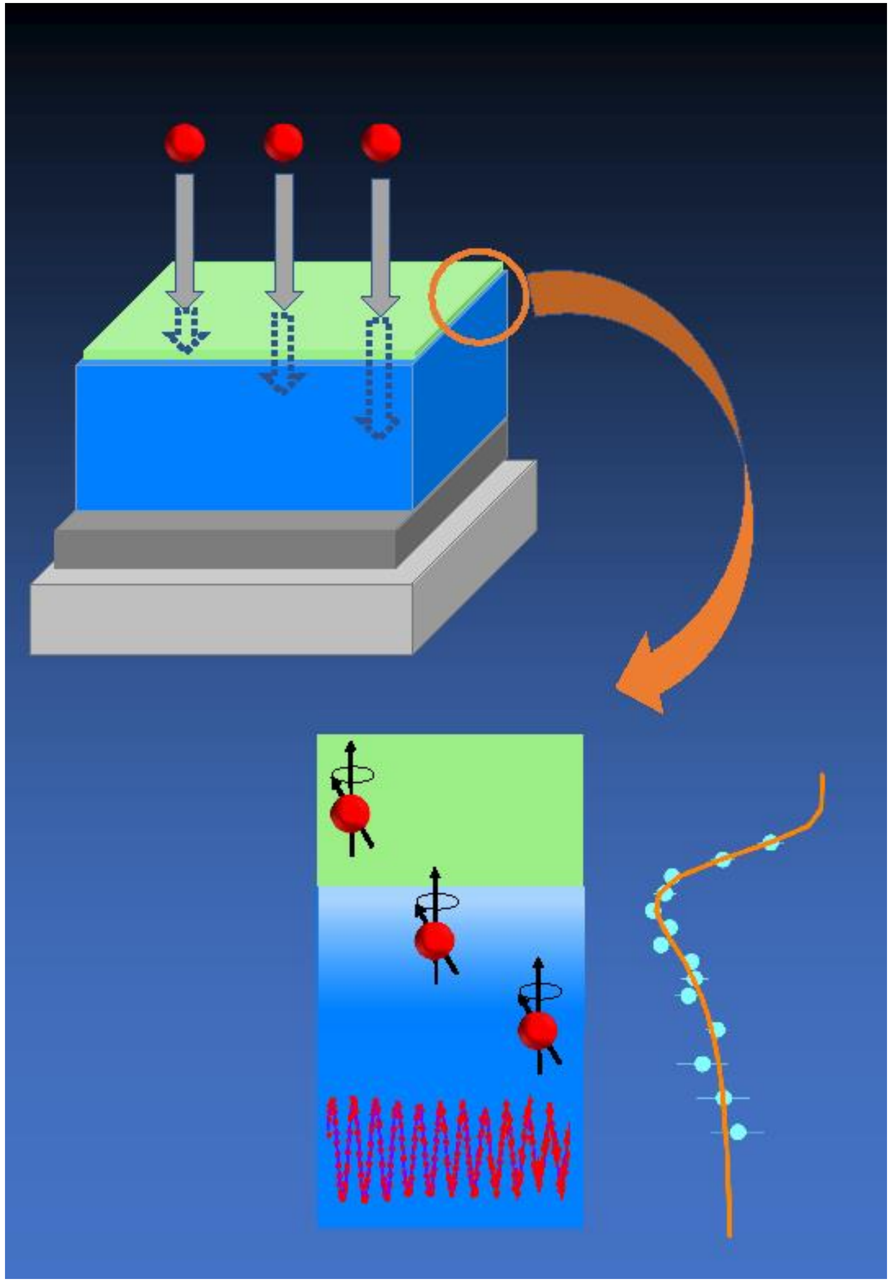


H : Mu = 1 : 1/9

- Behaves as a light isotope of hydrogen
- It is unstable: $\tau_\mu \sim 2.2\ \mu s$
- $Mu^0$, $Mu^+$ $Mu^-$ states and configurations similar to $H^0$, $H^+$ $H^-$ states and configurations
- Introduces donor and acceptor levels in the gap similar to the hydrogen levels
- Most of the existing information of isolated hydrogen in semiconductors was obtained from μSR



