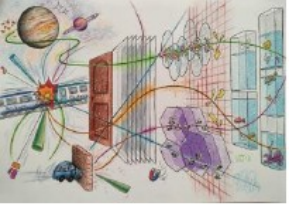


Assessment of electronic structure and metastabilities of complex defects in boron doped silicon samples following irradiation at high fluences

related to project proposal DRD3-2024-05

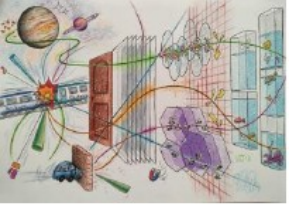
"Radiation damage in Boron-doped Silicon diodes and LGAD sensors "

Nicolae Filipoiu[1,2], Mihaela Cosinschi[1,2], Calin-Andrei Pantis-Simut[1,2], Amanda Teodora Preda[1,2], Ioana Pintilie[3] and George Alexandru Nemnes[1,2]

[1]Horia Hulubei National Institute for Physics and Nuclear Engineering, Magurele-Ilfov 077126, Romania (IFIN-HH)

[2]University of Bucharest, Faculty of Physics, Magurele-Ilfov 077125, Romania

[3]National Institute of Materials Physics, Magurele, Ilfov 077125, Romania



Outline

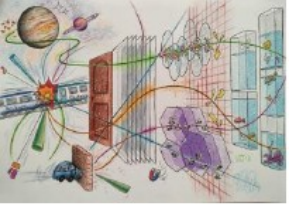
- **Objective of the project proposal:**
  Understanding radiation damage in silicon
  (in agreement with RG3.2 and RG3.4 within WG3)

- **Team expertise & resources (computational infrastructure) @ IFIN-HH**

- **Description of proposed activities and expected results:**
  → Complex defect dynamics (metastabilities):
  Molecular dynamics investigations using LAMMPS software
  → Electronic properties of defects in the context of co-doping (O, C and/or P impurities):
  Ab initio (atomistic) density funtional theory (DFT)

- **Challenges and open questions**

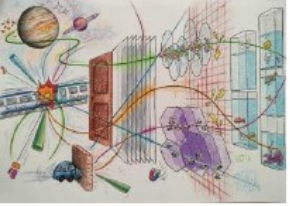
- **Final remarks**



Proposal objective

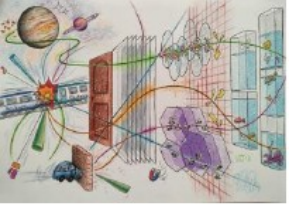
The research activities within the proposal *„Radiation damage in Boron-doped Silicon diodes and LGAD sensors"* are relevant to WP3, Task 3.3 – Extreme fluence in silicon detectors.

WP	Task	Title
1	1.1	MCMOS: spatial resolution
1	1.2	MCMOS: timing resolution
1	1.3	MCMOS: read-out architectures
1	1.4	MCMOS: radiation tolerance
2	2.1	4D tracking: 3D sensors
2	2.2	4D tracking: LGAD
3	3.1	Extreme fluence: wide band-gap materials (SiC, GaN)
3	3.2	Extreme fluence: diamond-based detectors
3	3.3	Extreme fluence: silicon detectors
4	4.1	3D Integration: fast and mask-less interconnect
4	4.2	3D Integration: in house post-processing for hybridization
4	4.3	3D Integration: advanced interconnection techniques for detectors
4	4.4	3D Integration: mechanics and cooling



WG3 Research goals

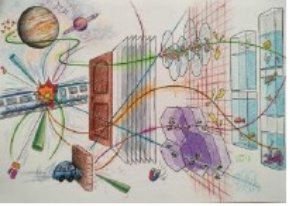
WG3 research goals <2027	
	Description
RG 3.1	Start of building up data sets on radiation-induced defect formation in WBG materials
RG 3.2	Continue developing silicon radiation damage models based on measured point and cluster defects
RG 3.3	Provide measurements and detector radiation damage models for radiation levels faced in HL-LHC operation
RG 3.4	Expand the measurements and models of silicon and WBG sensors properties in the fluence range 10^{16} to $1 \cdot 10^{18}$ n_{eq}/cm^2



