Localization and Correlations in Atomically Thin Dopant Chains in Silicon

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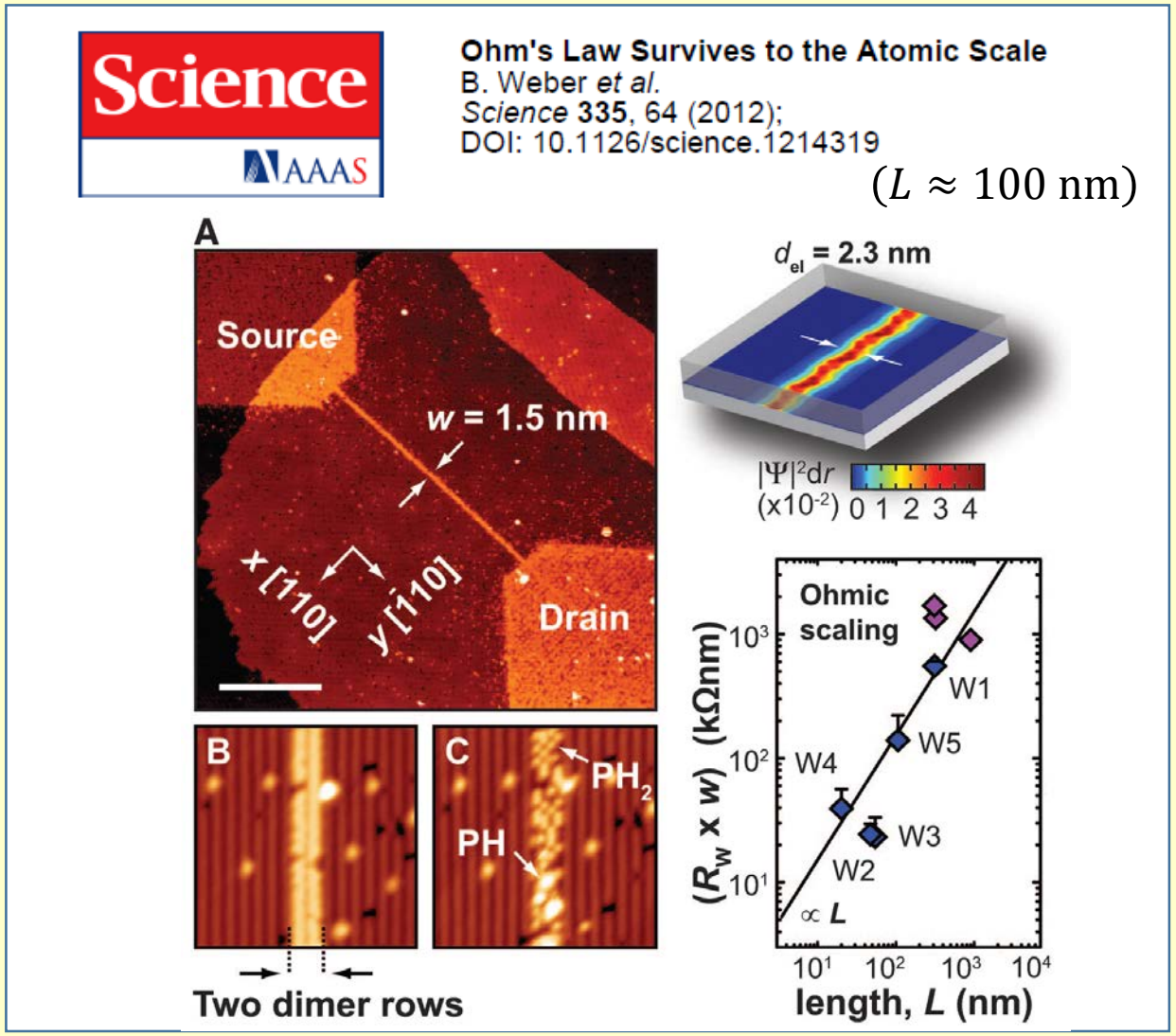
ATOMIC SCALE QUANTUM CIRCUITS IN SILICON-EXPERIMENTS



Metallic Behavior

B. Weber,
S. Mahapatra,
H. Ryu,
S. Lee,
A. Fuhrer,
T. C. G. Reusch,
D. L. Thompson,
W. C. T. Lee,
G. Klimeck,
L. C. L. Hollenberg,
M. Y. Simmons

ATOMIC SCALE QUANTUM CIRCUITS IN SILICON-EXPERIMENTS

nature nanotechnology

LETTERS

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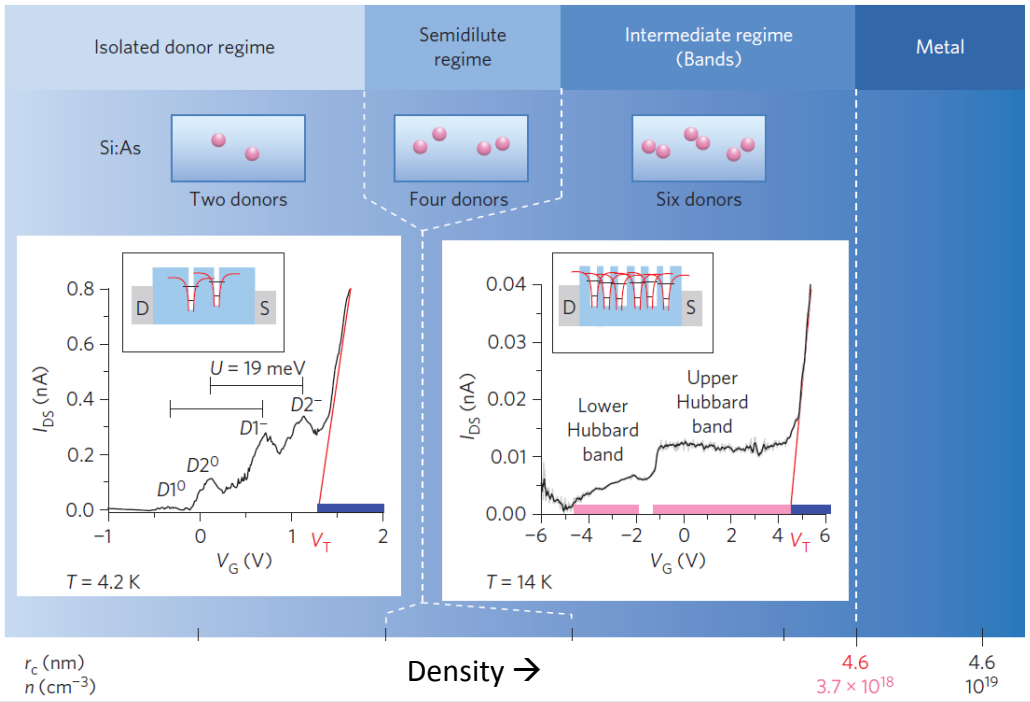
Anderson–Mott transition in arrays of a few dopant atoms in a silicon transistor

Enrico Prati[1]*, Masahiro Hori[2], Filippo Guagliardo[3], Giorgio Ferrari[3] and Takahiro Shinada[4†]*



Metal-Insulator Transition

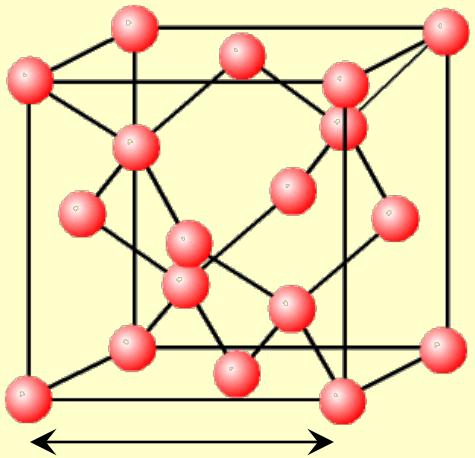
Enrico Prati,
Masahiro Hori,
Filippo Guagliardo,
Giorgio Ferrari,
Takahiro Shinada

Electrons in bulk Si: Bloch states

REAL SPACE

Lattice potential:

FCC lattice
Diamond structure



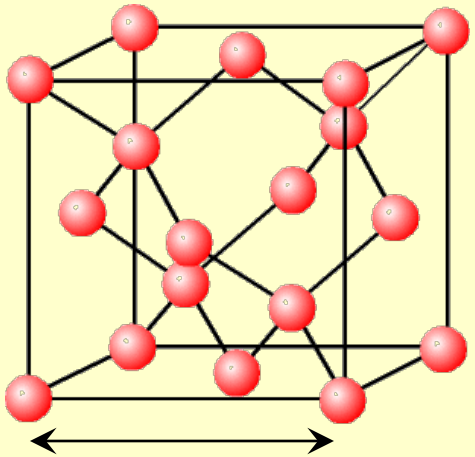
Cubic UNIT CELL

Electrons in bulk Si: Bloch states

REAL SPACE

Lattice potential:

