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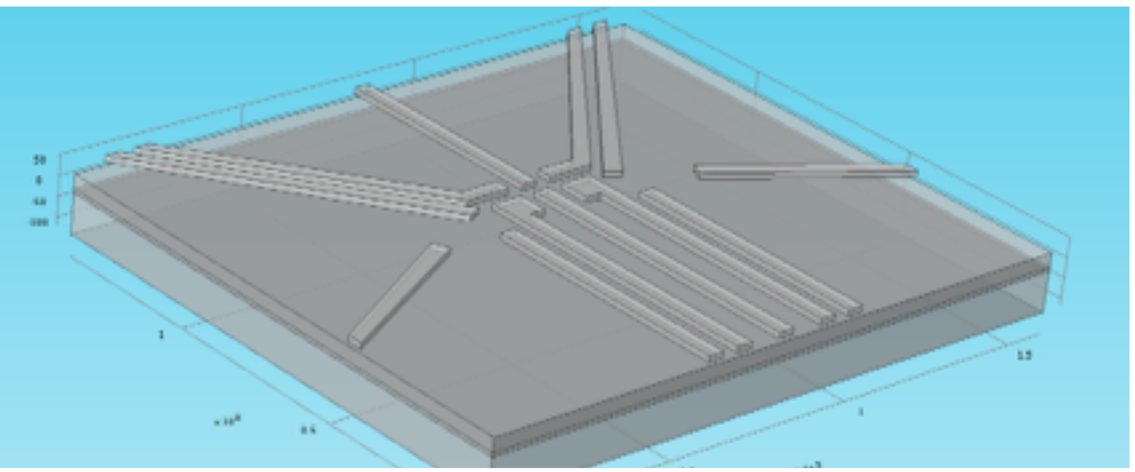

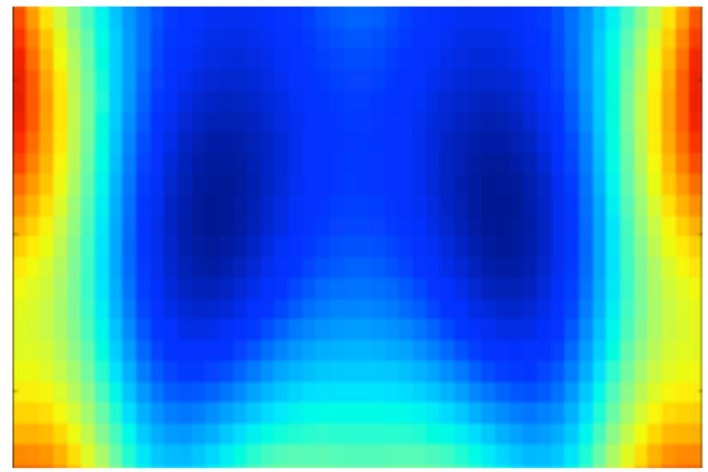

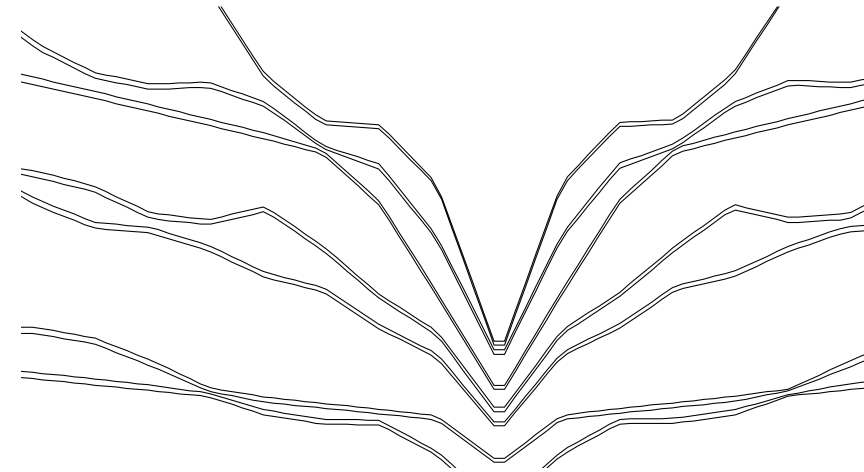

Full-scope modeling of semiconductor devices for quantum information processing

John King Gamble

Andrew D. Baczewski, Adam Frees, N. Tobias Jacobson, Inès Montaño, Richard P. Muller, Erik Nielsen

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Motivation: quantum computing in semiconductors

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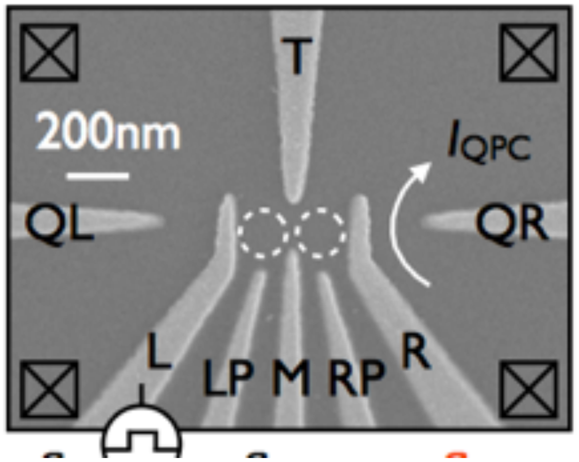

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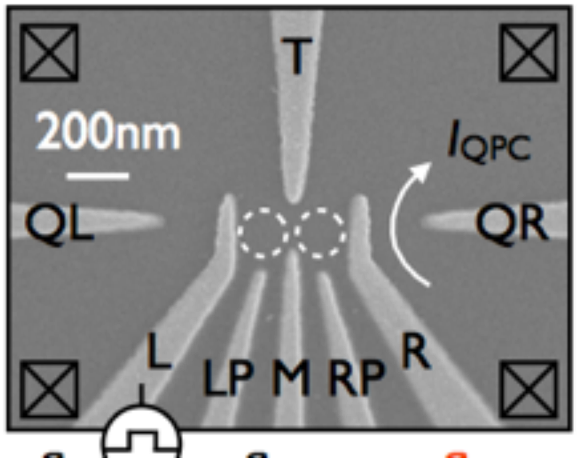

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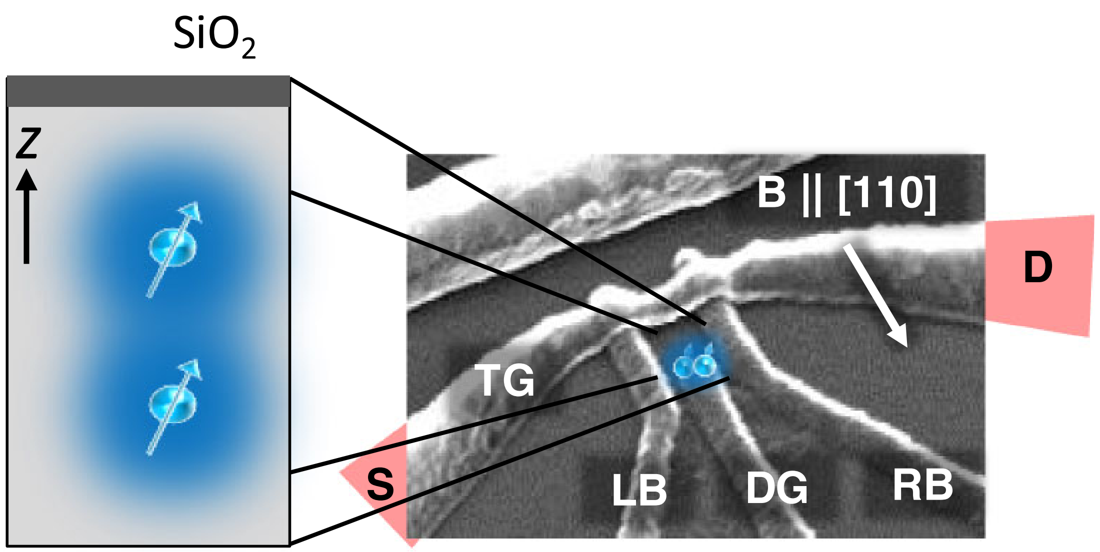

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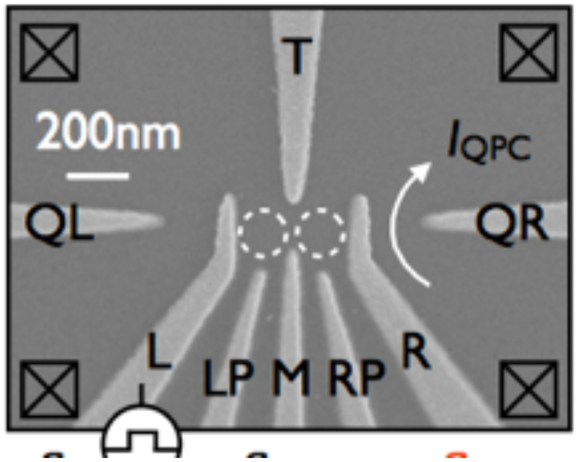

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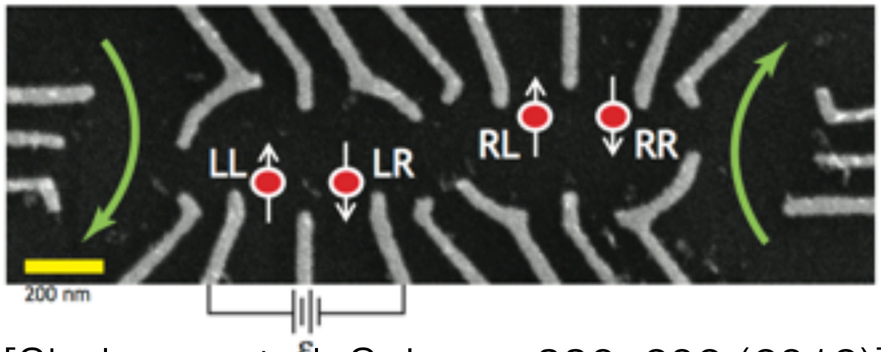

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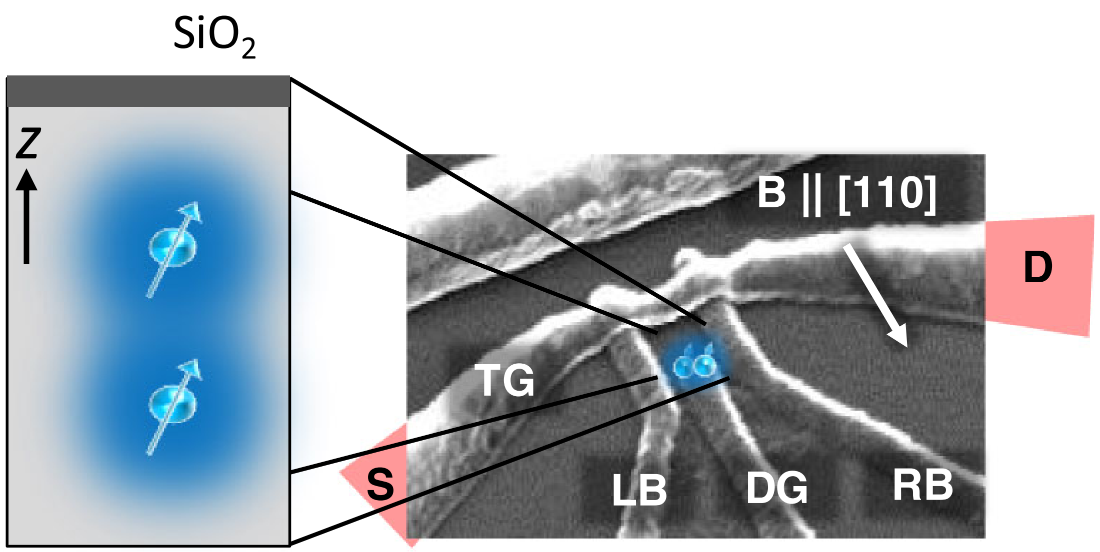

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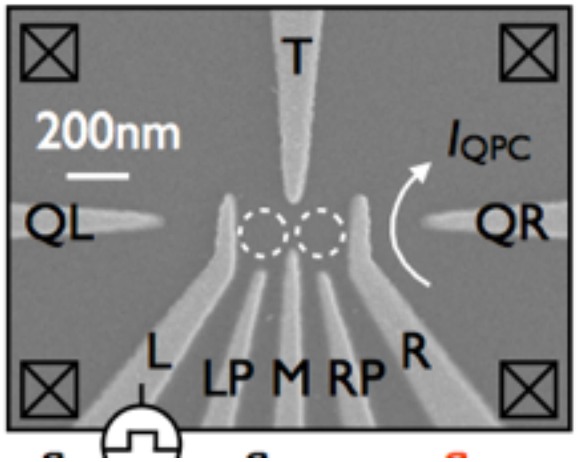

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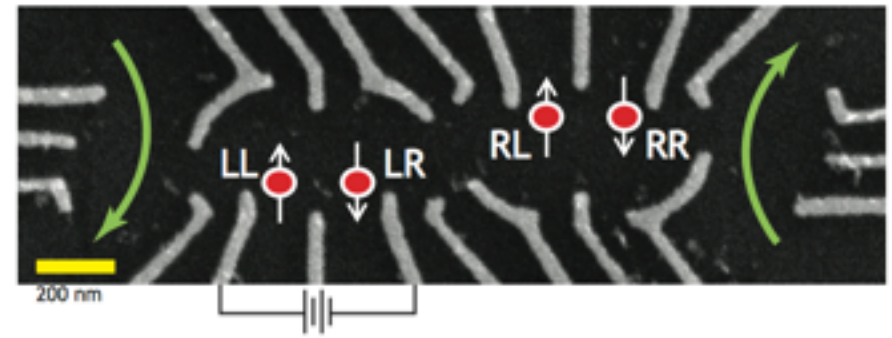

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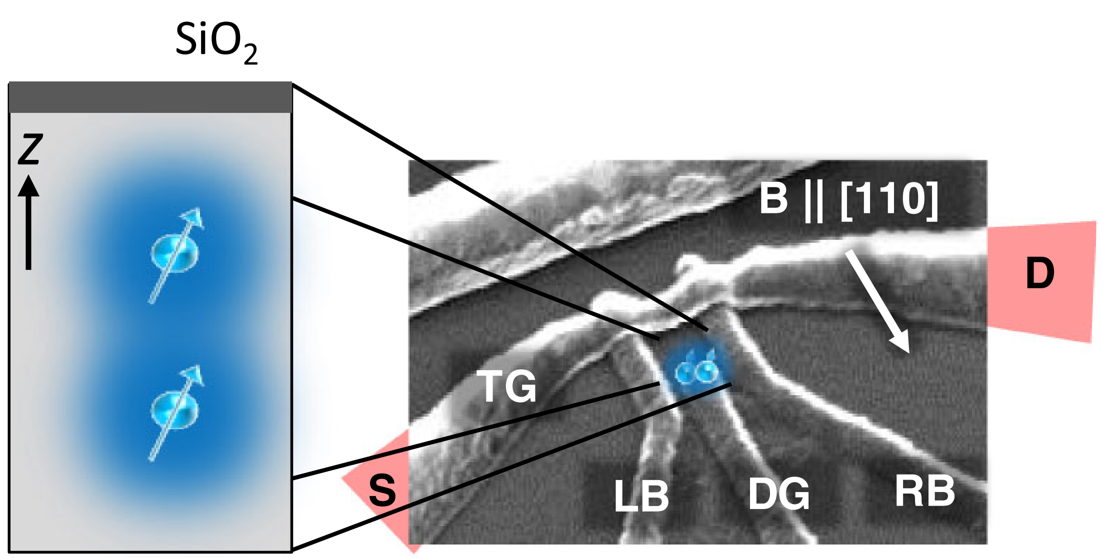