WP3 Tasks description

DRD3

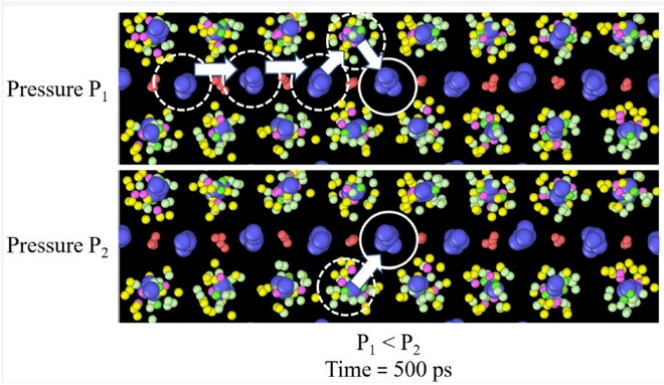
WP	Task	MS or D	Description	2024	2025	2026	2027-2029	> 2030
3	3.3.	MS3.7	Fabrication and testing of different defect engineered Si sensors (enrichment with O, C and/or P) mimicking the gain layer in LGADs	x				
3	2.2, 3.3.	MS3.8	Understanding the effect of co-doping with O, C and/or P on the radiation hardness of gain layers in LGADs and develop defect engineered strategies for improving the radiation hardness (pin diodes 2026) and then segmented detectors (2029).			x	x	



Competences in our group

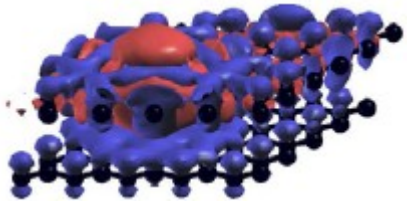
DRD3

- **Molecular dynamics (MD) using classical force-fields (LAMMPS):** investigation of annealing processes, defect migration (vacancies, intersitials), dynamics of complex defects (metastabilities).

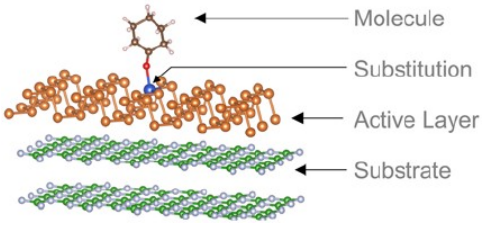


J. Phys. Chem. C 127, 7838 (2023)

- ***Ab initio* density functional theory (DFT) calculations (SIESTA):** formation energies of defects, electronic structure and type (p/n) of complex defects (mono, di-, tri-vacancy, extrinsic impurities, cluster defects etc).

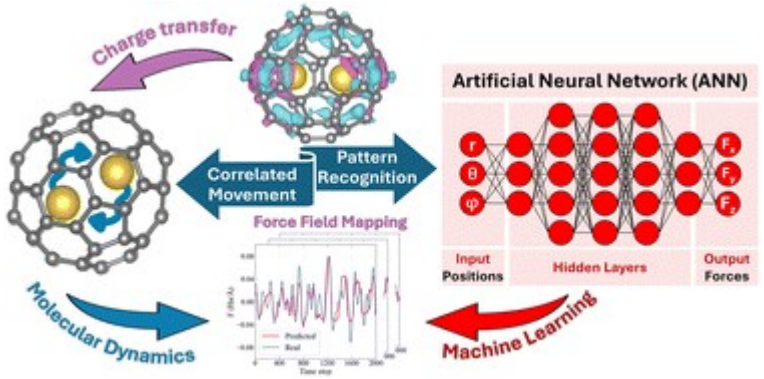


Comput. Mater. Sci. 155, 175 (2018)

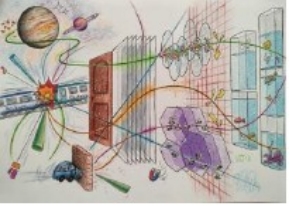


RSC Advances 14, 1803 (2024)

- **Machine learning (ML) techniques:** to efficientize high throughput calculations (DFT, device modeling), using regression & classification, image translation, inverse problems.



