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PIANO NAZIONALE DI RIPRESA E RESILIENZA

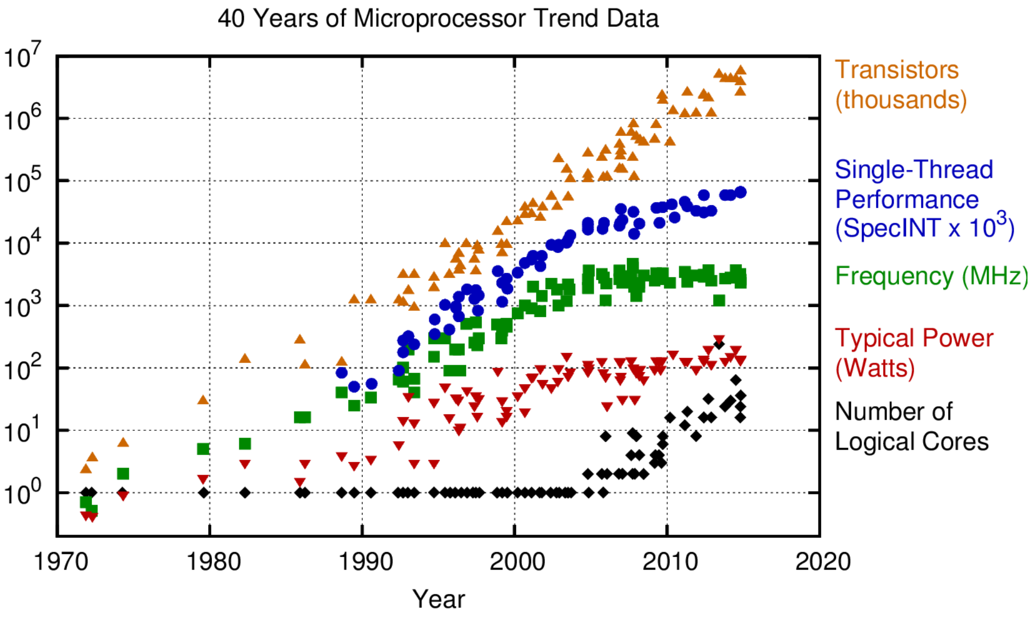
INFN
Istituto Nazionale di Fisica Nucleare
Laboratori Nazionali di Frascati

TCAD modeling of Ferroelectric Materials for Enhanced Electronic Device Efficiency

Arianna Morozzi
on behalf of the HiEnd collaboration

Negative Capacitance…
…Delving into the concept's origins

Do we need to reinvent the transistor?



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten
New plot and data collected for 2010-2015 by K. Rupp

Increase in performance:

Frenquency

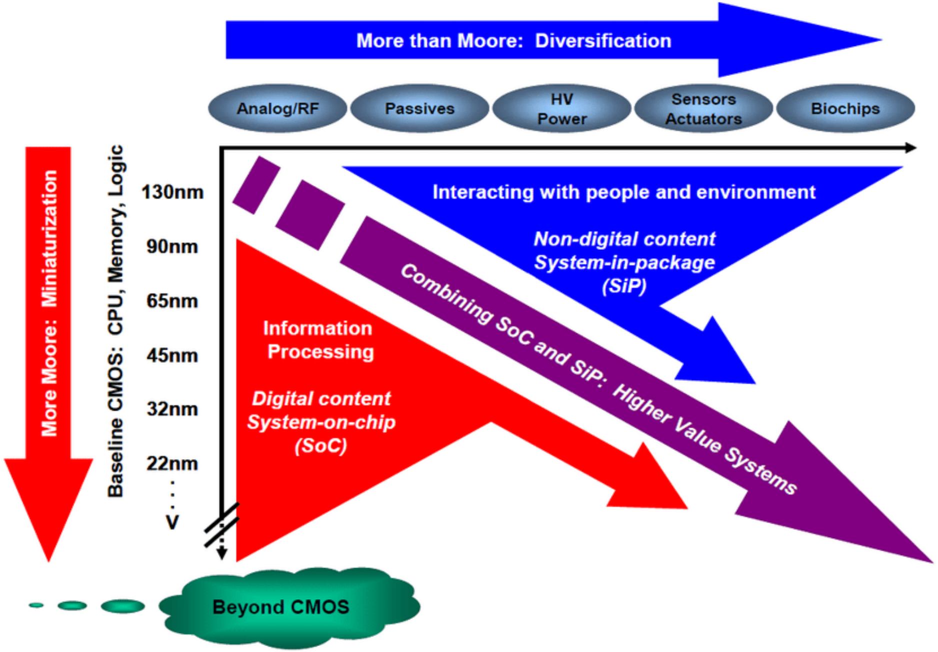
Speed

Drawback:

Power consumption

Heat generation

Do we need to reinvent the transistor?



Increase in performance:

Frenquency

Speed

Drawback:

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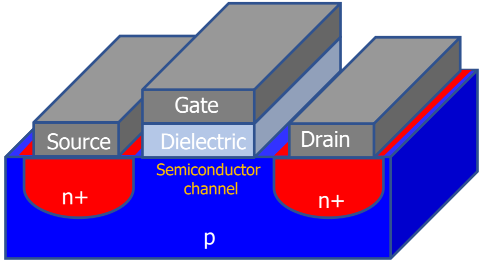
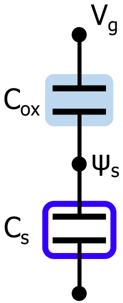
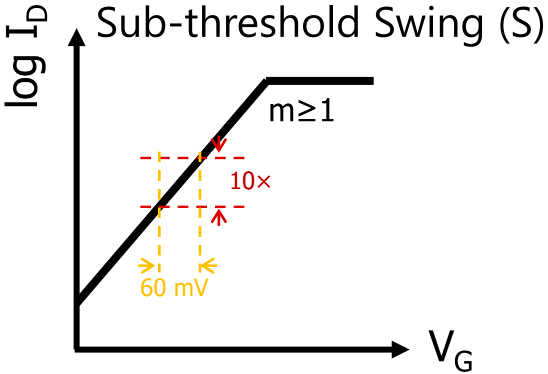
Heat generation

