Simulating displacement damages in electronic devices: from primary knock-on atom to electronic noise

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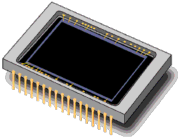
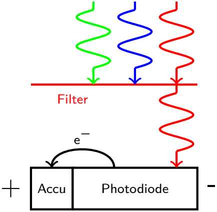
[2]STMicroelectronics, *Crolles, France*
[3]CIMI-DEOS, *ISAE SUPAERO, Université de Toulouse, France*
[4]CNR-IOM, *Democritos and Sissa, Trieste, Italy*
[5]CEA, DAM, DIF, *Arpajon, France*
[6]ZTF-IRB, *Zagreb, Croatia*
[7]CNES, *Toulouse, France*

November 29th 2023

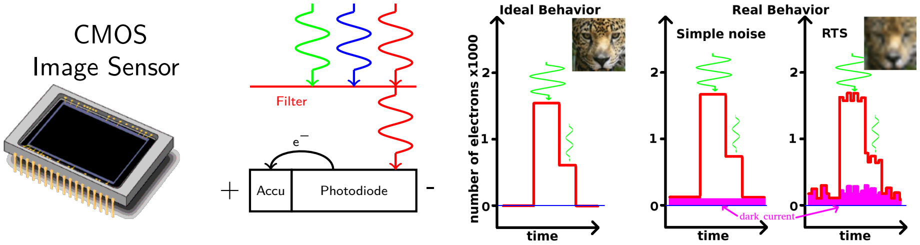
Context: leakage current, CMOS example

CMOS
Image Sensor





Context: leakage current, CMOS example



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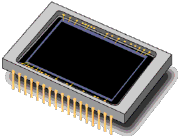
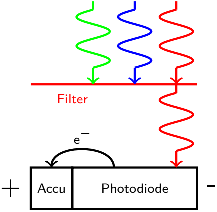
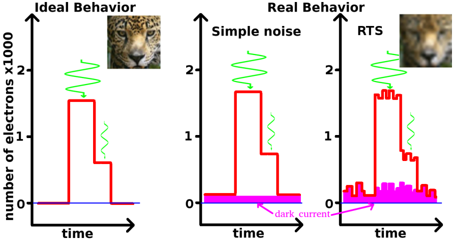
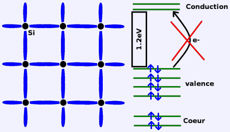




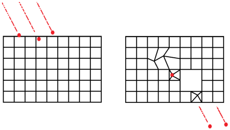


S-C ideal view

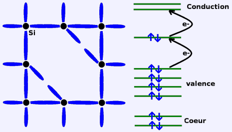


perfect device
noise ~ 0

irradiation
implantation
deposition



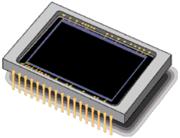
S-C real view

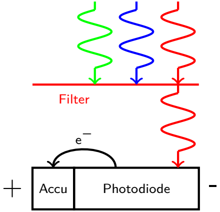


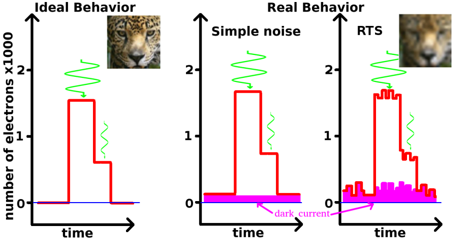
defective device
noise $\gg$ signal

Context: leakage current, CMOS example

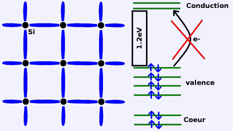
CMOS
Image Sensor







S-C ideal view



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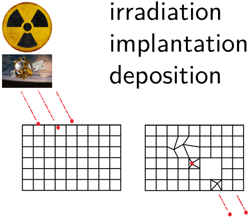
noise ~ 0



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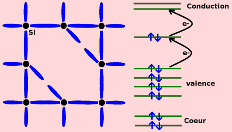
S-C real view

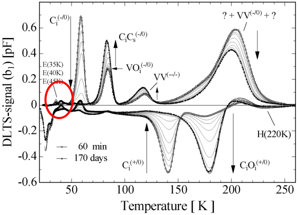


defective device
noise $\gg$ signal

Unpredictable: technological problem, challenging modelization

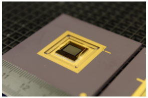
Why studying defects with image sensors?

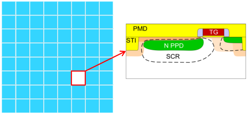
- Photoluminescence,
- Electron Paramagnetic Resonance
- Deep Level Transient Spectroscopy
- Raman and Infra-Red
  - stable defects
  - many IDENTICAL defects: $10^9/\text{cm}^3$



M. Moll, PhD thesis, 1999

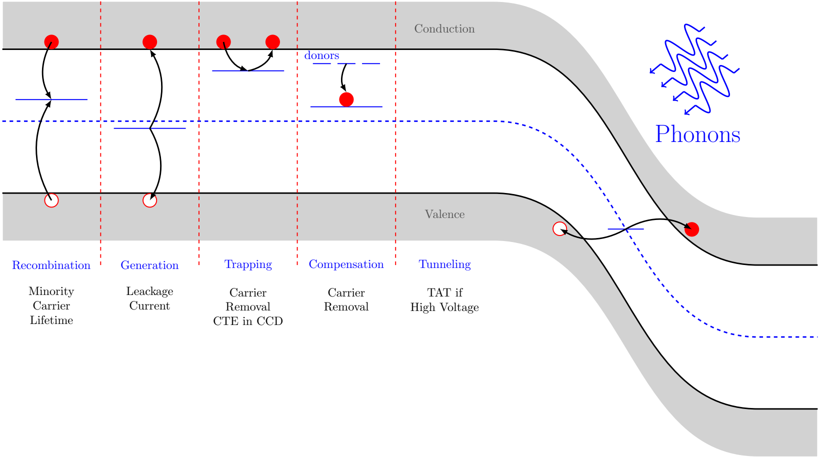
- Monitoring pixel array
  - metastable defects
  - 1 single defect
  - Statistics





Focus of the talk

Effect of Displacement Damage (not Total Ionizing Dose)
Reverse biased *pn* junction, bulk Silicon



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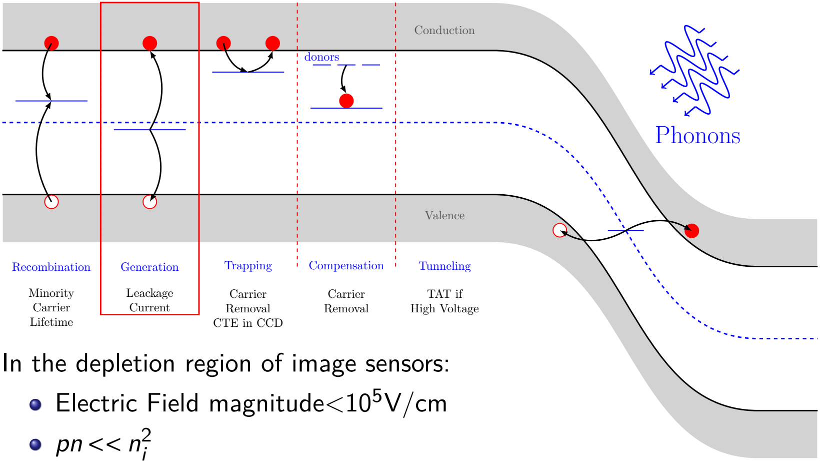


In the depletion region of image sensors:

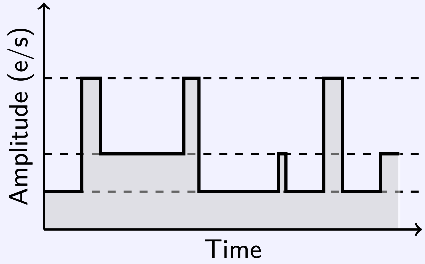
- Electric Field magnitude$<10^5$V/cm
- $pn << n_i^2$
- 1 single defect generation dominates the signal

