Radiation Damage: Integrated Atomistic-to-TCAD for Silicon (RADIANT-Si)

A bottom-up, physics-based prediction of radiation effects in silicon devices

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Collaboration: Laurent K. Béland (Queen’s University, Canada)

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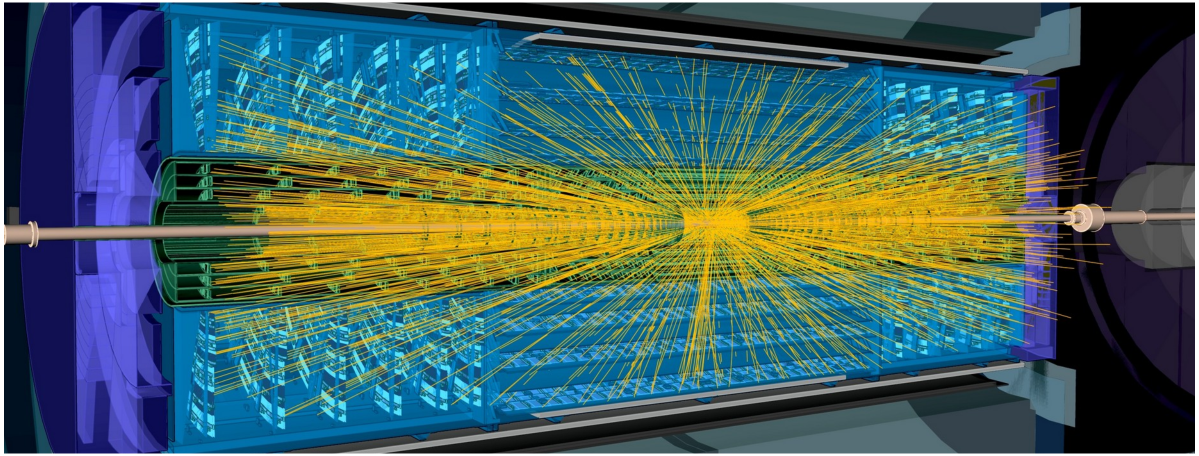
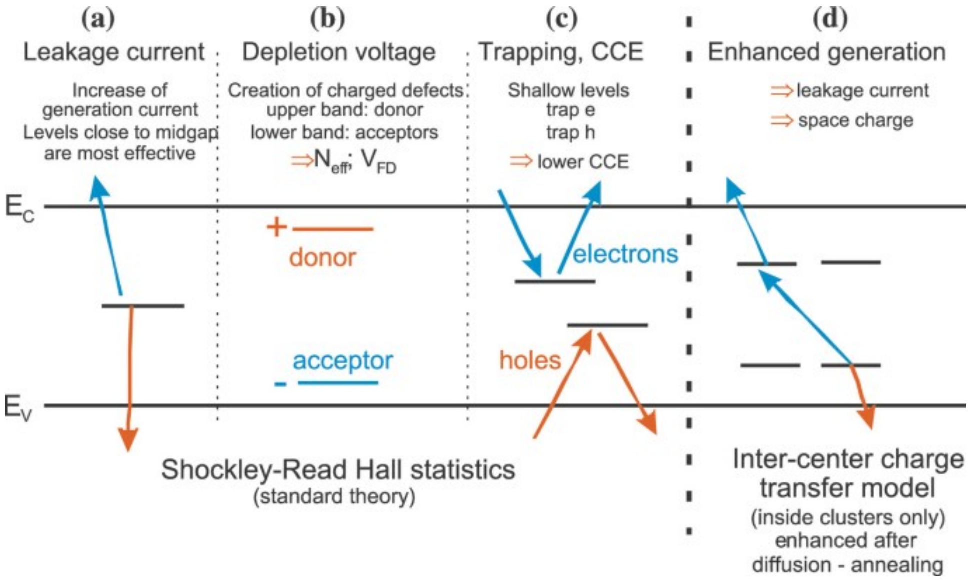
Motivation and applications