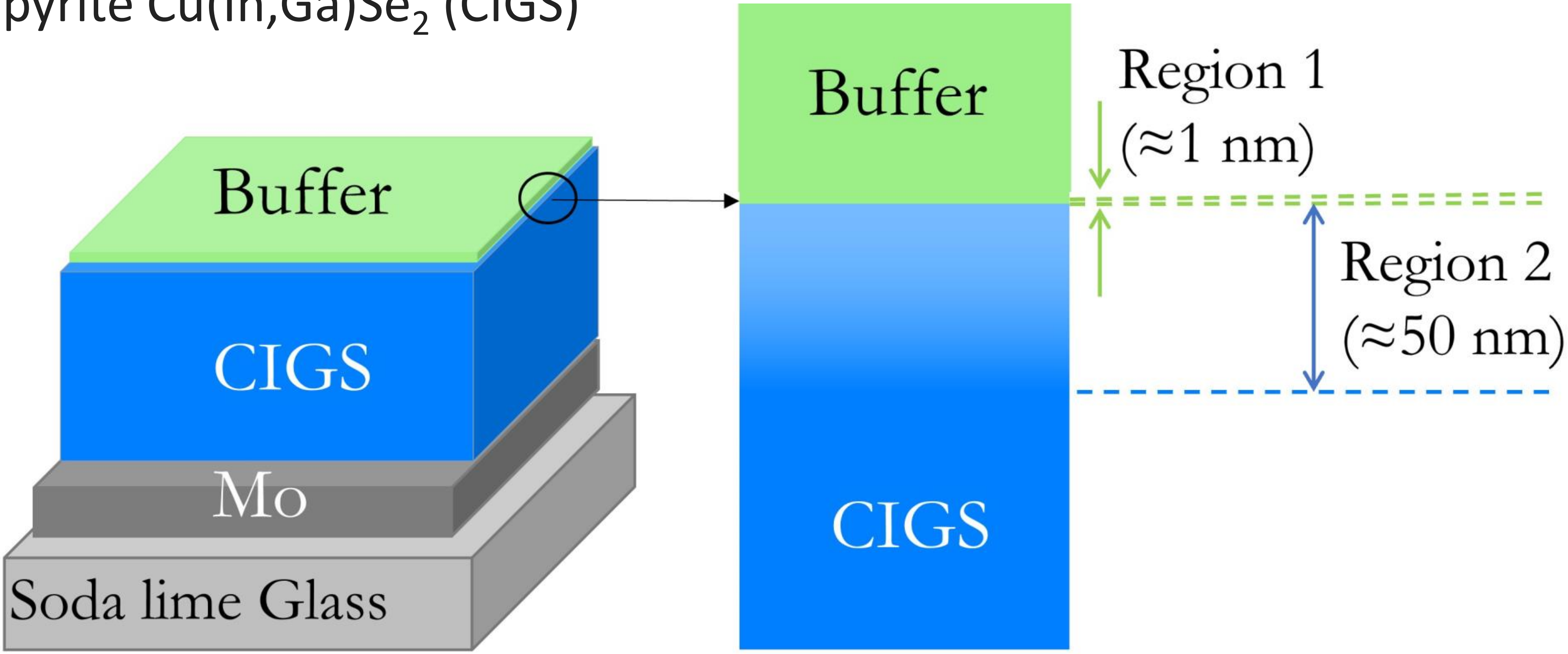
# Positive muons as probes to defect regions in semiconductors