Overview

Table of Contents

Random Telegraph Signal characteristics

Measured RTS



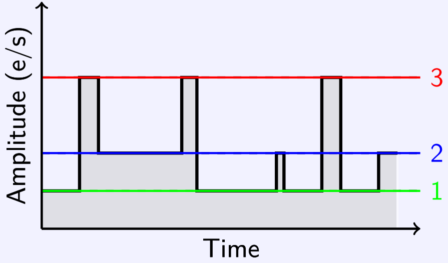
Observations

Characteristics:

- Number of levels
- Life times
- Activation Energies
- Amplitudes

Random Telegraph Signal characteristics

Measured RTS



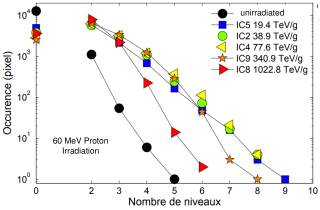
Observations

1 to 10 levels

$10=5\times 2$ or $10=2\times 5$ or $10=10\times 1$

Characteristics:

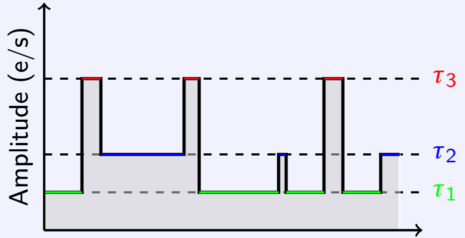
- Number of levels
- Life times
- Activation Energies
- Amplitudes



C. Virmontois, PhD thesis, 2012

Random Telegraph Signal characteristics

Measured RTS



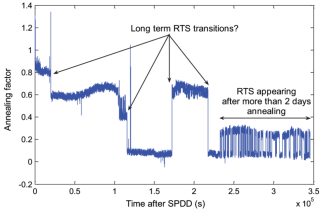
Observations

From ms to months

$$1/\tau \quad \sim \quad exp(-E/k_B T)$$

Characteristics:

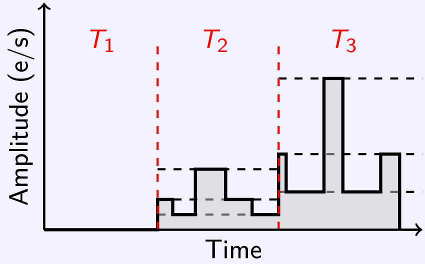
- Number of levels
- Life times
- Activation Energies
- Amplitudes



M. Raine *et al.*, IEEETNS, 2014

Random Telegraph Signal characteristics

Measured RTS



Observations

Need Temperature to activate

$$A \sim exp(-E_a/k_B T)$$

Characteristics:

- Number of levels
- Life times
- Activation Energies
- Amplitudes

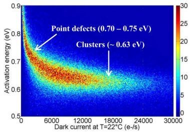
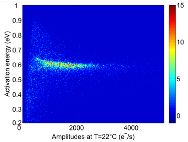


Fig. 3. Dark current activation energy in CIS 2 (10^{12} cm^{-2} 22 MeV neutrons). The color scale corresponds to the pixel occurrence.

Cst DC

J.M. Belloir, PhD thesis, 2017

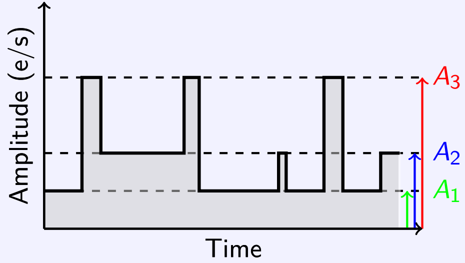


DC RTS

C. Durnez, PhD thesis, 2017

Random Telegraph Signal characteristics

Measured RTS



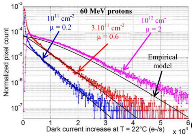
Observations

$$A_i - A_j > 10^3 \;\; e/s$$

Predictable exp. shape: f(DD, V_{dep})

Characteristics:

- Number of levels
- Life times
- Activation Energies
- Amplitudes



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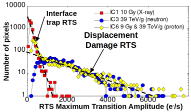
J.M. Belloir, PhD thesis, 2017



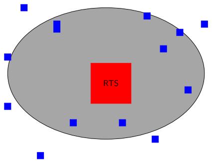
DC RTS

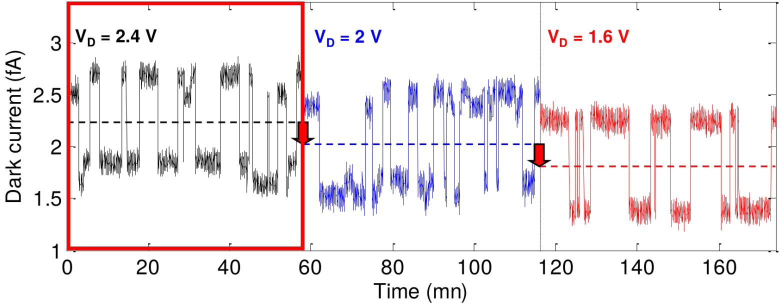
C. Virmontois, PhD thesis, 2012

Effect of electric field?

Small Voltage + low doping (no tunneling)

- Mean DC decreases
- No change in RTS amplitudes





see C. Durnez, PhD thesis, 2017 for larger voltages

Electric field not needed to explain large RTS relative amplitudes.

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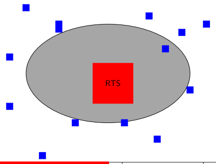

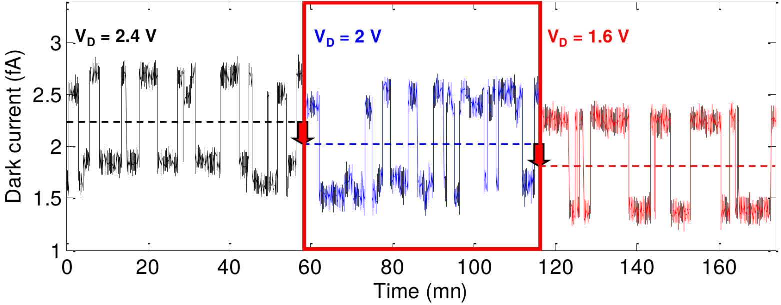

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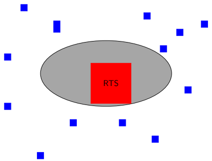
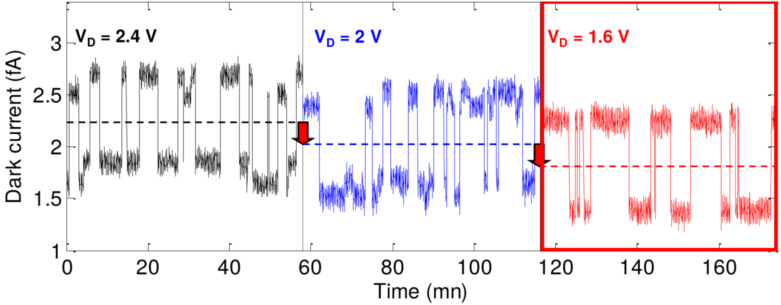




see C. Durnez, PhD thesis, 2017 for larger voltages

Electric field not needed to explain large RTS relative amplitudes.

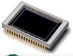
Technology? Material?

