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Quantum characteristics of electron and hole quasiparticles in silicon defects

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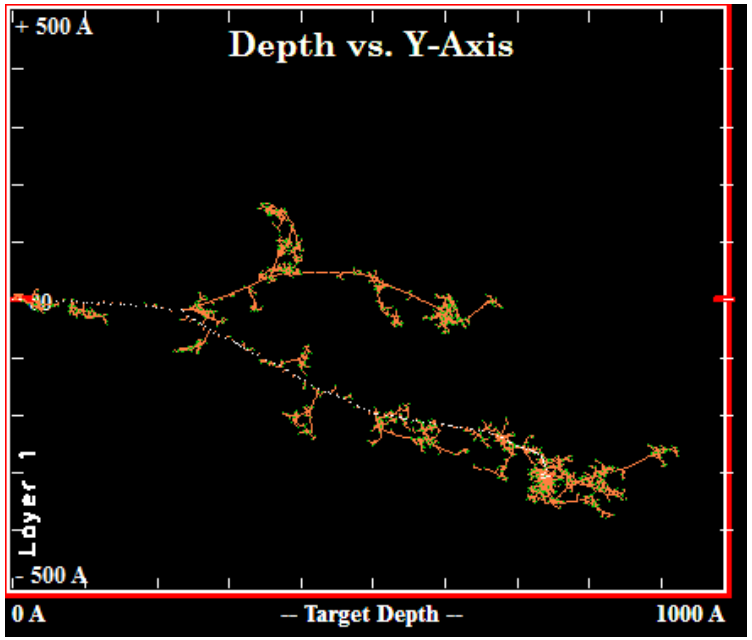
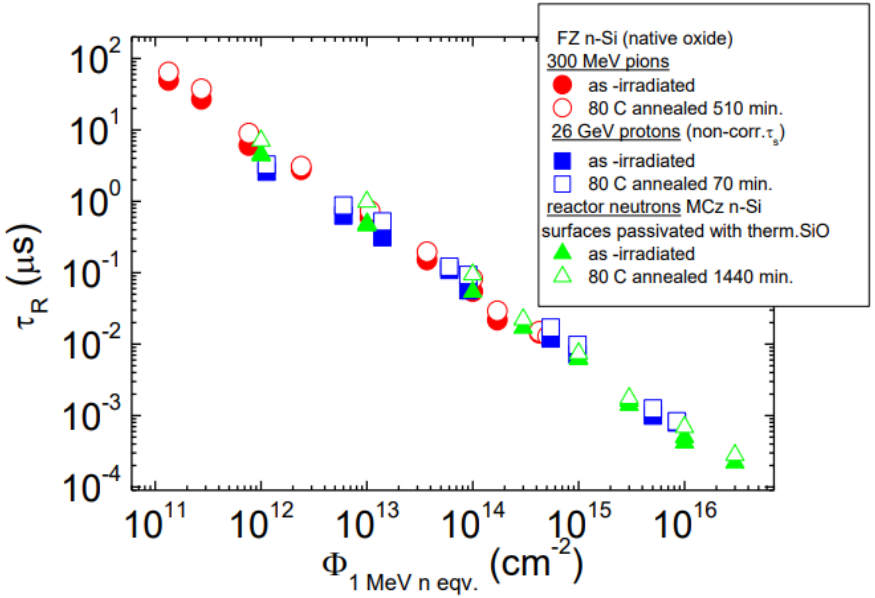
Defect network

1. Irradiation by high energy particles induces defect clusters
2. Irradiation reduces chage lifetimes,

what is directly related to irradiation doze.



24 th RD50 workshop



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Si lattice

$$n_{Si} = 4.99 \cdot 10^{22}\ \mathrm{cm}^{-1}$$

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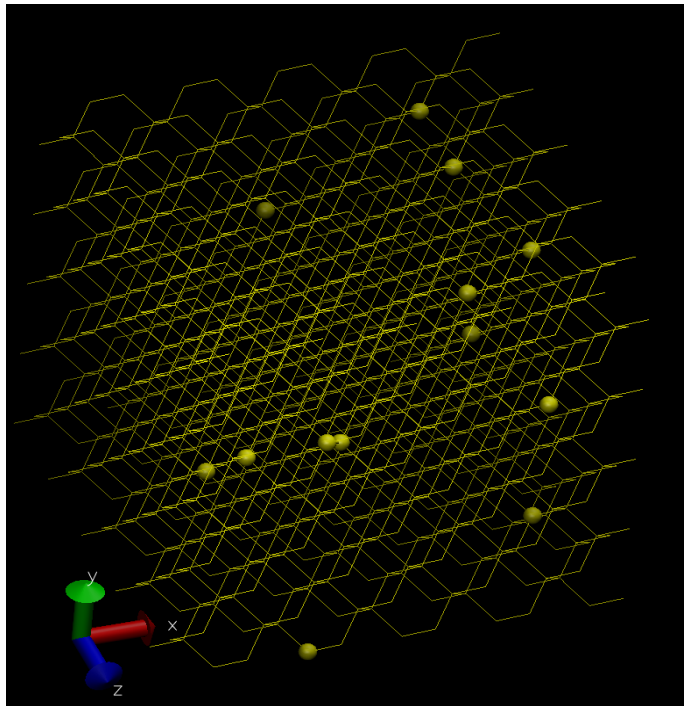
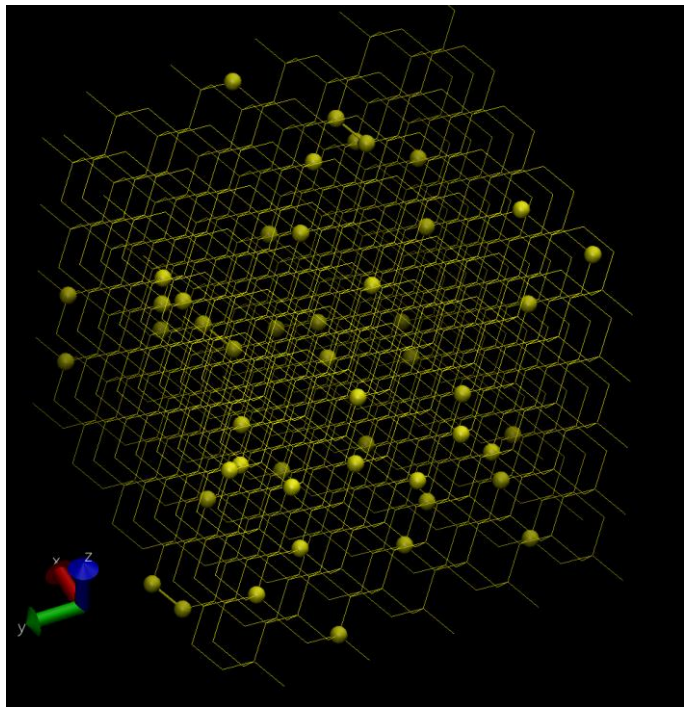
$$n = 10^{20}\mathrm{cm}^{-1}$$