Phys. Chem. Chem. Phys. 26, 22090 (2024)



Team & Resources

Nicolae Filipoiu
PhD

Amanda Preda
PhD student

Calin Pantis
PhD student

Alaa Allosh
PhD student

Mihaela Cosinschi
MSc student

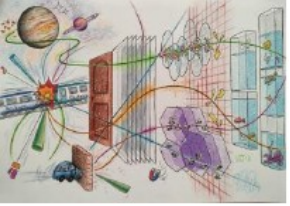
Computing infrastructure @ IFIN-HH / DFCTI

→ DFCTI is already participating in the LHC Computing Grid experiment, contributing with the RO-07-NIPNE grid site to the support of the ALICE, ATLAS and LHCb experiments, within the Worldwide LCG collaboration:

* DFCTI@IFIN-HH Grid computing infrastructure, 7,000 CPU cores, 8.5 PB storage

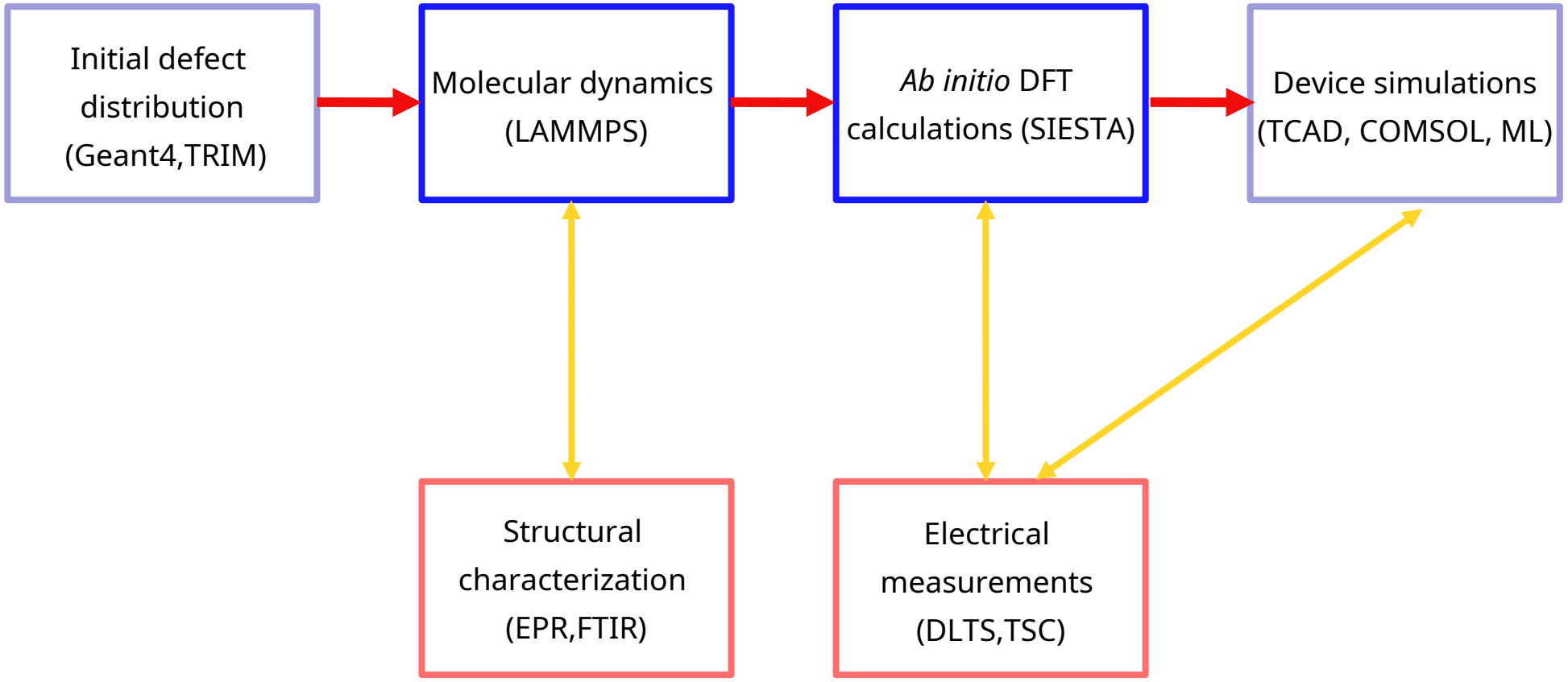
→ DFCTI@IFIN-HH Cloud computing infrastructure, CLOUDIFIN.1,000 CPU cores, Infiniband HDR100 100Gbps, 360 TB storage