All the components:

PV cells 

Fiber 

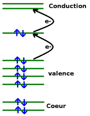
IR sensors 

CMOS 

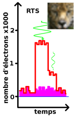
DRAM 

SPAD 

Same phenomenon:



⇒

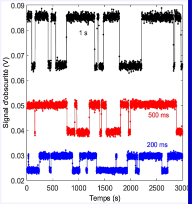


⇒

↘ efficacity, ↘ life time

Si

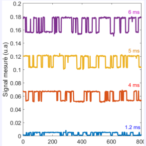
CMOS



C. Durnez thesis, 2017

InSb

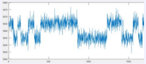
IR Photod



C. Durnez thesis, 2017

HgCdTe

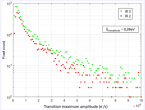
IR Photod



E. De Borniol, CEA LETI

InGaAs

IR Photod



Virmontois *et al.*,

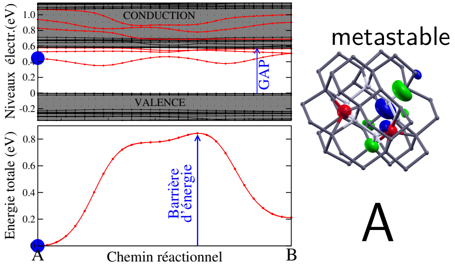
IEEETNS 2021

Constant and RTS leakage currents are everywhere

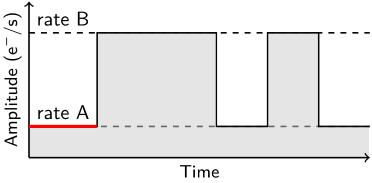
Table of Contents

State of the art

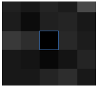
ab initio capacities



Observation in devices



CMOS example
Pixel flashes

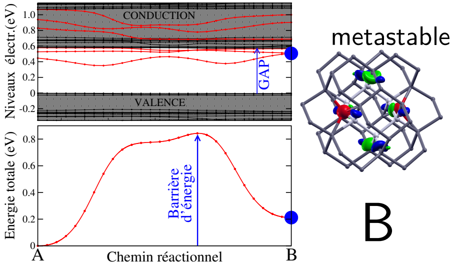


structure variation ⇒ noise variation=RTS

Challenge: Quantify the number of generated electrons

State of the art

ab initio capacities



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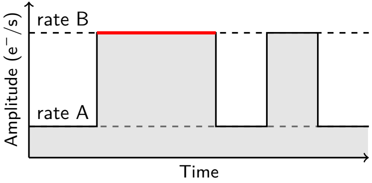

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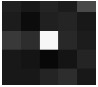

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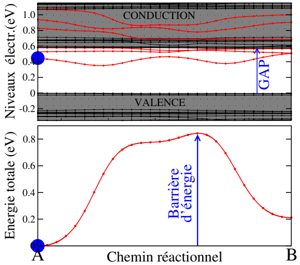
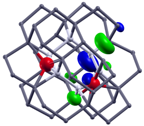
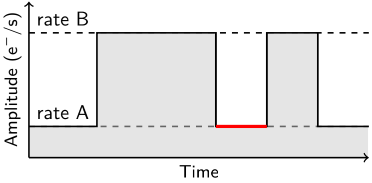


metastable



A

Observation in devices



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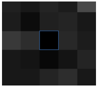

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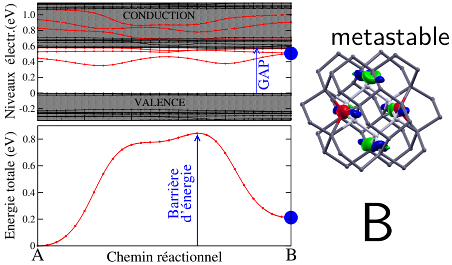

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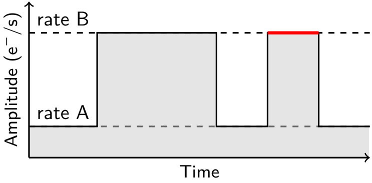

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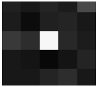

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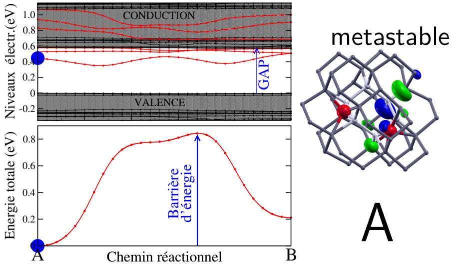

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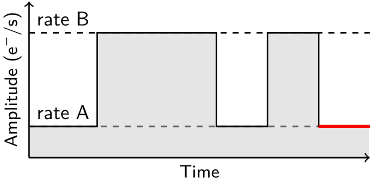

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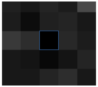
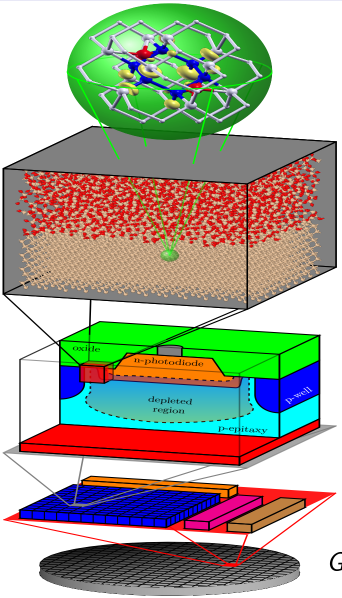


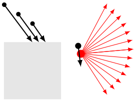
structure variation $\Rightarrow$ noise variation=RTS

Challenge: Quantify the number of generated electrons

Strategy to simulate the impact of irradiation/implantation



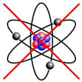
Problem : Apply Shockley Read Hall

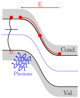


Rapidity Vs Precision

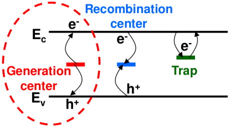
- -Incomplete mechanisms
- -Bad time scale
- -Not transportable

No atomic structure



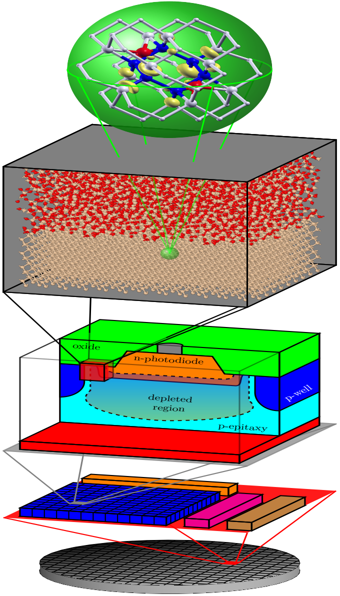


Neutrons, Dopants … → Primary knock on atom (KMC) → ~~SRH~~ → E-h: generation rate



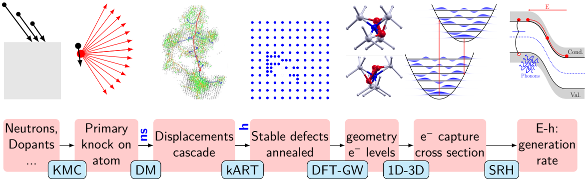
$$G_{SRH} = \frac{v_{th}\sigma_n\sigma_p(n_i^2 - np)}{\sigma_n[n + n_i exp(\frac{E_t - E_F}{k_B T})] + \sigma_p[p + n_i exp(\frac{E_t - E_F}{k_B T})]}$$

Strategy to simulate the impact of irradiation/implantation

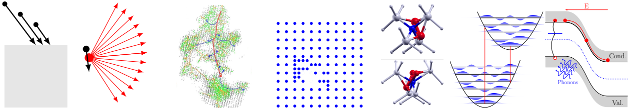


Problem : Apply Shockley Read Hall

Solution: Multi-scale model



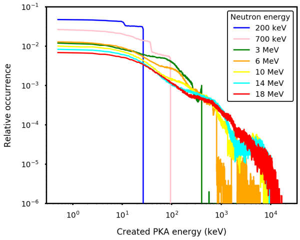
Step 1: get PKA energies

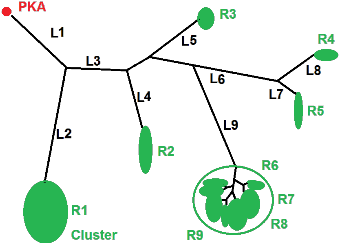


Neutrons, Dopants … → Primary knock on atom →ns→ Displacements cascade →h→ Stable defects annealed → geometry e^- levels → e^- capture cross section → E-h: generation rate