Typical MOSFET







Body factor Transport factor

$$S = \frac{\partial V_g}{\partial(log I_d)} = \frac{\partial V_g}{\partial \psi_s} \times \frac{\partial \psi_s}{\partial(log I_d)} \equiv m \times n$$

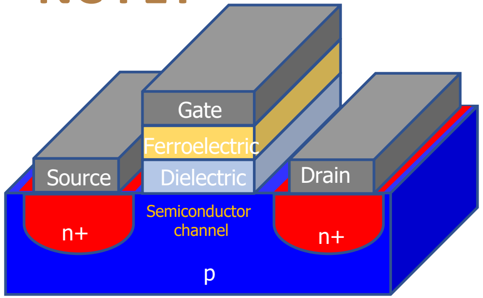
$$min\left(\frac{\partial \psi_s}{\partial(log I_d)}\right) = \ln(10) \times \frac{k_B T}{q} \approx 60\, \frac{mV}{decade}$$

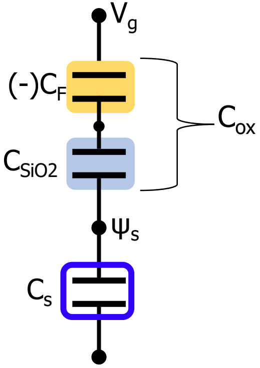
$$\partial \psi_s = \frac{C_{ox}}{C_{ox} + C_s} \partial V_g \longrightarrow m \geq 1$$

I_D increases at best by an order of magnitude per 60 mV of increase in V_G at room temperature due to Boltzmann statistics.

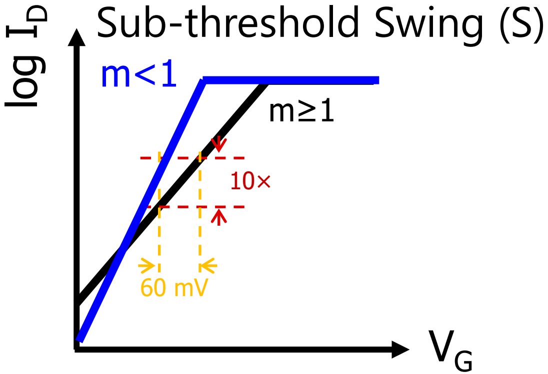
S ≥ 60 mV/decade typical MOSFET

NC FET





$\Psi_s > V_G$ if $C_F < 0$



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$$min\left(\frac{\partial \psi_s}{\partial(logI_d)}\right) = \ln(10) \times \frac{k_B T}{q} \approx 60\,\frac{mV}{decade}$$

$$\partial \psi_s = \frac{|C_{ox}|}{|C_{ox}| - C_s} \partial V_g \longrightarrow m<1$$

S < 60 mV/decade with NC-FET

Proposed solution: Negative capacitance (NC) FETs

IRDS
INTERNATIONAL ROADMAP FOR DEVICES AND SYSTEMS

INTERNATIONAL
ROADMAP
FOR
DEVICES AND SYSTEMS

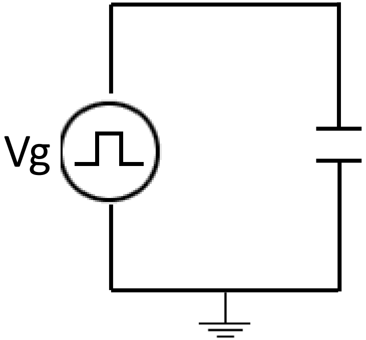
- By replacing the standard insulator with a ferroelectric insulator of the right thickness it should be possible to implement a step-up voltage transformer that will amplify the gate voltage thus enabling low voltage/low power operation
  → advantages in nano-electronics domain applications.

- **Exploring Negative Capacitance for the Future of HEP Detectors**
  - Would it be possible the concept of **pixelated detector with sufficiently small cells to be read out entirely by simple inverters exploiting the NC "self-amplification"?**
  - NC will foster particle detection with extremely thin layers and the fabrication of sensors with very low parasitic capacitances (intrinsic and extrinsic).

S. Salahuddin and S. Datta, Nano Letters, Vol. 8, No. 2, pp. 405-410 (2008), .

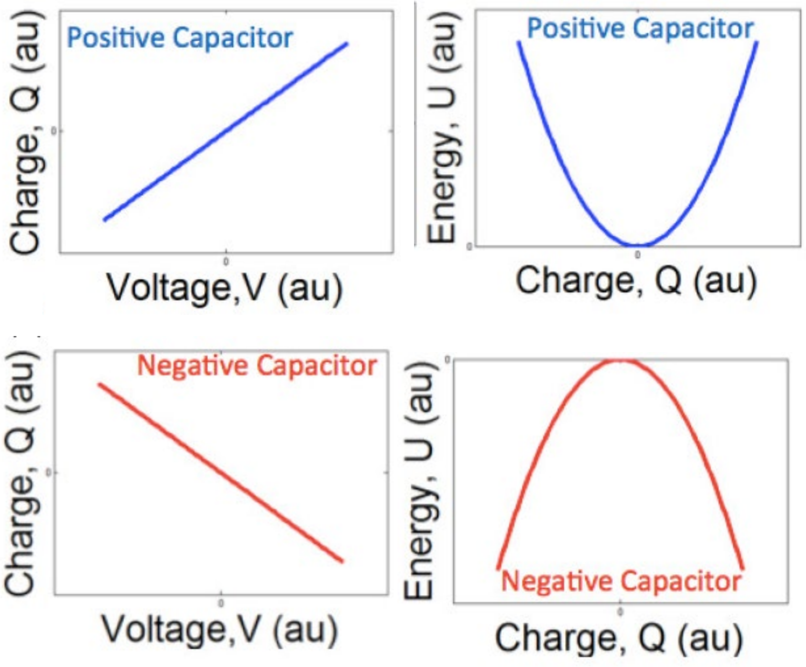
Negative Capacitance…
…Exploring the underlying principles