FCC lattice
Diamond structure

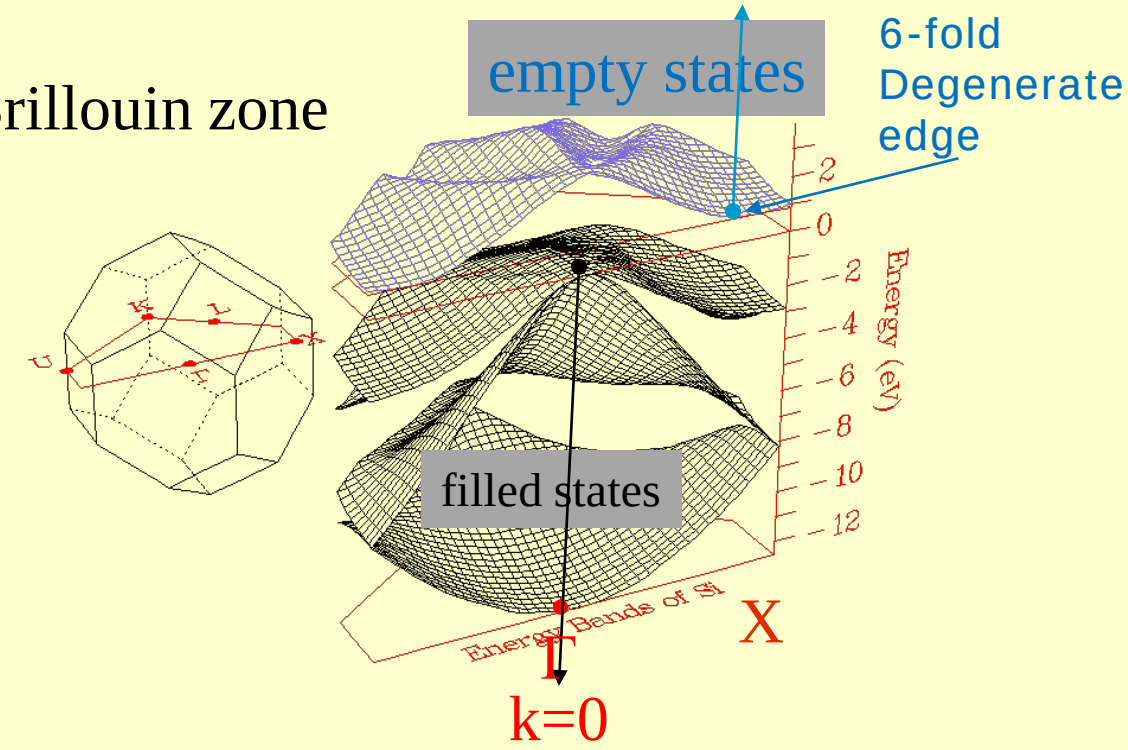


Cubic UNIT CELL

RECIPROCAL SPACE

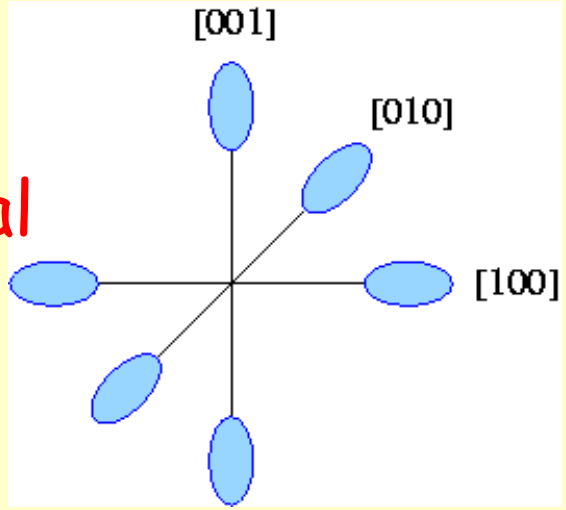
Spectrum: $\varepsilon_n(\vec{k})$

1st Brillouin zone



Si conduction-band edge

Reciprocal space



6 equivalent minima

$\vec{k}_\mu$ (μ = 1,2,…,6) =

(0,0,$\pm k_0$); (0, $\pm k_0$,0); ($\pm k_0$,0,0)

$k_0 = 0.85 \cdot 2\pi/a$

Eigenfunctions: 6 Bloch states:

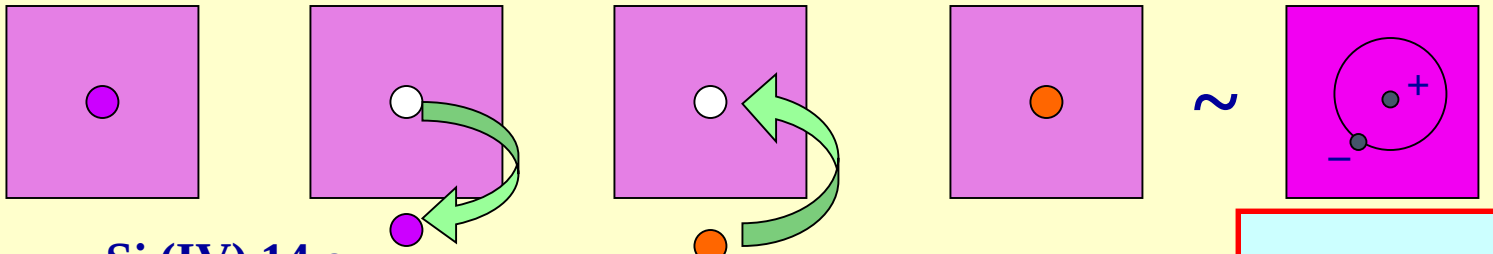
$$\phi_\mu(\vec{r}) = \boxed{\exp[i\vec{k}_\mu \cdot (\vec{r} - \vec{\varphi}_\mu)]} u_\mu(\vec{r})$$

Planewave-like part

Arbitrary phases

Periodic part $\Rightarrow$ pinned to the lattice

Hydrogenic model for P donors in Si



$$V(r) = \frac{-e^2}{\varepsilon\, r}$$

$$[-\hbar^2\nabla^2 / 2m^* + V(r)]\,\psi(r) = -E_d^*\,\psi(r)$$

$$\psi(r) = (1/\sqrt{\pi a^{*3}})\exp(-r/a^*),\ \ a^* = a_0\varepsilon(m_0/m^*) \approx 30\ \text{Å}$$

Single substitutional donor at R_0

perturbation potential:

$$V(\vec{r}) = -\frac{e^2}{\varepsilon\,|\,\vec{r} - \vec{R}_0\,|}$$

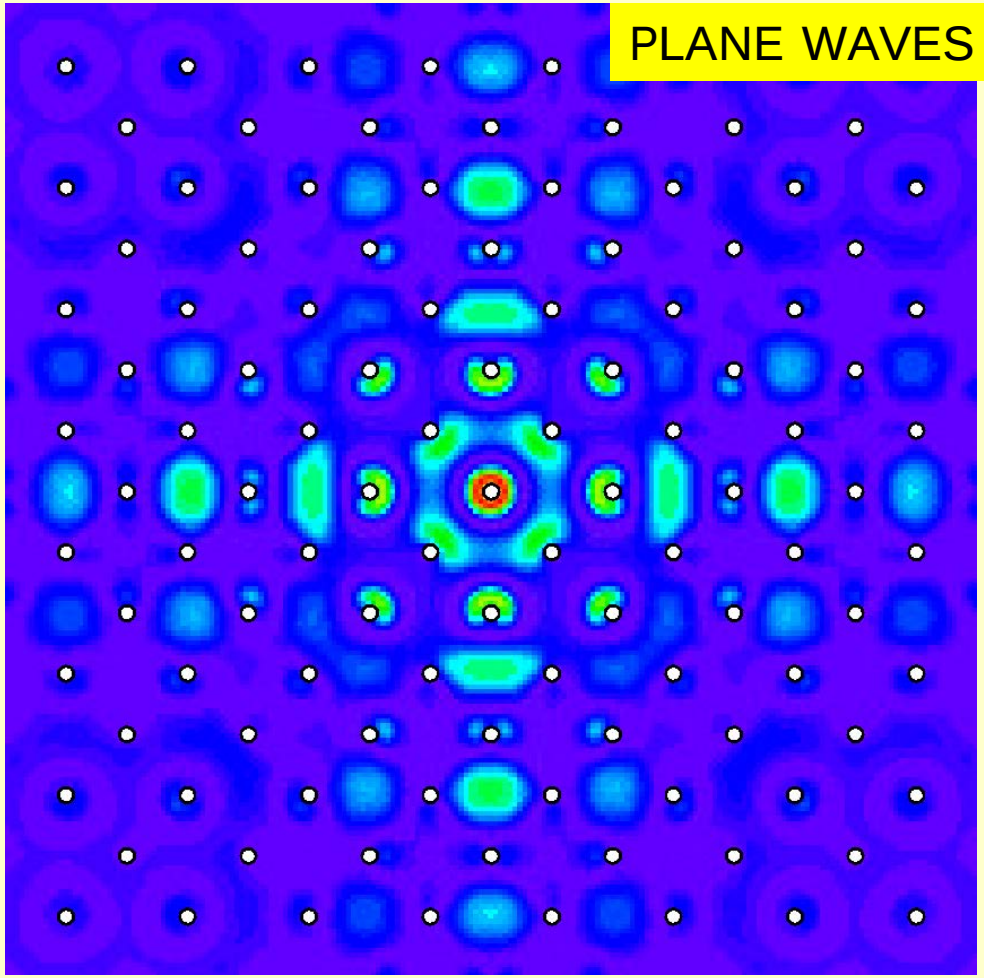
Kohn-Luttinger electronic ground state
A_1 symmetry $\Rightarrow$non-degenerate

$$\psi_{\vec{R}_0}(\vec{r}) = \frac{1}{\sqrt{6}} \sum_{\mu=1,6} F_\mu(\vec{r} - \vec{R}_0)\, u_\mu(\vec{r})\, e^{i\vec{k}_\mu \cdot (\vec{r} - \vec{R}_0)}$$

ENVELOPE FUNCTIONS (variational):
deformed 1S hydrogenic orbitals centered at donor site*

PLANE WAVES → interference!