Defects are independent



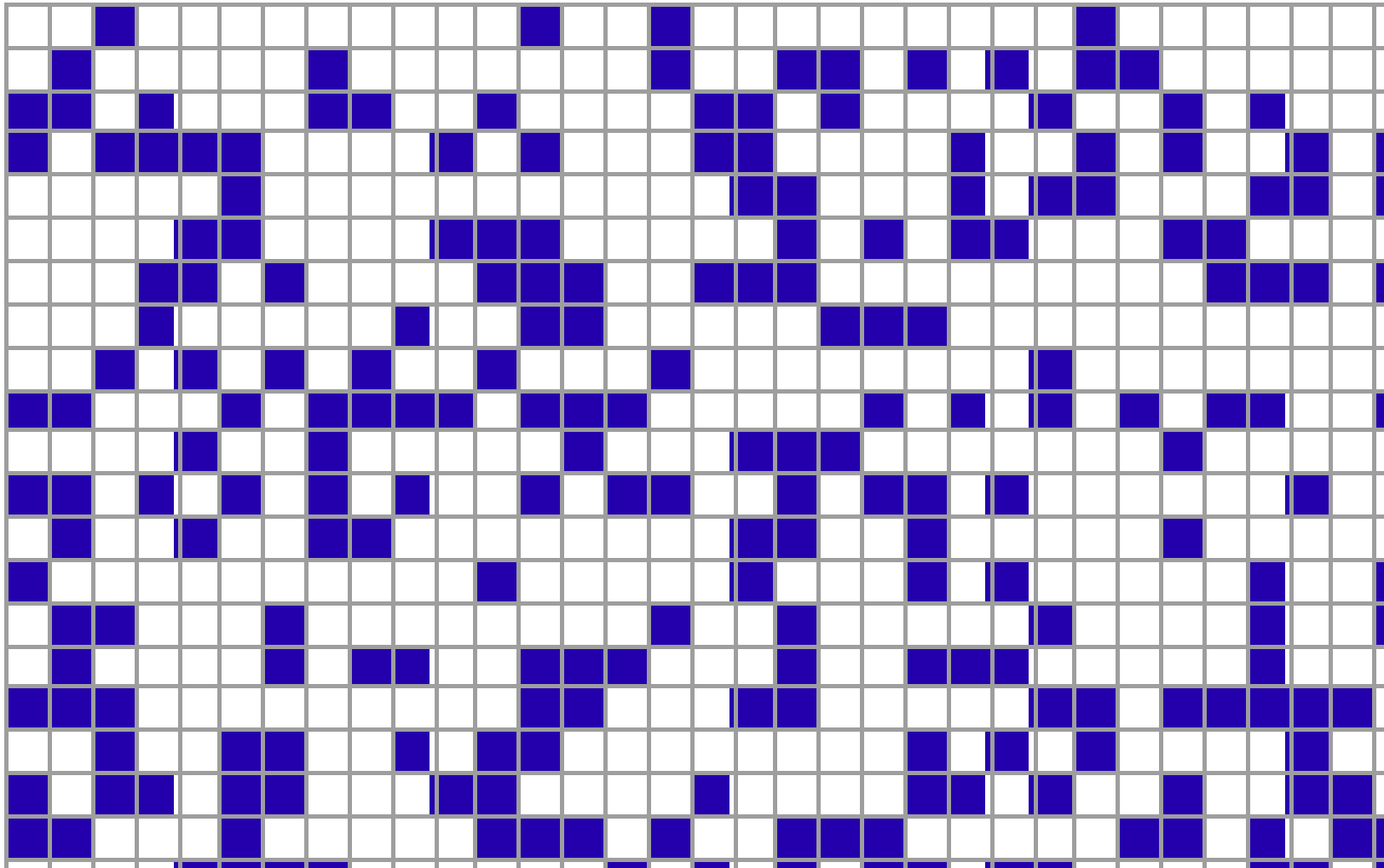
$$n = 5 \cdot 10^{20}\mathrm{cm}^{-1}$$

Defects form percolative clusters



Quantum percolation network

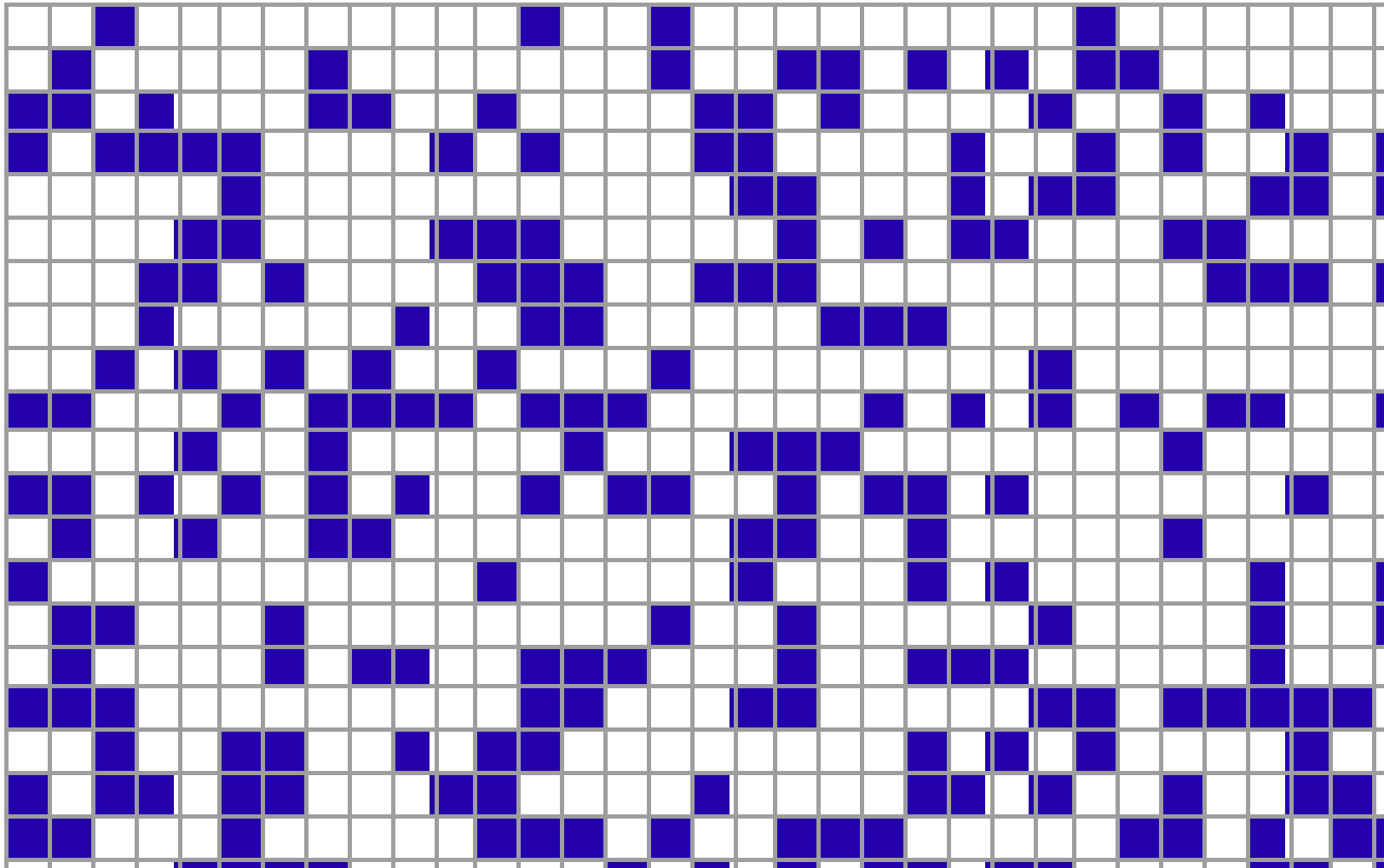
- Very sensitive to electron delocalization pattern



Quantum percolation network

- Very sensitive to electron delocalization pattern

- Clusters are distributed not homogeneously
- “sites” are not equivalent



Recombination model