Capacitance



$$C = \frac{dQ}{dV}$$

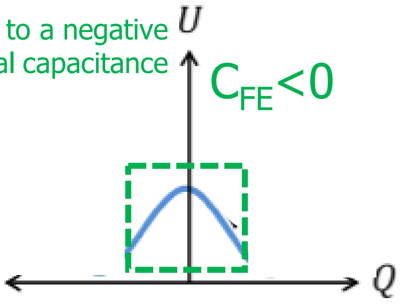
$$U = \frac{Q_c^2}{2C}$$



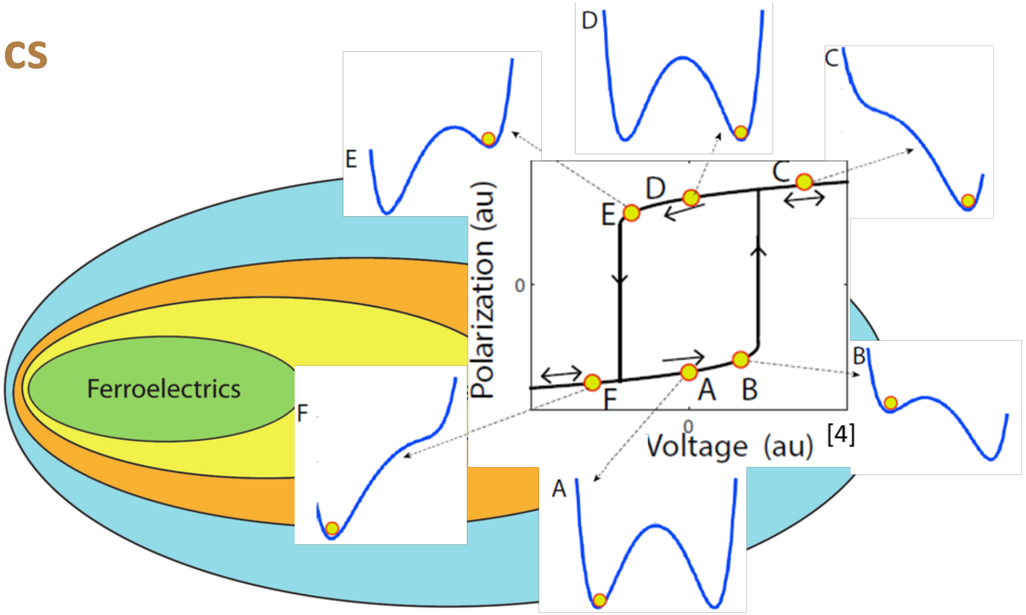
A.I. Khan, Ph.D. Thesis, University of California, Berkeley (2015).

C= capacitance
U= stored energy in a capacitor
Q= stored charge in a capacitor

Landau theory of ferroelectrics



NC refers to a negative differential capacitance



Free energy of a ferroelectric

$$\begin{cases} U_{FE} = \alpha Q^2 + \beta Q^4 + \gamma Q^6 - Q V_F \\ \rho \dfrac{dP}{dt} + \dfrac{dU}{dP} = 0 \end{cases}$$

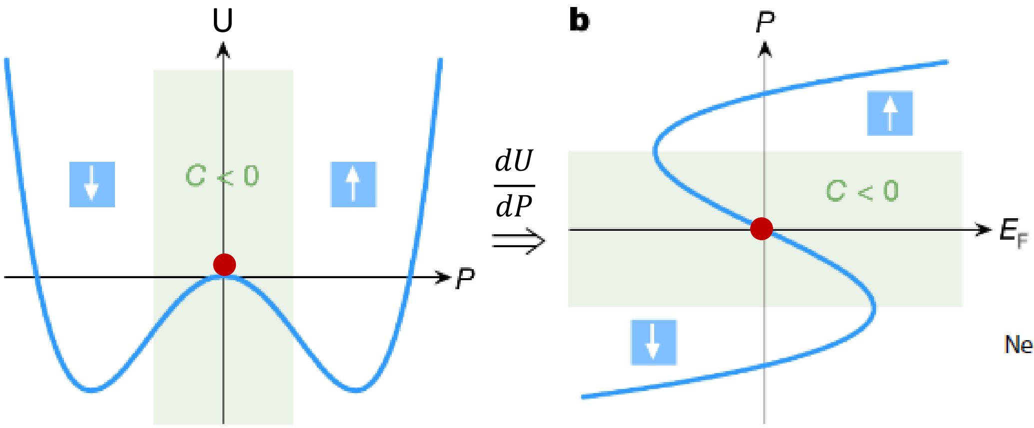
α (<0), β, γ= anisotropy constant

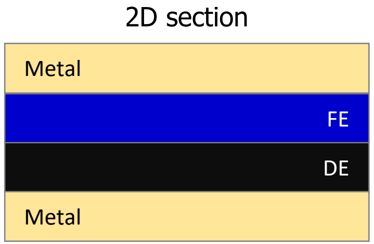
P,Q= Polarization E= Electric field

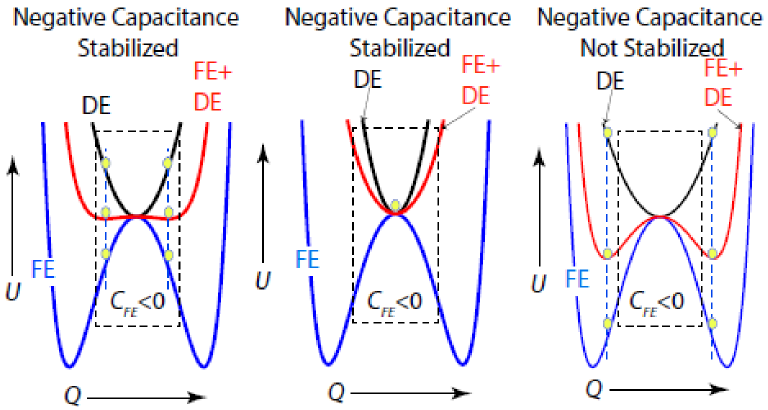
Landau, L. D. *Zh. Eksp. Teor. Fiz.* **7**, 19–32 , (1937).