- Silicon detectors are pivotal at CERN and in space/nuclear environments
- HL-LHC pushes radiation tolerance to extremes
- Accurate lifetime/performance predictions reduce risk and cost in detector upgrades
- Transferable methodology to other semiconductors and device geometries

Displacement damage: what matters

- High-energy particles create point defects, clusters and amorphous pockets in Si
- Defects induce band gap states, alter space charge, and trap carriers
- Device-level impacts: leakage current rise, depletion voltage shift, CCE loss, breakdown behavior
- Need defect-level fidelity to predict macroscopic device response [1]



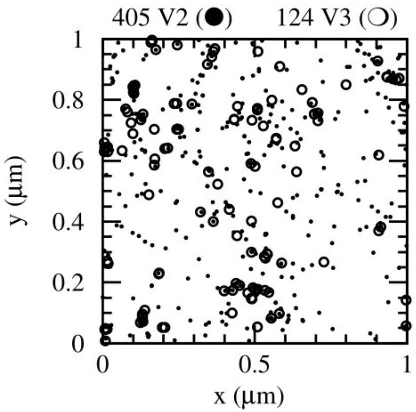
[Hartmann, F., in: Evolution of Silicon Sensor Technology in Particle Physics (2024) Springer]

[1] M. Moll, *IEEE Trans. Nucl. Sci.*, vol. 65, no. 8 (2018) pp. 1561-1582

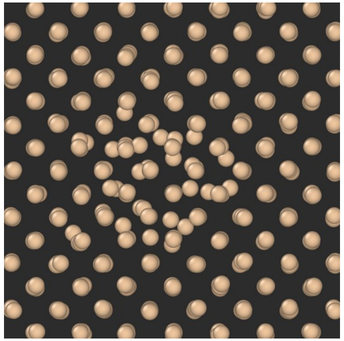
Limits of current practice (BCA & NIEL)

- Standard approaches based on binary collision approximation (BCA) damage predictions
  - Fast, but misses collective effects and amorphization [2]
- Poor capture of defect clustering, dopant interactions, and annealing behavior
- Uncertainties in NIEL scaling, and 1-MeV neutron equivalent at high fluence [2]
- Limits of Hamburg model applicability; need beyond-BCA physics [3] → full atomistic modelling

BCA



Molecular dynamics (MD)