Electron-hole lifetime is directly proportional to the irradiation dose.

Assumptions:

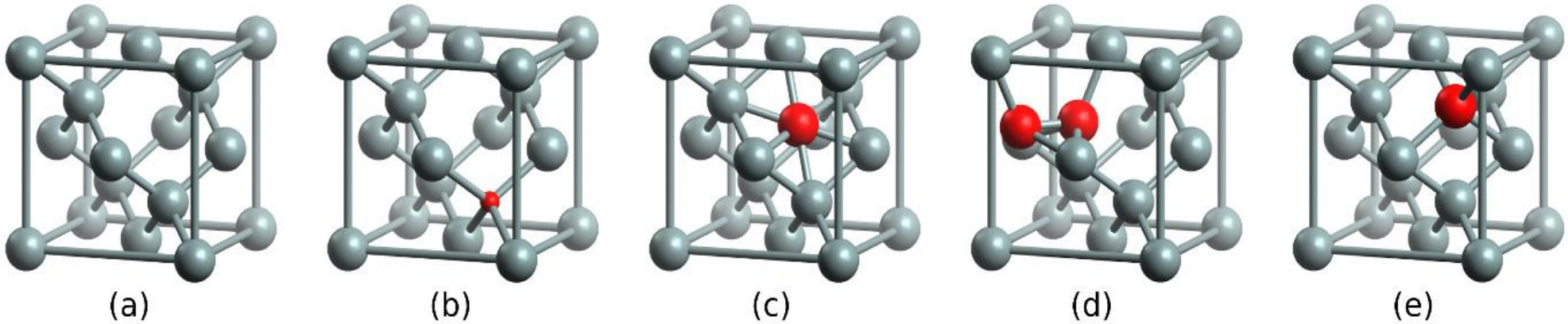
- defect concentration is proportional to irradiation dose
- defects are organized into high concentration clusters

1-st step: Understand the electron and hole fundamental properties

Motivation questions:

- Why single-exponential decay in heterogeneous system
- Whether microscopic organization is important
- What is the charge decay rate-limiting factor.