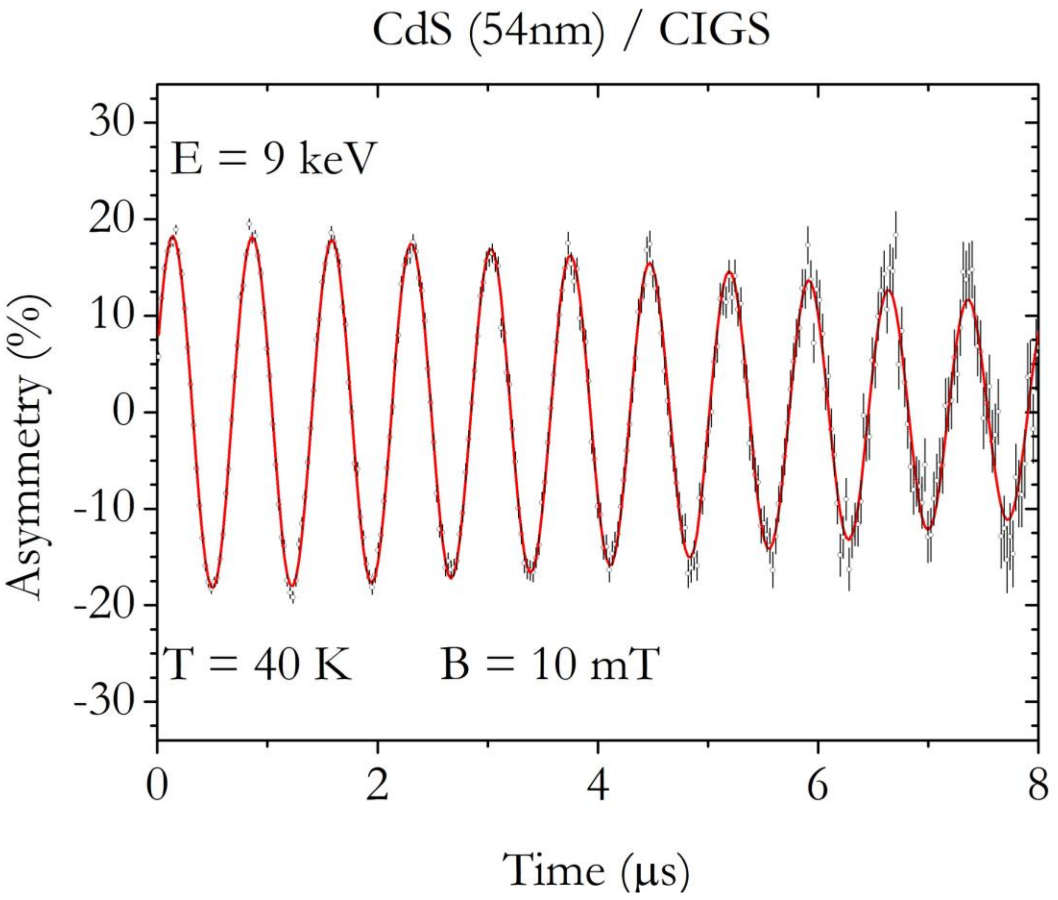
# Samples

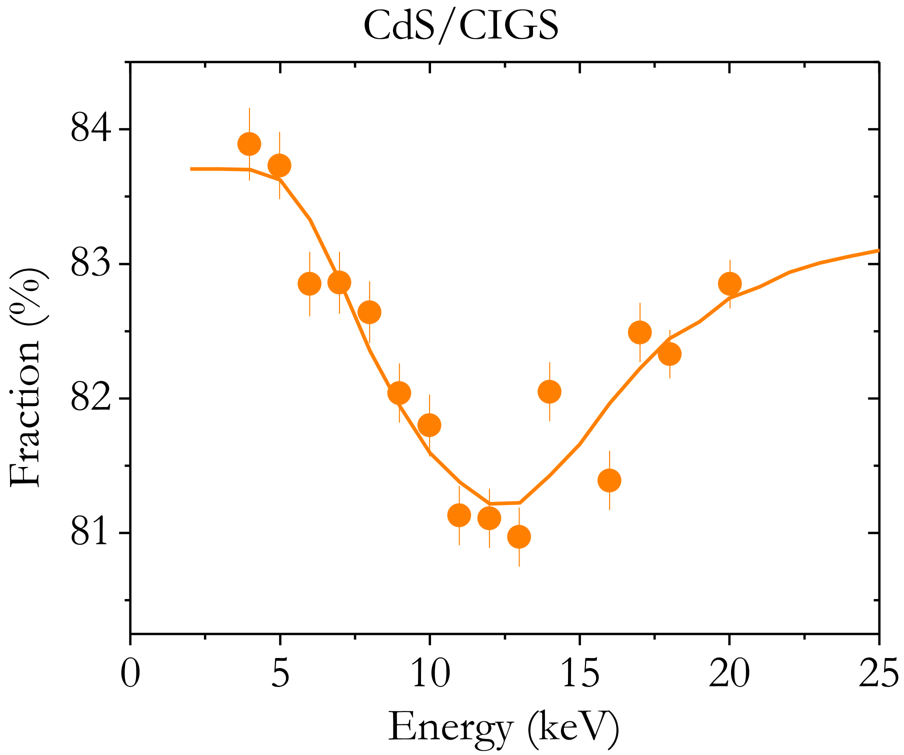
cover layer: CdS, ZnSnO, $Al_2O_3$ and $SiO_2$

Absorber: chalcopyrite $Cu(In,Ga)Se_2$ (CIGS)



# LEM measurements





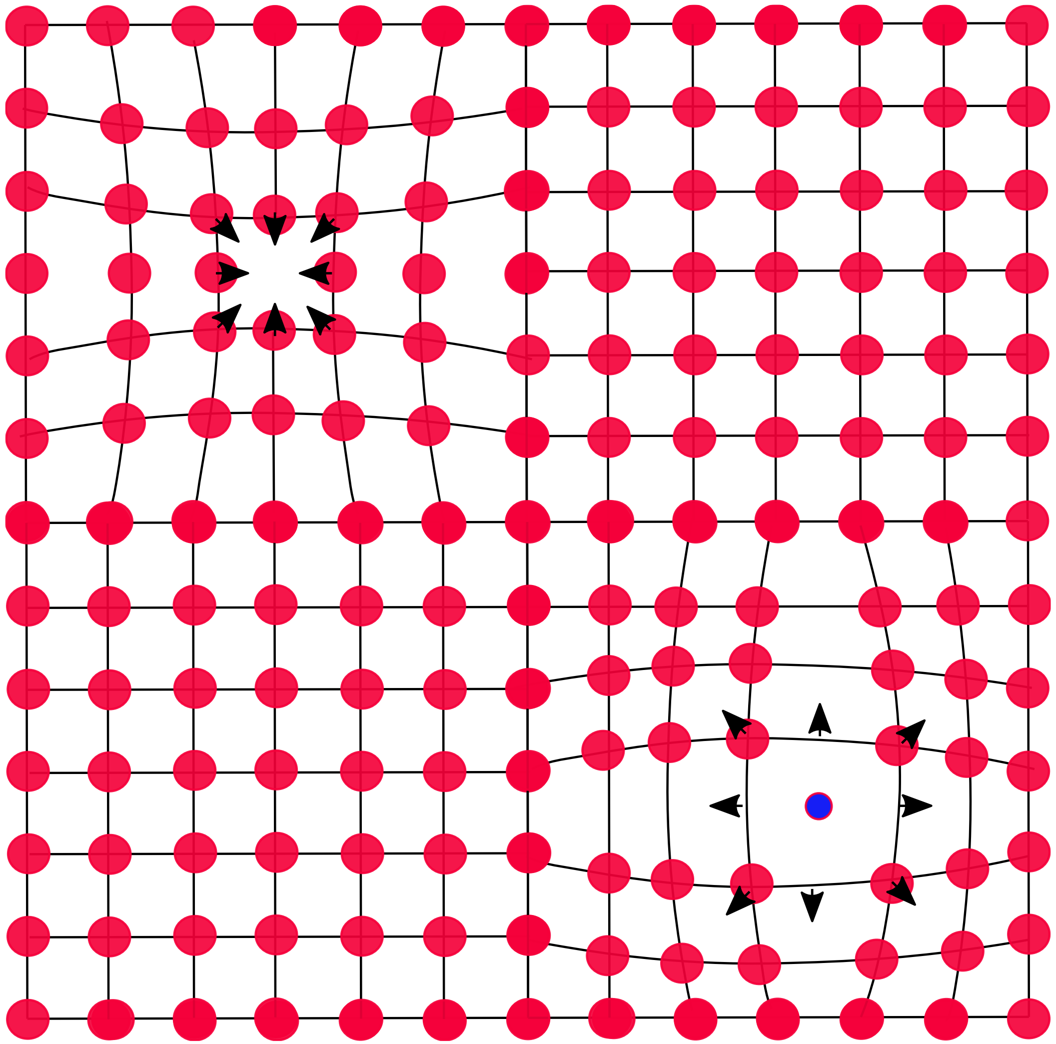
change of diamagnetic fraction with implantation energy

⬇

1.What causes the dip?