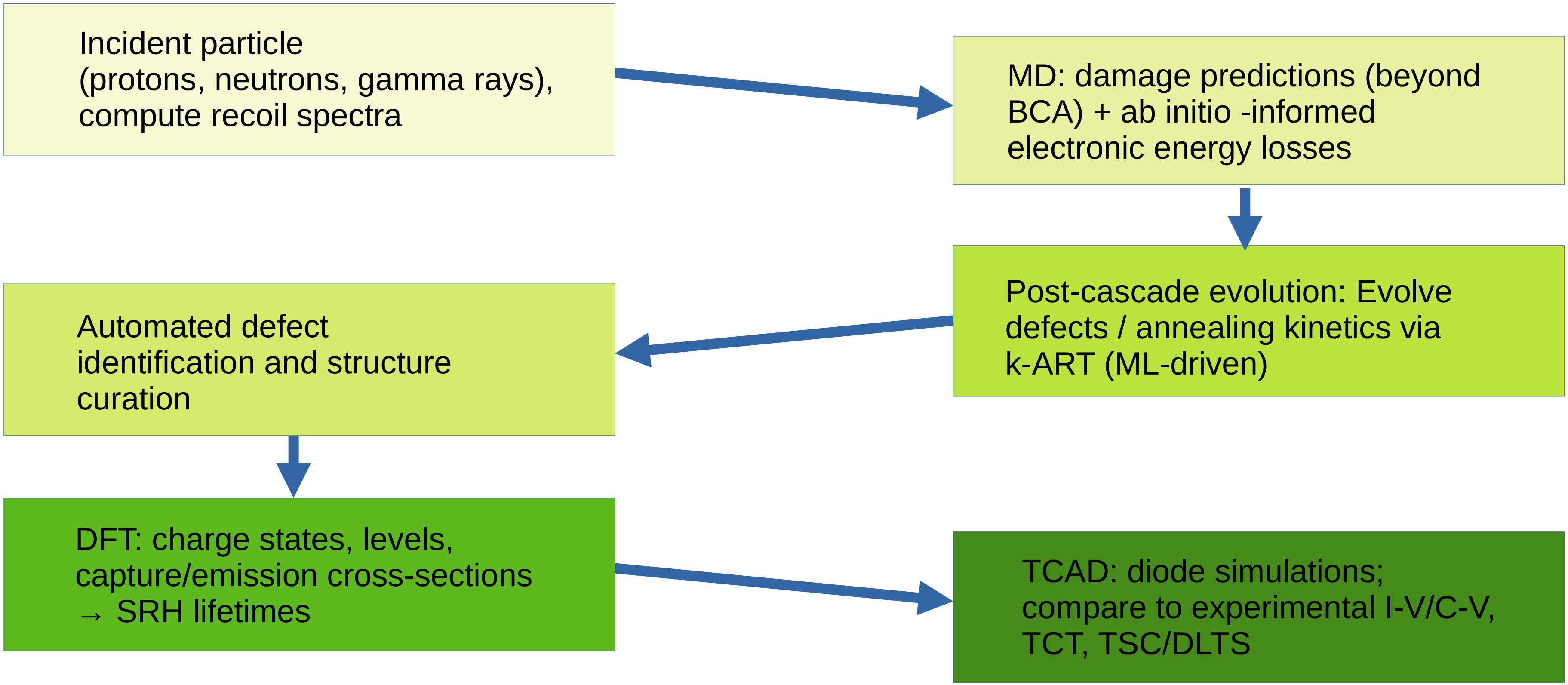
[2] M. Huhtinen, *Nucl. Inst. And Meth. A* 491 (2002) 194–215

[3] G. Kramberger, *et al*., *JINST* 9 (2014) P10016

RADIANT-Si objectives and impact

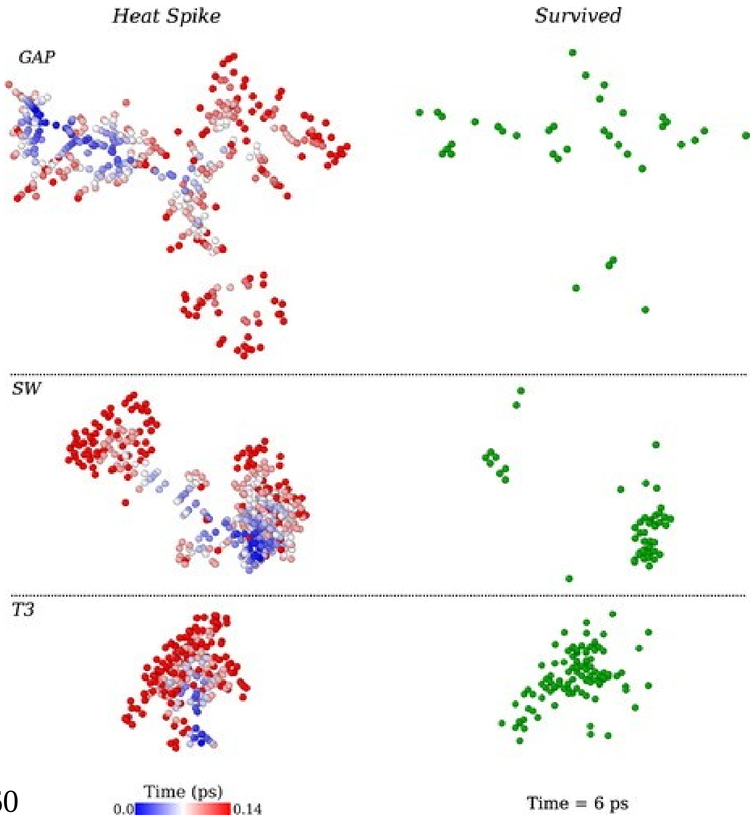
- Objectives
  - Build an atomistic-to-TCAD pipeline with ab initio fidelity at scale
  - Validate against controlled irradiations and device measurements
- Impact
  - End-to-end, bottom-up pipeline: First integrated chain from primary radiation events → atomistics → defect energetics/cross-sections → SRH parameters → TCAD device response, minimizing empirical tuning
  - High fidelity: Ab initio-informed electronic energy losses and DFT-level accuracy of ML potentials
  - Explicit treatment of clustered damage: Mixed representation (discrete centers + distributed trap spectra) grounded in atomistic statistics, addressing known failures of point-defect-only models at high fluence.