Landau and Khalatnikov, Dokl. Akad Nauk., 96, 85, 469472, (1954).

M. S. Islam, A. A. M. Mazumder, C. Zhou, C. Stampfl, J. Park and C. Y. Yang, IEEE J. Electron Devices Soc., 11, pp. 235-247, 2023.




2D section



A.I. Khan, Negative Capacitance for Ultra-low Power Computing, Ph.D. Thesis(2015)

- ✓ Ferroelectric oxides could give an effective NC.
- ✓ Spontaneous polarization
  → In equilibrium conditions, the ferroelectric material resides in one of the wells

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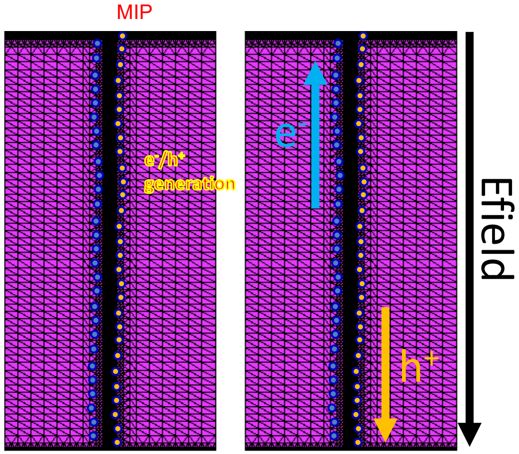
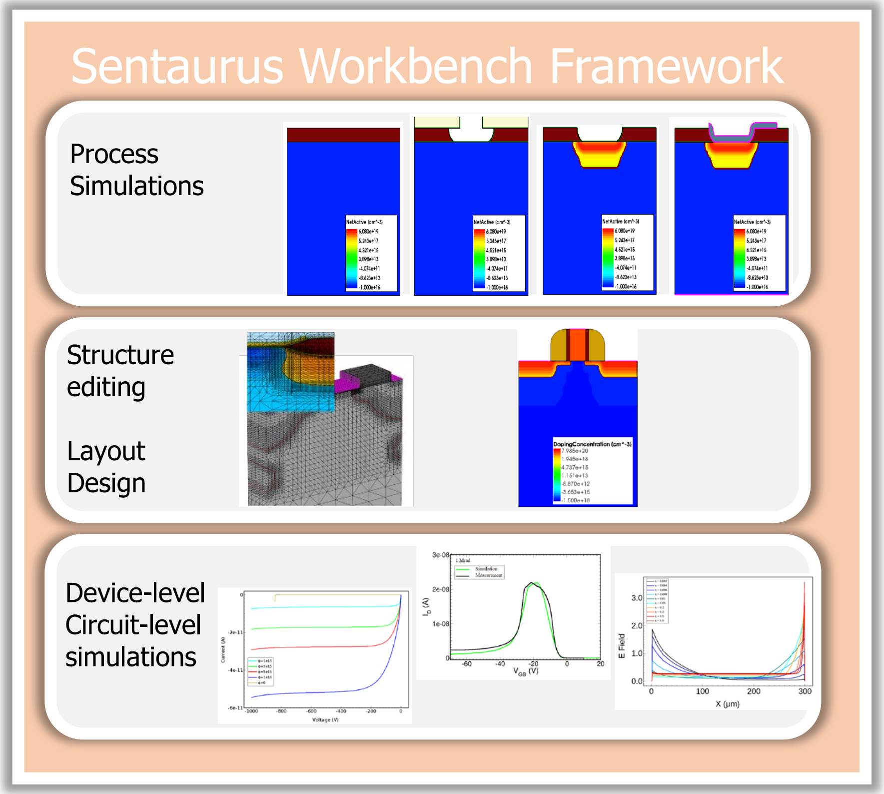
Negative Capacitance…
… Our perspective

Motivations



- ❑ Innovative Detectors for High-Energy Physics applications
  - ✓ High granularity, thin layers.
  - ✓ Radiation hardness.
  - ✓ Fast response.
- ❑ Continuous increasing in electronics performance demand
  - → Continuous scaling of transistors:
    - ✓ Increase of leakage currents.
    - ✓ Increase heat-up → high effort for cooling → thermal runaway.
    - ✓ Radiation resistance/tolerance.
- ❑ Low signals detection in thin layers:
  - ✓ minimum detectable signal is dominated by the switching threshold of a digital switch (e.g. ≈1 ke$^-$ for 28 nm technology, <100 e$^-$ for sub 10-nm technology).