Isolated defects



Silicon geometry configurations of conventional lattice (a) and various defects: vacancy (b) and hexagonal (c), split<110> (d), tetrahedral (e) interstitials.

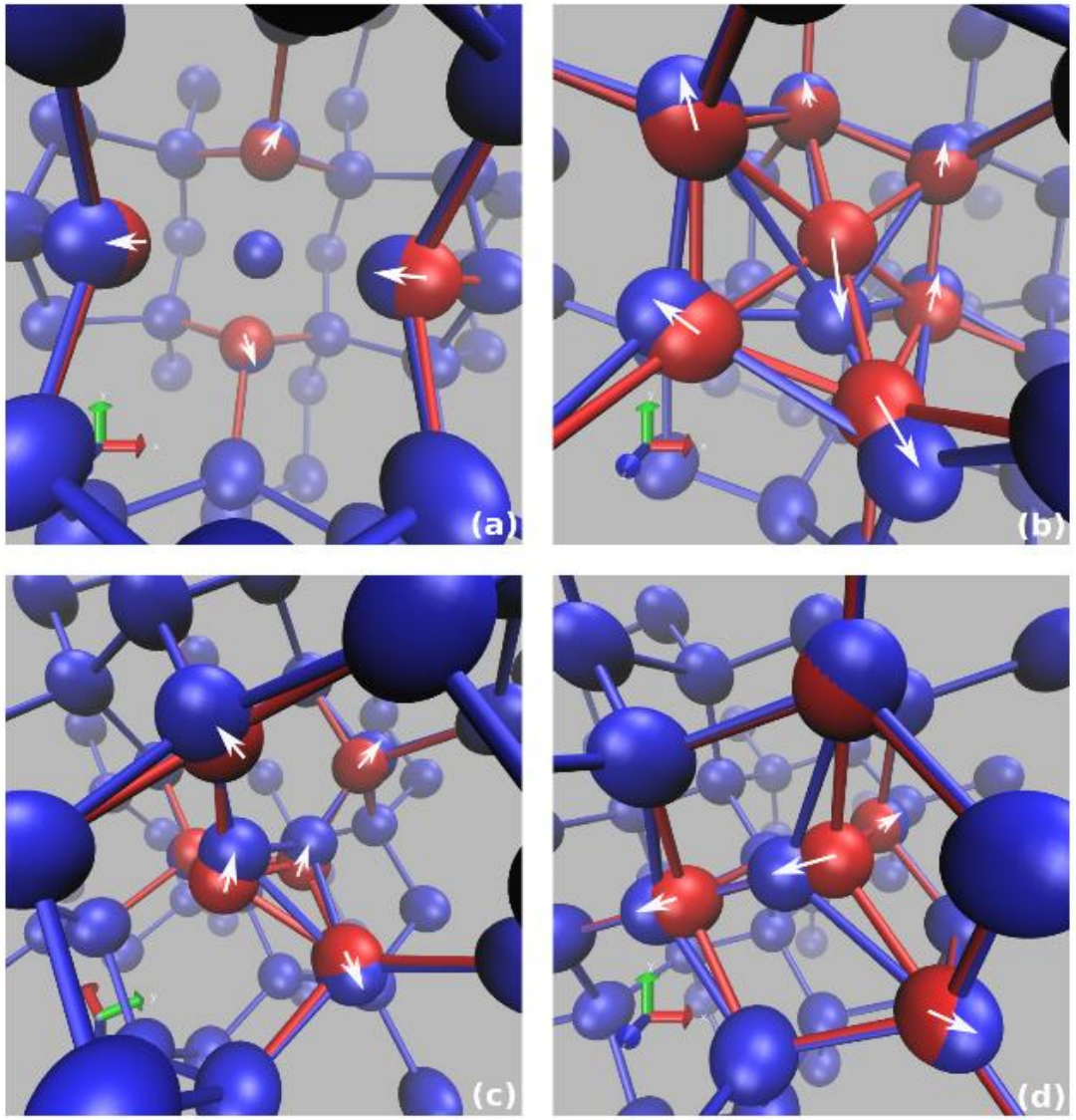
S. A. Centoni, B. Sadigh, G. H. Gilmer, Th. J. Lenosky, T. D. de la Rubia, Ch. B. Musgrave. *First-principles Calculation of Intrinsic Defect Formation Volumes in Silicon.* Phys. Rev. B, 72, 195206, 2005

Optimized geometries

vacancy (a),
hexagonal (b),
split-<110> (c)
tetrahedral (d)

Red atoms denote the initial configuration.

The arrows show the direction of atom relaxation to their optimal positions.



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All pictures were created by VMD program, https://www.ks.uiuc.edu/Research/vmd/

Charge densities

Defect-related electronic states are localized around the defect sites.