Integrated workflow overview



Atomistic damage with ML potentials

- Molecular dynamics (MD) cascade simulations with modern ML interatomic potentials for Si with near DFT accuracy [4,5]
  - Captures covalent bonding, defect relaxation, and clustering faithfully
- State-of-the-art efficient codes and HPC resources enable large-scale cascades with realistic statistics across energies and species
  - Quantify primary defect populations vs. PKA spectra with sufficient statistics



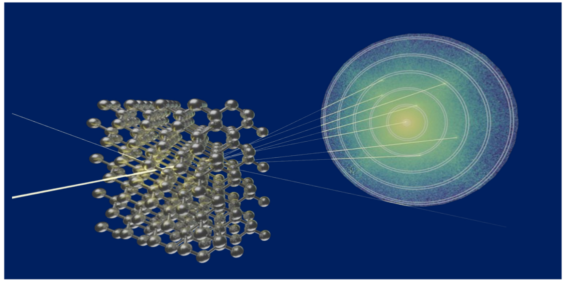
[A. Hamedani, et al., MRL 8 (2020) 364–372]

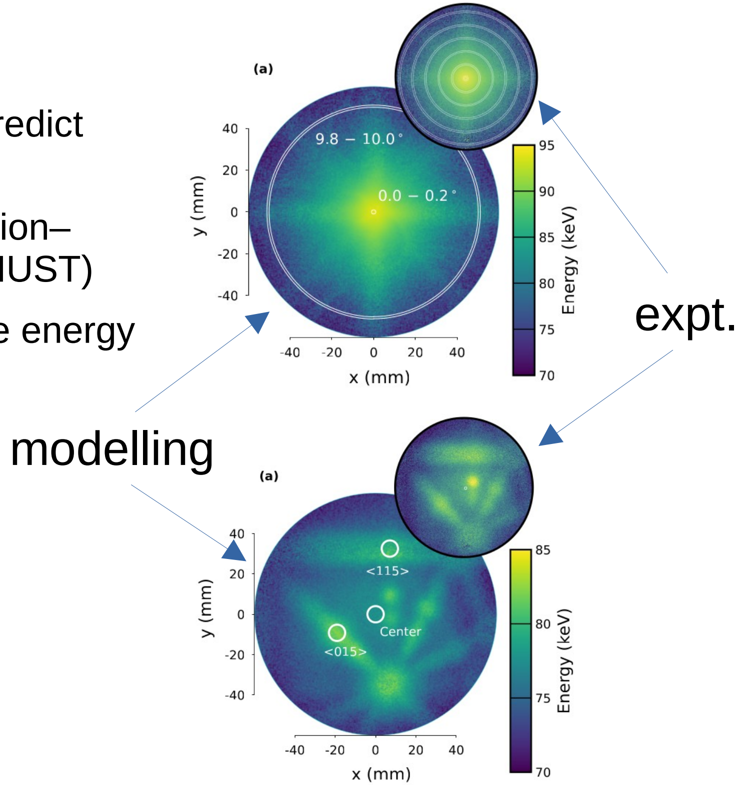
[4] A. Hamedani, et al., *Phys. Rev. Mat.* 5 (2021) 114603