→ **For DRD3 activities:** 4x server with min 48 CPU cores, min 256 GB DDR4 RAM, Infiniband HDR100, min 10 GbE (dual-port), 80 TB storage, that will be integrated in the CLOUDIFIN infrastructure and dedicated to the project.

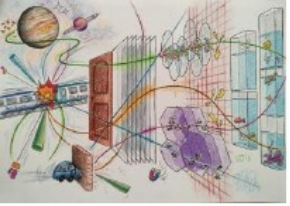


Project workflow

Numerical simulations

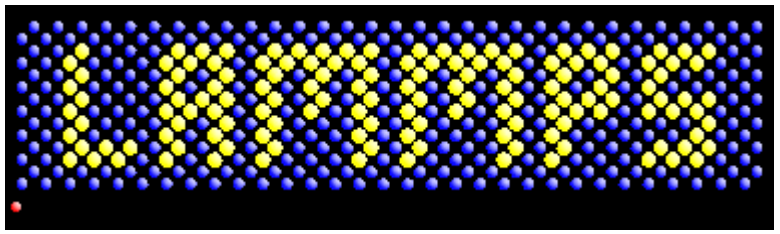


Experimental investigations



Molecular dynamics with LAMMPS

LAMMPS = Large-scale Atomic/Molecular Massively Parallel Simulator



→ Started calibration runs

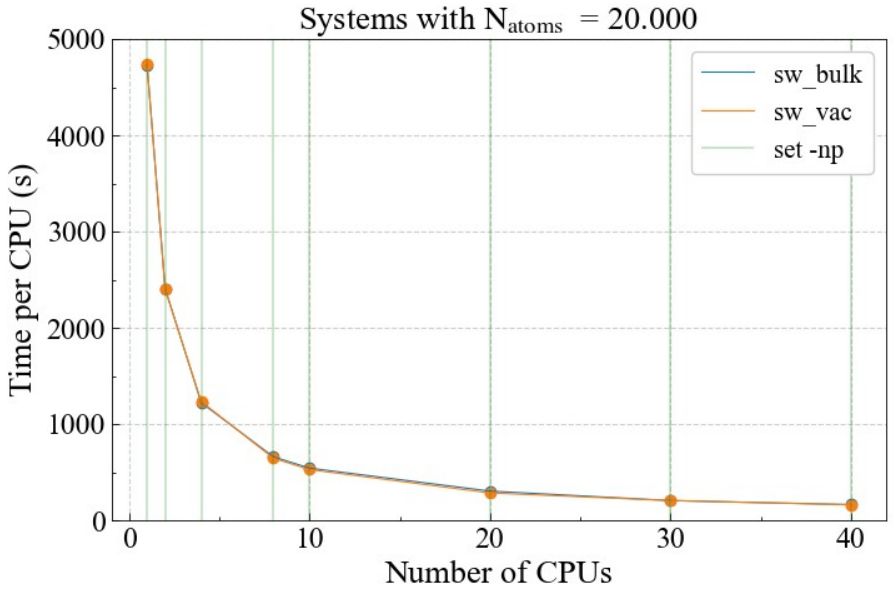
→ Bulk ideal Silicon (up to 100000 atoms)

→ Systems with vacancies (1%)