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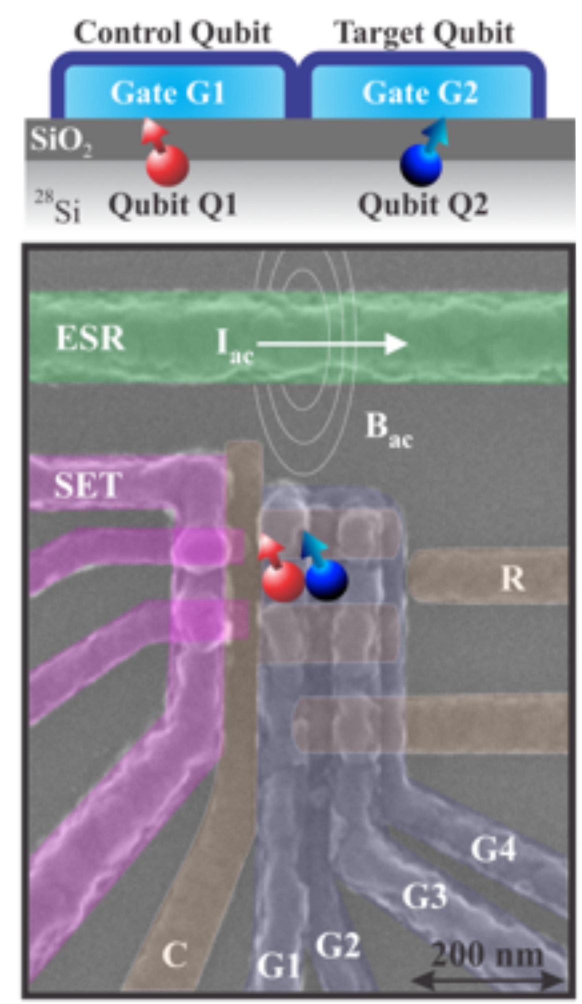

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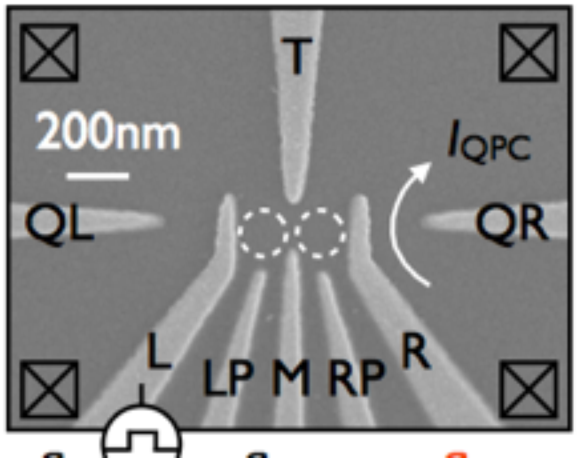

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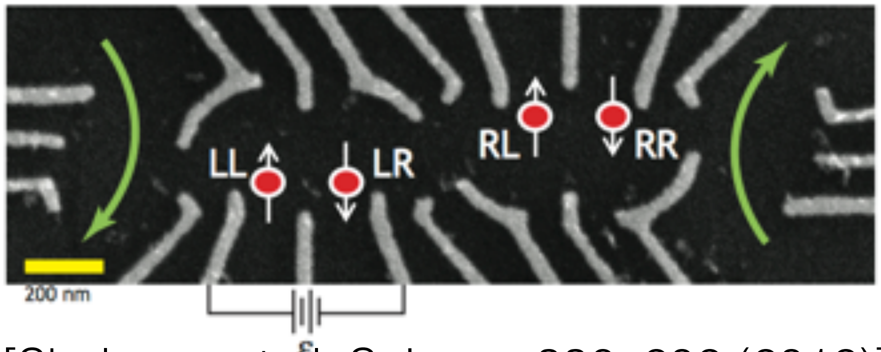

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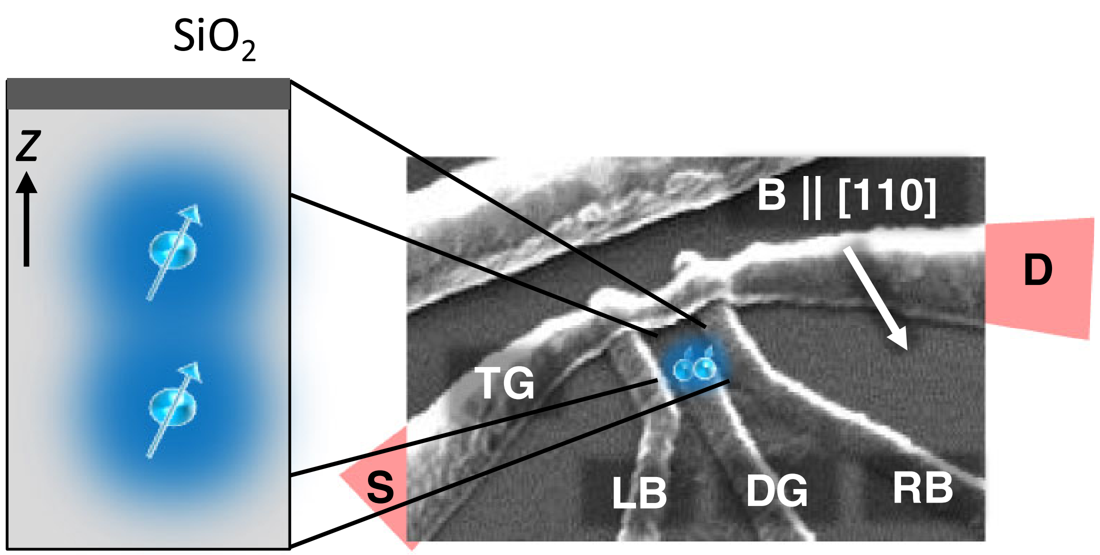

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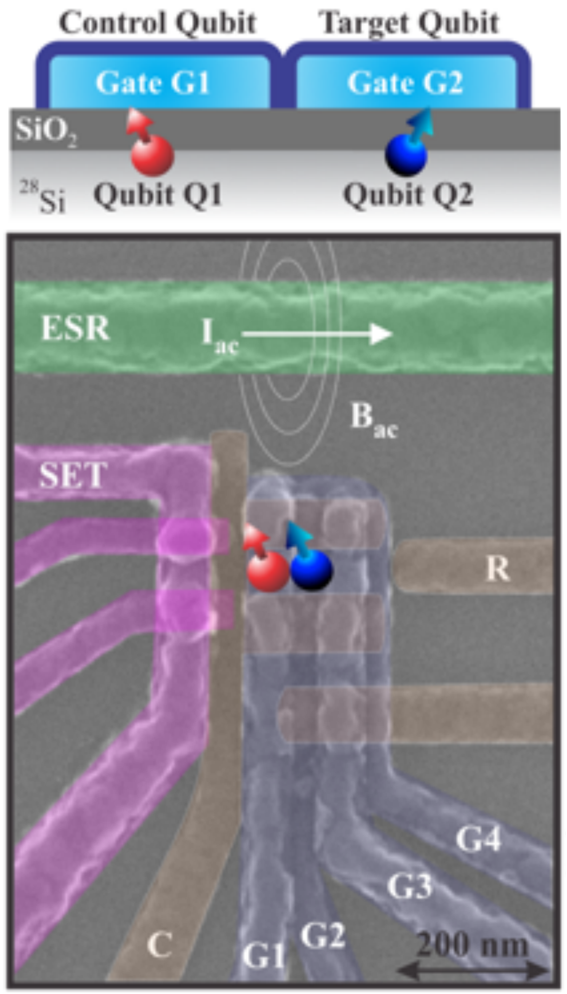

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Wow! These devices are getting pretty complicated…

Currently, many different techniques see use in modeling semiconductor QIP systems

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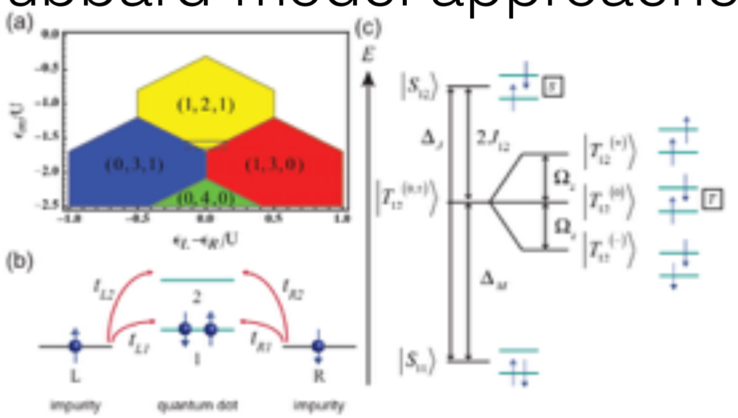
Hubbard-model approaches



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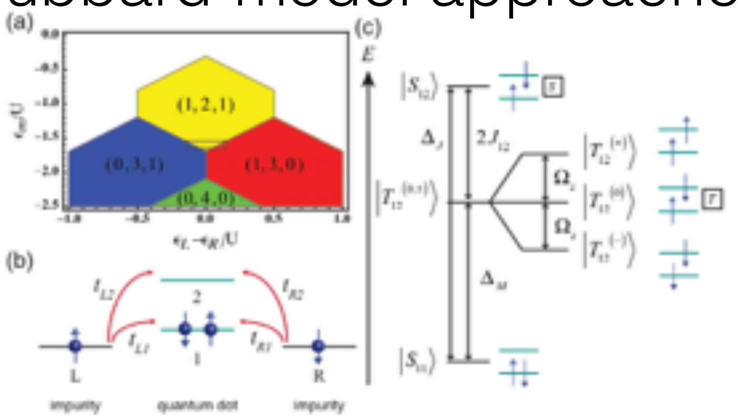

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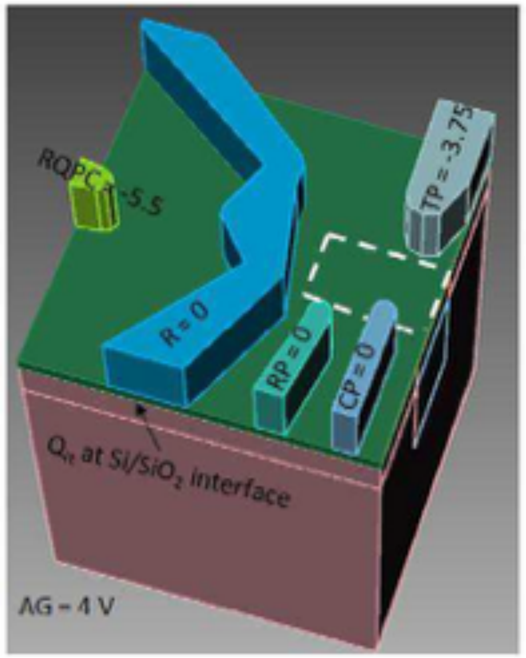
Device-scale methods



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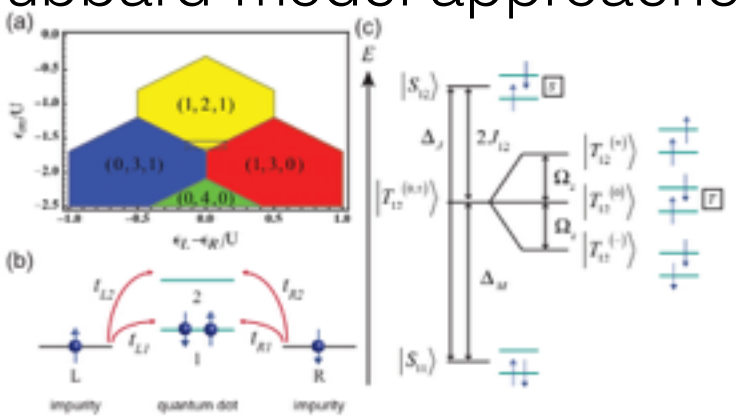

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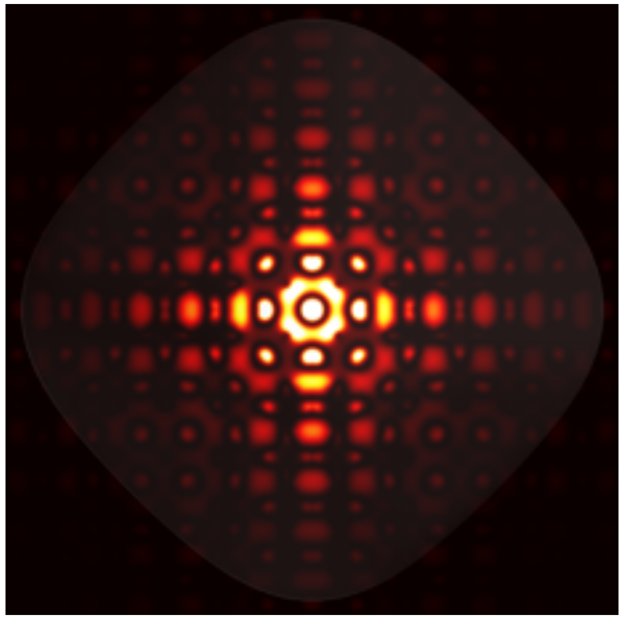
Effective mass theory



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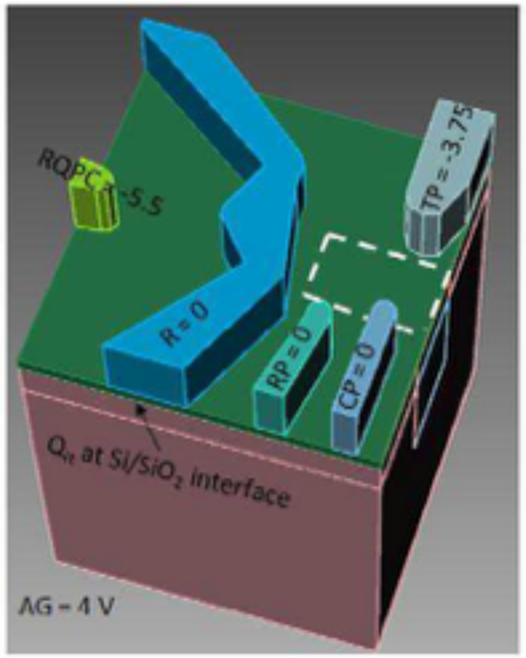