KMC DM kART DFT-GW 1D-3D SRH

GEANT4: binary collision approximation in $Si_{0.8}Ge_{0.2}$

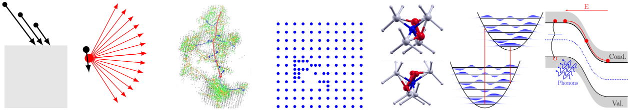




Raine *et al.*, IEETNS 2017

mean free path = cluster size → overlap

Step 2: Collision Cascades - method

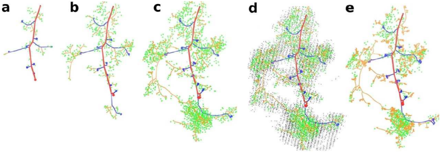


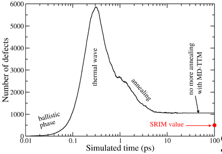
Neutrons, Dopants … → Primary knock on atom → Displacements cascade → Stable defects annealed → geometry e^- levels → e^- capture cross section → E-h: generation rate

KMC | DM (ns) | kART (h) | DFT-GW | 1D-3D | SRH

- Solve equation of motion
- 1 interatomic potential
- 1 million crystalline Si atoms
- 10 keV PKA

A. Jay, IEETNS 2017

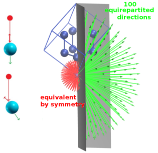


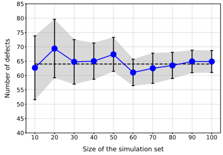


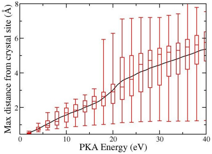
SRIM?

Step 2: Collision Cascades - improved

Stochasticity



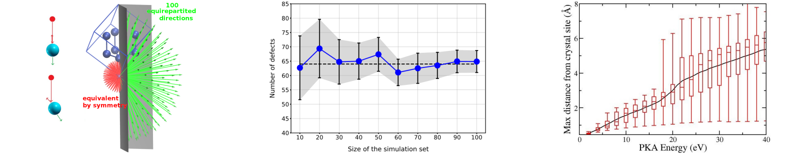




T. Jarrin *et al.*, NIMB 2021

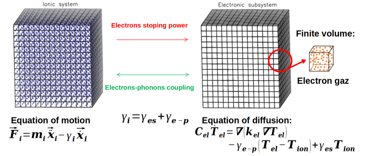
Step 2: Collision Cascades - improved

Stochasticity



T. Jarrin *et al.*, NIMB 2021

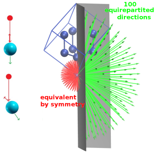
Electronic Stopping power

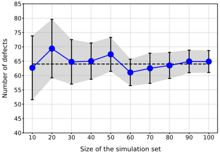


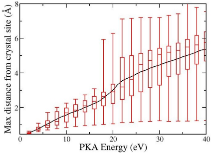
T. Jarrin *et al.*, NIMB 2020

Step 2: Collision Cascades - improved

Stochasticity

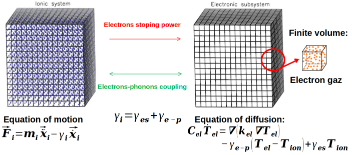






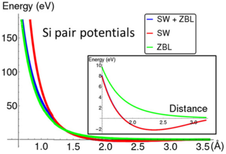
T. Jarrin *et al.*, NIMB 2021

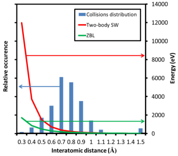
Electronic Stopping power



T. Jarrin *et al.*, NIMB 2020

Short Range interaction Potential

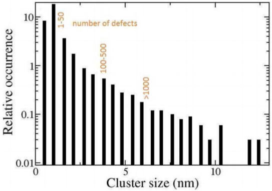


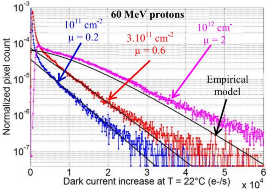


T. Jarrin *et al.*, IEETNS 2020

Step 2: Collision Cascade - results

Exponential Shape

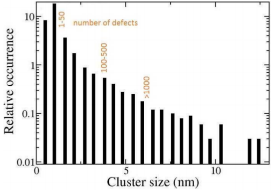


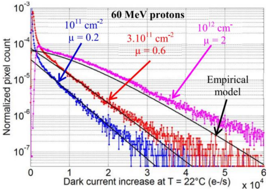


A. Jayet *al.* IEETNS 2017 ⚠correlation≠ causality → need more

Step 2: Collision Cascade - results

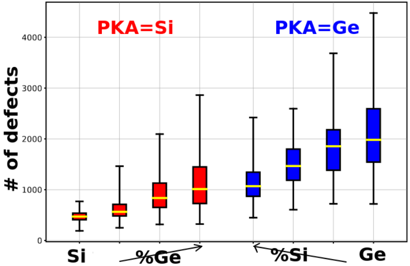
Exponential Shape





A. Jay*et al.* IEETNS 2017 ⚠correlation≠ causality → need more

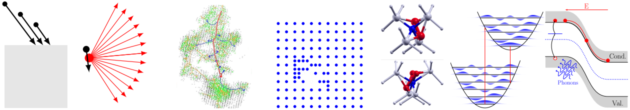
Different materials



- Ge PKA damage more the material than Si PKA
- The greater the % of Ge, the more defects are produced

T. Jarrin, PhD Thesis, 2021

Step 3: Long time annealing of the defects - method



Neutrons, Dopants … → Primary knock on atom → ns → Displacements cascade → h → Stable defects annealed → geometry e^- levels → e^- capture cross section → E-h: generation rate

KMC | DM | kART | DFT-GW | 1D-3D | SRH

Potential Energy Surface

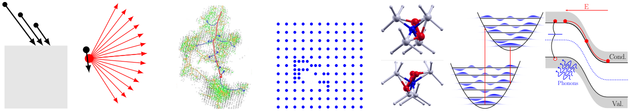
Find Transition State

- Stable structures = minima
- Transition states = saddle point
- Activation Relaxation Technique
- Init+Saddle+Final= event

A. Jay *et al.*, JCTC 2020

A. Jay *et al.*, CMS 2022

Step 3: Long time annealing of the defects - method



Neutrons, Dopants … → Primary knock on atom → ns → Displacements cascade → h → Stable defects annealed → geometry e^- levels → e^- capture cross section → E-h: generation rate

KMC | DM | kART | DFT-GW | 1D-3D | SRH

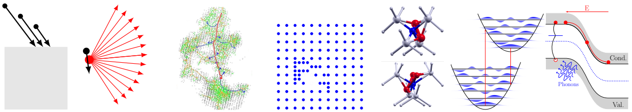
Potential Energy Surface

Stabilize the system

- Start from DM last structure
- Find all atomic events
- Choose 1 event and apply it
- Do it again

L.K. Béland *et al.*, PRE 2011

Step 3: Long time annealing of the defects - method



Neutrons, Dopants … → Primary knock on atom →(ns) Displacements cascade →(h) Stable defects annealed → geometry e^- levels → e^- capture cross section → E-h: generation rate

KMC | DM | kART | DFT-GW | 1D-3D | SRH

Structure evolution

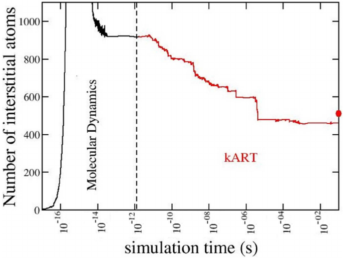
Change atomic positions

- Flickers appears= metastable states

A. Jay *et al.*, IEETNS 2016

Step 3: Long time annealing of the defects - results

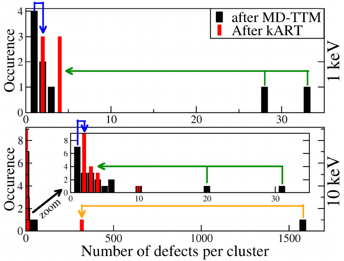
Potential Energy Surface



A. Jayet *al.*, IEETNS 2016

- Reach correct # of defects
- Reach experimental time scales

Potential Energy Surface



A. Jayet *al.*, IEETNS 2016

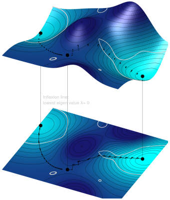
- Reduction of the clusters size
- Diffusion agglomeration of point defects

Step 3: Long time annealing of the defects - results

Number of levels problem!