Sentaurus Workbench Framework

Process Simulations

Structure editing

Layout Design

Device-level Circuit-level simulations

- √ State-of-the-art Synopsys© Sentaurus TCAD.
- √ TCAD simulation tools solve fundamental, physical partial differential equations, such as diffusion and transport equations for discretized geometries (finite element meshing).
- √ This deep physical approach gives TCAD simulation predictive accuracy.

$$\left\{ \begin{aligned} &\nabla \cdot \left(-\varepsilon_s \nabla \varphi\right) = q\left(N_D^+ - N_A^- + p - n\right) && \text{Poisson} \\ &\frac{\partial n}{\partial t} - \frac{1}{q}\nabla \cdot \vec{J}_n = G - R && \text{Electron continuity} \\ &\frac{\partial p}{\partial t} + \frac{1}{q}\nabla \cdot \vec{J}_p = G - R && \text{Hole continuity} \end{aligned} \right.$$

$$\vec{J}_n = -q\mu_n n \nabla \varphi + qD_n \nabla n$$

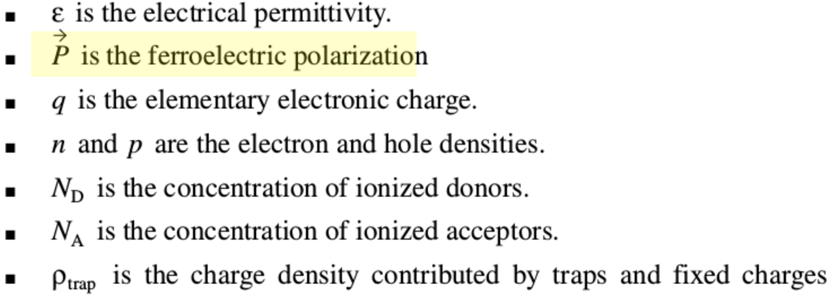
$$\vec{J}_p = -q\mu_p p \nabla \varphi - qD_p \nabla p$$

Setting-up the TCAD environment

- Development of TCAD library for ferroelectric-material physics model
  - Recently released version of Sentaurus TCAD has embedded two models aiming at simulating ferroelectric materials: **Preisach** models and **Ginzburg-Landau-Khalatnikov** equations.
  - Proper tuning with experimental assessed parameters.
  - **Methodology validation**: simulations vs measurements simple devices (MFM, MFIM).

Poisson equation

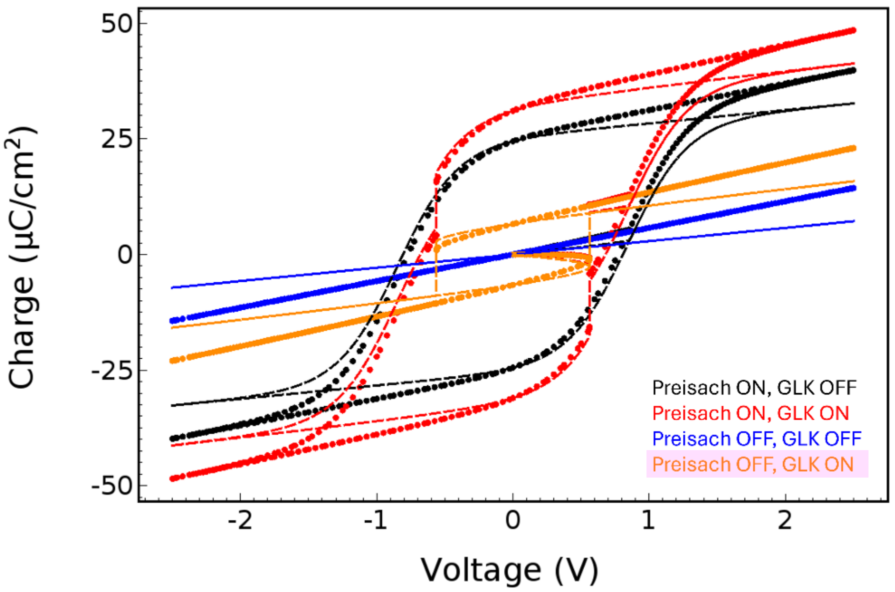
$$\nabla \cdot \left(\varepsilon \nabla \varphi - \vec{P}\right) = -q(p - n + N_D - N_A) - \rho_{trap}$$



- ε is the electrical permittivity.
- $\vec{P}$ is the ferroelectric polarization
- q is the elementary electronic charge.
- n and p are the electron and hole densities.
- N_D is the concentration of ionized donors.
- N_A is the concentration of ionized acceptors.
- ρ_{trap} is the charge density contributed by traps and fixed charges

Modeling a FE material within the TCAD

The polarization $\vec{P}$ depends nonlinearly on the electric field $\vec{F}$ (or $\vec{E}$)



Preisach model of hysteresis:

P_r remnant polarization

P_s saturation polarization

E_c coercive field

Ginzburg-Landau-Khalatnikov (GLK) equations

$$F = \int_{\Omega} \alpha_i P_i^2 + \beta_i P_i^4 + \gamma_i P_i^6 - g_{ij} \frac{\partial P_i}{\partial x_{ij}} - E_i P_i + \epsilon_0 E_i \, d\Omega \quad (1)$$

$$\rho \frac{dP_i}{dt} + \nabla_{P_i} F = 0 \quad (2)$$

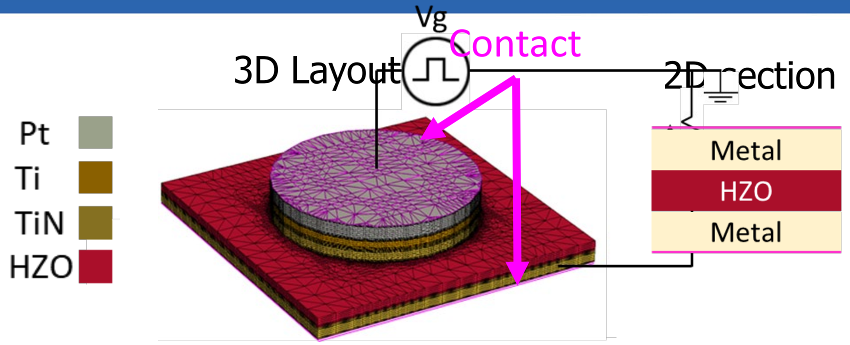
$$\rho \frac{dP_i}{dt} + 2\alpha_i P_i + 4\beta_i P_i^3 + 6\gamma_i P_i^5 - 2g_{ij} \frac{\partial^2 P_i}{\partial x_j^2} - E_i = 0 \quad (3)$$