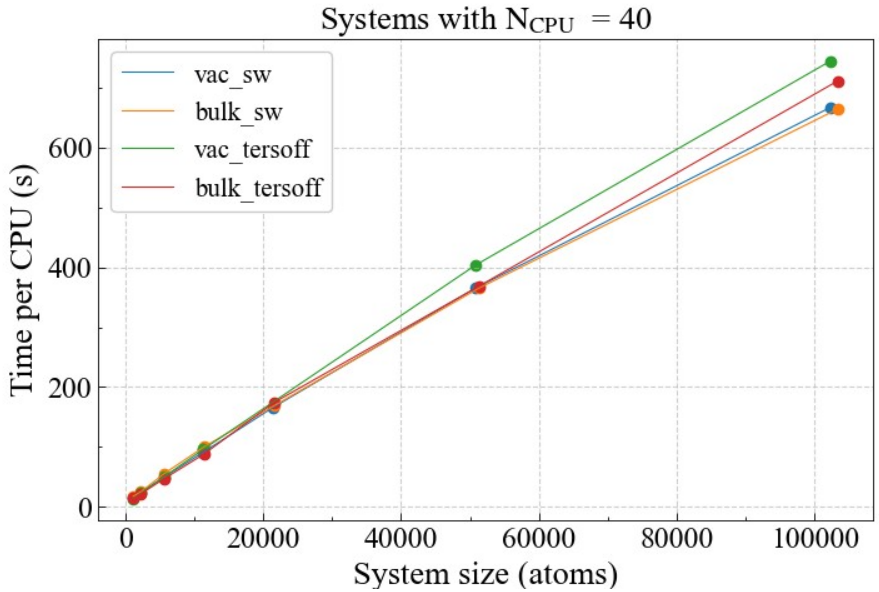
→ Simulation parameters: 10^5 steps, 1 fs timestep, T = 300K.

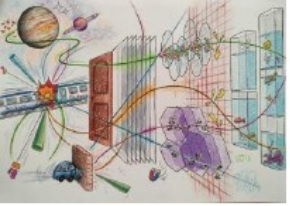
→ Timing tests (100 ps):

Number of cores (N_{atoms}=20000)



Number of atoms (N_{cores}=40)





LAMMPS – Vacancy migration

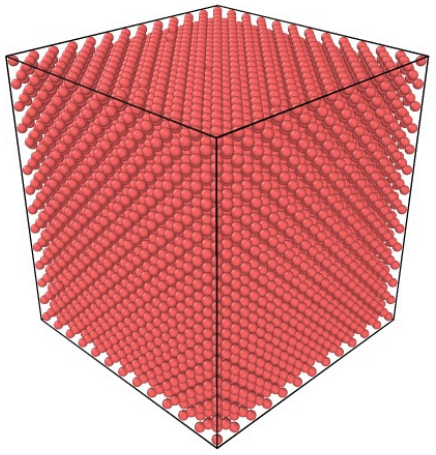
Characterized by Mean Square Displacement (MSD):

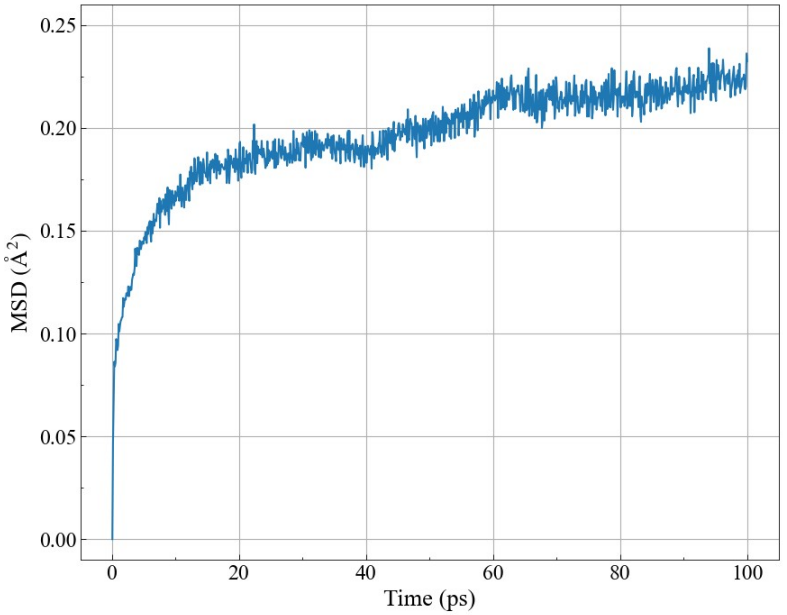
$$\mathrm{MSD}(t) = \frac{1}{N_\mathrm{I}} \sum_{i=1}^{N_\mathrm{I}} |\mathbf{r}_i(t) - \mathbf{r}_i(0)|^2$$