Bound electron ground state
electronic charge distribution



PLANE WAVES → interference

Koiller, Capaz, Hu & Das Sarma
PRB 70, 115207 (2004)

Hamiltonian – Chain of donors

Extended Hubbard-Kanamori Hamiltonian

$$H = \sum_{i,\sigma} \epsilon_i n_{i,\sigma} + \sum_{\langle i,j \rangle} t_{ij} c_i^+ c_j + \sum_i U_i n_{i,\sigma} n_{i,\bar{\sigma}} + \sum_{\langle i,j \rangle,\sigma,\sigma'} V_{ij} n_{i,\sigma} n_{j,\sigma'}$$

On-site Hopping — Single electron terms

Hubbard Direct — Electron-electron interaction terms

Linear Combination of Dopant Orbitals (LCDO) at impurity sites.

Ground State (A_1 Symmetry): $\psi_{A_1}(\boldsymbol{r} - \boldsymbol{R}_i) = \frac{1}{\sqrt{6}} \sum_{\mu} \phi_\mu$

*For simplicity, we assume isotropic s-like envelopes.

Single Electron Approach

Localization Length (ξ) definition: $\Psi(\mathrm{x} \to \infty) \sim e^{-\frac{|x|}{\xi}}$

Technical Procedure: Transfer Matrix Technique

Transfer Matrix

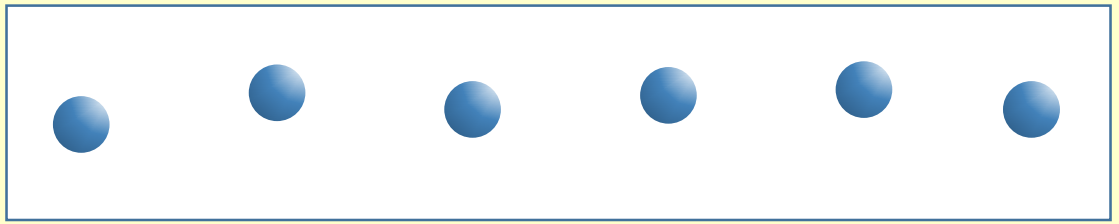
Lyapunov Exponents (γ_p)

Localization Length

$$\xi = \left|\gamma_0^{-1}\right|$$

(Minimum Lyapunov Exponent)

Localization Properties – 1D Disordered Chain



Unavoidable positioning disorder

↓

Off-Diagonal Disorder model

Monoelectronic Hamiltonian:

$$H = \sum_{i,\sigma} \epsilon_i n_{i,\sigma} + \sum_{\langle i,j \rangle,\sigma} t_{ij,\sigma} c^{+}_{i,\sigma} c_{j,\sigma}$$

Standard tight-binding procedure:

$$\epsilon_i \approx \langle i | \hat{H}_i | i \rangle = E_0^D$$

E_0^D → Single electron energy (onsite energy) in a single donor D (P, As, Sb, Bi)—Experimentally known with great accuracy.)

$$t_{ij} \approx \langle j | \hat{H}_i | i \rangle = E_0^D S(R, a_{cc})$$

Nearest neighbor hopping → Two models.

$S(R, a_{cc}) = \langle j | i \rangle$ → Wave-function Overlap (nearest neighbors)

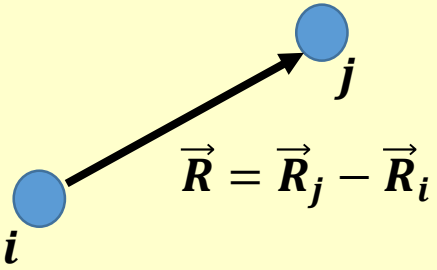
Fast hopping estimate preserving physical insight!

Two Hopping Models

Explore relevance of valleys plane wave components [$e^{i\vec{k}_\mu \cdot (\vec{r} - \vec{R}_i)}$]

- Single-valley model [no plane-waves components].

$$t_{ij}^{sv} = E_0 e^{-\frac{R}{a_{cc}}} \left(1 + \frac{R}{a_{cc}} + \frac{R^2}{3a_{cc}^2}\right) \qquad R = |\vec{R}|$$



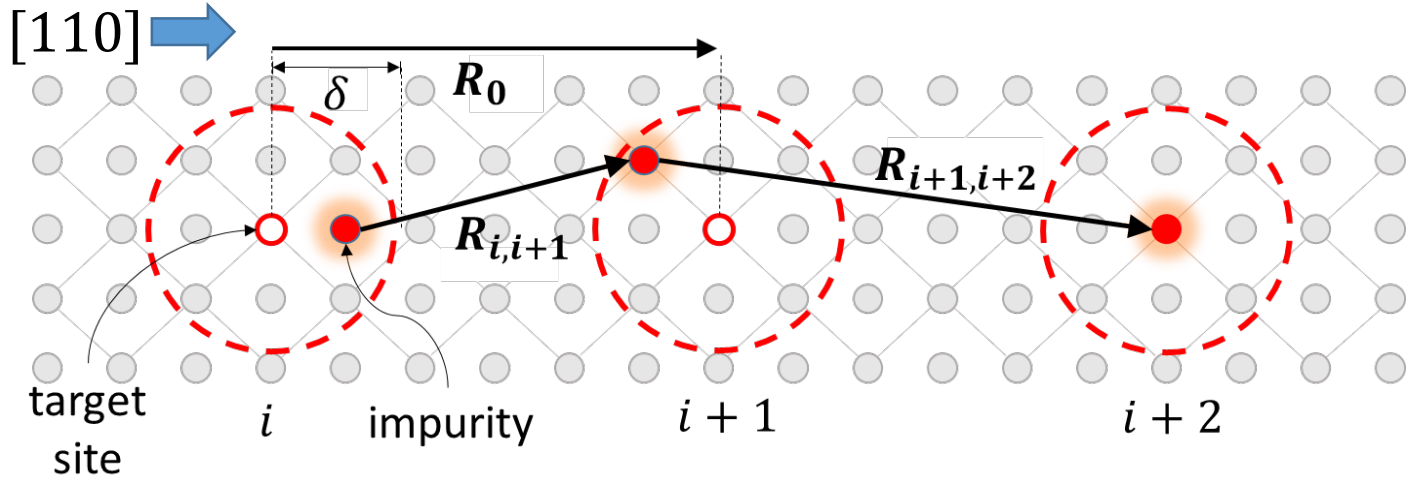
- Multi-valley model.

$$t_{ij}^{mv} = t_{ij}^{sv} \left\{ \frac{1}{3} \left[\cos(k_0 R_x) + \cos(k_0 R_y) + \cos(k_0 R_z) \right] \right\}$$

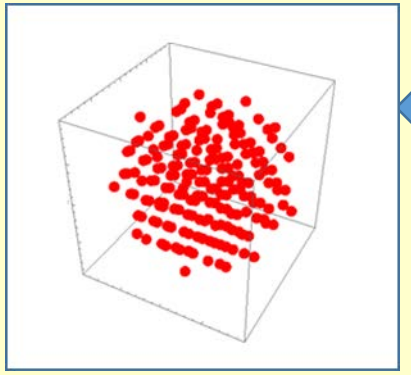
cos terms come from valleys plane-waves interference.

Given the relative position vectors, both models lead to off-diagonal disordered H, with specific values for the hoppings. Fixed bound disorder distributions.

Disorder: uncertainty radius δ

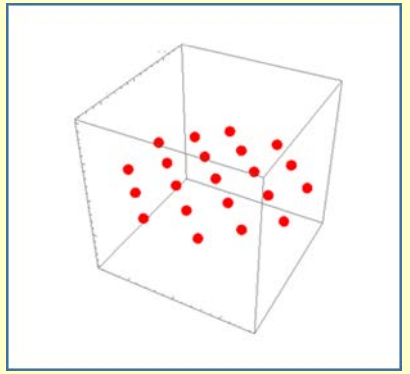


One donor in one of the substitutional sites within each sphere or disk centered at each target site with equal probability.



3D disorder → δ Sphere radius

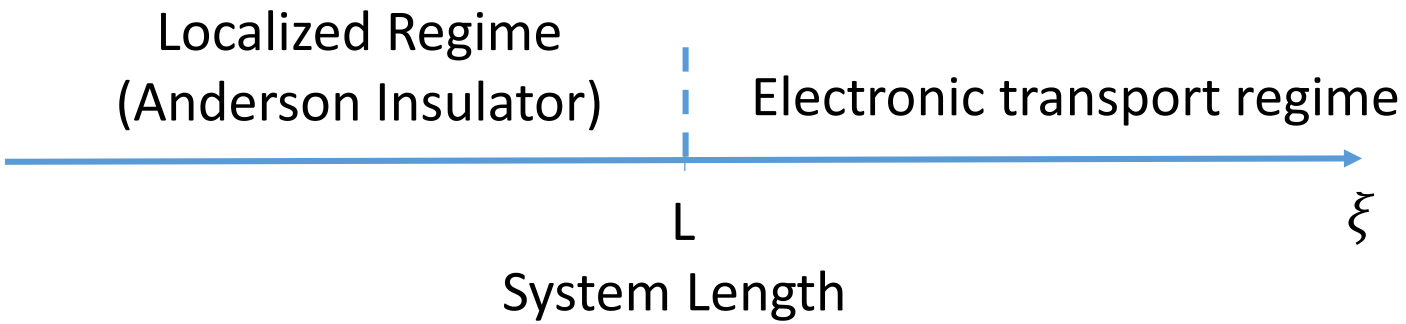
2D disorder → δ Disk radius



Criterion for electronic transport in finite chains

Decay Length (ξ) definition: $\Psi \sim e^{-\frac{|x|}{\xi}}$

ξ ➔ generalized localization length for finite chains.