[5] U. Saha, A. Hamedani, M.A. Caro, A.E. Sand, *Comp Mat Sci* 267 (2026) 114560

Electronic stopping: rt-TDDFT-informed

- Electronic energy losses are trajectory-dependent [6]
- Real-time time-dependent density functional theory (rt-TDDFT) can predict local energy losses in any environment [7]
- We have developed and will use rt-TDDFT-derived spatially resolved ion–electron coupling for Si in Si (results from ongoing ERC StG project MUST)
- Coupling embedded into multi-million atom MD simulations to improve energy loss physics and defect yields [8]
- Coupling parametrization for Si validated against ion energy loss measurements



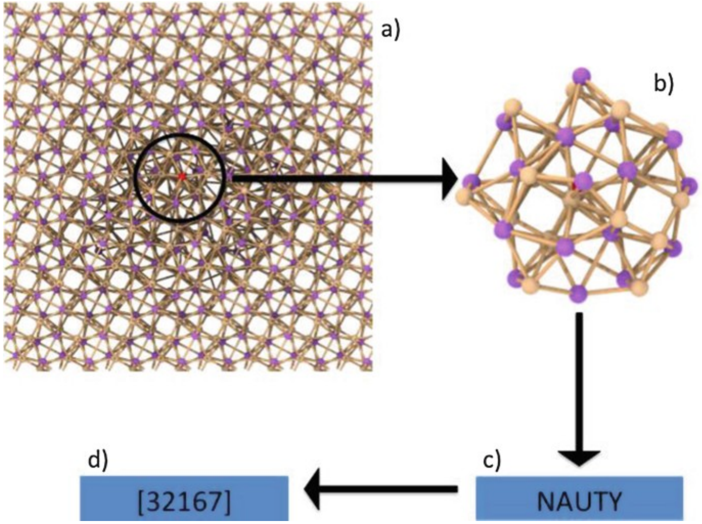


[6] S. Lohmann, et al., *Phys. Rev. A* 102 (2020) 062803
[7] R. Nuñez-Palacio, A.E. Sand, *Communications Materials* 6 (2025) 109
[8] A.E. Sand, *et al.*, *Phys. Rev. Mater.* 9 (2025) 053603

Defect evolution and annealing (k-ART)

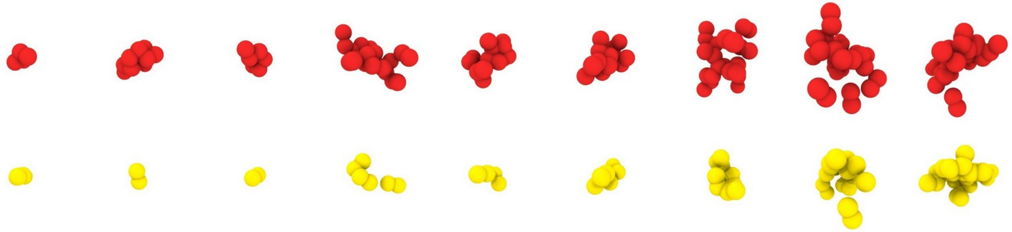
in collaboration with L. K. Béland

- Kinetic Activation-Relaxation Technique (k-ART) explores long-timescale events, beyond MD [9]
- Temperature/time protocols matching experiments
- Track cluster growth/dissolution, extendable to dopant/oxygen interactions (later phase)
- Output: stable defect spectra vs. fluence and anneal history



Local topological analysis procedure and cataloging accelerates energy barrier search