2. Where is the dip situated (in CIGS? in the cover layer? in both?) ?

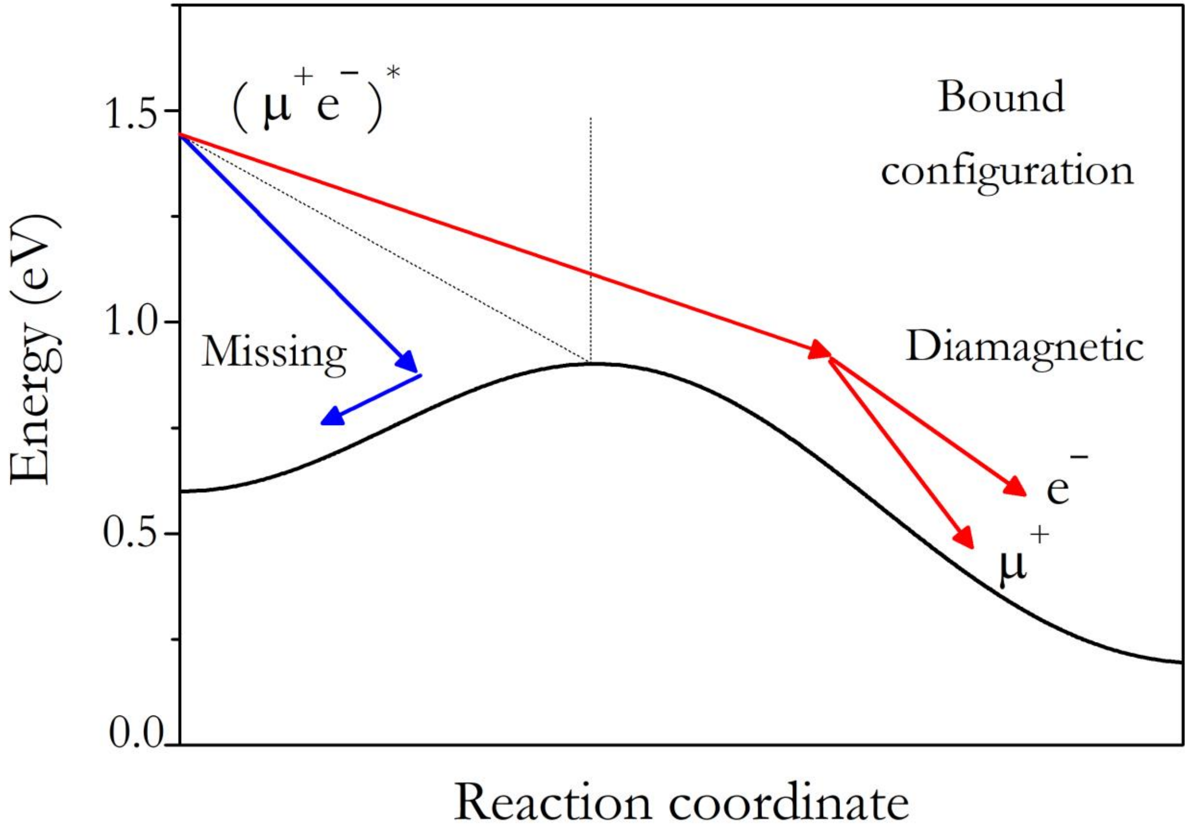
# Defect-induced strain



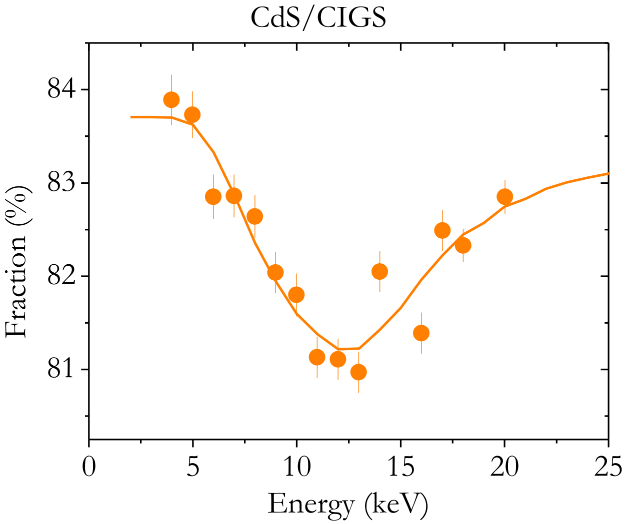
- *The muon probe may be sensing effect of charges at the interface or may be sensing defects.*
- *No evidences for an effect of charges*
- Formation of the diamagnetic configuration requires rearrangement of the lattice around the muon
- It occurs more easily in an ordered lattice than in a distorted lattice.
- Defects (such as vacancies or interstitials) induce a long-range disturbance of the lattice which affects the formation probability of the diamagnetic signal.
- we use the diamagnetic fraction as a measure for defect induced strain.

# The model

- The formation of the diamagnetic bound state requires lattice rearrangement, which can be described as a potential barrier.
- Lattice strain induced by defects increases the barrier height and reduces the formation probability of the bound diamagnetic state.
- That is the origin of the dip in the diamagnetic signal: the muon probe is sensing a defect region.