Only nonequilibrium electronic properties are of interest

Electron density in general

$$\sigma_e(\boldsymbol{r}) = \int d^3\boldsymbol{r}_1 \ldots \int d^3\boldsymbol{r}_{N-1} \, |\Phi_0(\boldsymbol{r}_1 \ldots \boldsymbol{r}_{N-1}\boldsymbol{r})|^2$$

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Difference charge densities

Electron quasiparticle charge density

$$\sigma_e(\mathrm{r}) = \int d^3r_1 \ldots \int d^3r_{N-1} \left(\int d^3r_N \, |\Phi_e(\mathrm{r}_1 \ldots r_N, r)|^2 - |\Phi_0(\mathrm{r}_1 \ldots r_{N-1} r)|^2 \right)$$

Hole quasiparticle charge density

$$\sigma_h(\mathrm{r}) = \int d^3r_1 \ldots \int d^3r_{N-2} \left(|\Phi_h(\mathrm{r}_1 \ldots r_{N-2}, r)|^2 - \int d^3r_{N-1} \, |\Phi_0(\mathrm{r}_1 \ldots r_{N-1} r)|^2 \right)$$

Gaussian orbitals to represent atomic orbitals,
Only valence orbitals responsible for electronic properties.
Effective core pseudopotential approach (Stuttgart – Cologne pseudopotentials - Cologne university data base)

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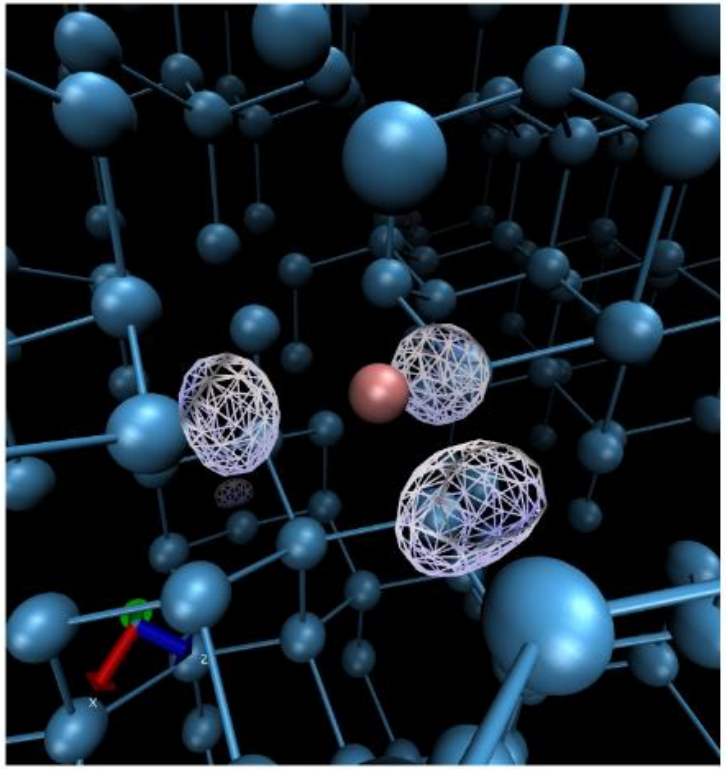
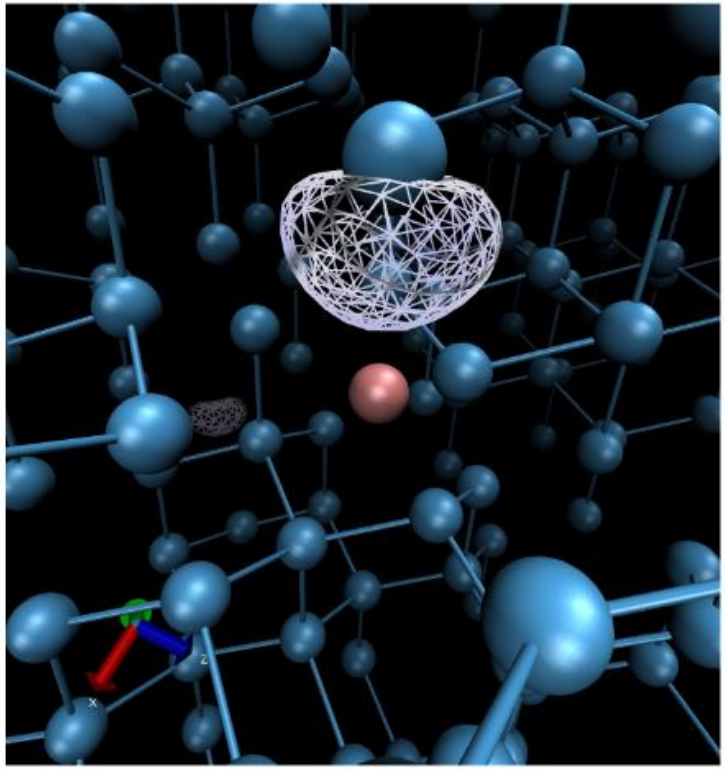
Vacancy defect