Ensemble of Chains with fixed
- δ
- R_0
- Hopping Model (SV or MV)
- Disorder Model (2D or 3D)

Ensembles of ~10,000 Chains

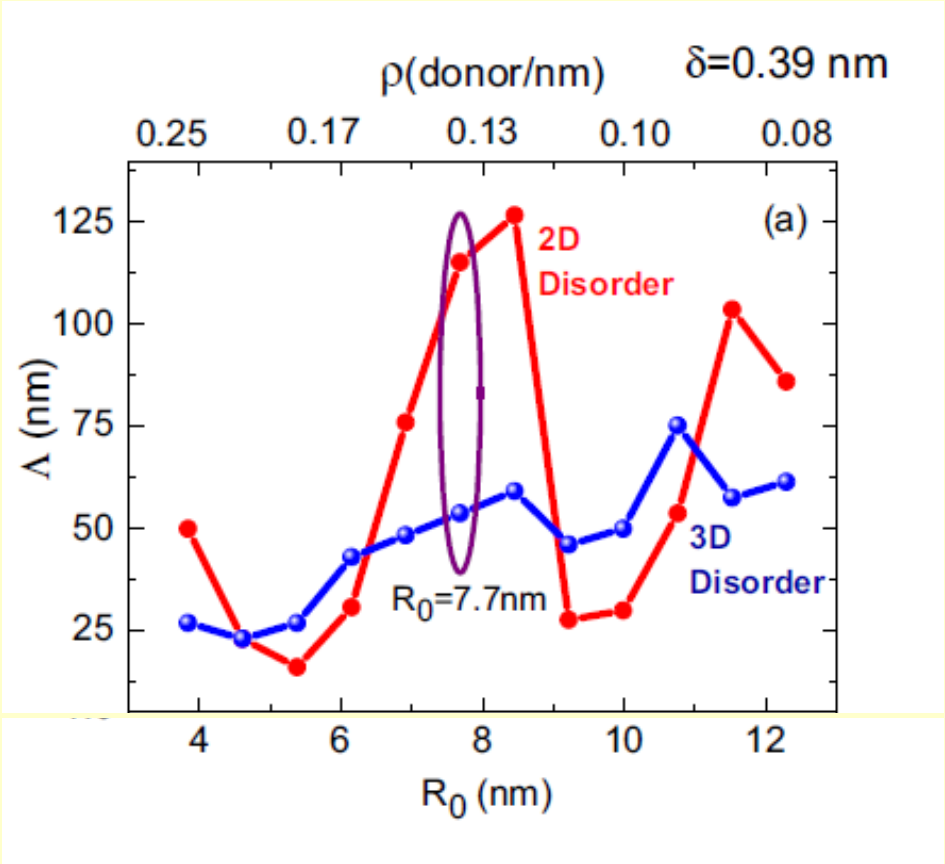
$\xi(\delta, R_0)$ is calculated for each disorder realization
→ Ensemble averages are performed

Maximum size of conductive chain

$\Lambda(\delta, R_0)$ ⇒ Upper limit of a chain lenght that sustains electronic transport.

$L < \Lambda \Longrightarrow \langle \xi(E) \rangle > L \Longrightarrow$ conductive

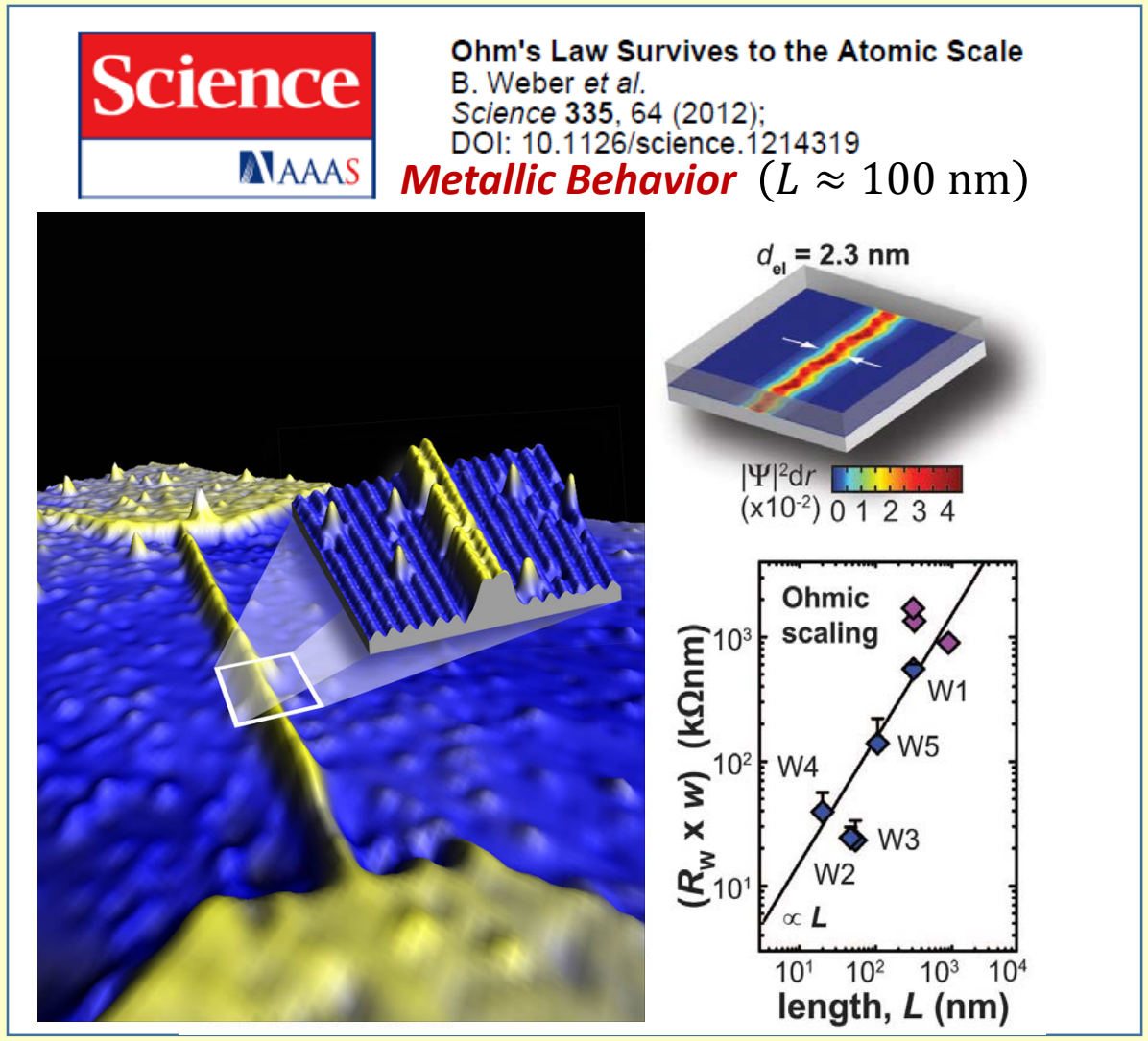
$\langle \ldots \rangle$ → ensemble average.

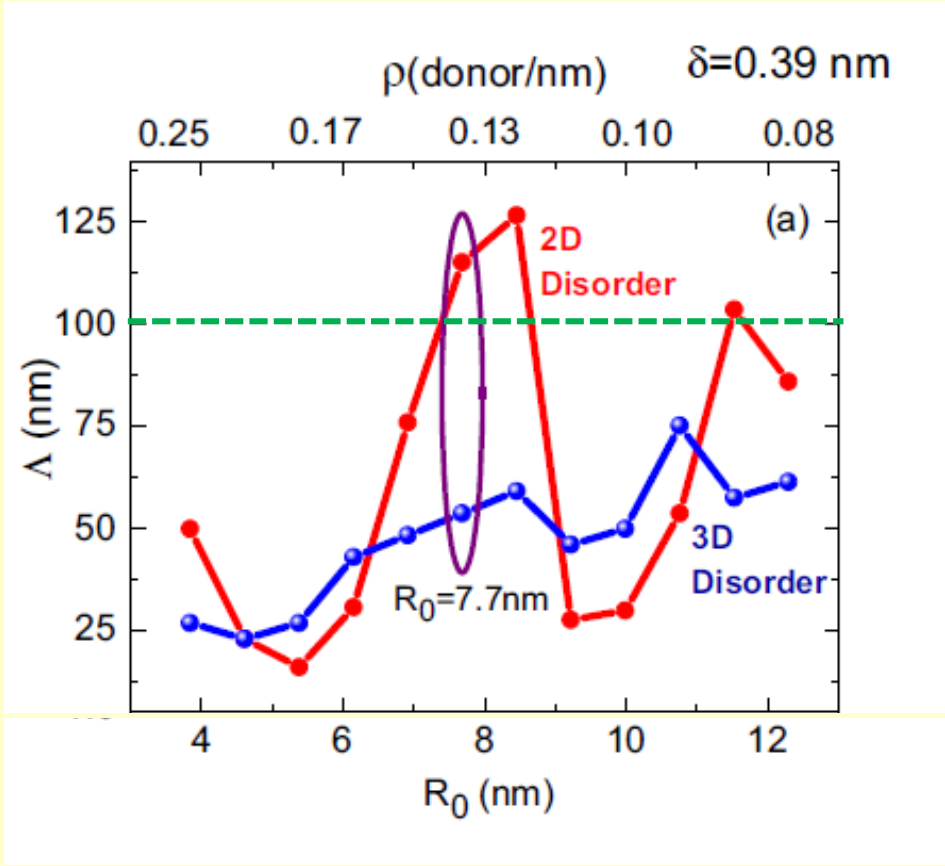


The figure is for a fixed δ, $E = E_0$ (band center) and several values of R_0:

$\langle \xi(E_0) \rangle > L$ below each curve

Maximum size of conductive chain





The figure is for a fixed δ,
$E = E_0$ (band center)
and several values of R_0:

$\langle \xi(E_0) \rangle > L$ below each curve

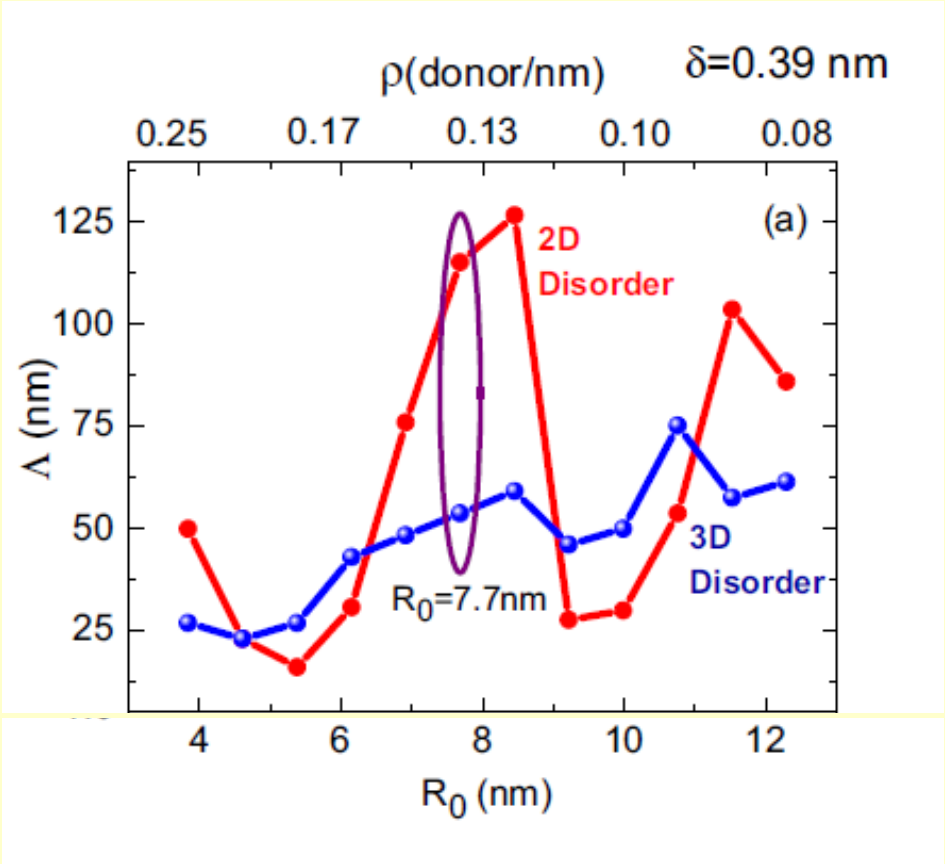
Maximum size of conductive chain:

Non-monotonic fluctuations – Why?

Hopping t :
- larger absolute values → favor transport;
- broad distribution of values (disorder)
→ hinder transport.

Empirical "Figure of Merit":

$$Q \propto \frac{\langle |t| \rangle}{\sigma(|t|)}$$



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Maximum size of conductive chain:

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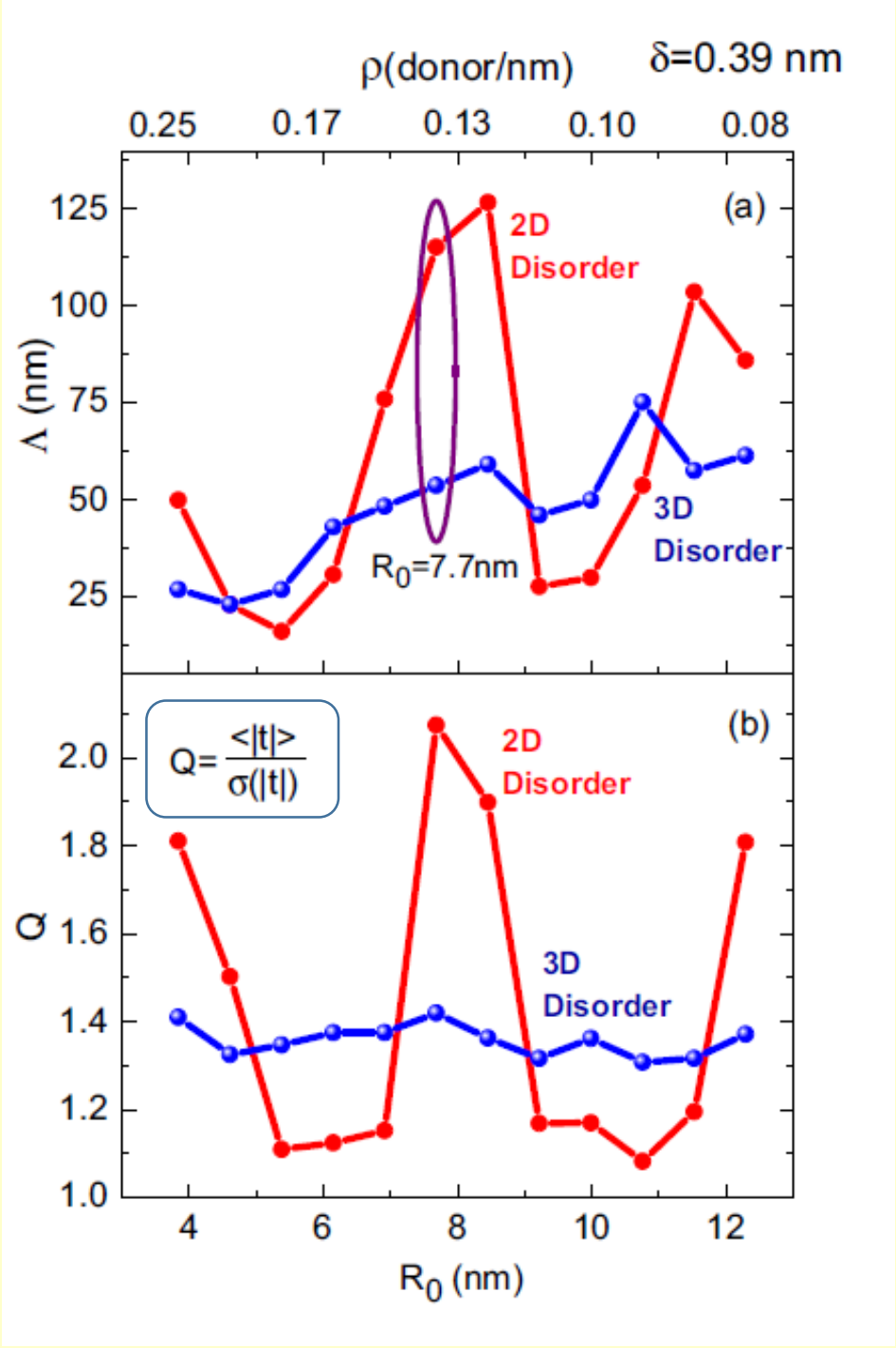
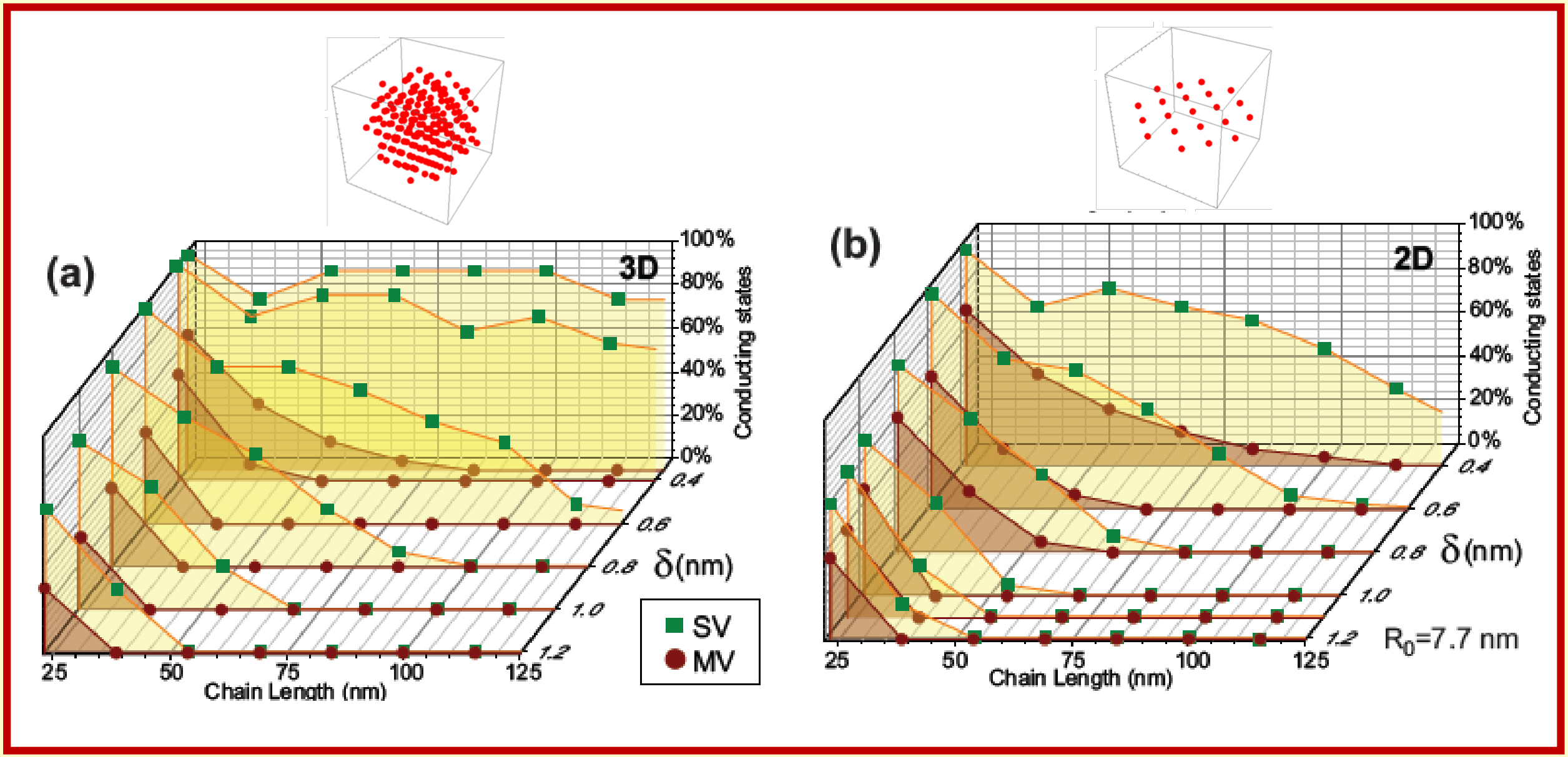