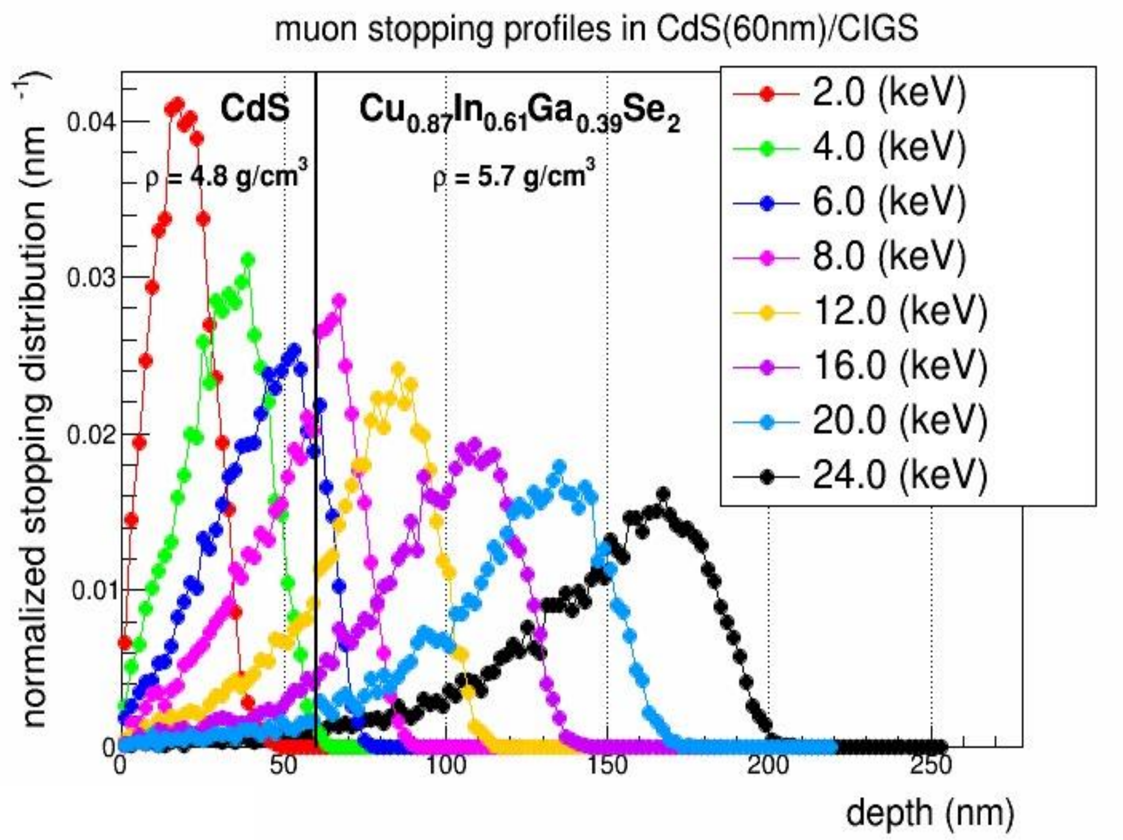
# Where is the dip situated?
# Using resolution information from TRIM.SP



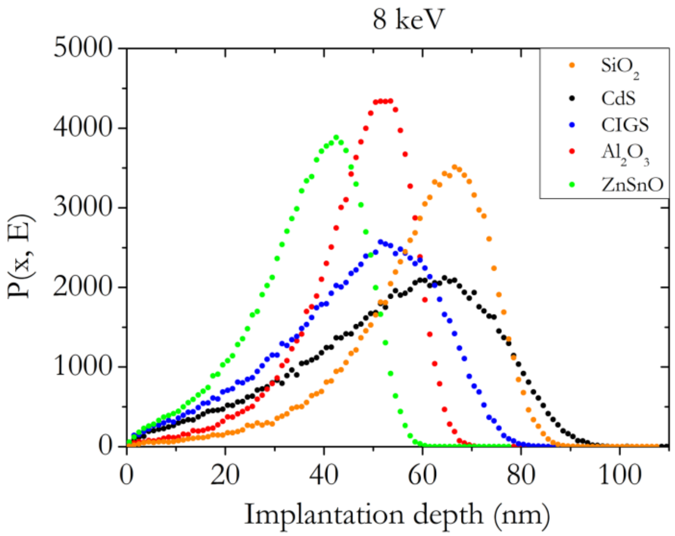
$$f_{\text{dia}}^{\text{exp.}}(E) = \int_0^\infty P(x,E)\, f_{\text{dia}}(x)\, dx$$

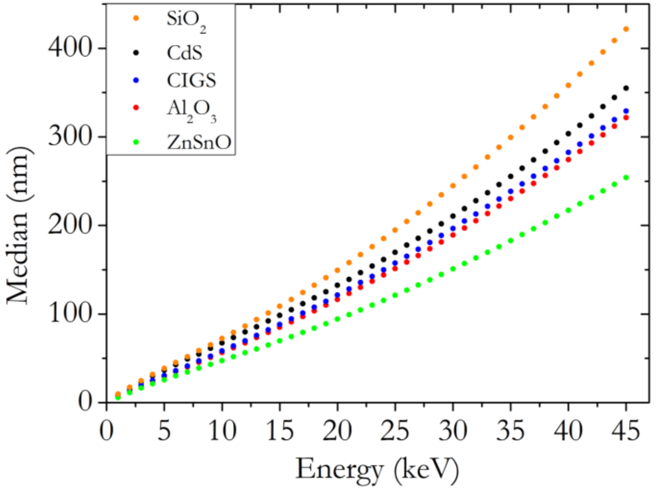
- The experimental $f_{\text{dia}}(E)$ is the result from a convolution of the real $f_{\text{dia}}(x)$ with the normalized stopping distribution P($x$,$E$), obtained by Monte Carlo simulations (TRIM.SP).