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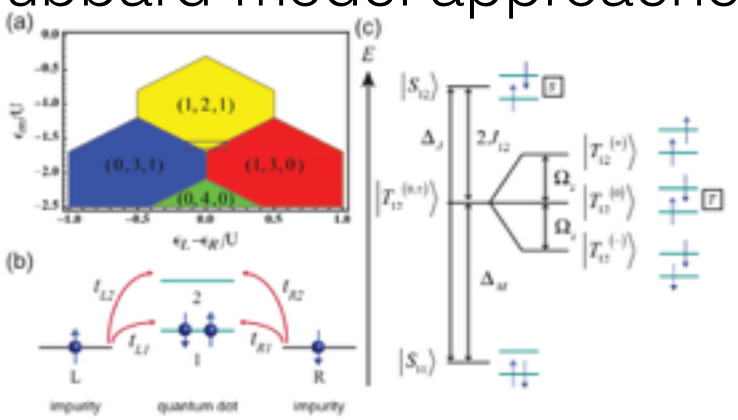

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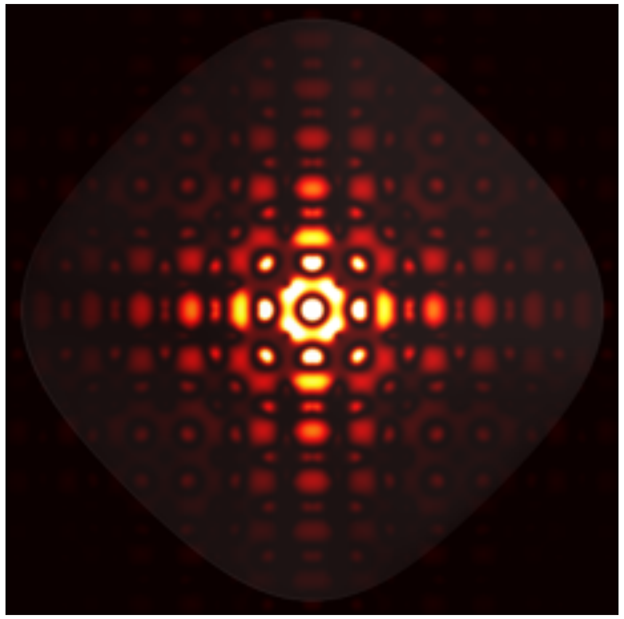

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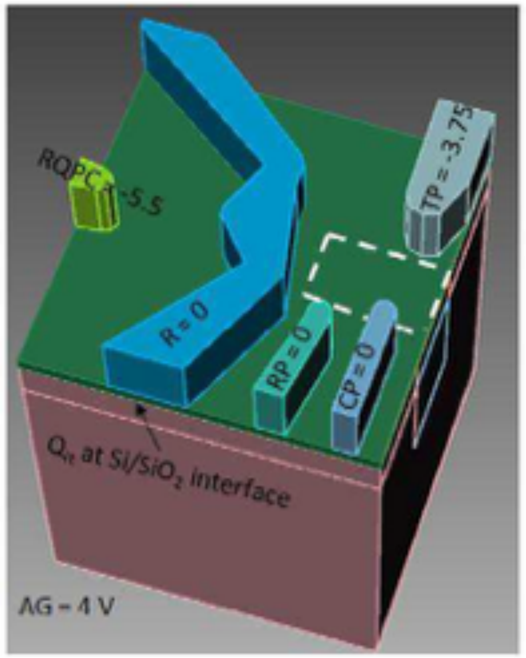

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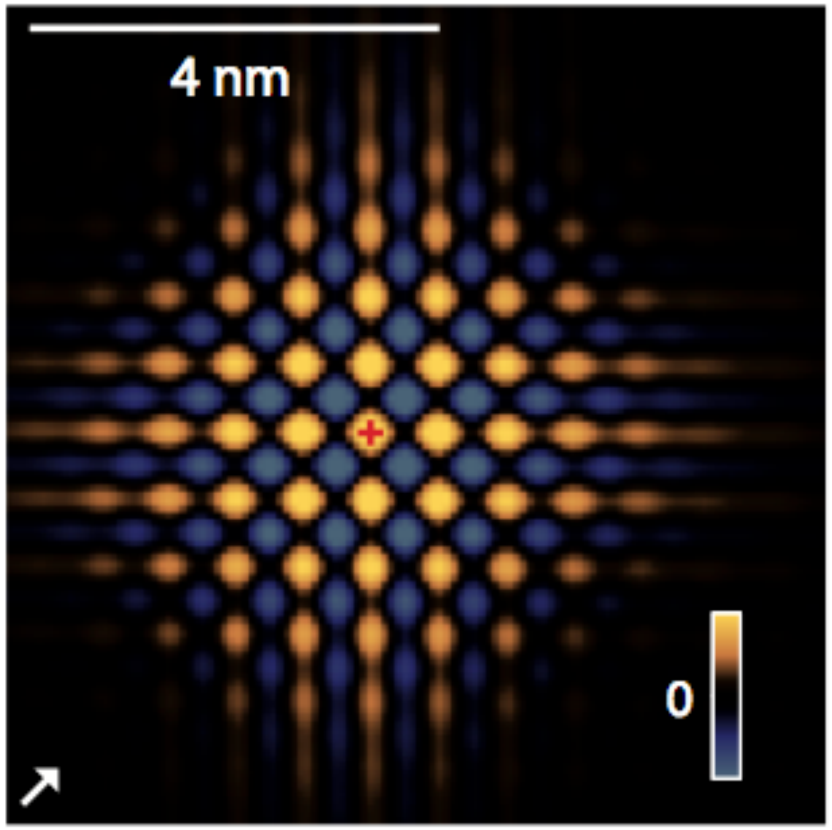
Atomistic tight-binding



[Salfi, et al. Nat. Mat. 13, 605-610 (2014)]

Our approach: ‘full-scope’ effective mass framework that handles device-level + small-feature physics

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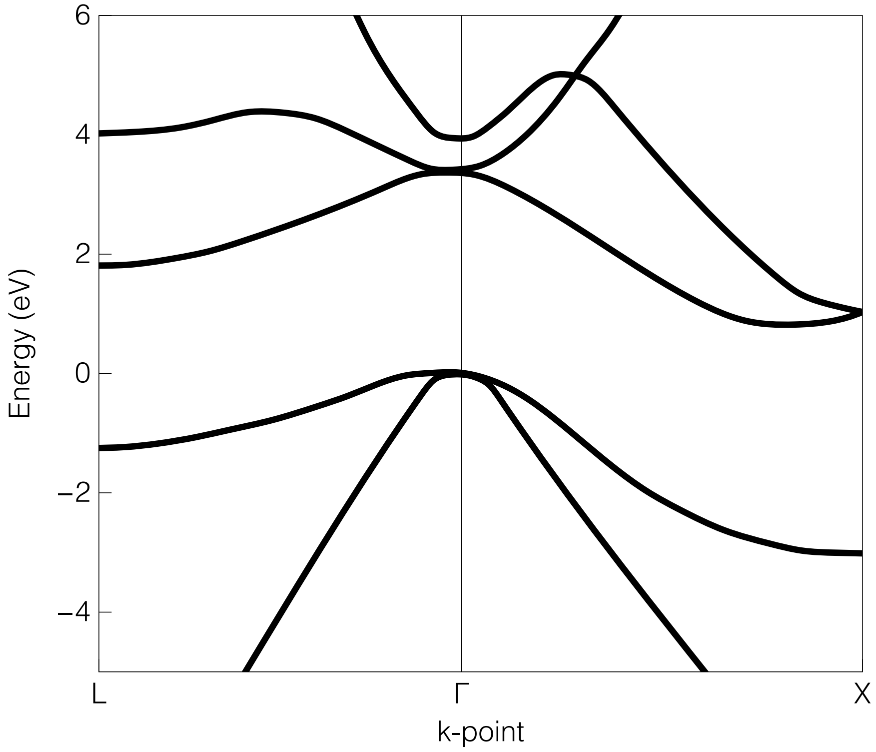
band structure of bulk silicon



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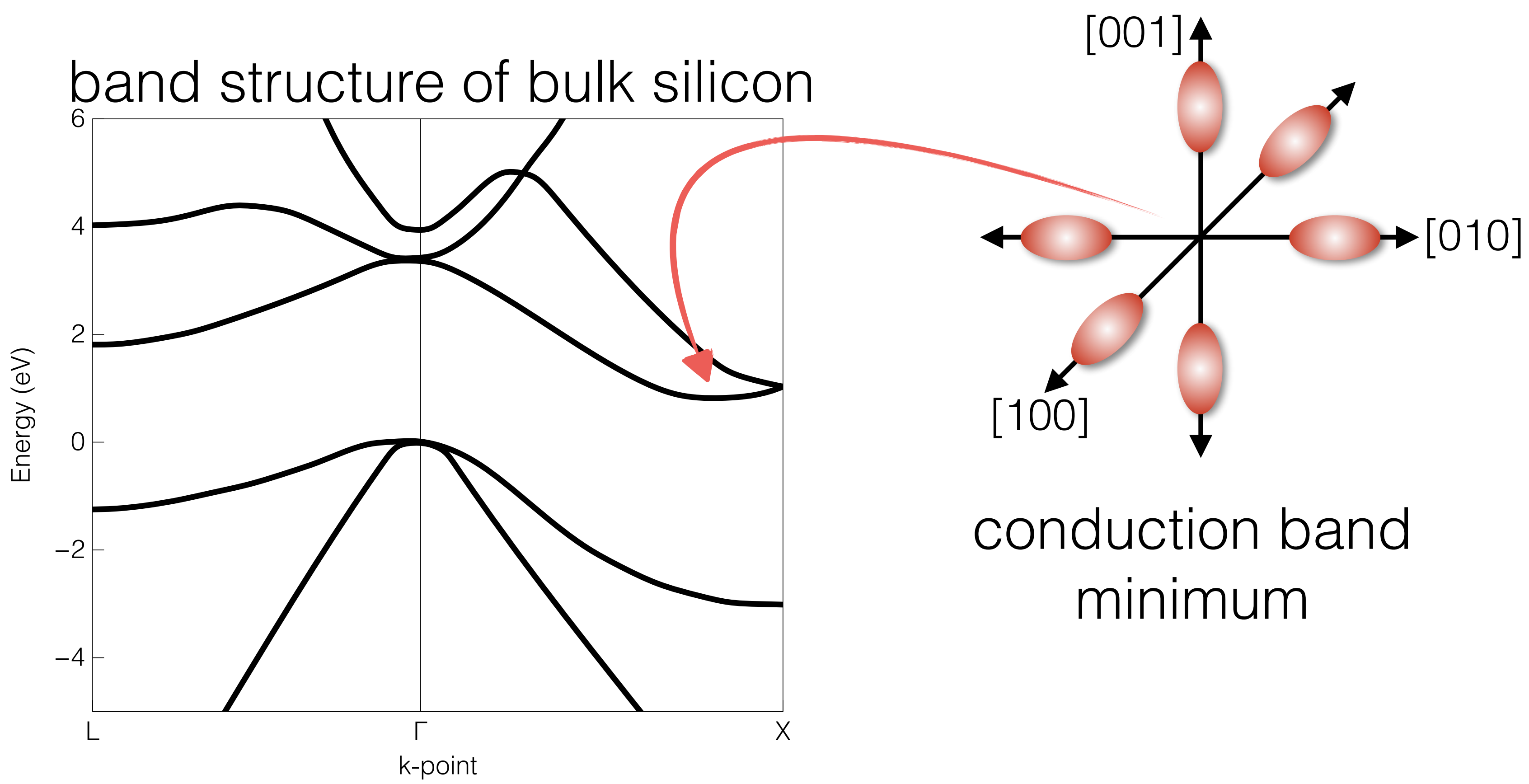

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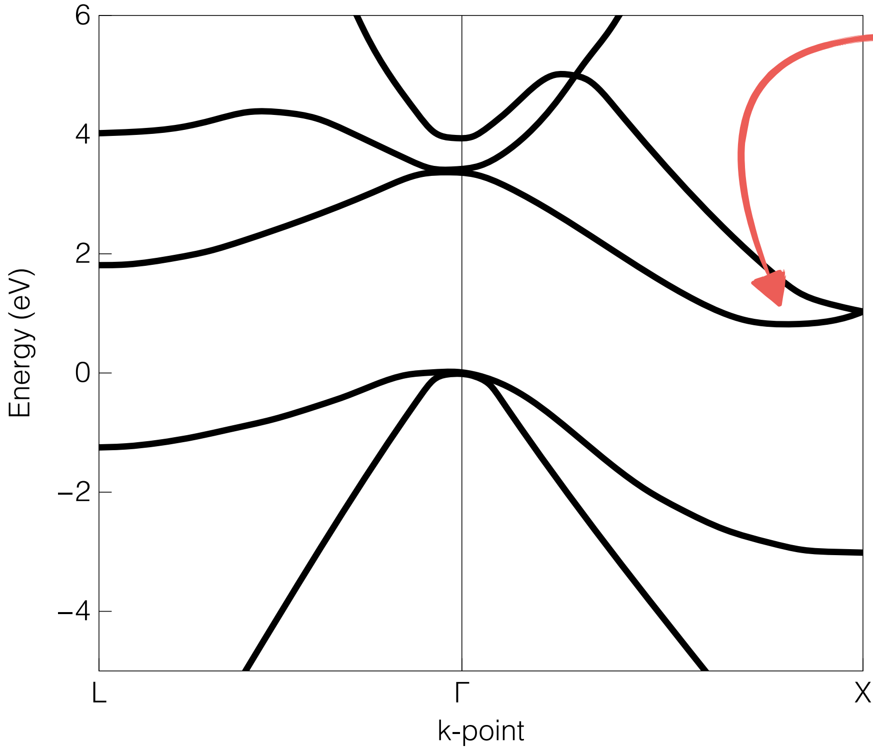

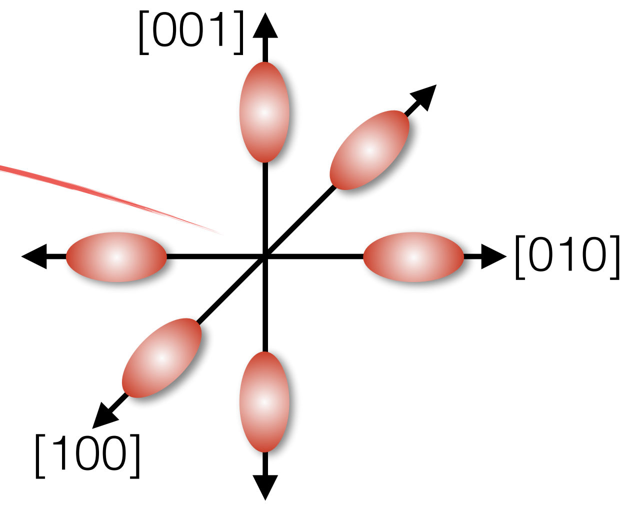

conduction band minimum

$$\psi(\mathbf{r}) = \sum_j F_j(r) e^{i\mathbf{k}_0^j \cdot \mathbf{r}} u_{\mathbf{k}_0^j}(\mathbf{r})$$