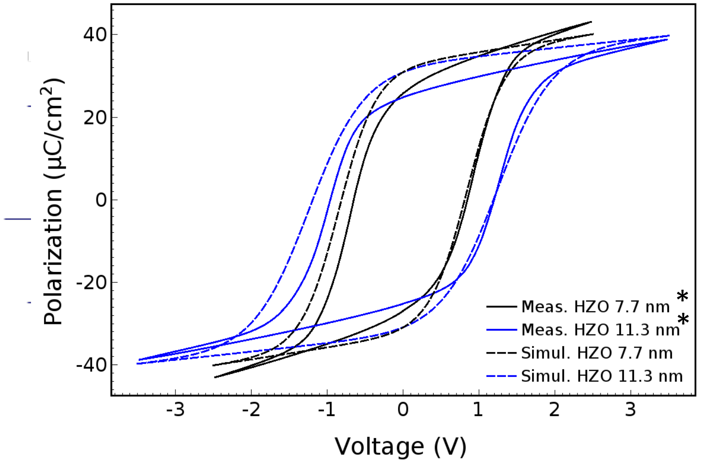
Simulation of MFM structures

- ✓ MFM structure.
- ✓ TCAD Preisach model of hysteresis.
- ✓ Different thicknesses for the ferroelectric HZO thin film.
- ✓ The experimental setup has been implemented within the TCAD environment.
- ✓ Simulations & measurements: Key to model/method validation.

- ✓ remnant polarization
  Pr = 31 μC/cm^2
- ✓ saturation polarization
  Ps = 33 μC/cm^2
- ✓ coercive field
  Ec =1.1 MV/cm

for both 7.7 nm and 11.3 nm thin HZO films.

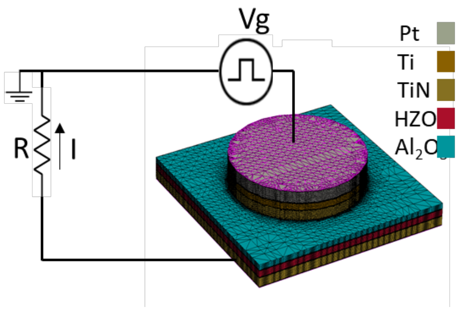




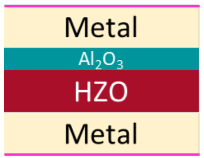
* M. Hoffmann, et al., 2018 IEDM (2018), doi:10.1109/IEDM.2018.8614677

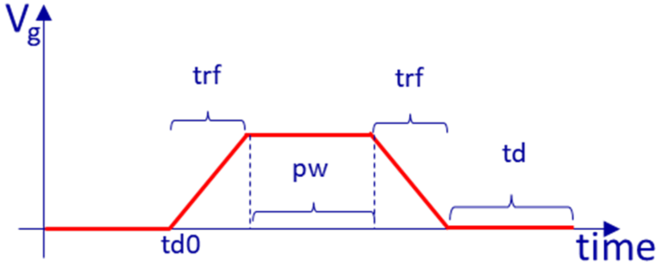
Simulation of MFIM structures

- ✓ MFIM structure.
- ✓ GLK equations model hysteresis-free operation
- ✓ Different thicknesses for the ferroelectric HZO and Al_2O_3 thin films.
- ✓ The experimental setup has been implemented within the TCAD environment.
- ✓ Simulations & measurements:
  Key to model/method validation.
- ✓ The results obtained for MFIM capacitors can be extended to the study of NC-FETs.