The real profile $f_{\text{dia}}(x)$ is washed out because not all muons stop at the same depth.



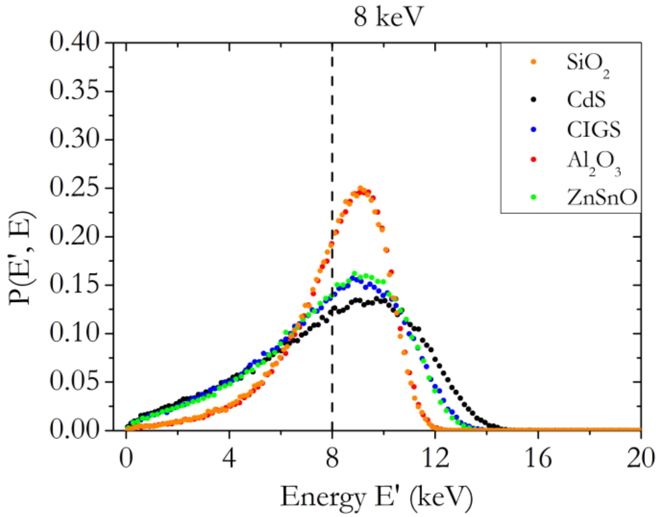
# Unfolding the depth profile





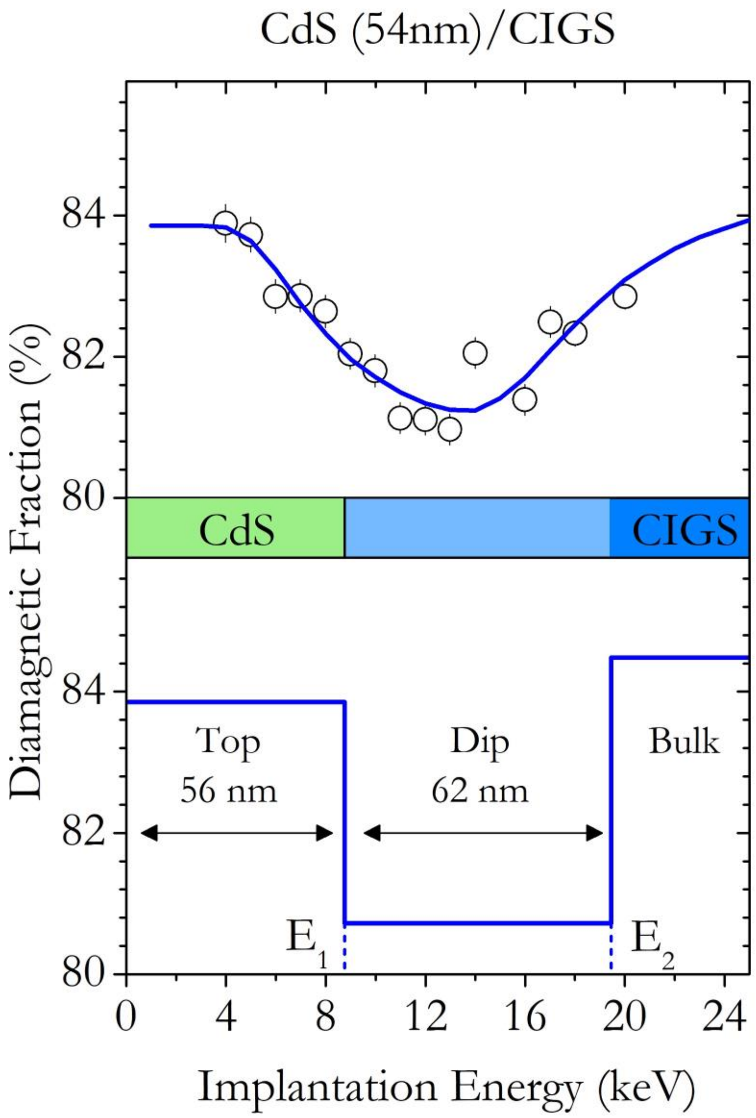
x = f(E')

$$P(E',E)\,\mathrm{d}E' = P(x,E)\,\mathrm{d}x = P(x,E)\frac{\mathrm{d}x}{\mathrm{d}E'}\,\mathrm{d}E'$$



$$f_{\mathrm{dia}}^{\mathrm{exp.}}(E) = \int_0^\infty P(E',E)\, f_{\mathrm{dia}}(E')\, dE'$$

# results



$$f_{\rm dia}^{\rm exp.}(E) = \int_0^\infty P(E', E)\, f_{\rm dia}(E')\, dE'$$

- the trial function for $f_{\rm dia}(E')$ is a simple three step function with 5 adjustable parameters. A fit is performed to obtain the parameters that lead to the best description of the experimental data $f_{\rm dia}^{\rm exp.}(E)$

- the relation x = f(E’) is used to convert $E_1$ and $E_2$-$E_1$ in widths measured in nm.