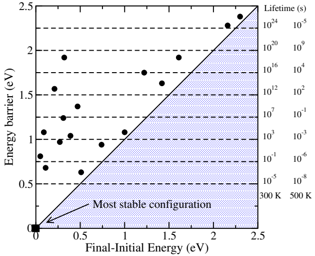
- point defects are simple: small number of topologies
- Clusters are complicated: many topologies

1 RTS level = 1 stable configuration



PES Exploration with ARTn-DFT

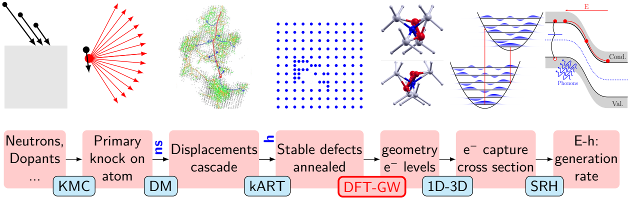
14I cluster PES



A. Jayet *al.*, SISPAD 2021

A cluster exists in many different configurations!

Step 4: *Ab initio* - method

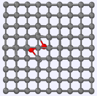


solve Hamiltonian $H|\Psi_i\rangle = E|\Psi_i\rangle$

- Get total E and Forces → minimization
- Get electronic states (corrected by GW)

Step 4: *Ab initio* - Si defects bestiary

compacts V, 2V, 3V, 4V, 5V, 6V

I1

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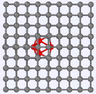
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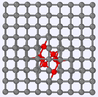
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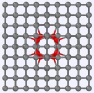
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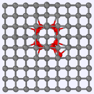
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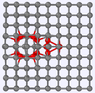

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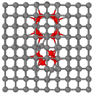
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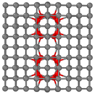
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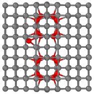
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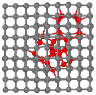
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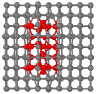
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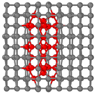
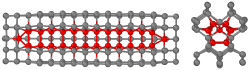
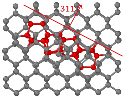
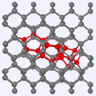


Chain-like


rod-like 311


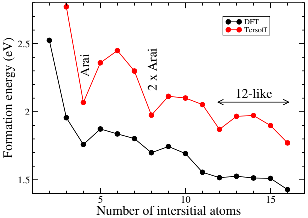
Amorphous


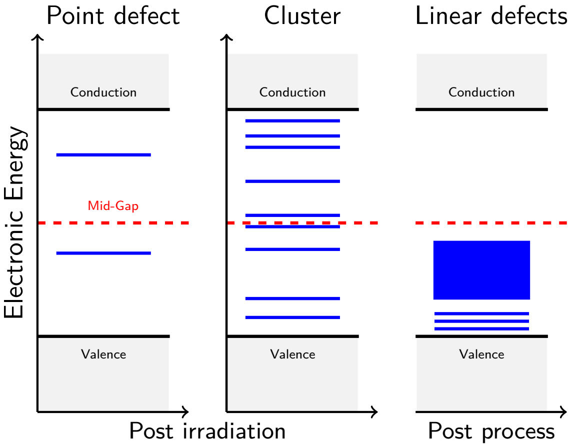
dislocation loop

⚠POST-IRRADIATION ≠ POST-IMPLANTATION+ANNEALING

Step 4: *Ab initio* - results on annealed clusters

Lower E_f = more stable





Step 4: *Ab initio* - results on simple DC

Case: simple DC

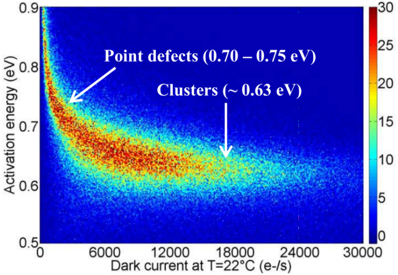


Fig. 3. Dark current activation energy in CIS 2 (10^{12} cm^{-2} 22 MeV neutrons). The color scale corresponds to the pixel occurrence.

$$E_{act} > \frac{E_{GAP}}{2}$$

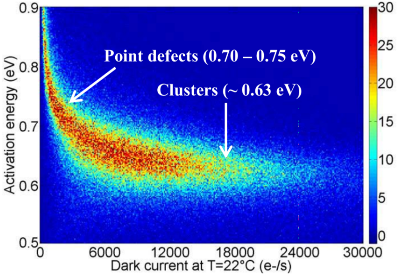
WORST= midgap

Proba ~ 0 Proba = ?

Observed crossing through 1 level

Step 4: *Ab initio* - results on simple DC

Case: simple DC



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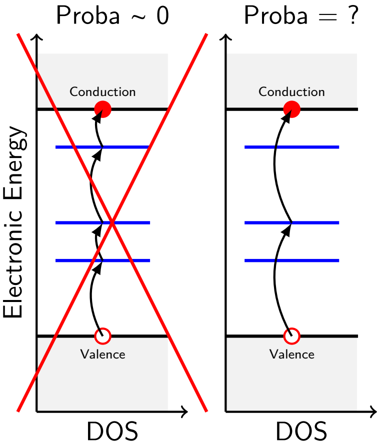
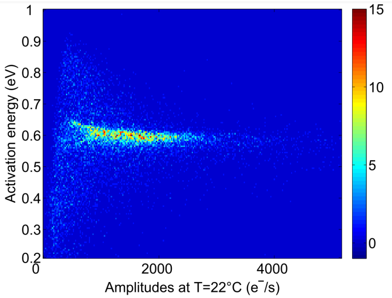
WORST$=$ midgap



Observed crossing through 1 level

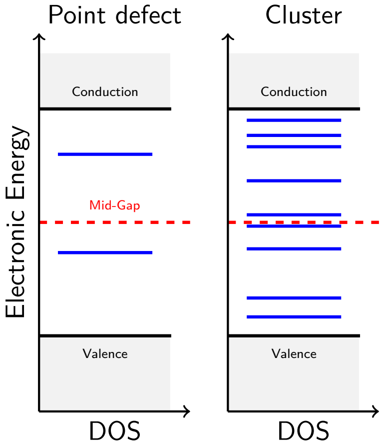
Step 4: *Ab initio* - results on DC-RTS

Case: DC-RTS



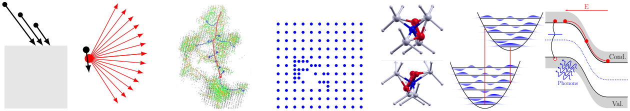
$$E_{act} \sim \frac{E_{GAP}}{2}$$

Many levels → 1 is midgap



Clusters have many electronic levels in the band gap

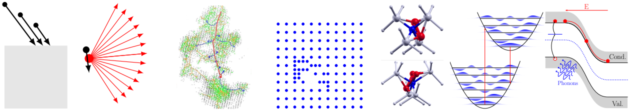
Step 5: Electronic capture rate - Amplitude problem