Electron quasiparticle charge density



Hole quasiparticle charge density



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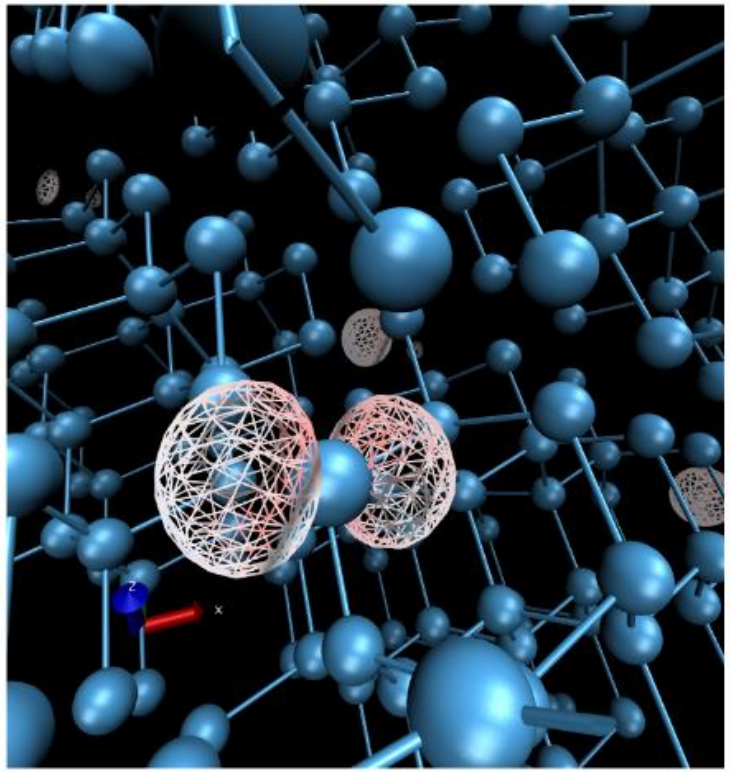
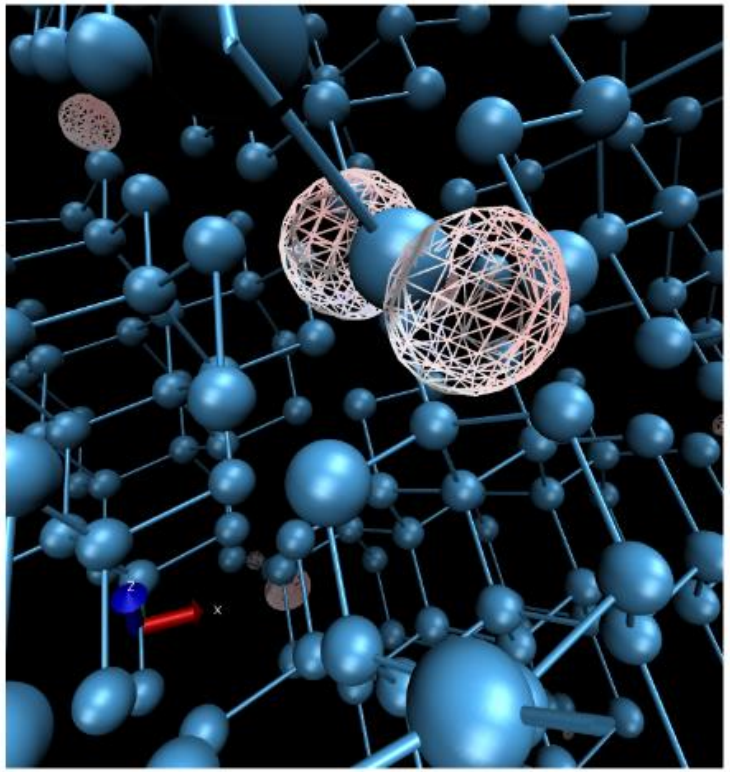
All electron density calculations were done by CRYSTAL program with periodic boundary conditions

Hexagonal defect

Electron quasiparticle charge density



Hole quasiparticle charge density



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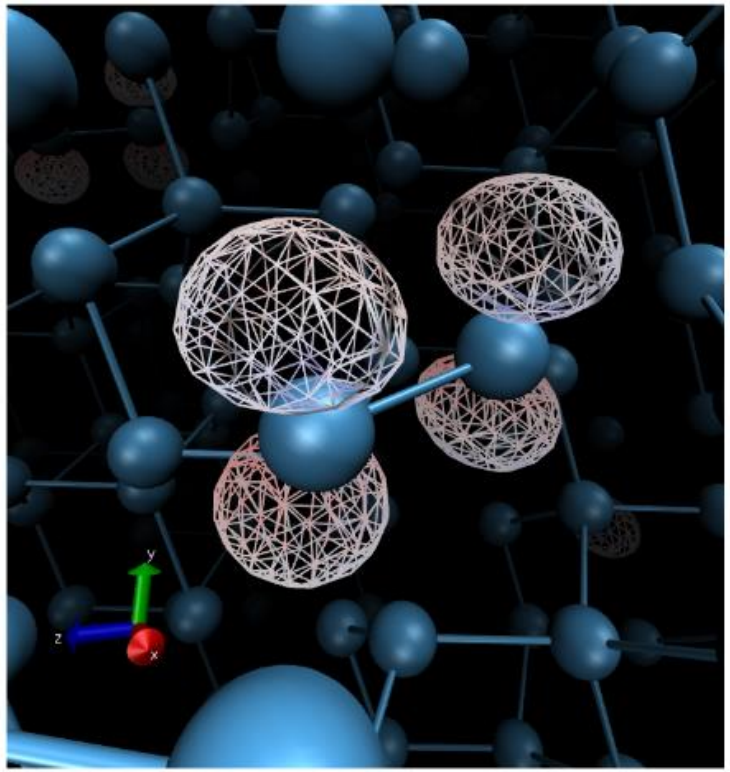
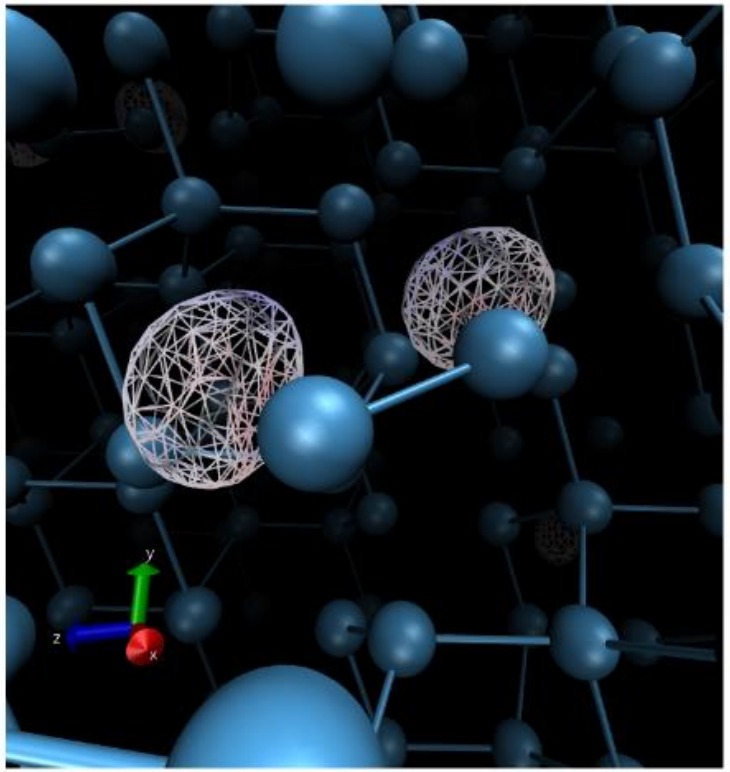
Split-<110> defect