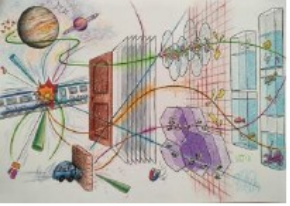
Diffusion coefficient: $$D = \frac{1}{6} \lim_{t \to \infty} \frac{\mathrm{MSD}(t)}{t}$$

Simulation box:

15000 atoms, 1% vacancies





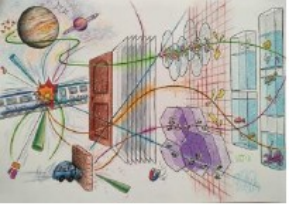


MD/LAMMPS – Proposed activities

1. MD simulations shall be used to evaluate **defect dynamics** after irradition (initial defect distributions can be provided by Geant/TRIM).

2. MD simulations will be used to capture **defects metastability**, in particular boron containing defects, also in the context of **co-doping with impurities (O, C, and/or P)** and irradiation fluence.

3. The **relevant defect configurations** will be identified and assigned for further investigations of electronic properties by *ab initio* calculations. This will be performed in close correlation with experimental characterization techniques (EPR,FTIR).



DFT calculations using SIESTA

DRD3

Spanish Initiative for Electronic Simulations with Thousands of Atoms

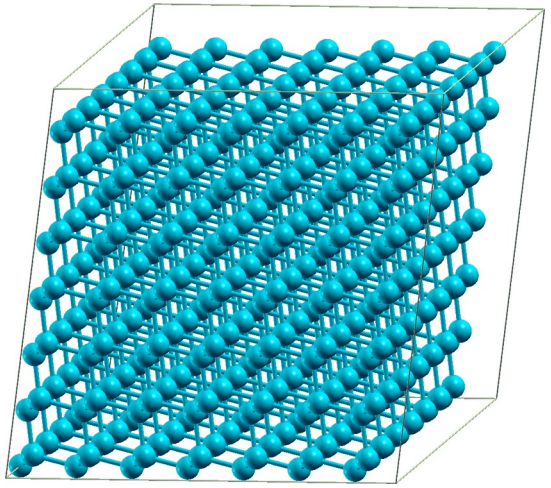
Density Functional Theory (DFT) calculations provide:

Total energy and charge density in the ground state.

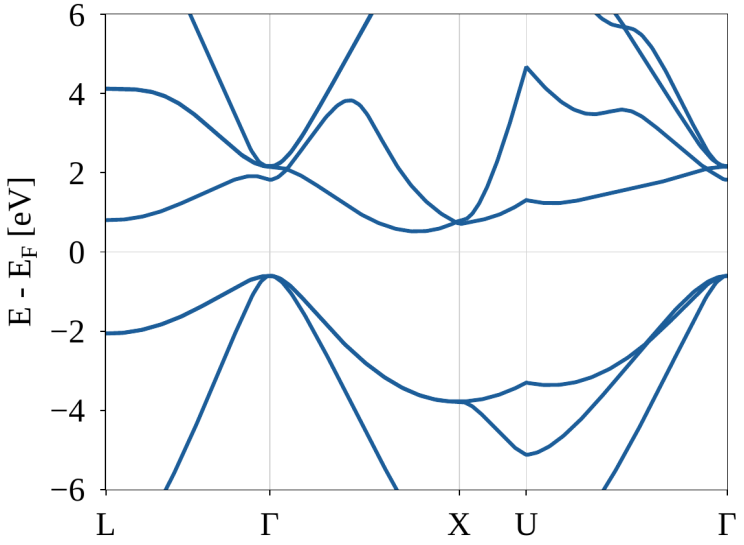
SIESTA features:

- Strictly localized numeric atomic orbitals (NAOs) → linear scaling of the computational time with the system size → large supercells
- Pseudopotential approach → core electrons are frozen, only valence electrons are included in the calculations

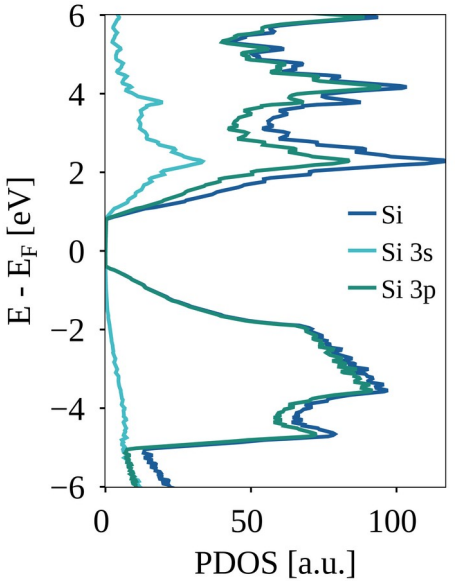
Silicon (7x7x7 supercell)

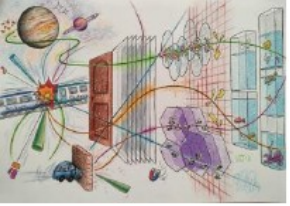


Band structure



Projected density of states





Defect formation energies and transition levels

Neutral and charged defect formation energies:

$$E^f[X^q] = E_{tot}[X^q] - E_{tot}[ideal] - \sum_i n_i\mu_i + q(E_{VBM} + \mu_e) + E_{corr}$$

→ Defect concentrations:

$$c = N_{\text{sites}}\ N_{\text{config}}\ \exp\left(-E^f/k_{\text{B}}T\right)$$

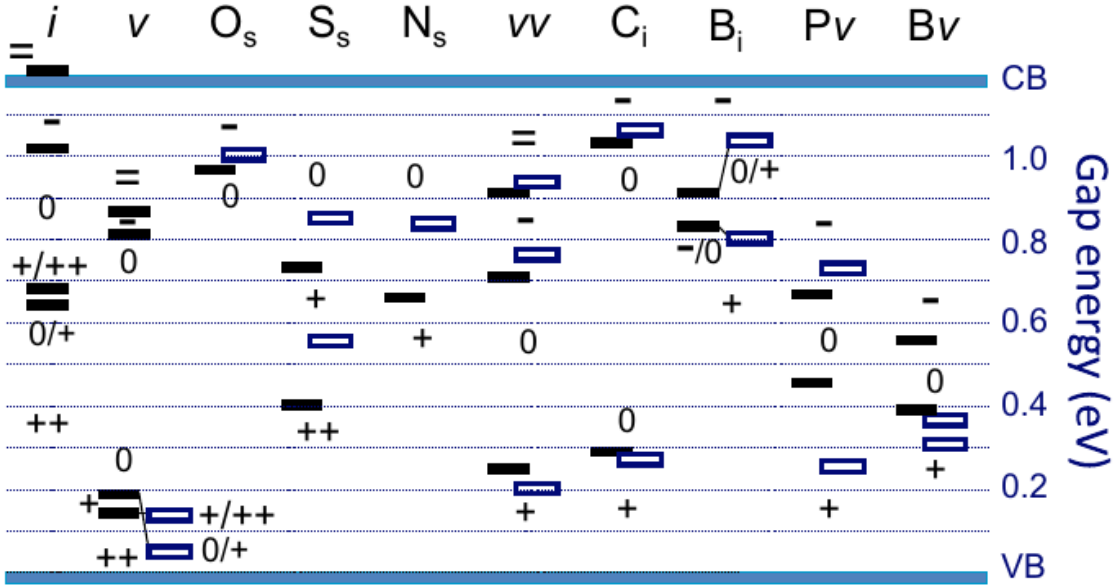
C.G. Van der Walle et al., *J. Appl. Phys.* 95, 3851 (2004)