Conduction trends diagrams

Fraction of conducting states (all energies)

$$\mathcal{F} = \int DOS(E)\langle\xi(E)\rangle\theta(\langle\xi(E)\rangle - L)\, dE$$

Conduction trends diagrams



Conclusions – Localization

- Electronic transport possible for fairly diluted 1D chains in size comparable with experimental results ($L \approx 100\ \mathrm{nm}$).

- This behavior is expected to be enhanced for chains with smaller disorder radius and if restricted to a plan (2D disorder).

- Possibility of control by design of electronic transport.

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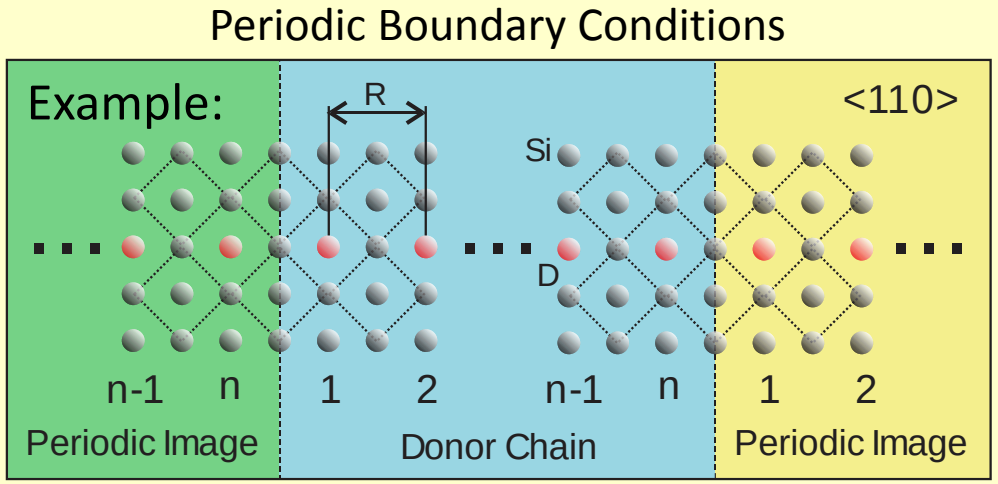
Mitigating valley-driven localization in atomically thin dopant chains in Si

Amintor Dusko,* A. L. Saraiva, and Belita Koiller
Instituto de Física, Universidade Federal do Rio de Janeiro, Caixa Postal 68528, 21941-972 Rio de Janeiro, Brazil
(Received 31 March 2016; revised manuscript received 8 August 2016; published 19 September 2016)

Many-Body: complete extended Hubbard Hamiltonian (no disorder)

Substitutional Donors array (D) in Si



Configuration Interaction

↓

Direct Diagonalization

Magnetic Properties?

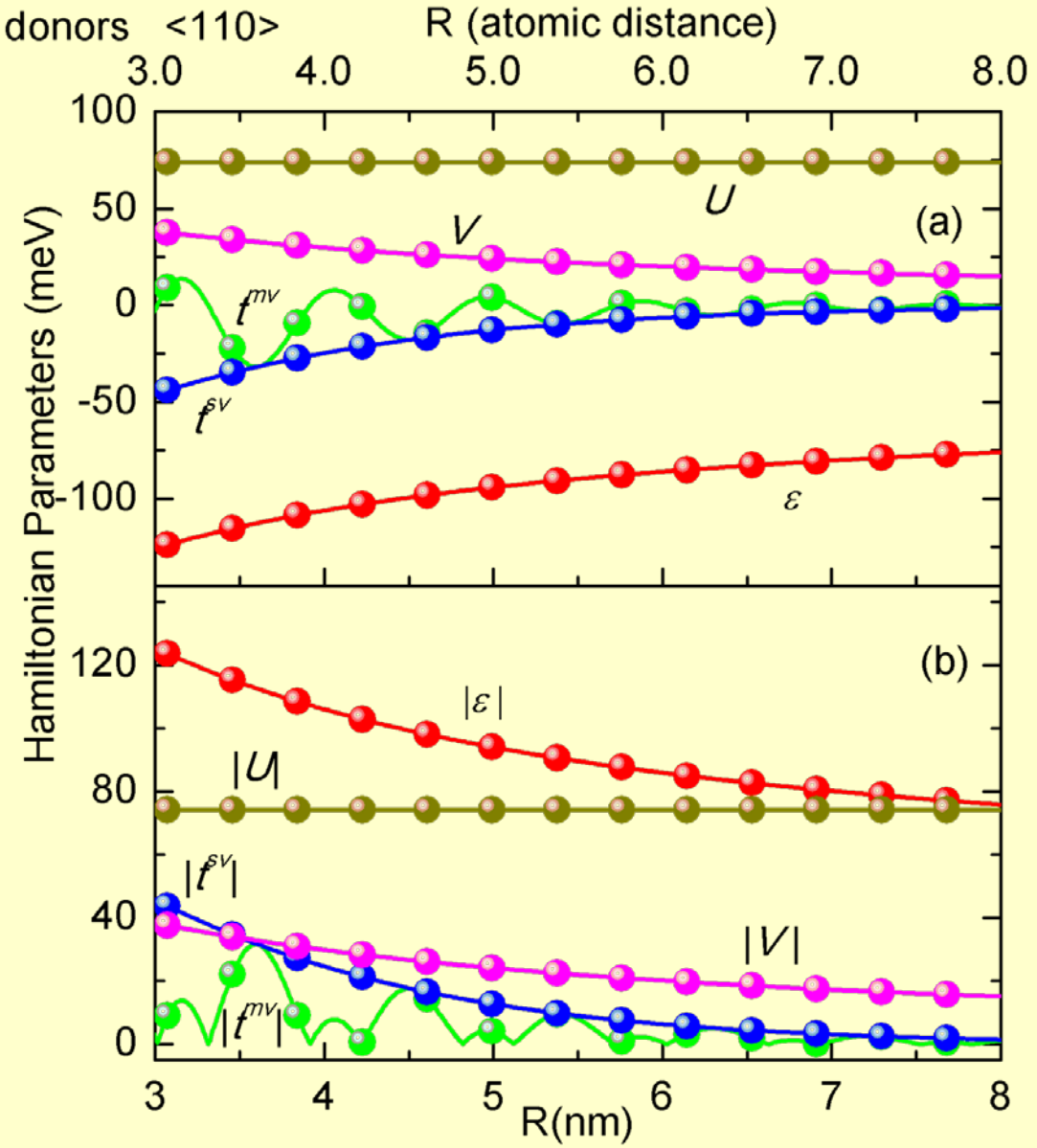
1D ordered Chain
Extended Hubbard Hamiltonian.