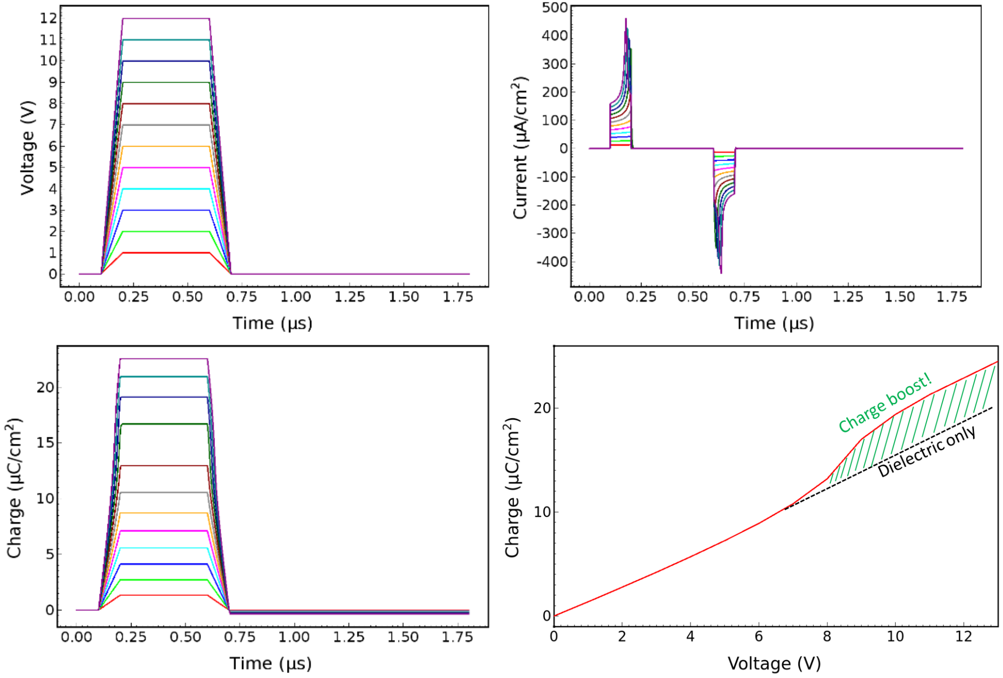


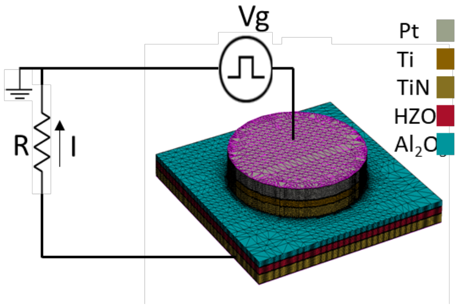
2D section

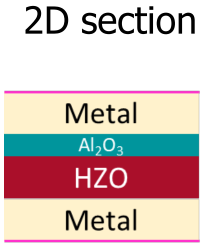


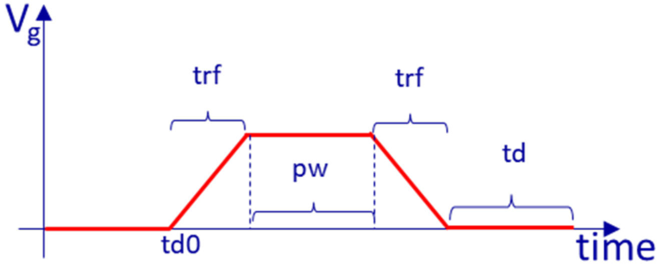


Simulation of MFIM structures



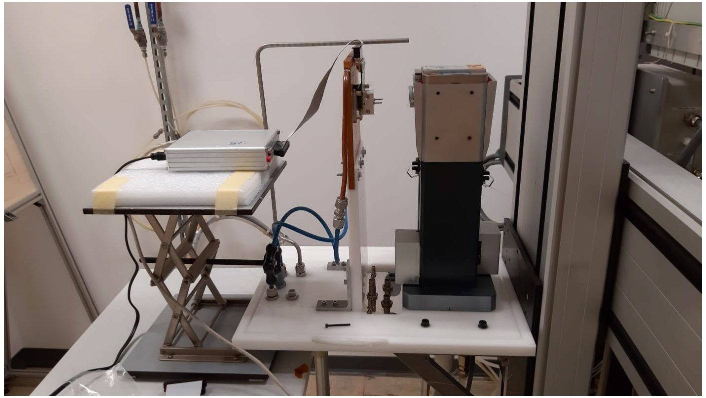




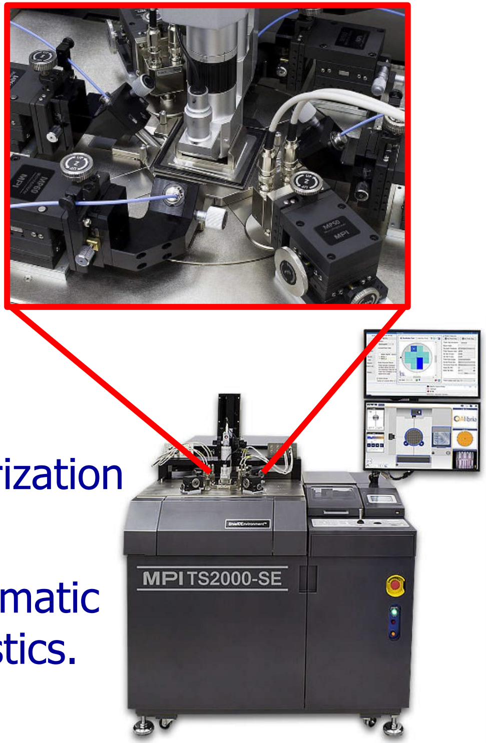


X-ray facility and test structure characterization

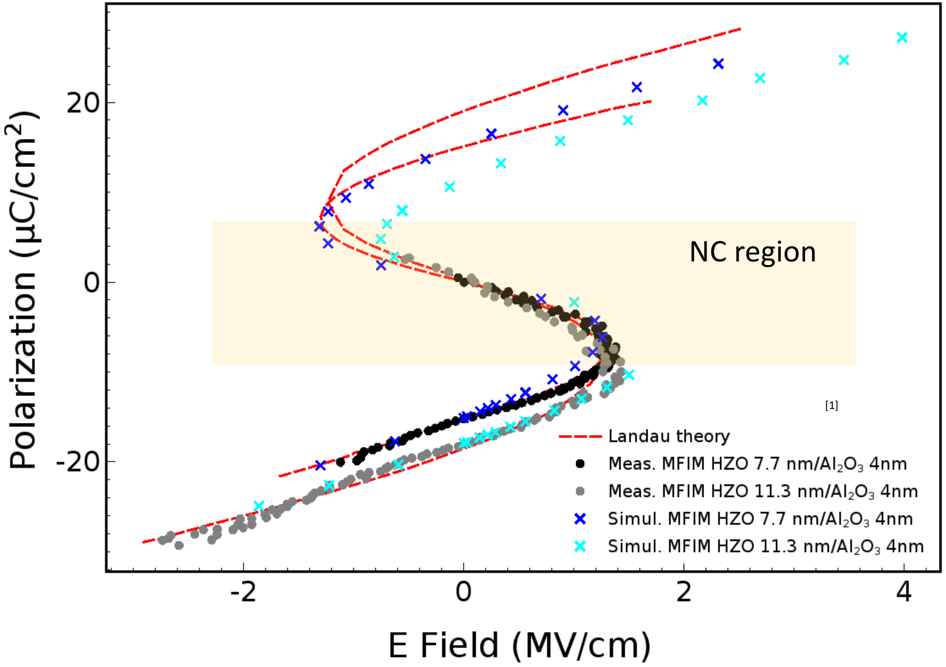
- Irradiation campaign at INFN Genova X-ray facility.
- Typical dose rate is about 3 Mrad/h in 2 cm^2.



- Test structures characterization at INFN Perugia.
- MPITS2000 SE semiautomatic Probe station characteristics.