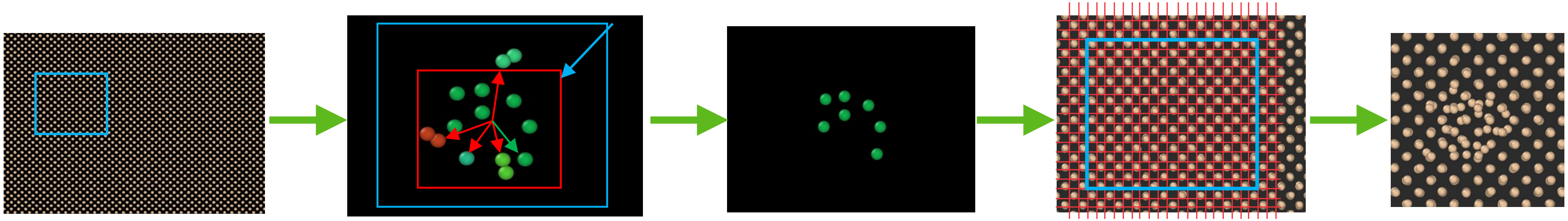
5 ns annealing with MD; before (red) → after (yellow)



[9] L. K. Béland, Phys. Rev. E **84** (2011) 046704

Ab initio defect properties

- DFT supercells from annealed and extracted structures
  - finite-size and charge corrections (Freysoldt, Neugebauer, and Van de Walle (FNV) [10])



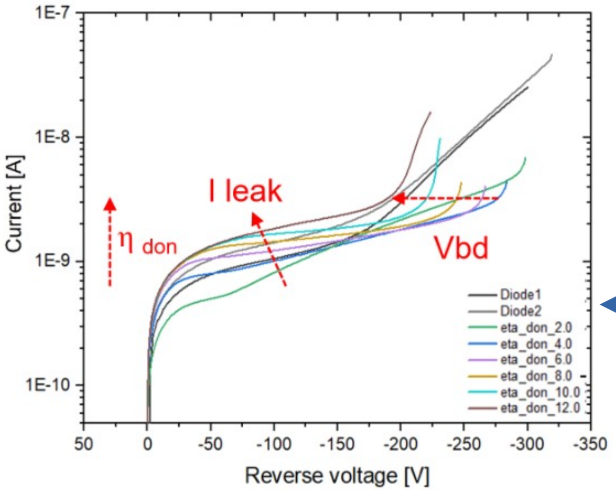
- Hybrid functional for accurate band gap description
- Compute thermodynamic/optical levels, charge transition levels
- Electron/hole capture and emission cross-sections → Shockley-Read-Hall parameters
- Build defect libraries indexed by species, fluence, and annealing

[10] C. Freysoldt, J. Neugebauer, and C. G. Van de Walle, Phys. Rev. Lett.102, 016402 (2009).

TCAD integration and device targets

with Eric Brücken (HIP)

- Start with simple planar Si diode as proof of concept
- Source defect libraries into TCAD (trap concentrations, energy levels, capture cross sections σ_e/σ_h)
- Simulate I-V, C-V, depletion voltage, leakage, breakdown, and CCE
- Compare pre/post-irradiation and annealing scenarios

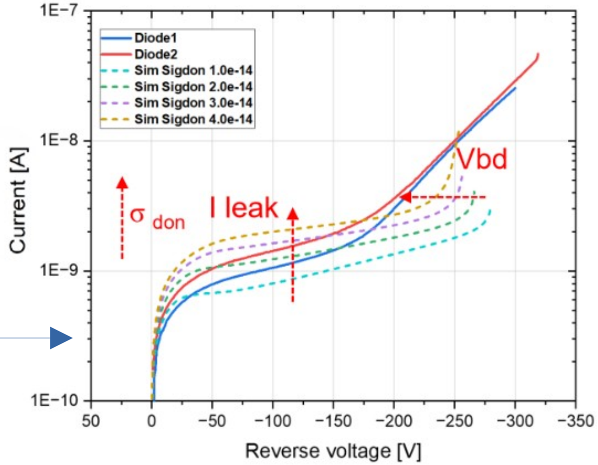


Examples of TCAD predictions of effects of irradiation induced donor trap state on I-Vs simulated at -25°C of 50×50 3D detectors irradiated at 1×10^{16} n_{eq}/cm^2