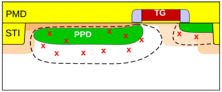
Neutrons, Dopants … → Primary knock on atom → Displacements cascade → Stable defects annealed → geometry e$^-$ levels → e$^-$ capture cross section → E-h: generation rate

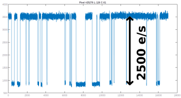
KMC | ns | DM | h | kART | DFT-GW | 1D-ND | SRH

Step 5: Electronic capture rate - Amplitude problem



Neutrons, Dopants … → (KMC) → Primary knock on atom → (DM) ns → Displacements cascade → (kART) h → Stable defects annealed → (DFT-GW) → geometry e^- levels → (1D-ND) → e^- capture cross section → (SRH) → E-h: generation rate





SRH generation rate:

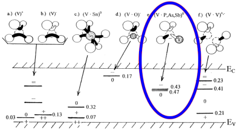
$$A \approx \frac{\sigma v_{th} n_i}{2cosh\left(\frac{E_t - E_{mg}}{k_B T}\right)}$$

σ= e^- cross section

v_{th}=2.7×10^{7}cm/s

n_i=1.45×10^{10}/cm^3

Worth known point defect

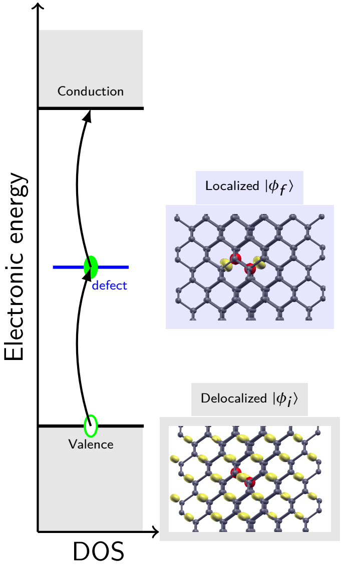


PV:Phosphorus-Vacancy in Silicon

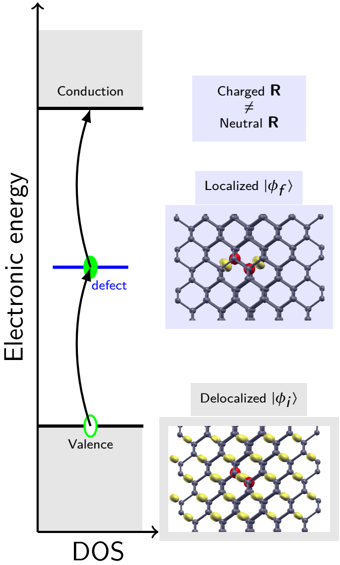
$$\left.\begin{aligned} \sigma &= 10^{-15}\ cm^2 \\ E_t - E_{mg} &= 0.07 eV \end{aligned}\right\} 20\ e/s\ (300\ \text{K})$$

$\boxed{\text{Need larger } \sigma}$

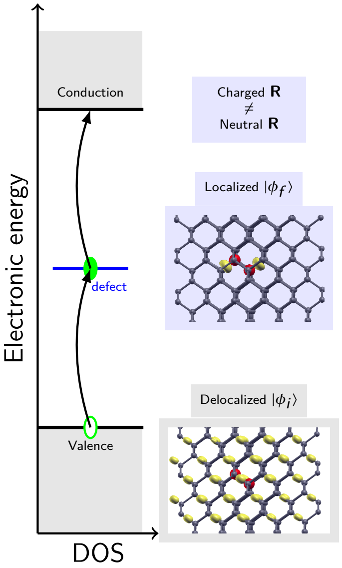
Step 5: multiphonon excitation - method



Step 5: multiphonon excitation - method

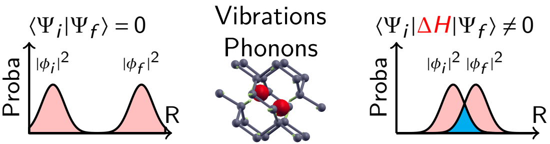


Step 5: multiphonon excitation - method



Fermi's Golden rule = overlap

$$\Gamma_{i \to f} \sim |\langle \Psi_i | \Delta H | \Psi_f \rangle|^2$$



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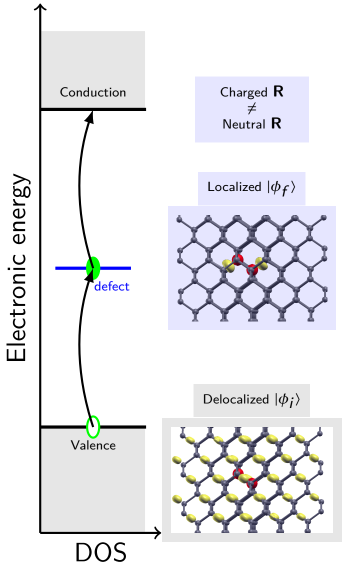

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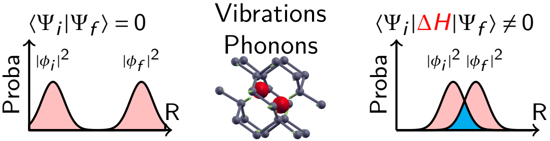


Born-Oppenheimer

$$\Psi_n(\mathbf{r},\mathbf{R}) = \phi_n(\mathbf{r},\mathbf{R})\chi_n(\mathbf{R})$$

Taylor 1rst order

$$\Gamma_{i\to f} \sim$$

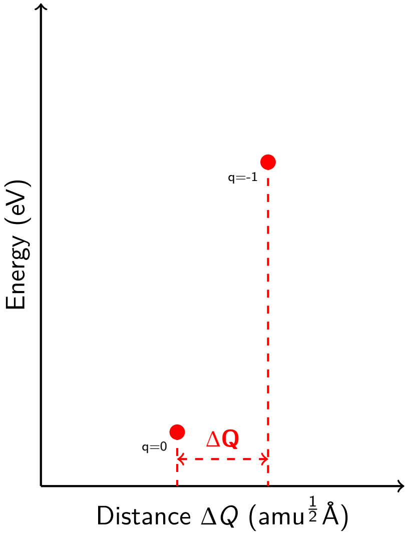
$$|\sum_k^{N_{modes}} \underbrace{\langle\phi_i|\frac{\partial H}{\partial \mathbf{Q_k}}|\phi_f\rangle}_{electrons} \underbrace{\langle\chi_{im}|\Delta\mathbf{Q_k}|\chi_{fn}\rangle}_{ions}|^2\Delta E$$

need ~10 phonons → multiphonon

Step 5: Electronic part - method : 1D model

Approximation:
1 fictive phonon is responsible of the transition

- Relax $\mathbf{R_i}$ at $q=0$ and $q=1$
- E_{tot} for $\mathbf{R^{q=0}_{0\rightarrow 1}}$ and $\mathbf{R^{q=1}_{0\rightarrow 1}}$
- Fit the curvature: $\omega = \frac{\partial^2 E}{\partial \mathbf{Q}^2}$
- Deduce number of needed phonons $n\hbar\omega$
- $\langle \phi_i | \frac{\partial H}{\partial \mathbf{Q}} | \phi_f \rangle$ (back up slides)