Electron quasiparticle charge density



Hole quasiparticle charge density



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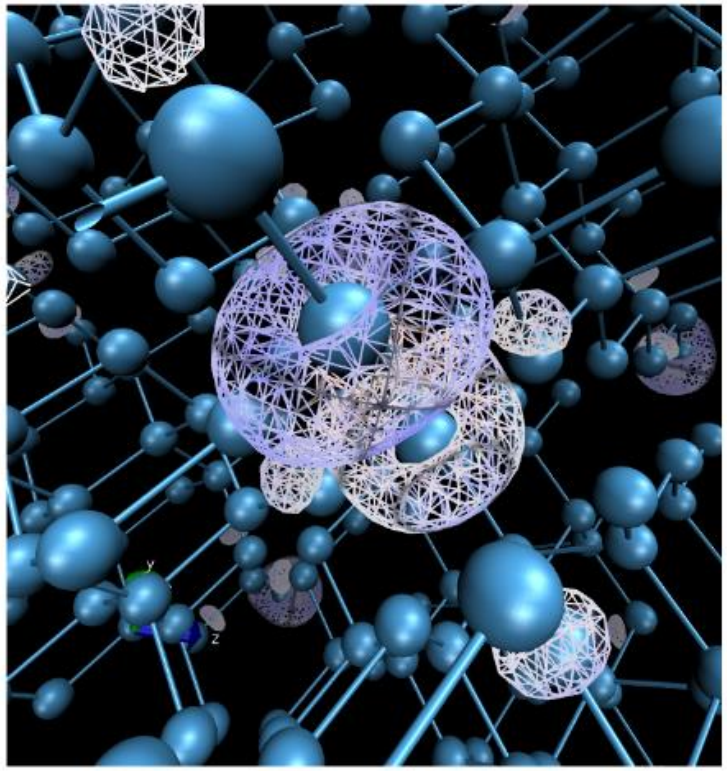
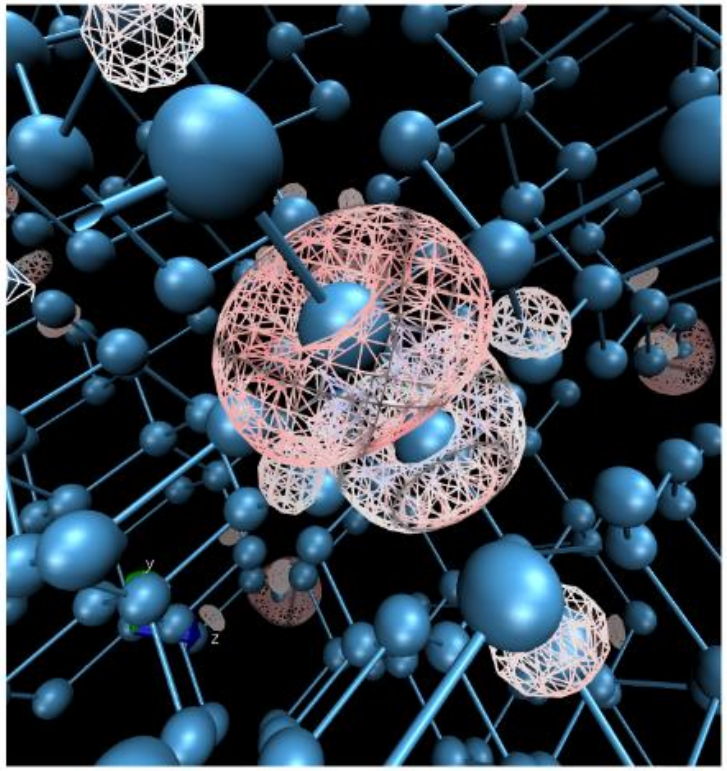
All electron density calculations were done by CRYSTAL program with periodic boundary conditions

Tetrahedral defect

Electron quasiparticle charge density



Hole quasiparticle charge density



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All electron density calculations were done by CRYSTAL program with periodic boundary conditions

Tight binding model

$$\begin{aligned}\hat{H} &= \sum_n t^{(e)}_{mn}\hat{c}^\dagger_m\hat{c}_n + t^{(h)}_{mn}\hat{d}^\dagger_m\hat{d}_n \\ &+ \sum_{mn} V_{mn}\hat{c}^\dagger_m\hat{c}_m\hat{d}^\dagger_n\hat{d}_n \\ &+ \sum_m\sum_k \left(R_m\hat{c}^\dagger_m\hat{d}^\dagger_m f_k + \hat{c}_m\hat{d}_m f^\dagger_k\right) + \sum_k \hbar\omega_k(\hat{f}^\dagger_k\hat{f}_k + \frac{1}{2})\end{aligned}$$

Why electron and hole wave functions are important?