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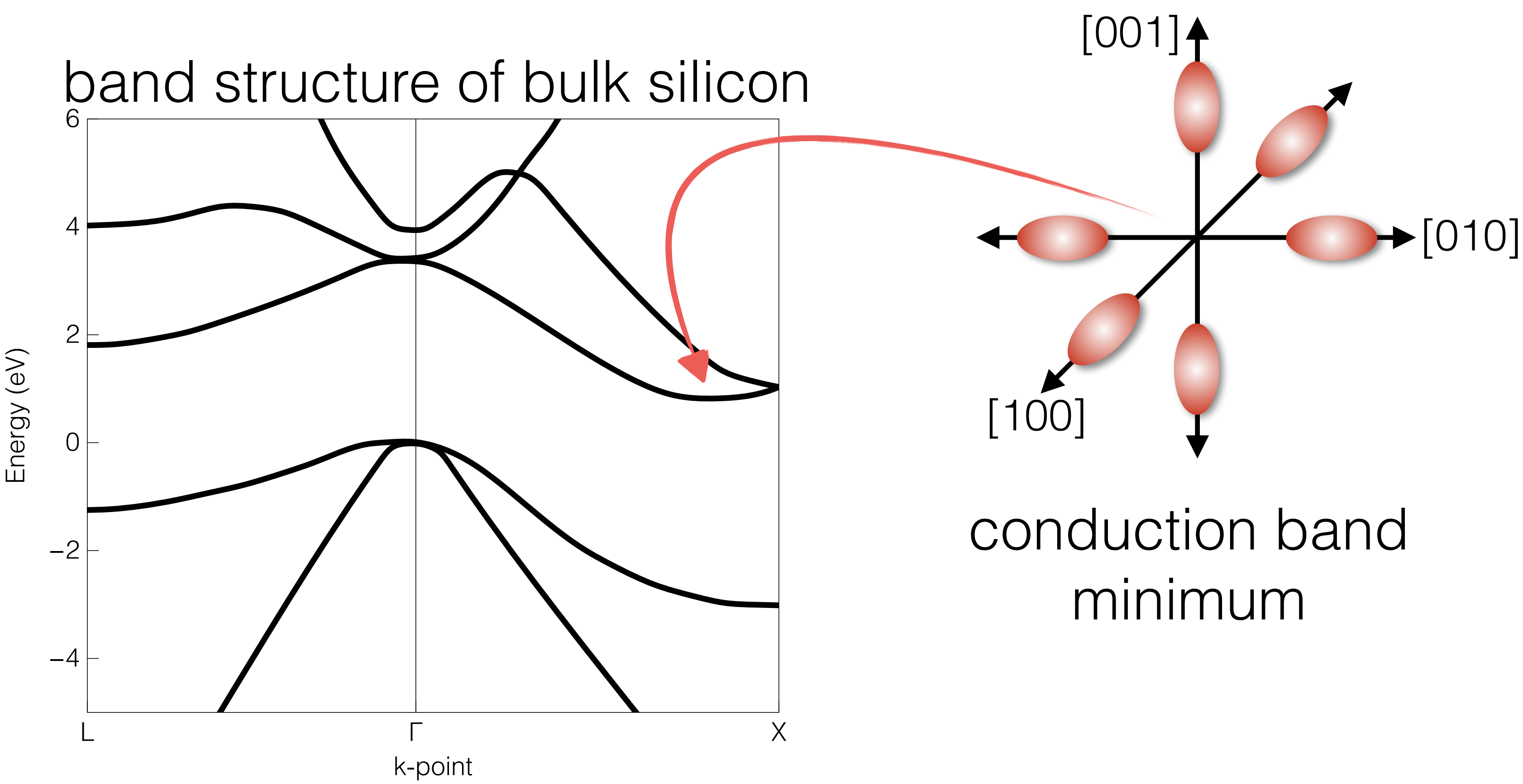

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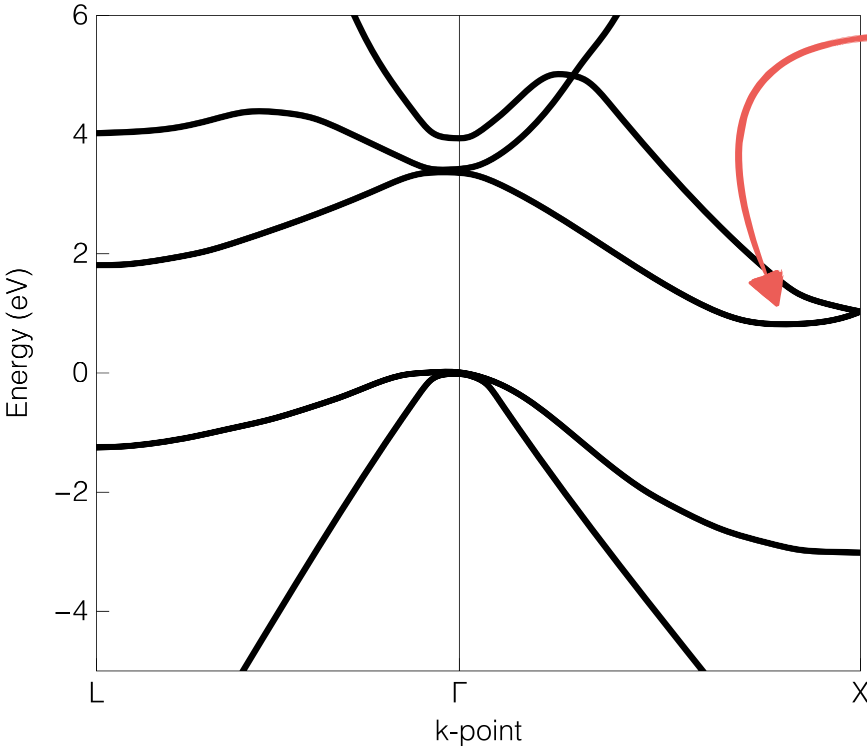
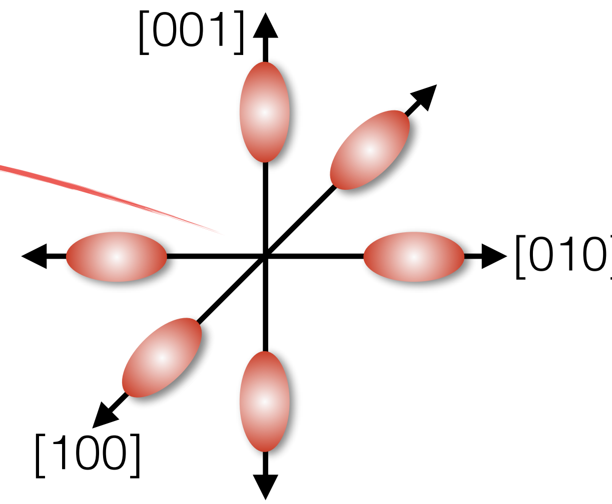
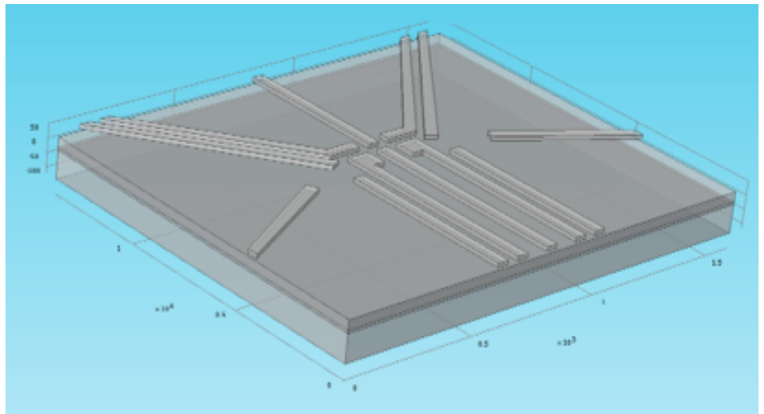




conduction band minimum

Finite element model



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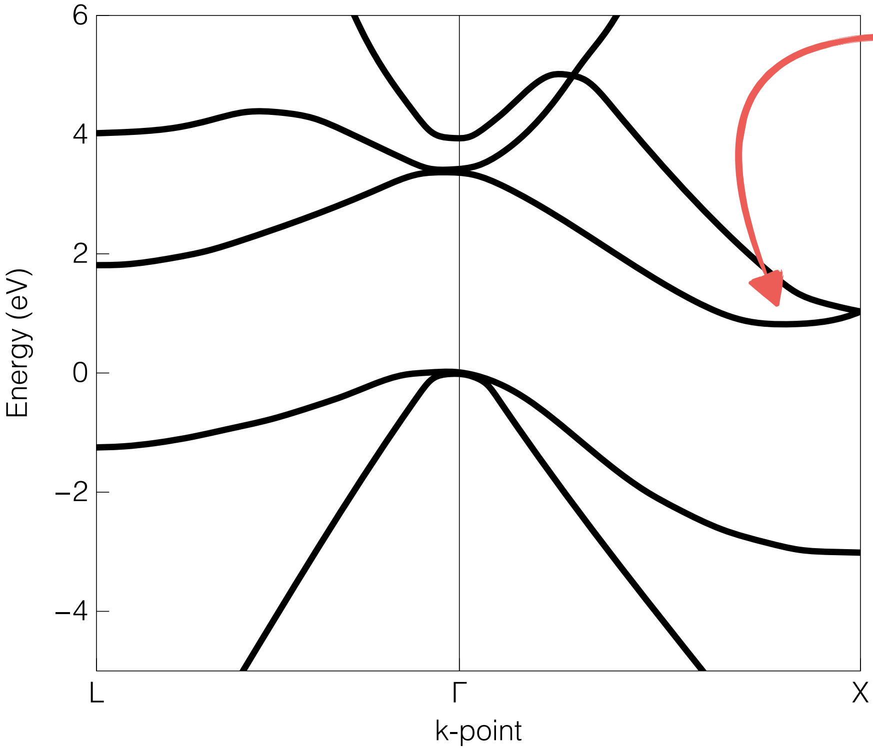

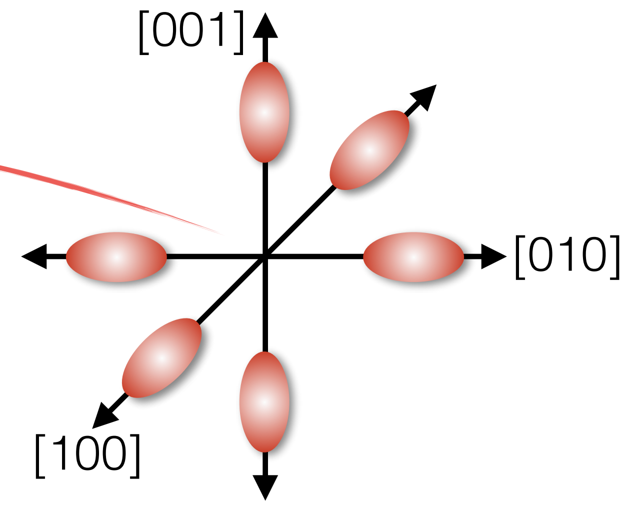

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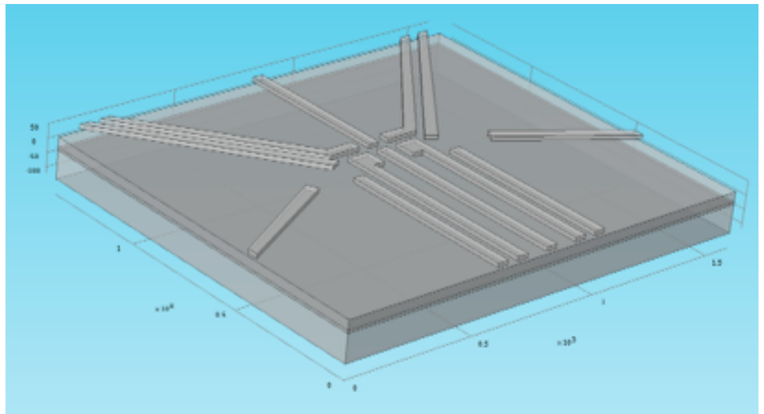
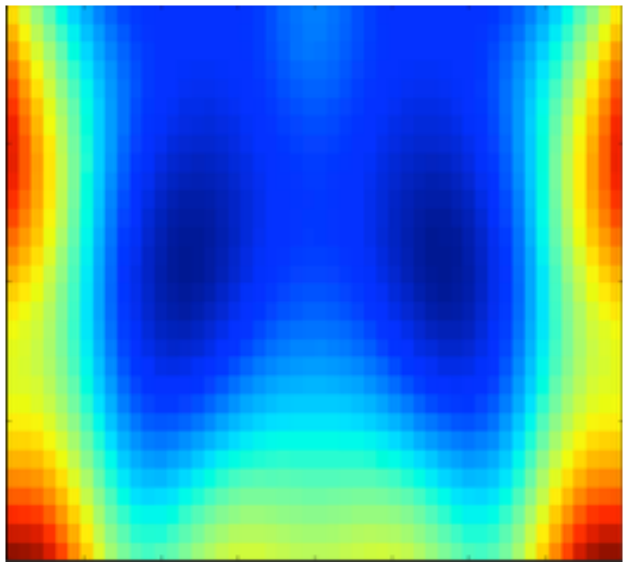


electrostatic landscape



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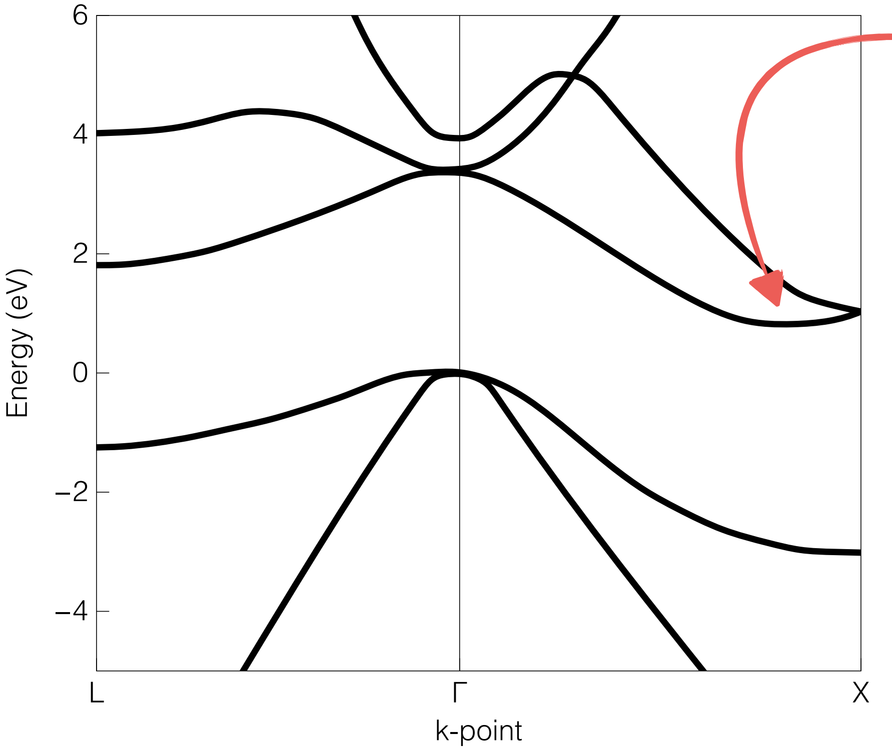