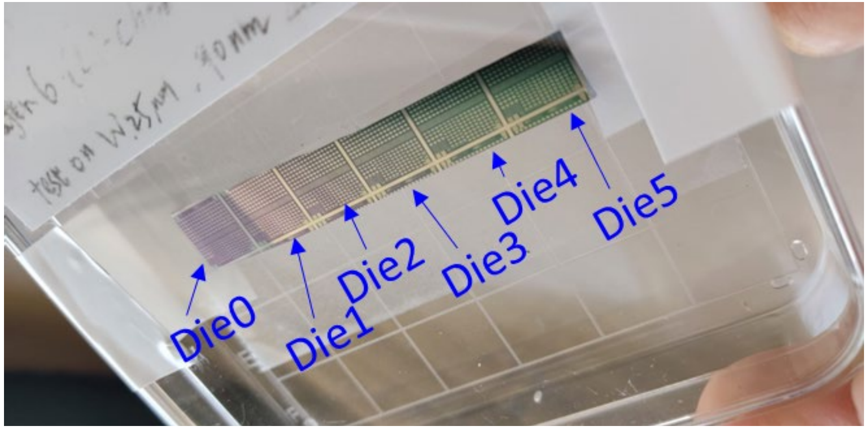
Model Validation

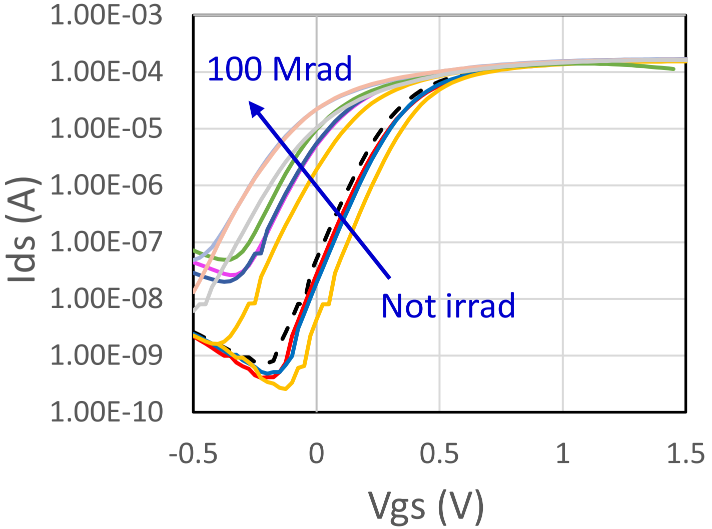


- ✓ Pulsed Q-V measurements are necessary to access the FE NC region during switching by preventing charge injection.
- ✓ EF is the electric field across the ferroelectric material while the total polarization has been assessed as P = QD + Qint.
- ✓ The NC region corresponds to the negative slope of the S-shaped Landau P-E curve.

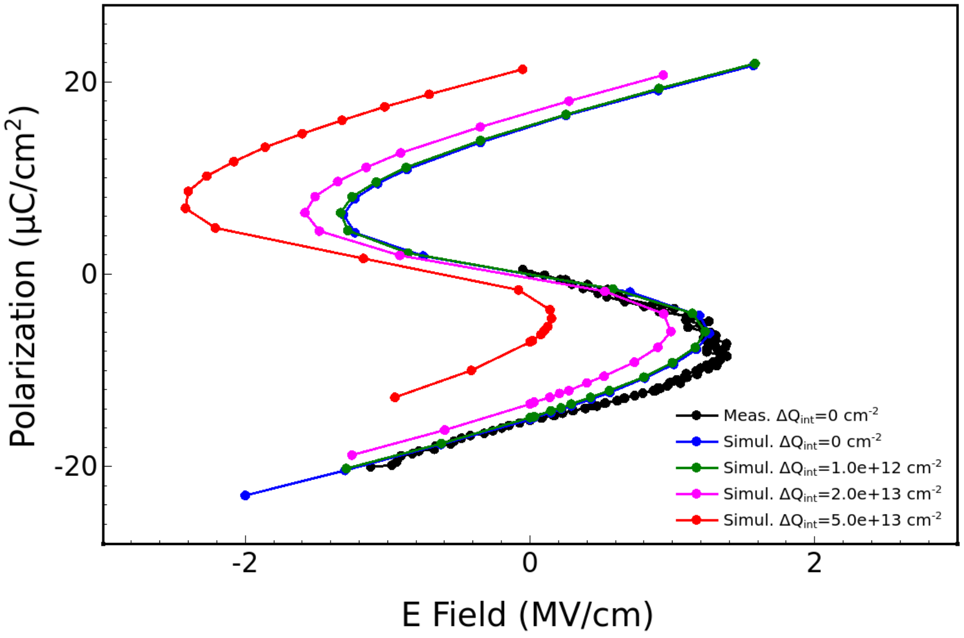
- MFIM structure HZO 7.7 nm/Al2O3 4 nm.
- Qint = -15/-18 µC/cm^2 for 7.7/11.3nm HZO.

NC-FET manufactured at Univ. Berkely





Modeling the radiation damage effects



Modeling of additional fixed charge Qint(ϕ) at the HZO/Al_2O_3 interface of increasing values, aiming at mimicking increasing X-ray doses (ϕ).

$$Q_{int}(\phi) = Qint(0) + \Delta Qint(\phi)$$

Qint(0)=-15/-18 μC/cm2

Conclusion

- ✓ The use of NC materials in HEP detectors is an area of ongoing research with potential benefits:
  - **Increased sensitivity** and **reduced noise**.
  - **Lower power** consumption for larger-scale experiments
  - **Faster signal** processing for real-time analysis

What's next?

- ✓ Further research is crucial to explore:
  - Integration of NC technology into complex detector systems
- ✓ Collaboration is key to unlocking the full potential of NC for HEP.

HiEnD

Development of **Hi**gh **En**ergy Efficient Electronic **D**evices Based on Innovative Ferroelectric Materials

Thanks for the attention!