The simplest recombination operator:

$$\hat{R} = |e\rangle\langle h|\hat{Q}_{ph}.$$

The phonon coordinate operator

The corresponding recombination rate is then given by Fermi Golden Rule

$$K = \frac{2\pi}{\hbar}\left|\langle e|\hat{R}|h\rangle\right|^2 \int_0^\infty d\omega_{ph}\,\rho(\omega_{ph})\delta(\omega_{eh} - \omega_{ph}).$$

Here $\rho(\omega_{ph})$ is the phonon spectral density.

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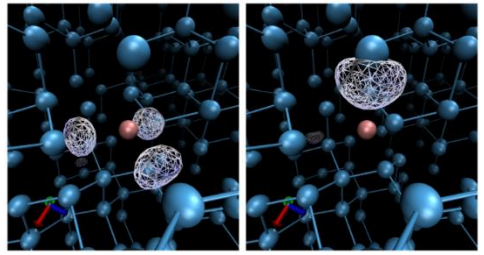
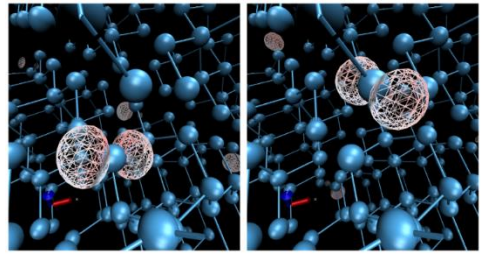
Recombination center candidate

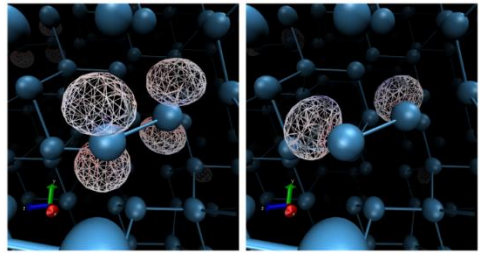
vacancy

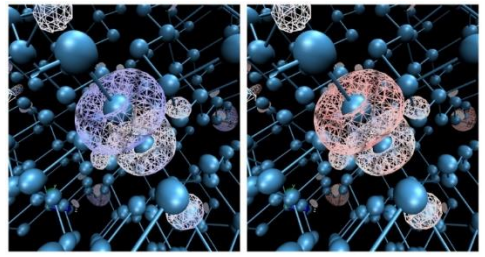




hexagonal

Split





tetrahedral

vacancy	tetrahedral	split110	hexagonal
-4.9741E-01	-2.5794E-01	-1.1941E-01	-5.7073E-01

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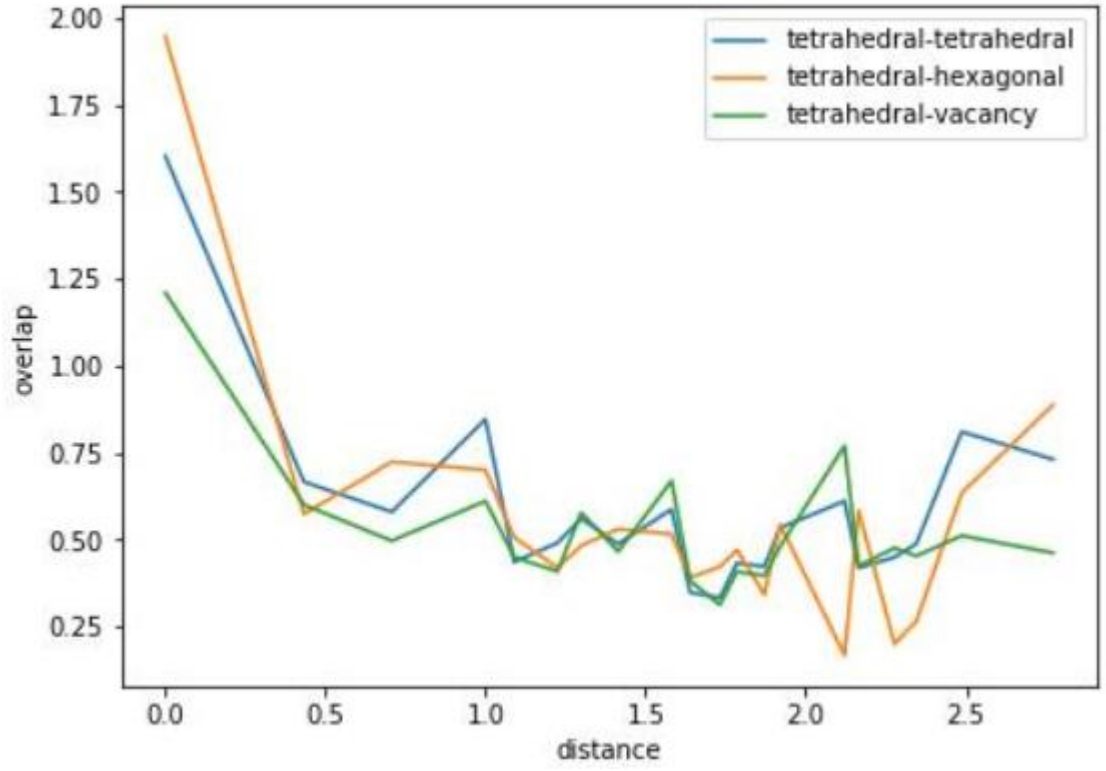
Hole hopping elements

Non-exponential decay
with the separation distance



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Conclusions

Optimized defect geometries show existence of local minima with reduced symmetry.

Only few types of defects demonstrate close overlap of the electron and hole densities. Concentration of specific defects is responsible for recombination.

The electron lifetime contains two components: the transition time required to reach the recombination center and the electron/hole lifetime on the defect.

Acknowledgement

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