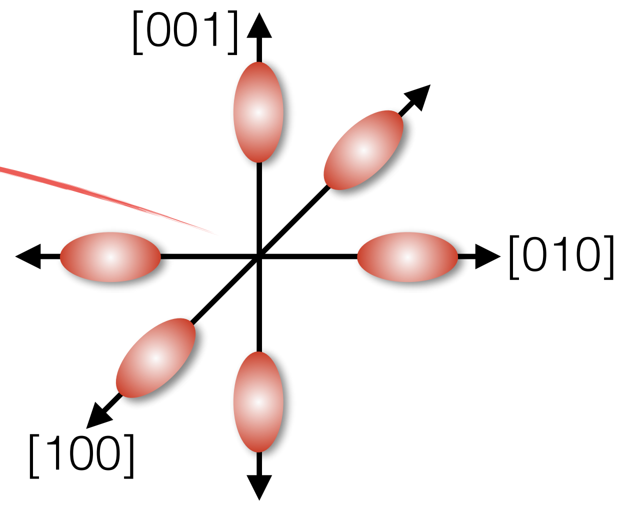

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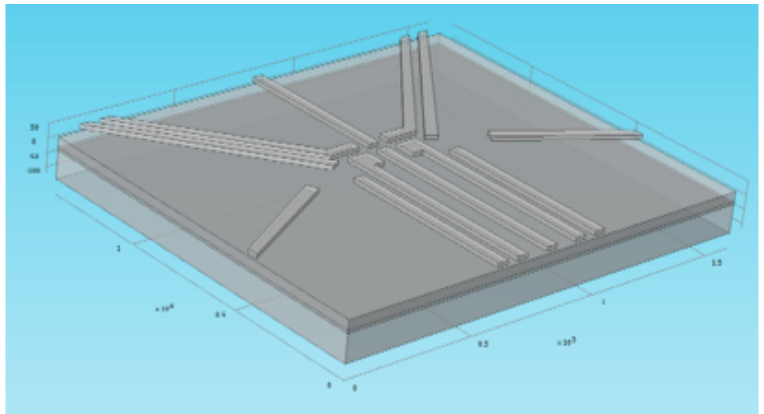

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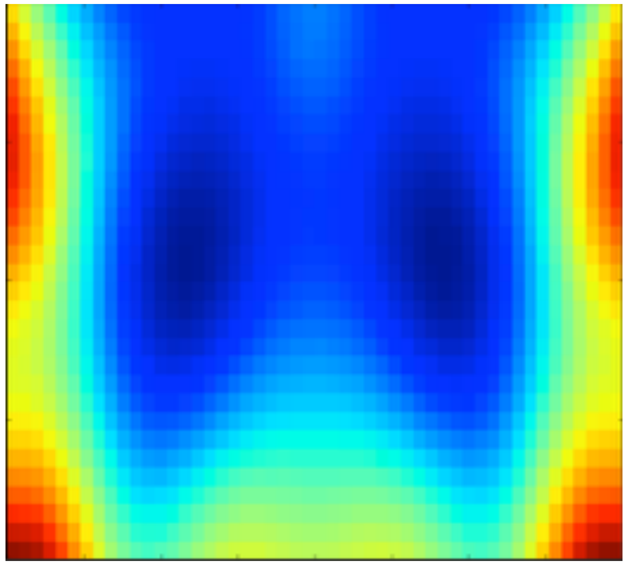

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1. Lay down a (3D) grid of Gaussians
2. Construct (local) overlaps with potential
3. Build generalized eigenvalue problem

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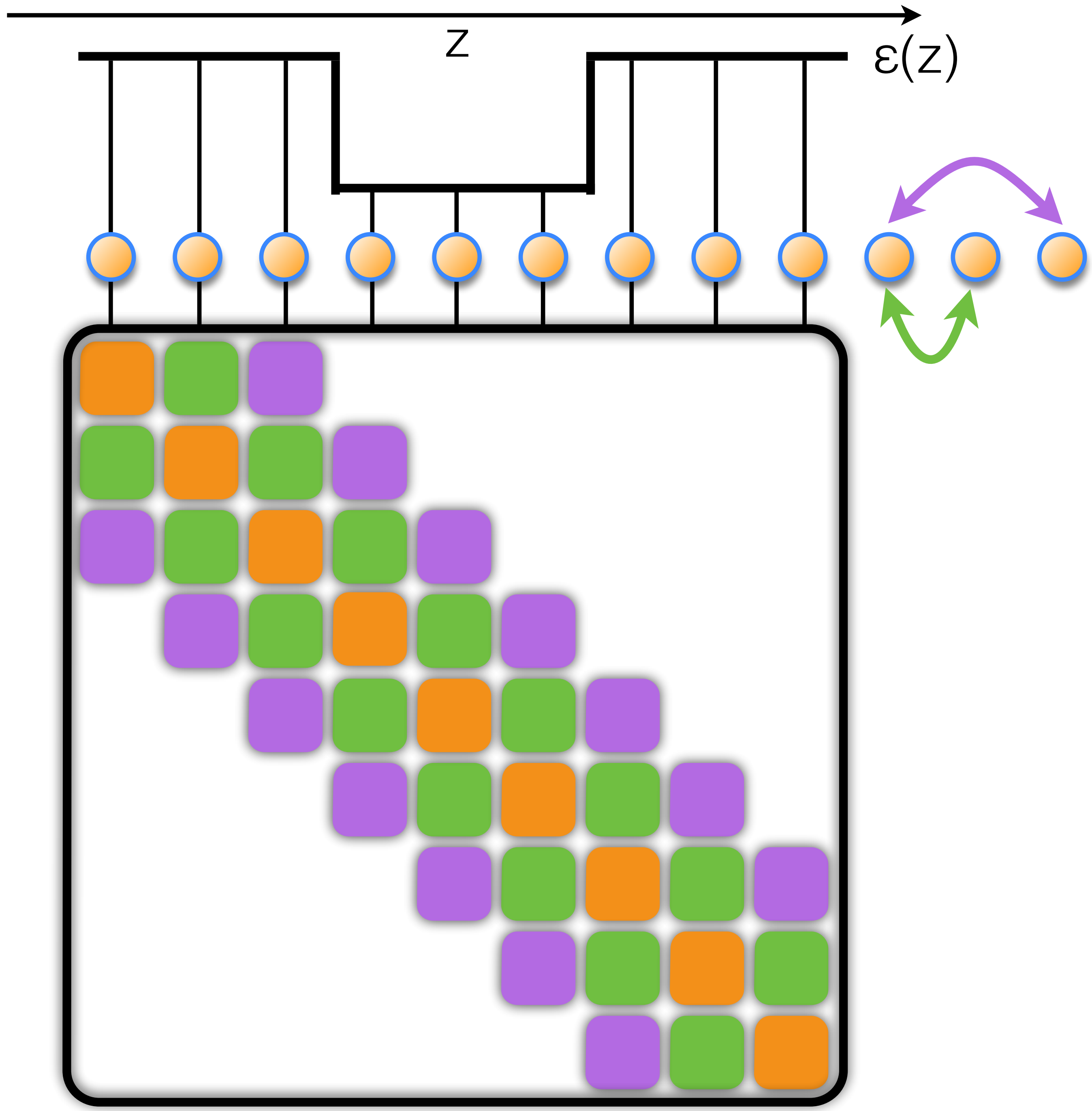

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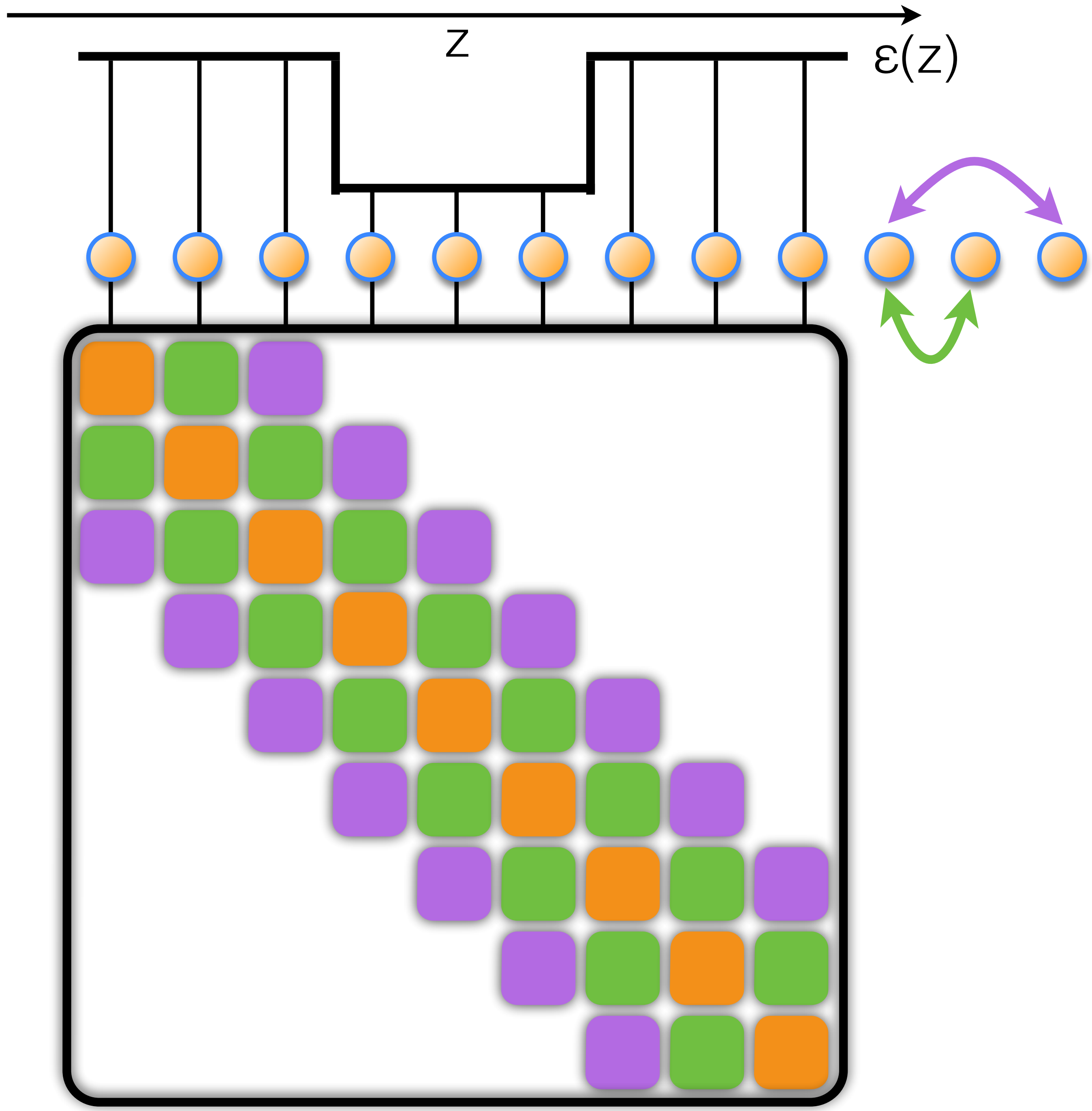

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potential +
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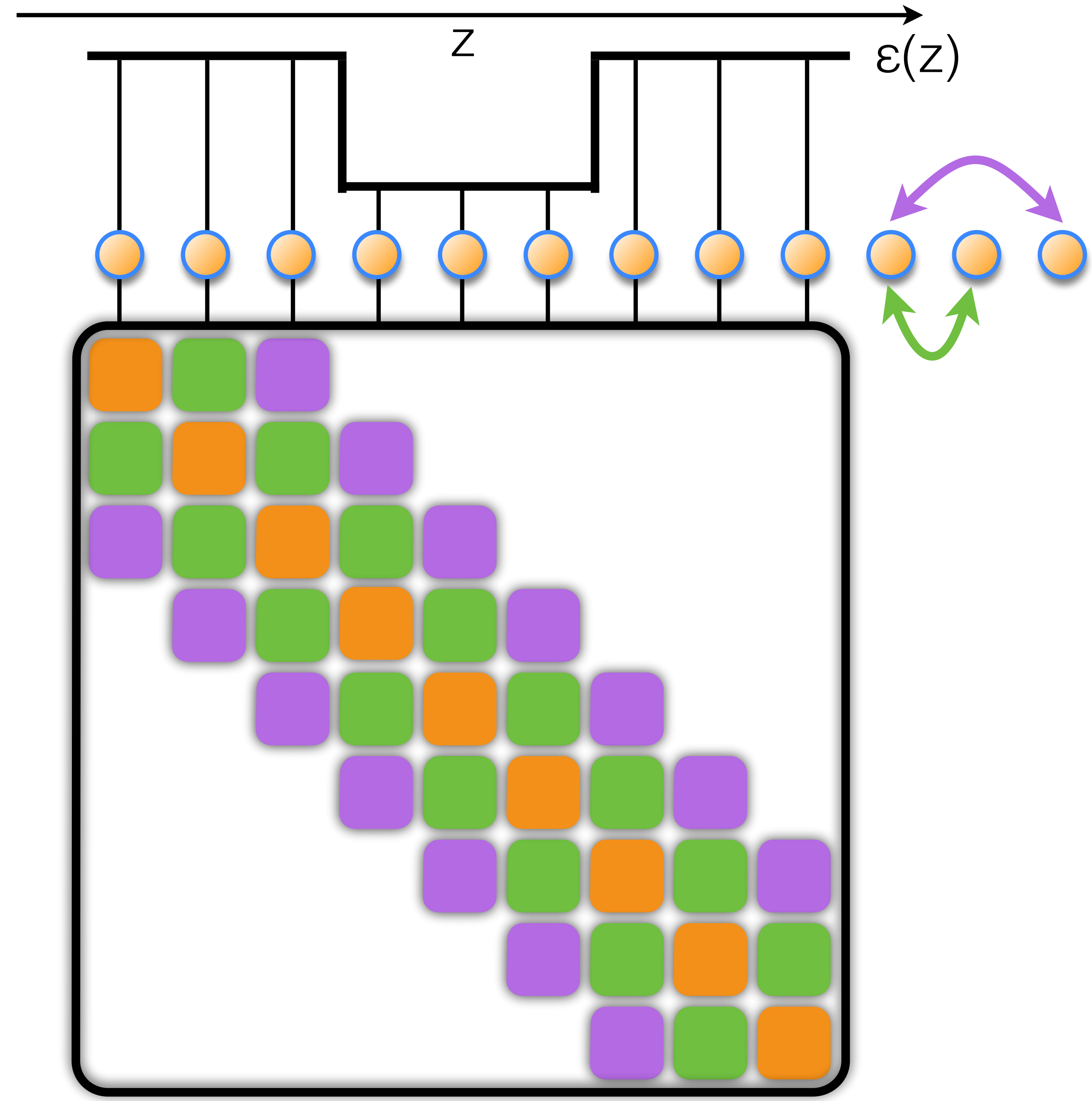
overlap matrix