A. Alkauskas *et al.* JAP 2016

Step 5: Electronic part - method : 1D model

Approximation:
1 fictive phonon is responsible of the transition

- Relax $\mathbf{R_i}$ at $q = 0$ and $q = 1$
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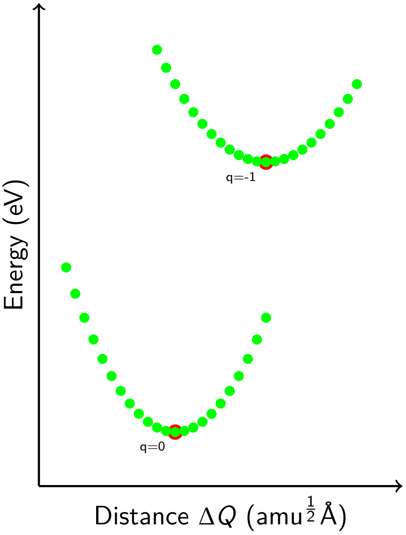

A. Alkauskas *et al.* JAP 2016

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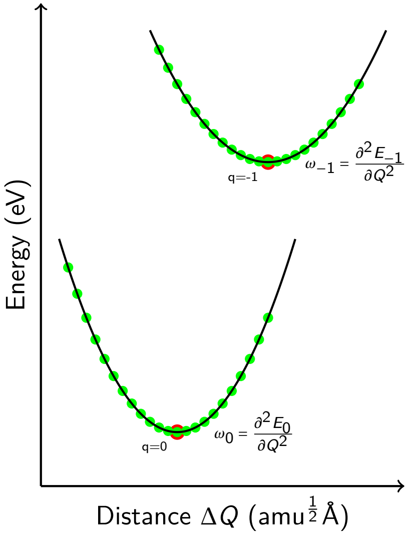

A. Alkauskas *et al.* JAP 2016

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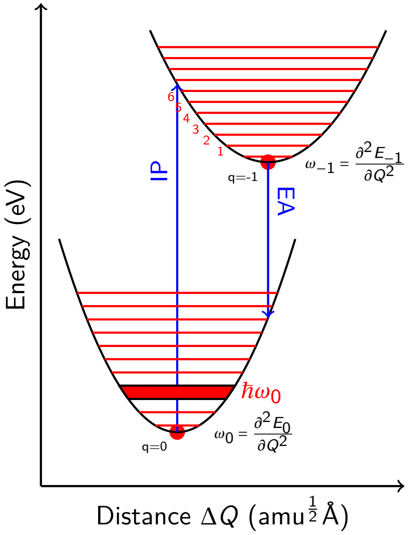

A. Alkauskas *et al.* JAP 2016

Step 5: Electronic part - method : 1D model

Approximation:
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  for $\mathbf{R^{q=0}_{0\rightarrow 1}}$ and $\mathbf{R^{q=1}_{0\rightarrow 1}}$
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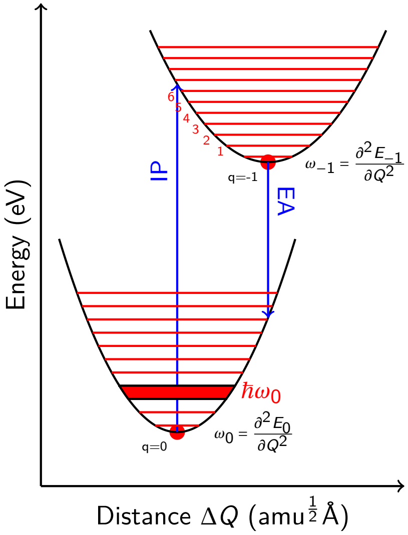
  (back up slides)



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Step 5: Ionic part - method 1D vs ND

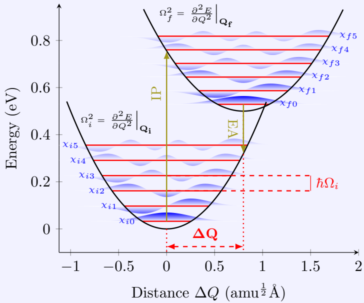
$$H^{ion}|\chi_n(\mathbf{R})\rangle = E_n|\chi_n(\mathbf{R})\rangle$$

1 dimension

Analytic solutions

Hermite polynomials order n

$$n = \frac{1}{exp(\hbar\omega/k_B T) - 1} \text{ (BE)}$$



N dimensions

Sol: 2^{nd} quantification

Huang, Prog. Phys., **1**, 31 (1981)

Borrelli, J. Phys. Chem. A **116**, 9934 (2012)

No direct solution

Xiao, Sci. China Phys. Mech. Astron. **63**, 277312 (2020)

Work in progress (backup)

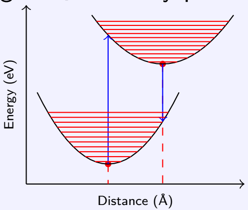
A. Jay *et al.*, SISPAD 2023

Step 5: Electronic cross section - results

$$\sigma_{cluster} \sim 1000\sigma_{single\ \ defect}$$

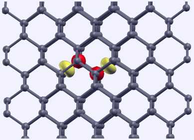
Point defects

Large $\Delta Q \Rightarrow$ many phonons



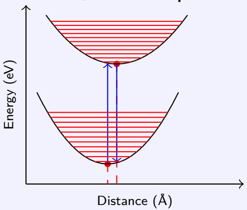
Reason: Localized $|\phi_i\rangle$

No hybridization



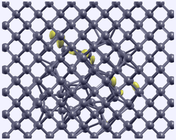
Clusters of defects

Small $\Delta Q \Rightarrow < 1$ phonon



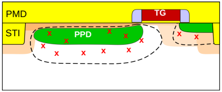
Reason: Extended $|\phi_i\rangle$

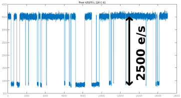
high hybridization



A. Jay *et al.*, SISPAD 2021

Step 5: Electronic cross section - results





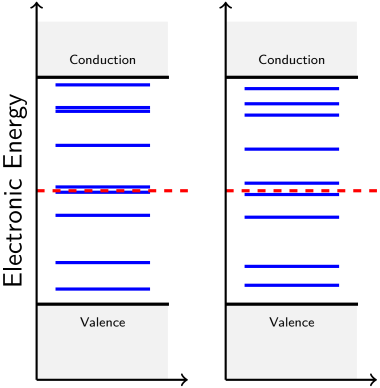
SRH generation rate:

$$DC_{SRH} \approx \frac{\sigma v_{th} n_i}{2cosh\left(\frac{E_t - E_{mg}}{k_B T}\right)}$$

Large $\sigma = 10^{-12}\mathrm{cm}^2$

small structure change ⇒
small elec. level change ⇒
Large DC variation

Solve Amplitude problem



E_t-E_{mg}=0.05
DC=55000e/s

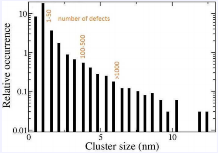
E_t-E_{mg}=0.1
DC=8000e/s

Table of Contents

Conclusion - Question answered

WHY clusters of defects correspond to observed DC and DC-RTS ?

Exponential Shape

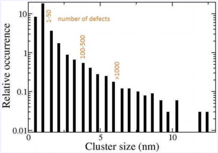


Same amplitude distribution

Conclusion - Question answered

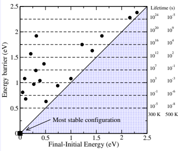
WHY clusters of defects correspond to observed DC and DC-RTS ?

Exponential Shape



Same amplitude distribution

Highly Metastable

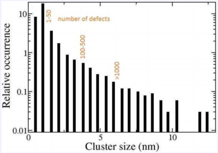


Multilevel RTS, all τ

Conclusion - Question answered

WHY clusters of defects correspond to observed DC and DC-RTS ?

Exponential Shape



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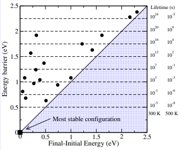
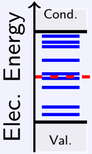


Multilevel RTS, all τ

Many electronic states

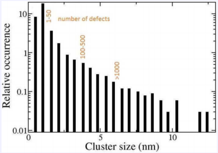


Midgap activation energies

Conclusion - Question answered

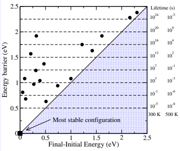
WHY clusters of defects correspond to observed DC and DC-RTS ?