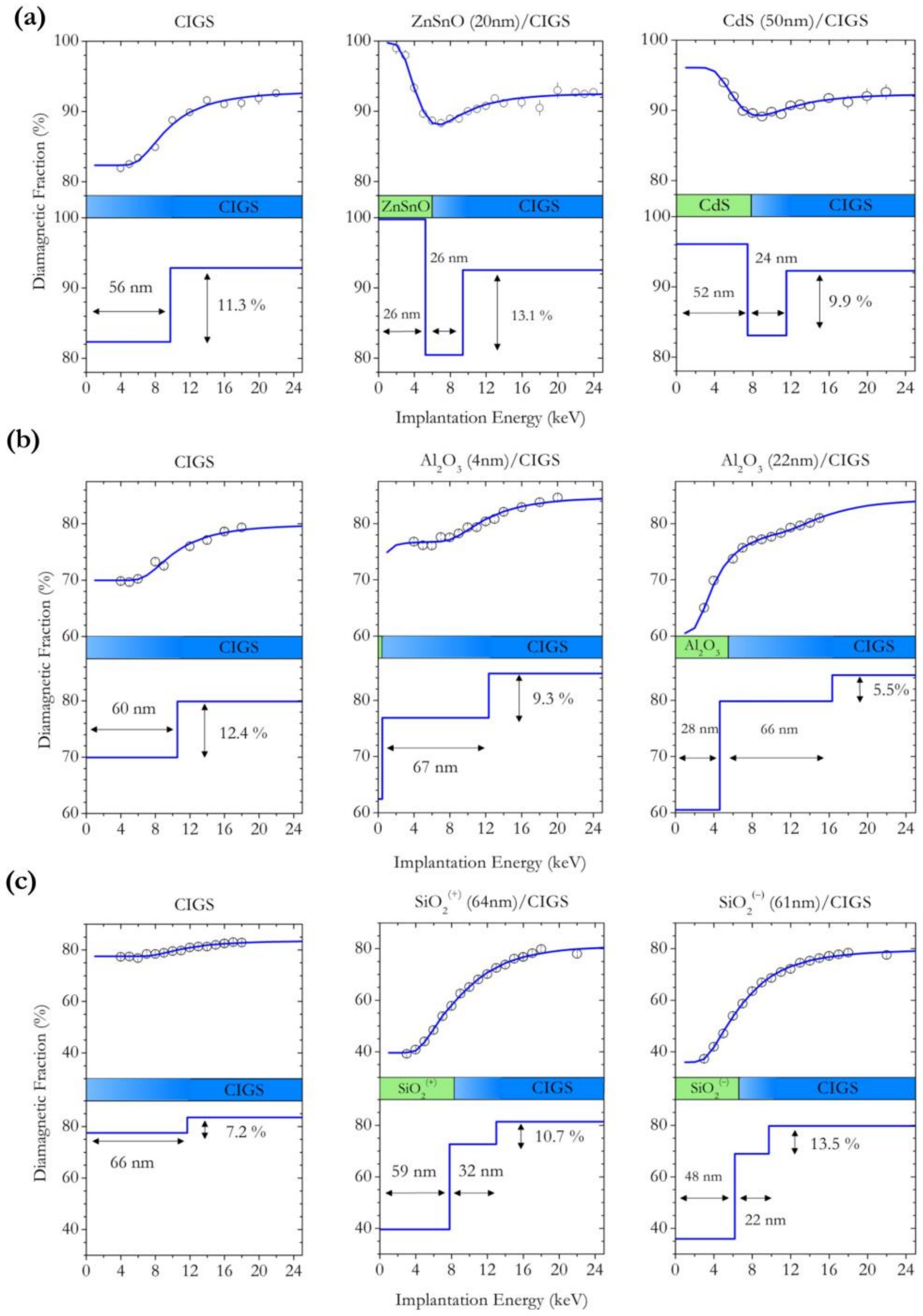
- The best fit to the trial function shows that the lattice is more perturbed **in the near-interface region, on the side of the absorber**, than further inward in the sample.