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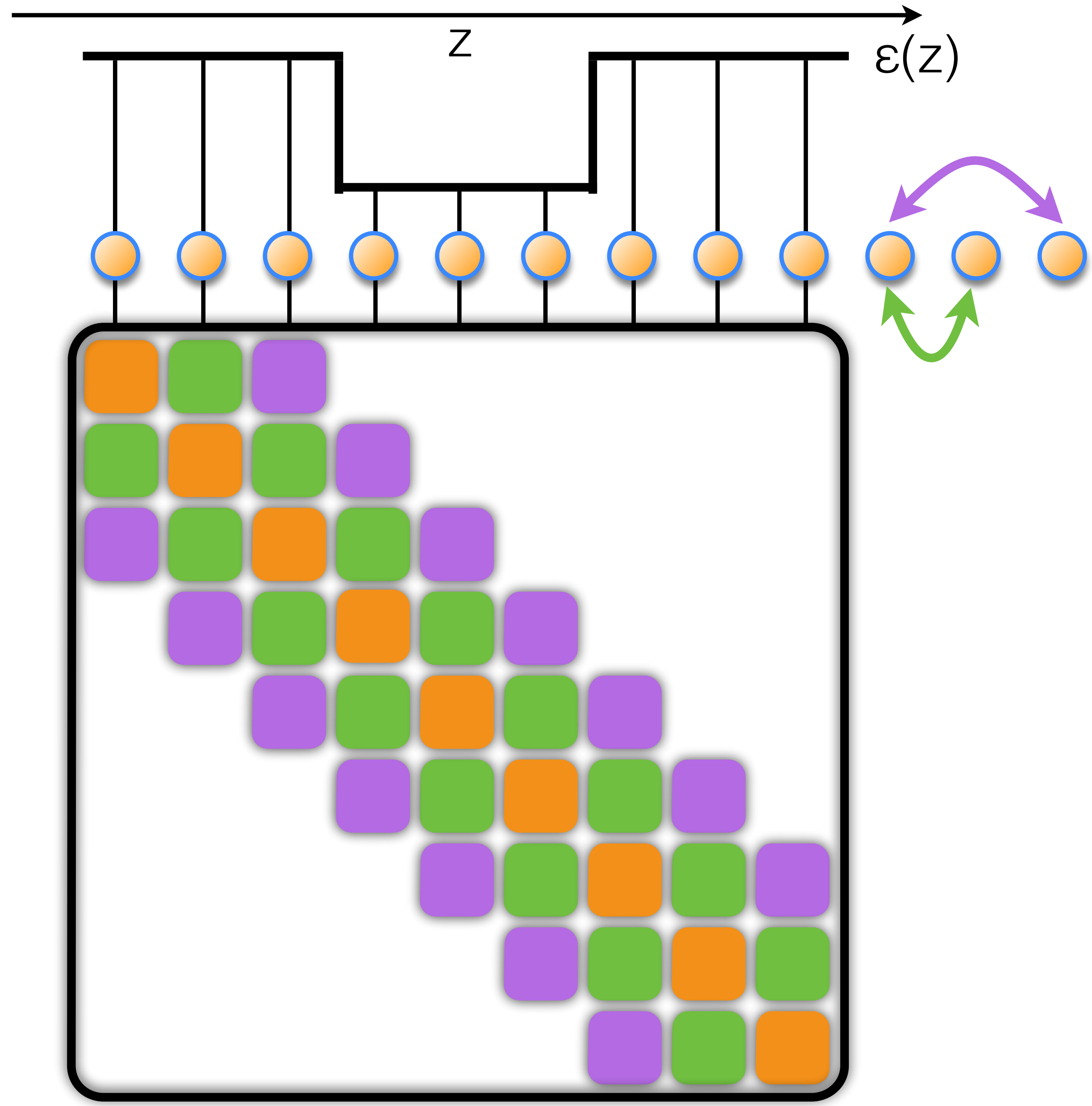
We'll use *anisotropic* gaussians on an example problem: valley splitting in a quantum dot



Valley splitting in silicon - ‘traditional’ approach

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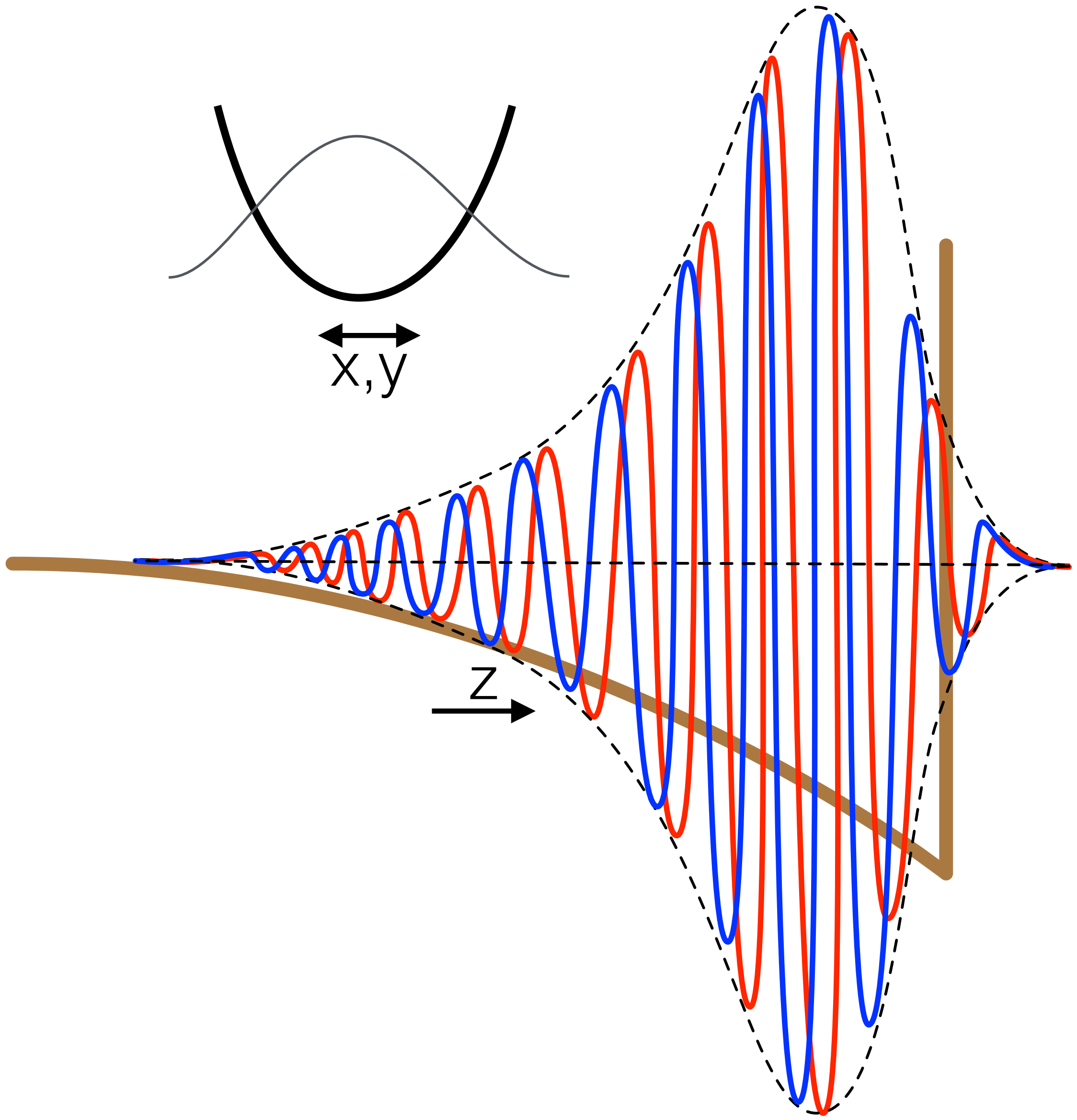

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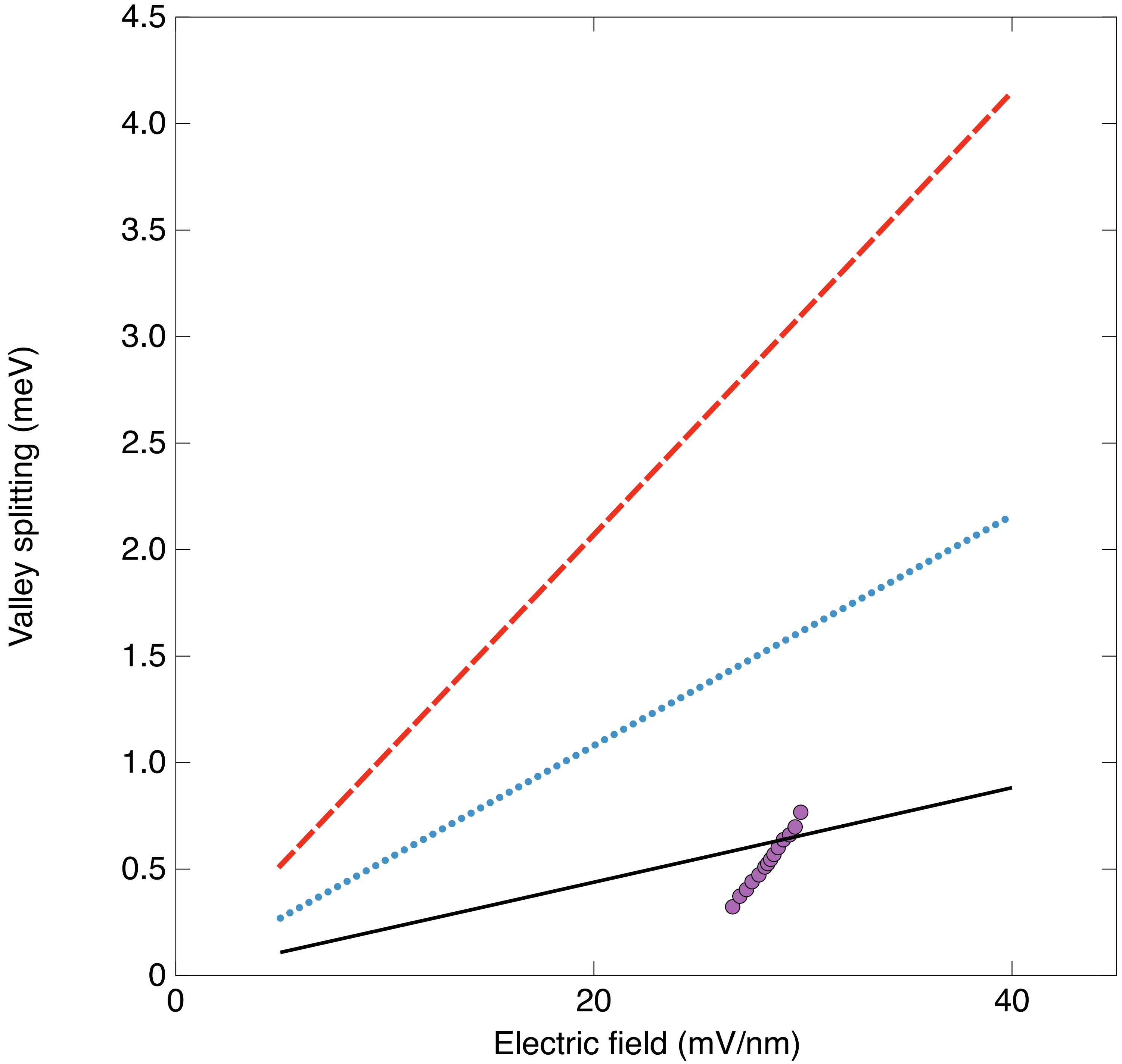