Effect of the introduction rate

Effect of the capture cross section

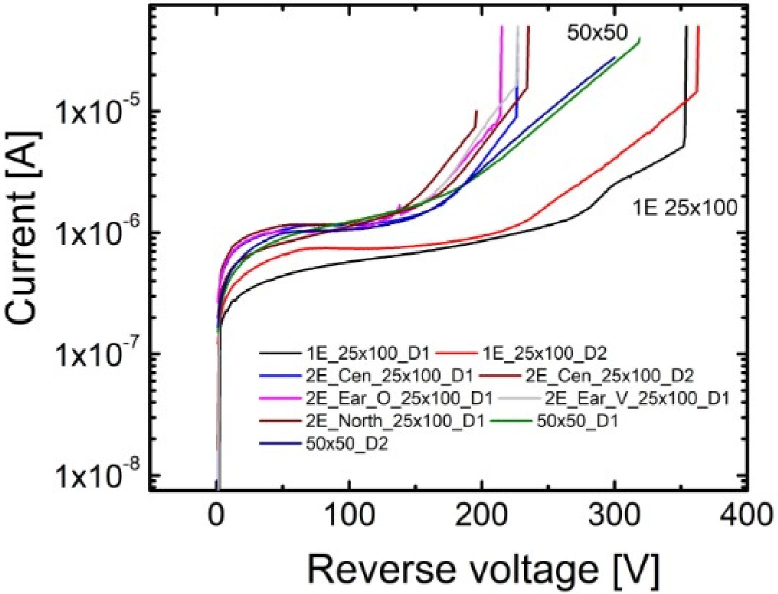
[F. Moscatelli, et al., JINST 20 (2025) C09006]



Experimental validation

with Eric Brücken (HIP)

- Species: protons, neutrons, gamma rays
  - Fluences: 1e13–1e16 n_{eq}/cm^2
- Facilities: UH Accelerator Lab (10 MeV p), Proton Irradiation Facility at Paul Scherrer Institute, Switzerland (up to 590 MeV p), Triga Mark II reactor at Jozef Stefan Institute, Slovenia (n), Co-60 irradiator at Ruder Boskovic Institute, Croatia (γ)
- Controlled annealing protocols to map time/temperature effects
- I-V/C-V: effective doping concentration, full depletion voltage, reverse leakage current, breakdown voltage, forward voltage efficiency
- TCT: effective doping concentration, electric field profiles, trapping times, charge collection efficiency, annealing curves, etc
- TSC/DLTS: defect spectroscopy to refine trap models and cluster fingerprints
- Close loop: Probe and refine defect libraries and TCAD parameters from measurements



I-Vs measured at -25°C on different 3D layout irradiated at 1×10^{16} n_{eq}/cm^2

[F. Moscatelli, et al., JINST 20 (2025) C09006]

Impact, deliverables, risks, and outlook

- Impact: Physics-based predictions beyond NIEL; address Hamburg model limits; transferable pipeline
- Key deliverables:
  - Reusable defect library; DFT cross-sections and TCAD decks: Machine-readable, species/fluence/anneal-indexed libraries enabling rapid scenario generation and portability to other geometries/devices
  - Benchmark validation dataset
- Risks/mitigations: Potential accuracy gaps (use uncertainty quantification, cross-potential benchmarking); computational cost (HPC + surrogate models); defect complexity (prioritize dominant centers)
- High-level timeline:
  - Y1 recoil spectra calculations + MD + k-ART + defect extraction + DFT; irradiations
  - Y2 MD to higher fluence, additional DFT; first TCAD modelling and additional experimental results
  - Y3 full validation + dissemination + preliminary dopant/oxygen extensions
- Outlook: Extendable to include dopants/oxygen and new materials/interfaces: Same pipeline accommodates dopant/oxygen interactions and can be ported to other semiconductors and segmented detector geometries

Thank you!