Parameters:

$$H = \sum_{i,\sigma} \boldsymbol{\varepsilon_i} n_{i,\sigma} + \sum_{\langle i,j\rangle,\sigma} \boldsymbol{t_{ij,\sigma}} c^{+}_{i,\sigma} c_{j,\sigma}$$

$$+ \sum_{i,\sigma} \boldsymbol{U_i} n_{i,\sigma} n_{i,\bar{\sigma}} + \sum_{\langle i,j\rangle,\sigma,\sigma'} \boldsymbol{V_{ij}} n_{i,\sigma} n_{j,\sigma'}$$

ϵ_i, t_{ij}, U_i and V_i are all obtained analytically



Spin-Spin Correlations – 1D N-sites Chain

$$S_i^z = \frac{1}{2}\left(c_{i,\uparrow}^{+}c_{i,\uparrow} - c_{i,\downarrow}^{+}c_{i,\downarrow}\right)$$

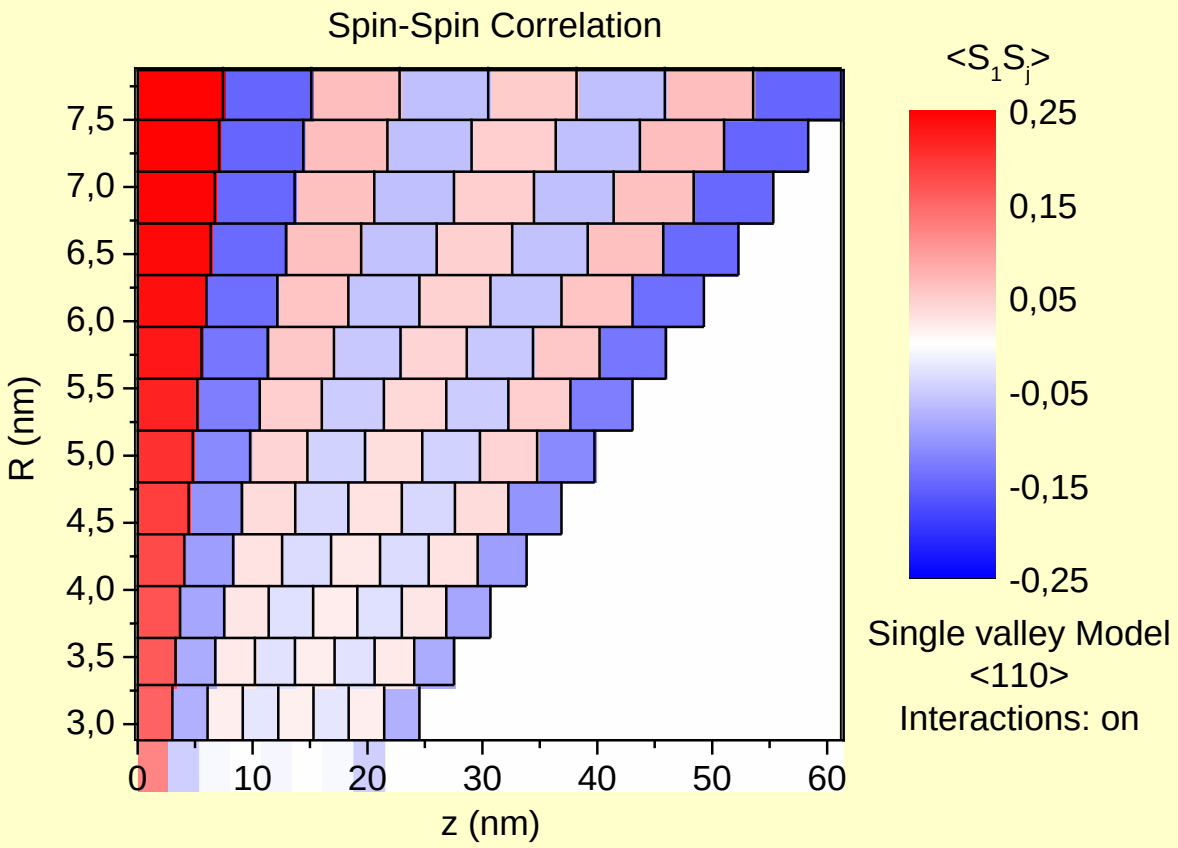
$$\left\langle S_i^z S_j^z \right\rangle = \frac{1}{4}\left(c_{i,\uparrow}^{+}c_{i,\uparrow} - c_{i,\downarrow}^{+}c_{i,\downarrow}\right)\left(c_{j,\uparrow}^{+}c_{j,\uparrow} - c_{j,\downarrow}^{+}c_{j,\downarrow}\right)$$

In 1D and $N \to \infty$ there is no magnetic order for $T \neq 0$!

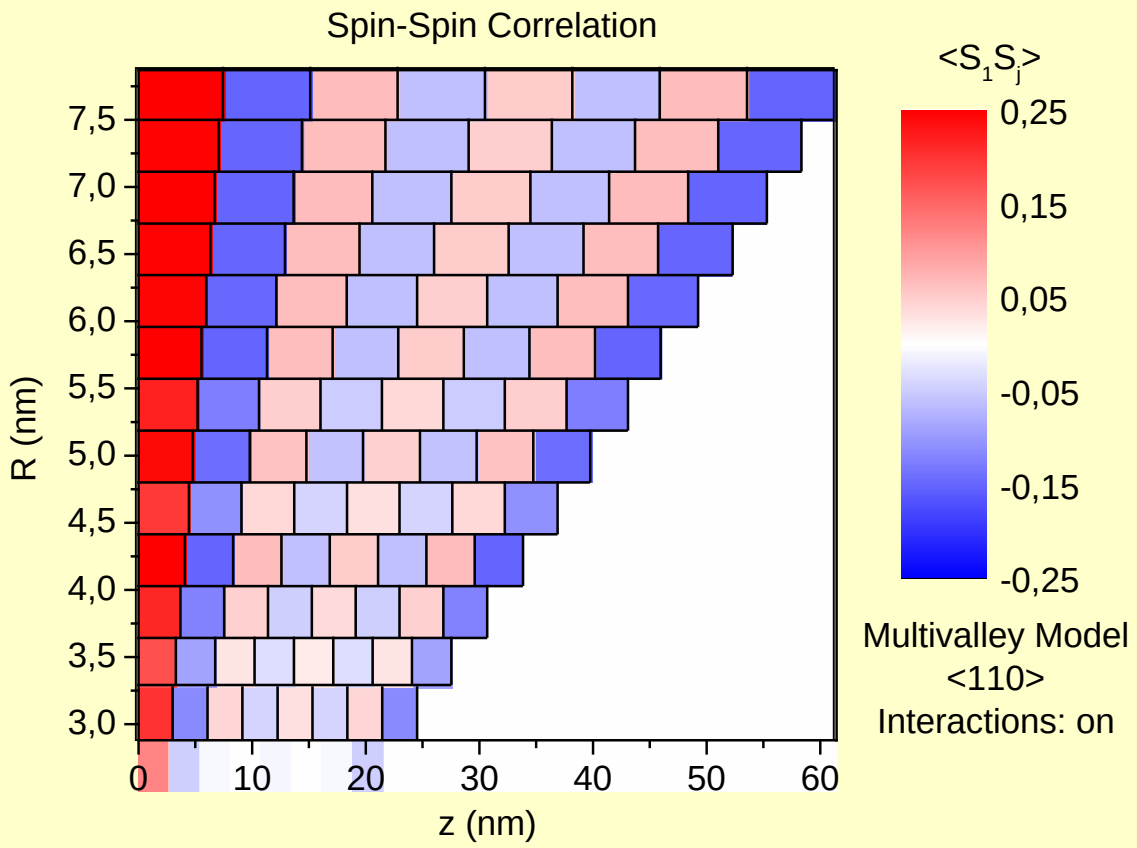
We consider here finite size chains (not in the thermodynamic limit).