→ Defect transition levels:

$$\epsilon(q/q') = \frac{E^f[X^q] - E^f[X^{q'}]}{q' - q}$$

Broberg et al., *npj Comput. Mater.* 9, 72 (2023)

PBE/DFT calculations in good agreement with experiment (~0.1 eV average error)



P.A. Schultz et al., *Nucl. Instrum. Methods Phys. Res. B* 327, 2 (2014)

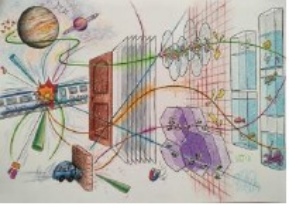
In recent years, several complex defects have been analyzed by DFT:

→ CsCs & CsCsV

[*Silicon* 16, 703 (2024)]

→ $CiOi(Si_I)_2$

[J Mater Sci: Mater Electron 28, 10296 (2017)]



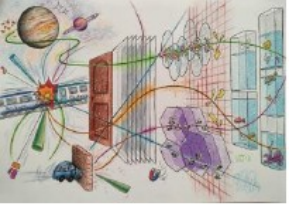
DFT – Proposed activities

1. A supercell approach will be employed in order to establish the **defect reactions**.

2. Evaluate the **formation energies of complex defects** (di-, tri-vacancies etc, cluster defects) in the context of extrinsic impurities (O, C and/or P). Neutral and charged defects shall be considered.

3. Determine the (potential) **local minima configurations and saddle points**:
Nudged Elastic Band (NEB) and molecular dynamics at DFT level.

4. The donor character of **Boron containing defects (BCD)** will be investigated in connection with the **acceptor removal process (ARP)**.



Machine learning (ML) approaches

A short note on ML approaches:

1. Objective: Efficientize computationally demanding simulations (*ab initio*, MD, device simulations).

2. Steps:

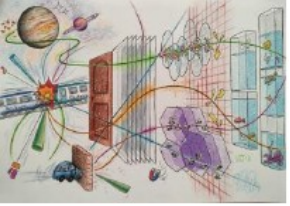
→ Construct the data sets by high throughput calculations (*ab initio*, MD, device simulations);

→ Identify features (e.g. defect configuration) for targeted property (e.g. formation energy).

→ Perform the mapping (e.g. using artificial neural networks -- ANNs)

→ Validate the model on a test set.

3. Methodologies: Besides „classical“ ML approaches, like conventional ANNs, one can employ other techniques such as time series prediction for MD, image-to-image translation procedures for inverse (device) design.



Challenges and open questions

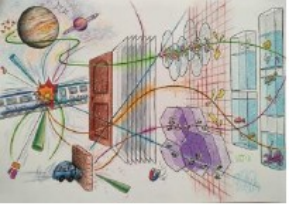
1. Identification of relevant complex defect structures and their electronic properties → to be achieved by high throughput MD and *ab initio* calculations in correlation with experimental studies.

2. Some of the force field parametrisations for LAMMPS (e.g. for extrinsic impurities) are not known → they can be determined from DFT calculations.

3. Low doping densities require large supercells → supercell size scaling analysis and interpolation is needed, DFTB approach can extend the size of the supercell.

4. Mitigation of acceptor removal process → to be achieved by defect engineering.

5. Complex and resource consuming simulations (in particular DFT & device simulations) → develop machine learning techniques based on existing data sets.



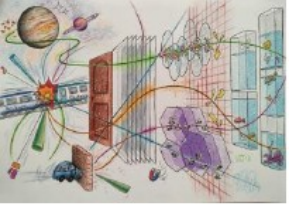
Final remarks

→ Our project proposal is focused is on WP3 / RG3.2 & RG3.4: radiation damage at high fluences

→ Primary goal: Understanding the radiation damage at microscopic level, in particular the acceptor removal process (ARP) in connection with boron containing defects, following irradiation.

→ Methodologies: first principle calculations (SIESTA), molecular dynamics (LAMMPS) in connection with experimental results.

→ The fundamental understanding and mitigation of ARP – will enable a predictable behavior of LGAD devices.



DRD3

Thank you for your attention !