# Changing cover layers

(a)  : unconvered CIGS and the effect of ZnSnO and CdS covers

(b) : effect of Al2O3 with different widths on the same uncovered CIGS

(c) : effect of SiO2 with different surface charges on the same uncovered CIGS

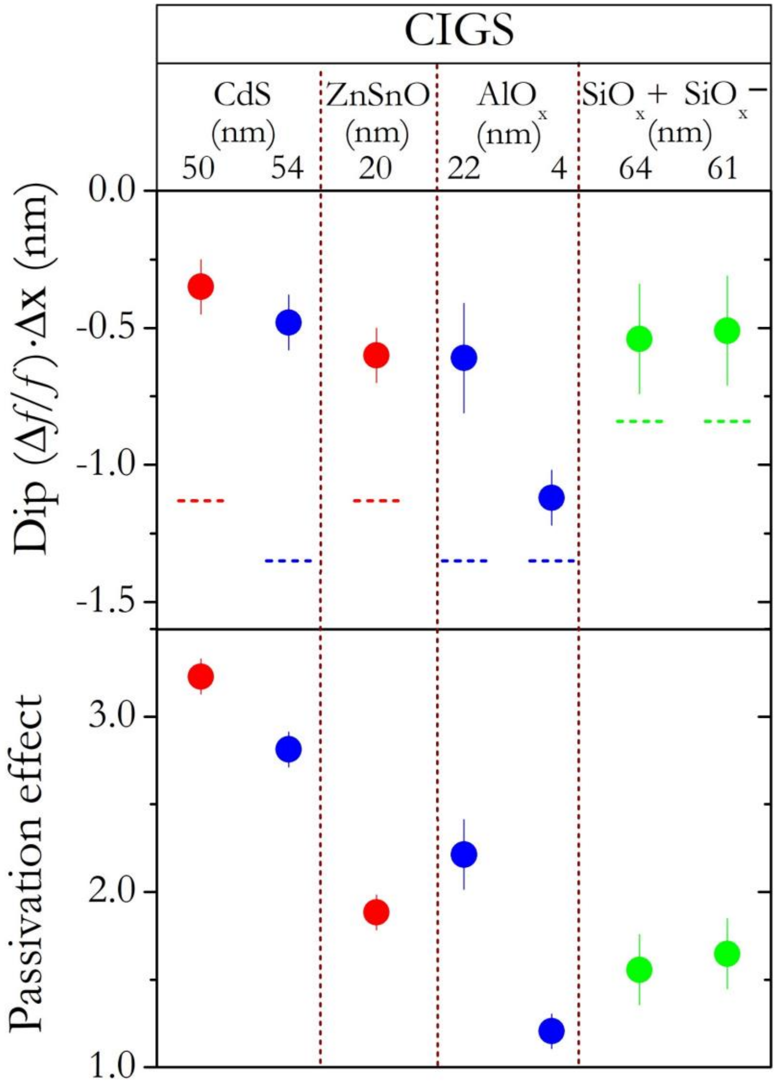


# Measuring passivation of bulk defects near the p-n junction

- the passivation effect near the p-n region is quantified : it is defined as the dip size of the uncovered film divided by the dip size of the covered film.

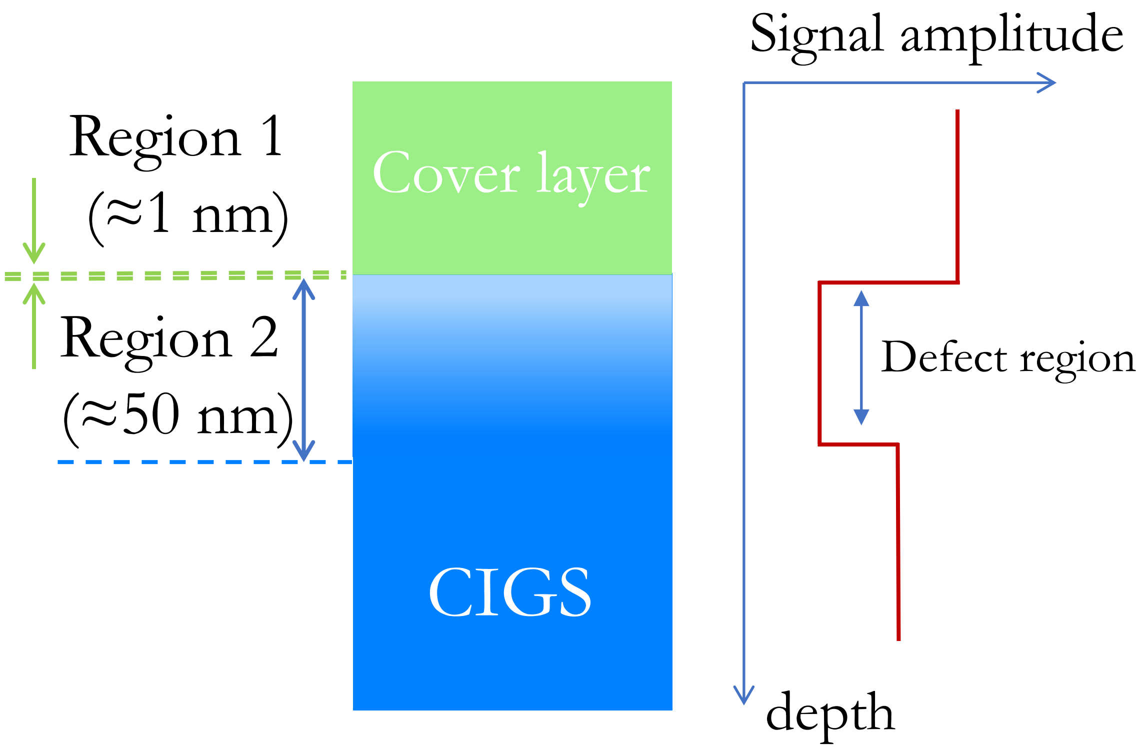
- CdS provides the best defect passivation.

- Oxide materials are less effective.



# Conclusions

- Slow muons are sensitive only to a region near the p-n interface (region 2) , which is more disturbed than the inner part of CIGS.
- A disturbed interface region is associated with interface recombination losses, affecting the device efficiency. It is important to distinguish contributions from regions 1 and 2.
- Slow muons allows us to separate contributions from region 1 and 2, not possible with other techniques.
- Using slow muons, it is possible to make a quantitative characterization of the effect of various buffer/cover layers on the passivation of bulk defects in this region.



# Open Questions

- How does the disturbed interface region observed by muons relate to interface recombination losses?
- Does this disturbed interface region affect ion diffusion (namely Cd) into CIGS? If yes, how?
- How does the disturbance in this region relate to macroscopic parameters such as quantum efficiency, open circuit voltage in the operating solar cell?

# Project SolarCells@CFisUC

- First step : workshop INL@CFisUC next week 30 Nov 2022, after café com Física

## Program

- 15:15-15:20 (5 minutos) Welcome ; project SolarCell@CFisUC
- 15:20 - 15:40 (20m) - Introduction to the International Iberian Nanotechnology Laboratory (INL) and the Nanofabrication for Optoelectronics Application group (NOA), by Pedro M.P. Salomé
- 15:40 - 15: 50 (10m) - Nanofabrication for ultrathin CIGS solar cells novel architectures, by Jennifer P. Teixeira
- 15:50 - 16:00 (10 m) - Passivation strategies for CIGS solar cells – by Marco A. Curado
- 16:00 - 16:20 (20 m) Optical Simulations of CIGS solar cells, by A. J. N. Oliveira
- 16:20 - 16: 40 (20m) - SCAPS 1D electrical simulation software, A. Violas
- 16:40- 17:00 (20 m) – Questions and discussion
- 17: 00 - coffee break

## Participants so far

- 16 students
- Coimbra group+ NOA