Results for 8 electrons – 8 sites

A) Single valley – Electron-electron interactions

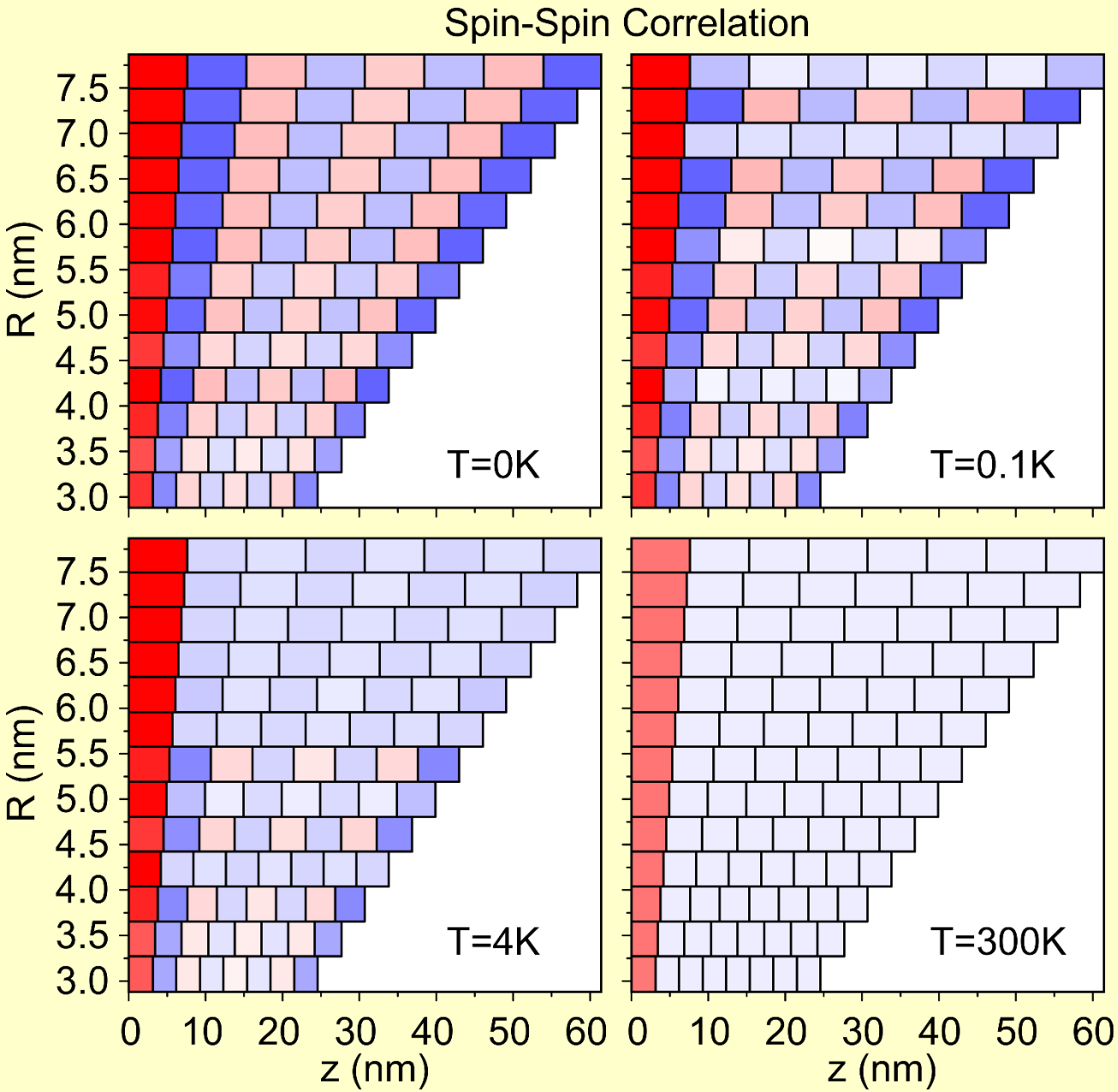


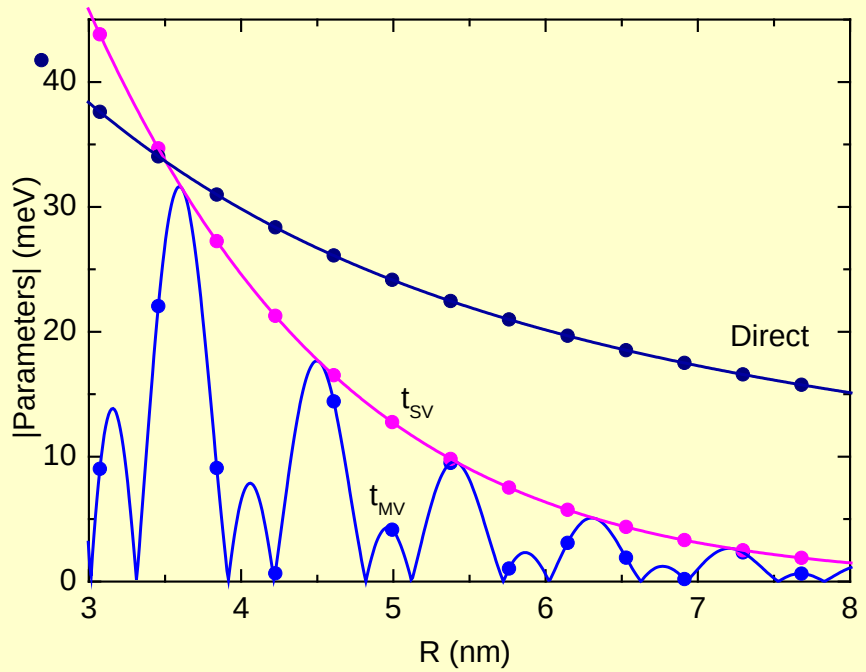
B) Multivalley – Electron-electron interactions



AF behavior for T=0K

B) Multivalley – Electron-electron interactions – Temperature effects





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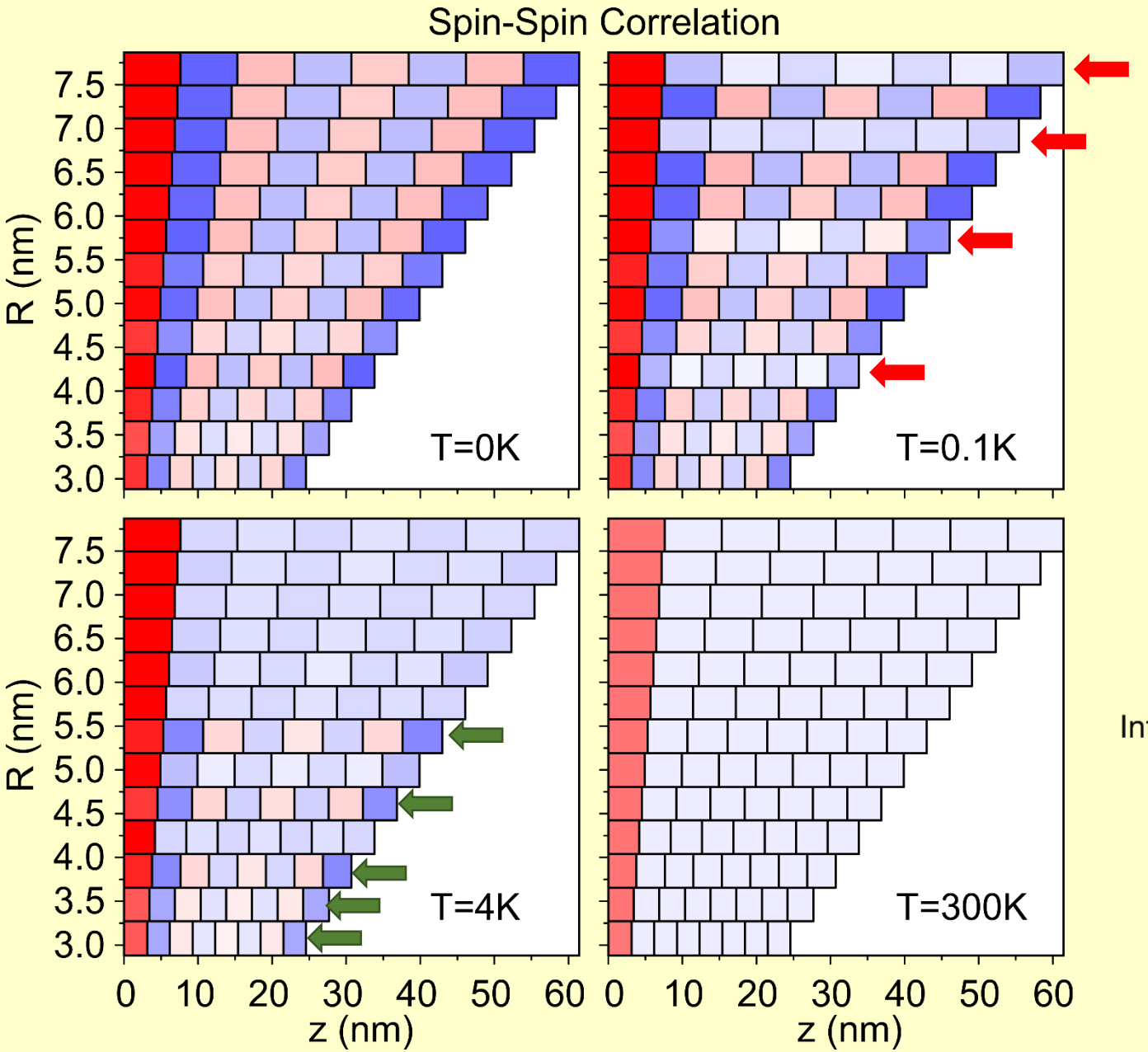

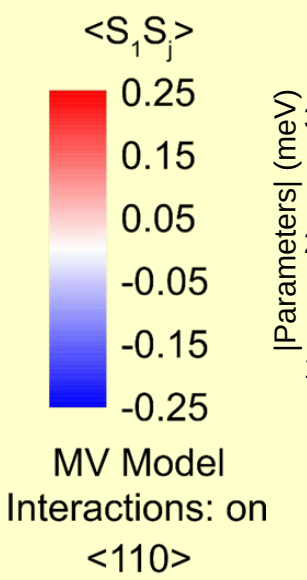

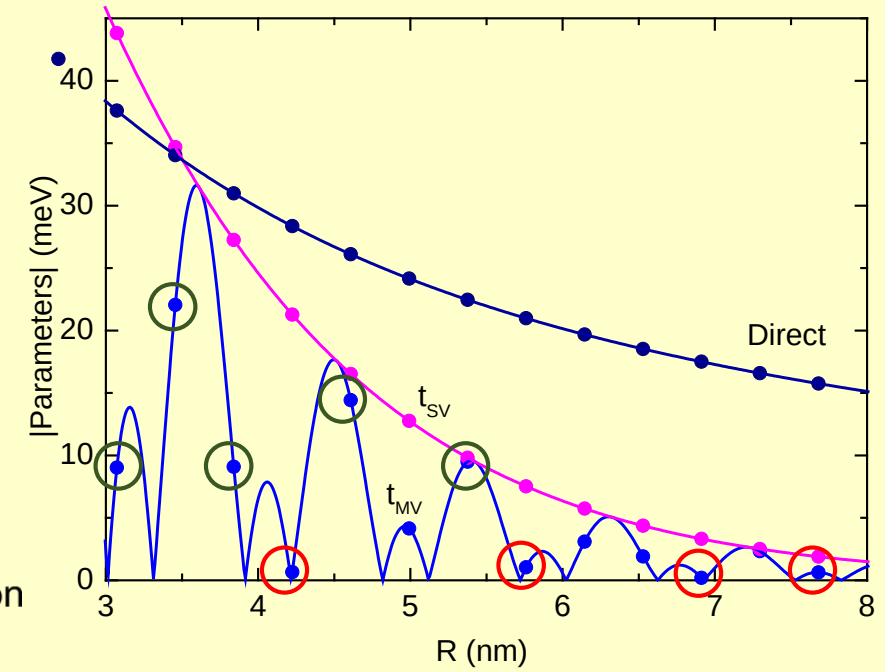

- Finite Samples show non-zero spin-spin antiferromagnetic-like correlation.

- The MV hopping opens possibility for systems with magnetic properties chosen by design, even around T=4K.

- A Hubbard lab?

Thank you!