Exponential Shape



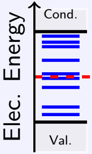
Same amplitude distribution

Highly Metastable



Multilevel RTS, all τ

Many electronic states

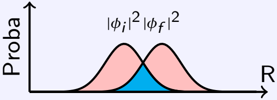


Midgap activation energies

Large cross sections

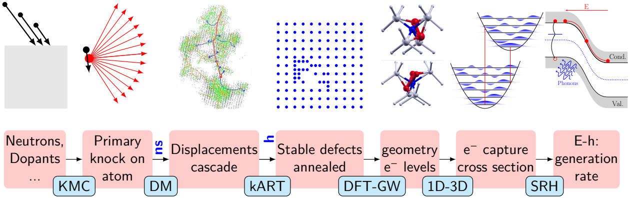
small $\Delta \mathbf{R}$

$$\langle \Psi_i | \Delta H | \Psi_f \rangle \neq 0$$



Large variation of amplitude

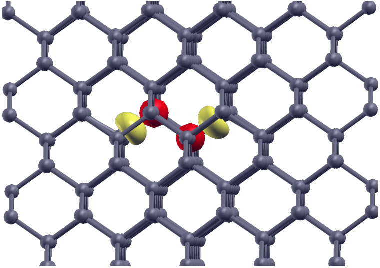
Conclusion - ongoing works



- Si & Ge Vs large (GaN, SiC) and small (InGaAs, HgCdTe) gap sc
- Ponctual defects → RTS?
- Si/SiO_2 interface → RTS?
- Same statistics for simu. than exp.
- Inter-defects distance to define a cluster?
- Better model for the cross sections (real time TDDFT)
- Temperature dependance of the cross sections
- Other impacts of clusters (carrier trapping, recombination...)
- Include these results into predictive softwares

Questions time

Italy



ajay@laas.fr

France

Thank you for your attention

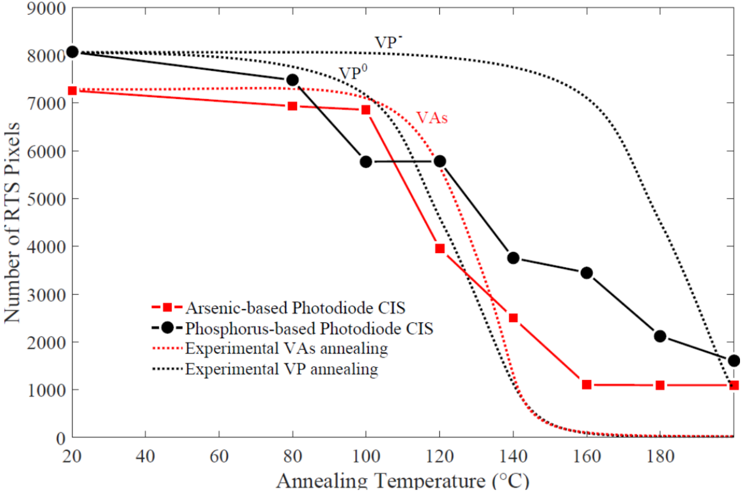
questions

suggestions

Table of Contents

Effect of dopants?

Annealing of RTS pixels Vs E centers



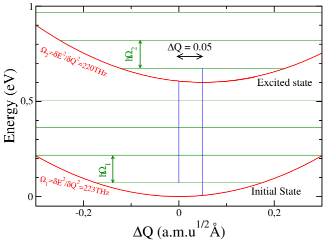
Dopants are not at the origin of DC-RTS.

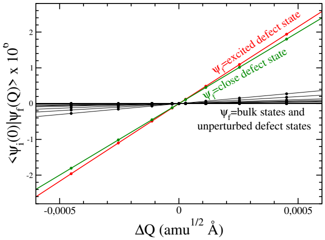
Electronic cross section: scalar product

$$\langle\psi_i|\frac{\delta h}{\delta Q}|\psi_f\rangle = (\epsilon_h-\epsilon_i)\langle\psi_i|\frac{\delta\psi_f}{\delta Q}\rangle$$
$$= (\epsilon_h-\epsilon_i)\frac{\delta\langle\psi_i|\psi_f\rangle}{\delta Q}$$

$$|\psi_f(\mathbf{R})\rangle = \sum_{k,nG} c_n e^{2i\pi(\mathbf{G}+\mathbf{k}).\mathbf{R}}$$

$$\langle\psi_i|\psi_f\rangle = \sum_{k,nG} c_i c_f^*$$





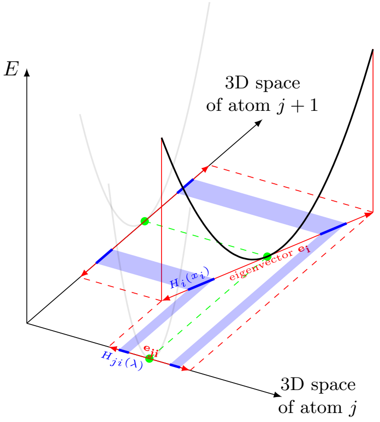
Representation of NDim ionic wf

- Harmonic approximation: Solve Dynamical matrix and get eigenmodes $\mathbf{e_i}$
- Split ND H along each 1D $\mathbf{e_i}$: $\hat{H}^{ions} = \hat{H}_1 \otimes \hat{H}_2 \otimes \cdots \otimes \hat{H}_{3N_{at}}$
- The exact solution is then $\chi(\mathbf{R}) = \prod_{i=1}^{3N_{at}} H_i(x_i)$

Approximation

Project the 1D solution on the 3D space of each atom
memory $=$ N$\times 100^3$ tabular

ionic wf do not overlap
Lose the relative motion between atoms (not needed)



Representation of NDim ionic wf

$\forall$ atom j, $\forall$ mode i:

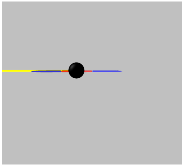
$$\chi_0^j(\mathbf{R}) = \begin{cases} 1 & \text{if} \quad \mathbf{R} = \mathbf{R}_{at_j} \\ O & \text{if} \quad \mathbf{R} \neq \mathbf{R}_{at_j} \end{cases}$$

$$\chi_{i+1}^j(\mathbf{R}) = \int \chi_i(\mathbf{R} - \lambda \mathbf{e_{ji}}) H_{ji}(\lambda) d\lambda$$

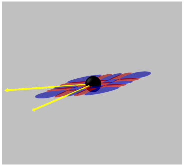
$$\chi^j(\mathbf{R}) = \chi_{3N_{at}}^j(\mathbf{R})$$

Example:
6 highest contribution modes.
yellow= eigenmode
blue/red= +/- wf

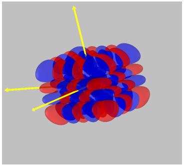
i=1 n=4



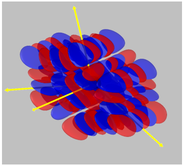
i=2 n=4



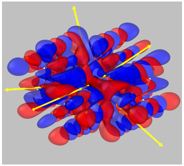
i=3 n=3



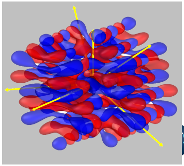
i=4 n=2



i=5 n=2



i=6 n=1



Ionic scalar product

no overlap between ions →
The full ionic wf is the sum of each ionic projected contribution

$$\chi^{proj}(\mathbf{R}) = \sum_{j=1}^{N_{at}} \chi^j(\mathbf{R}) \tag{1}$$

The final scalar product is:

$$\langle \chi_{im} | \Delta \mathbf{Q_k} | \chi_{fn} \rangle \sim \sum_{j=1}^{N_{at}} \langle \chi_i^j | \mathbf{Q_{jk}} | \chi_f^j \rangle \tag{2}$$