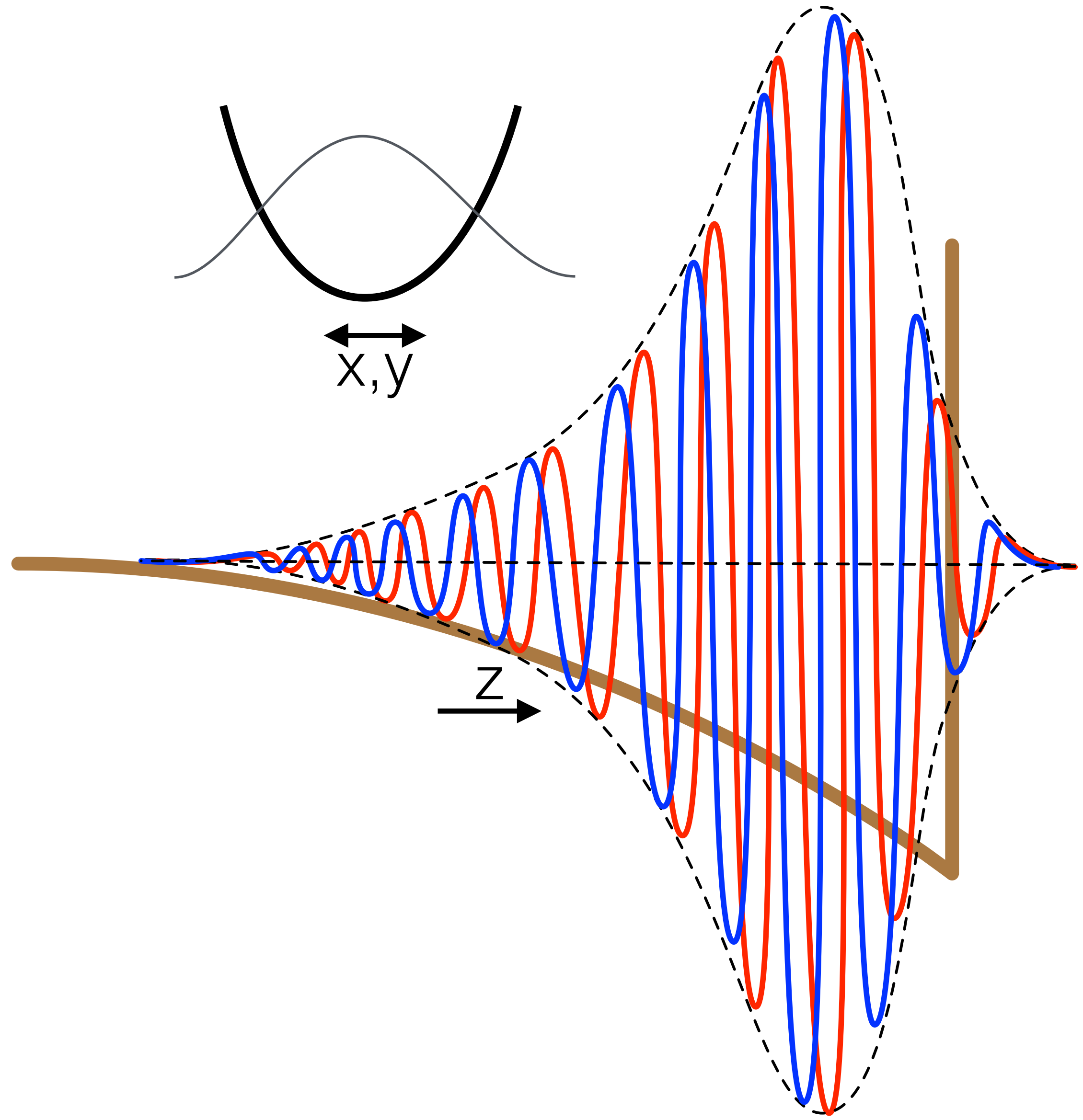

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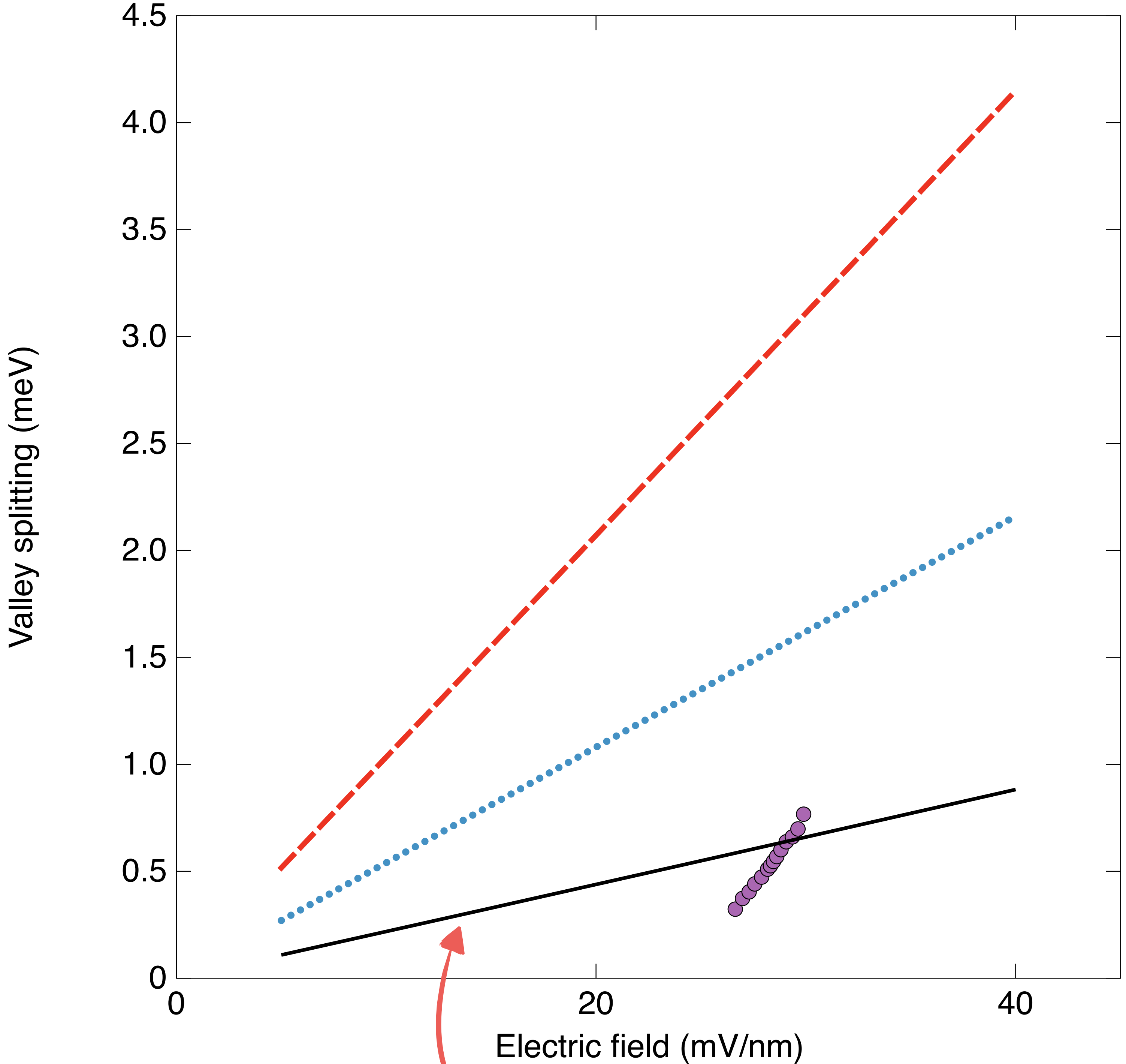
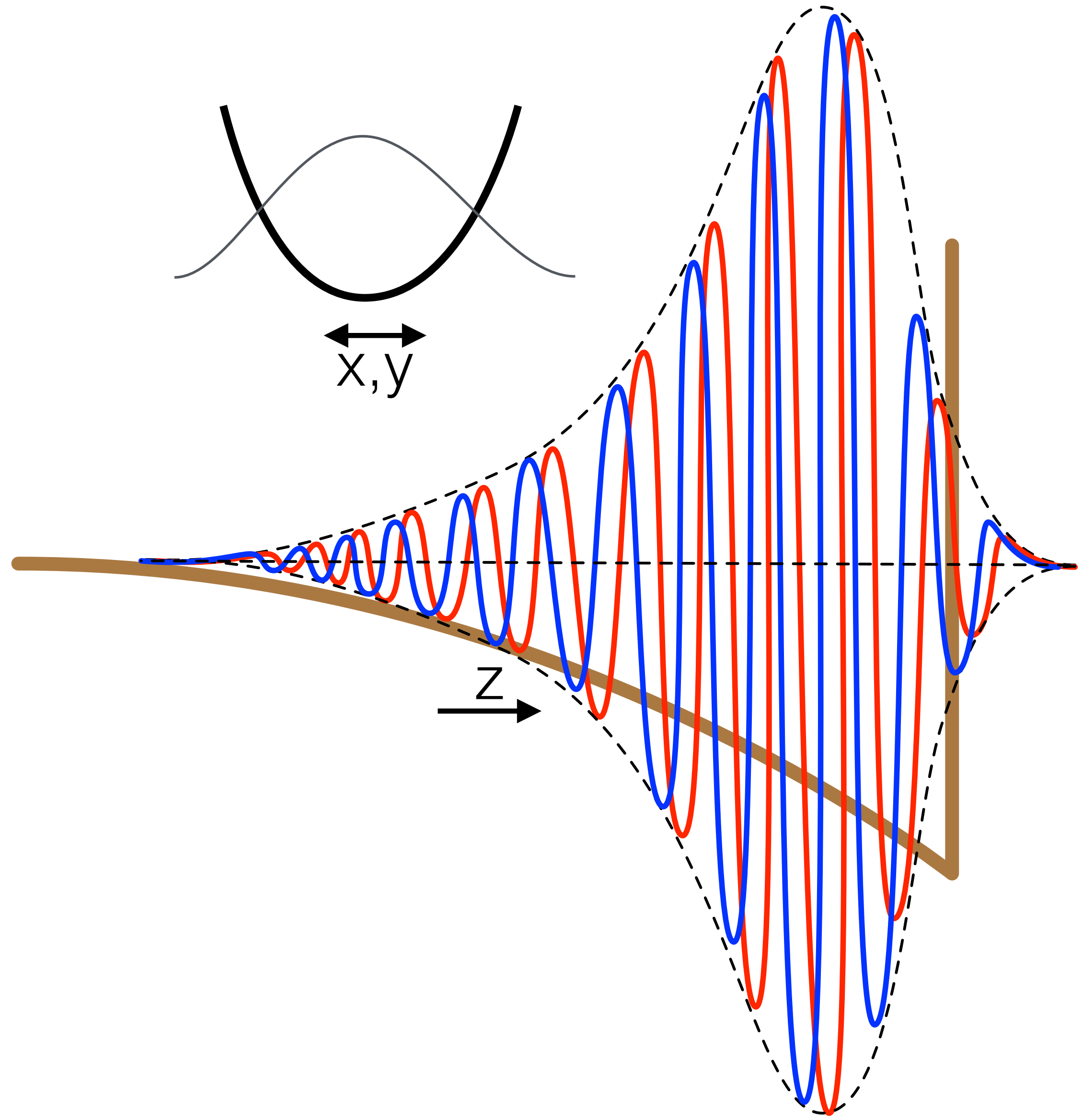
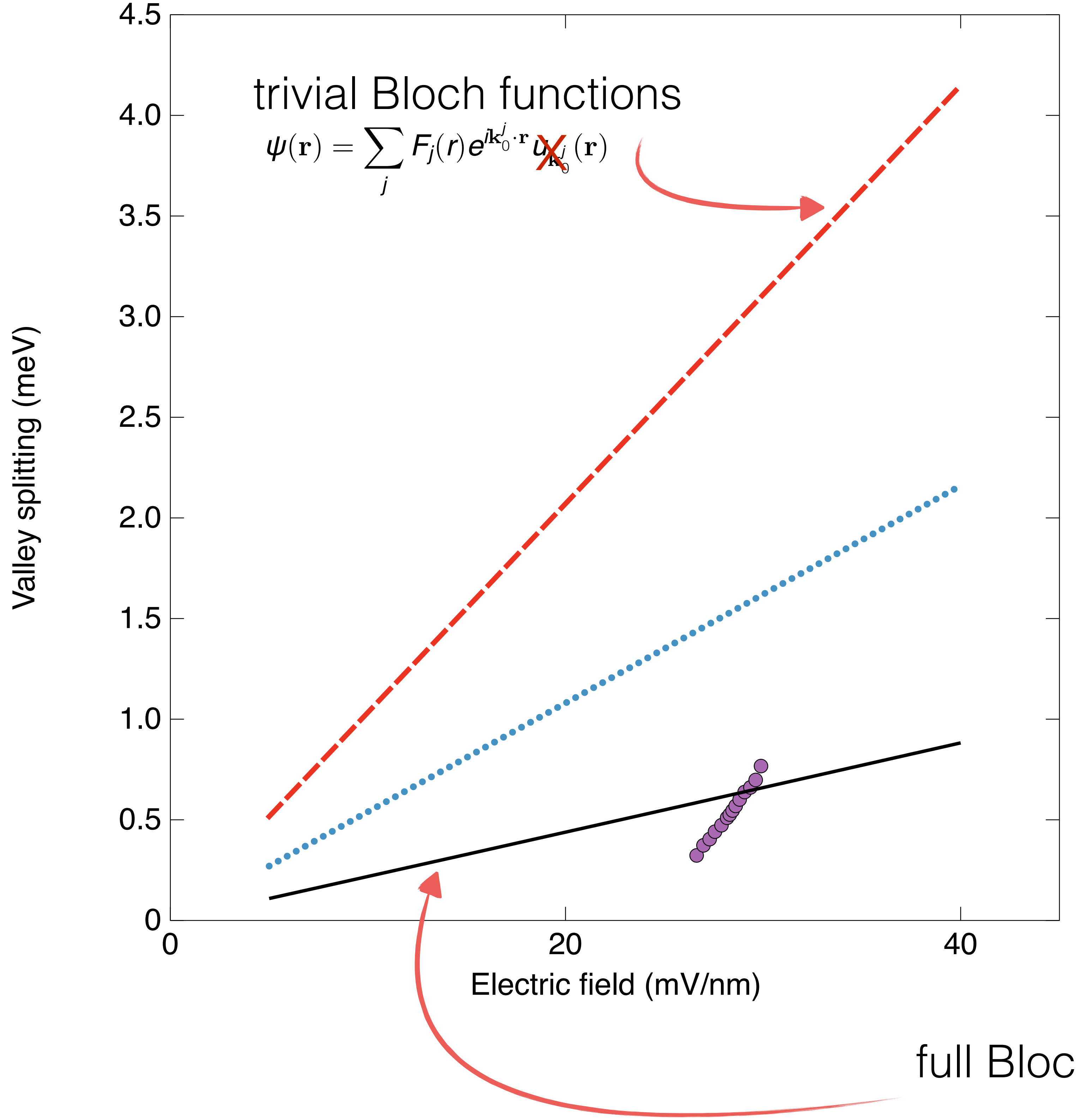
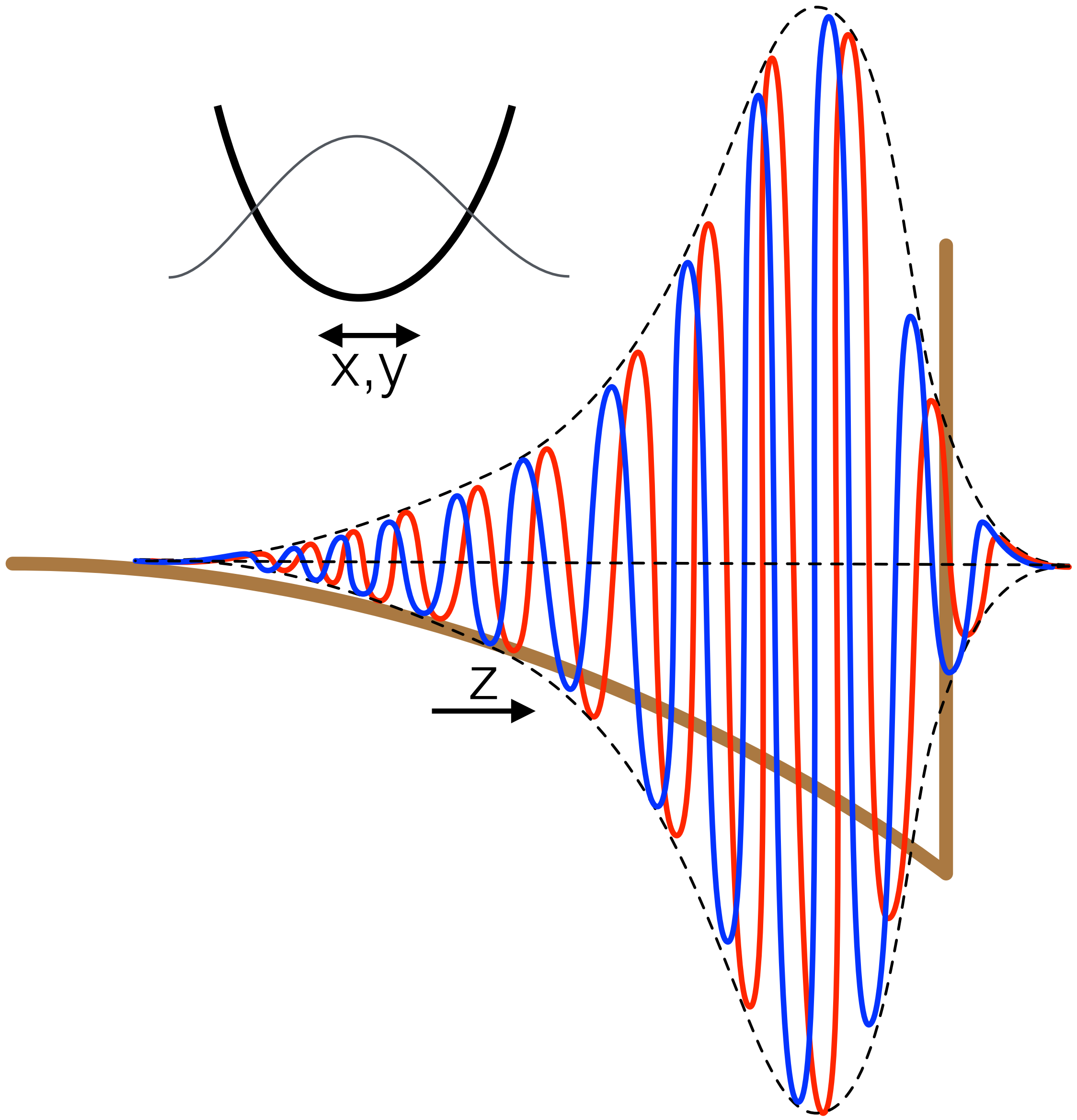




full Bloch functions

Valley splitting in silicon - 'traditional' approach





full Bloch functions

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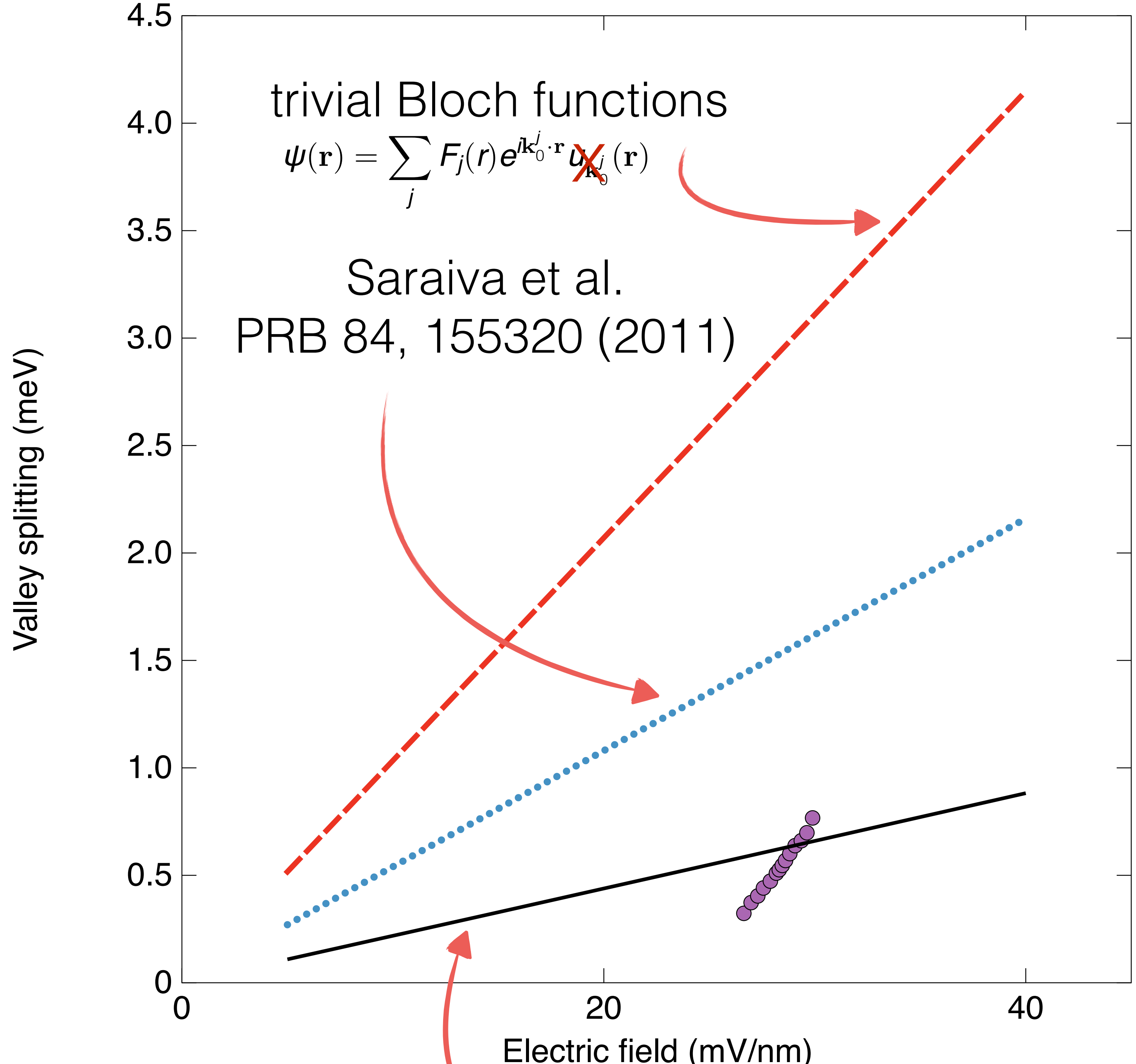

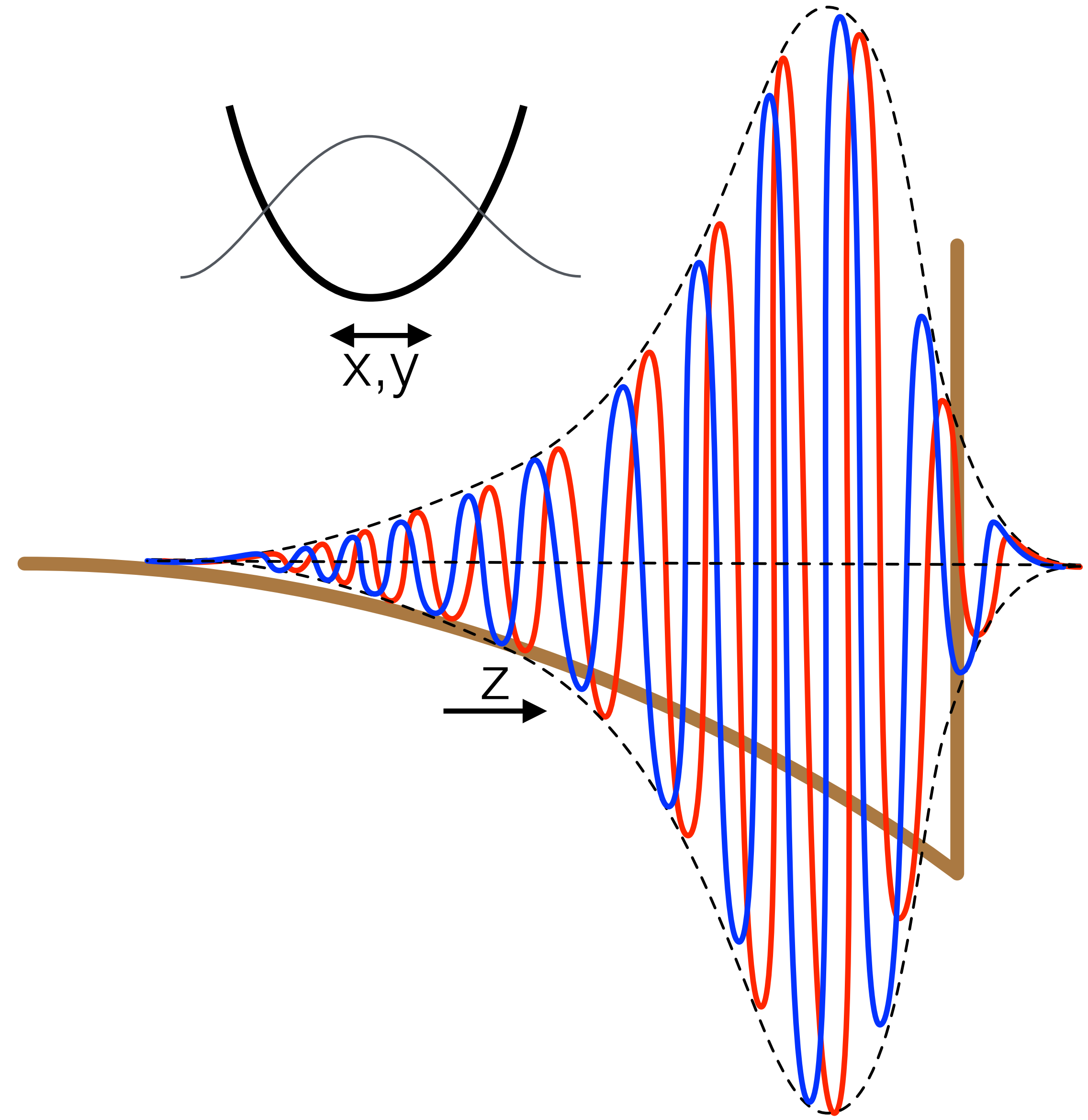

full Bloch functions

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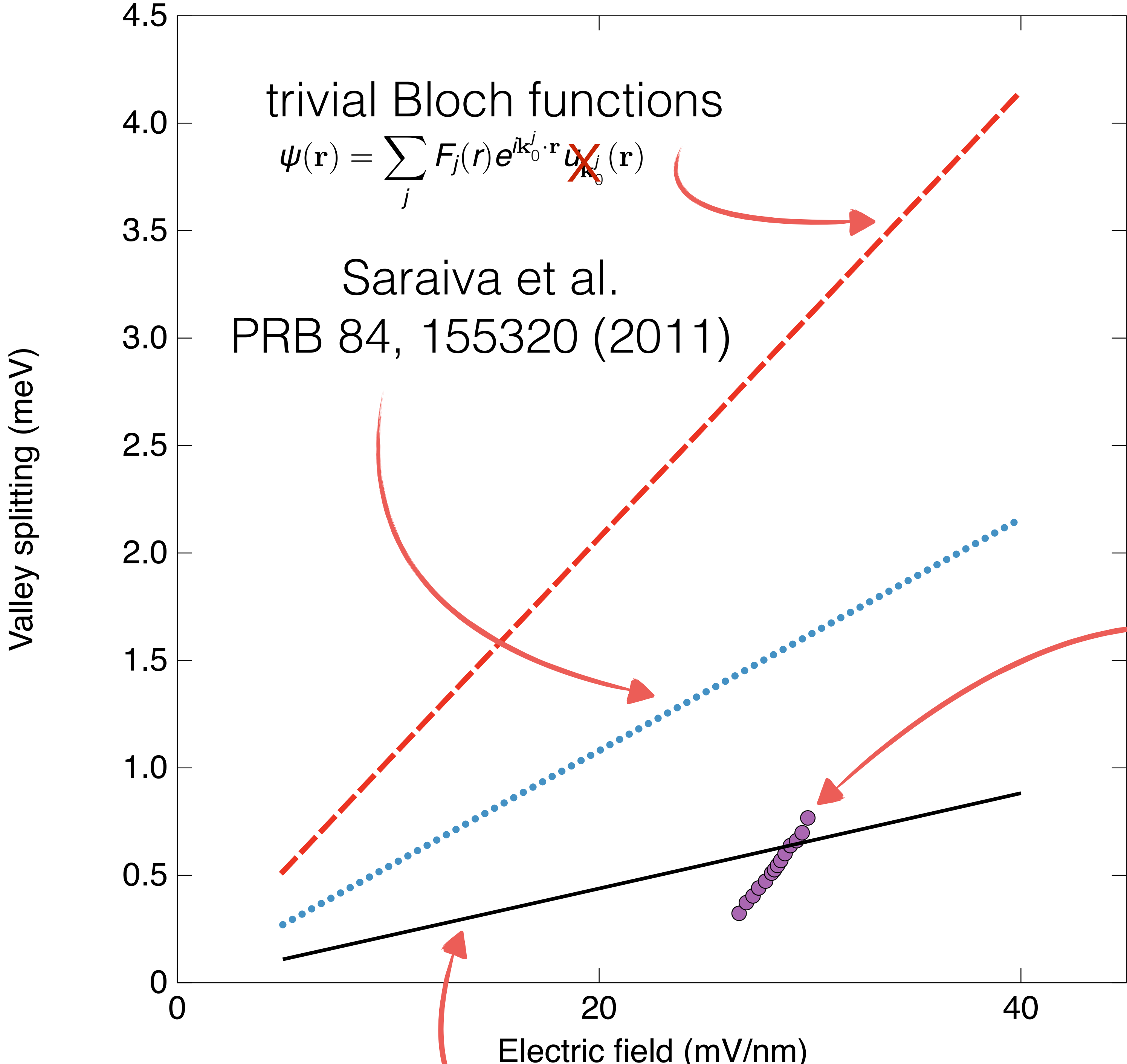
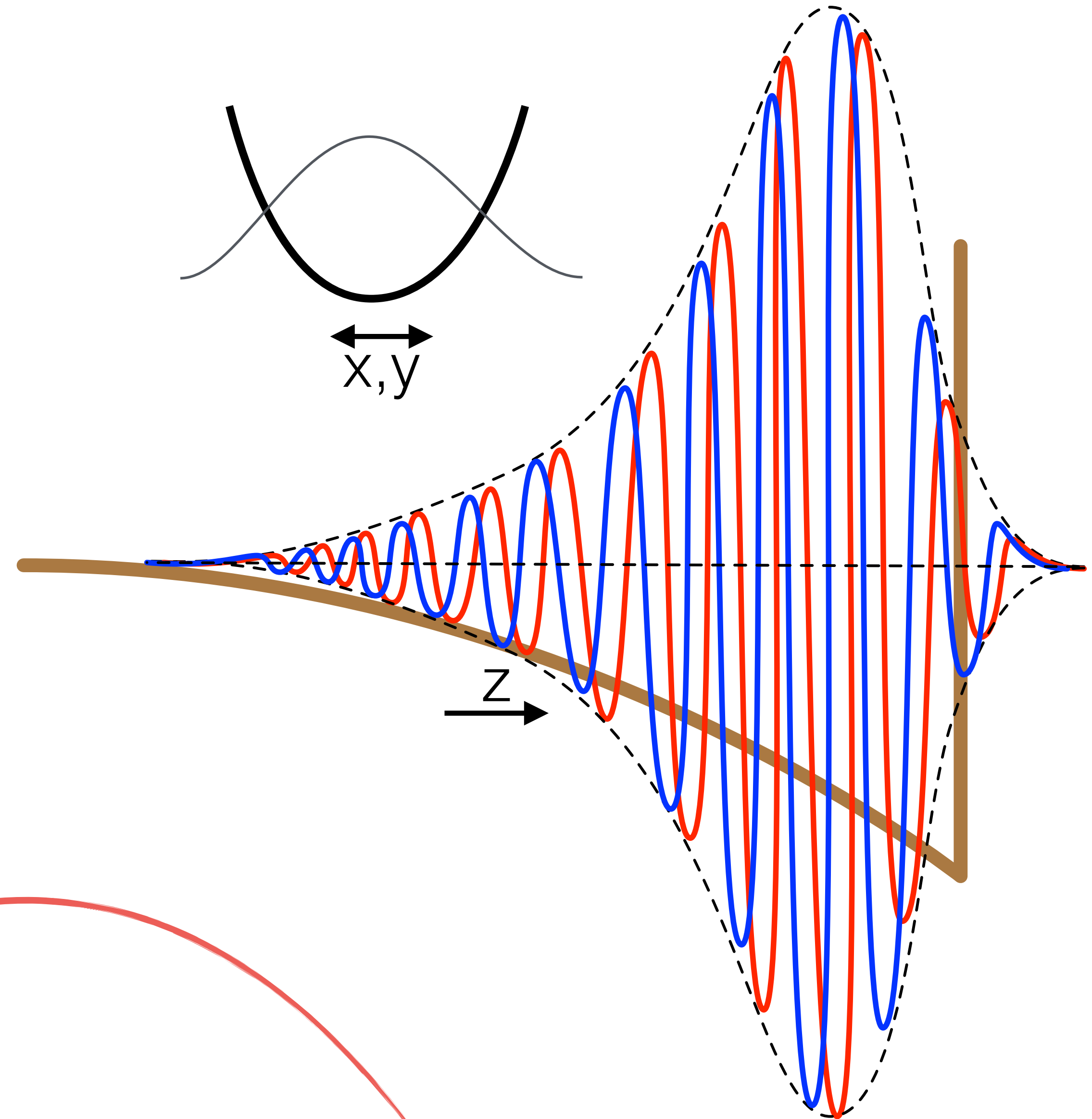
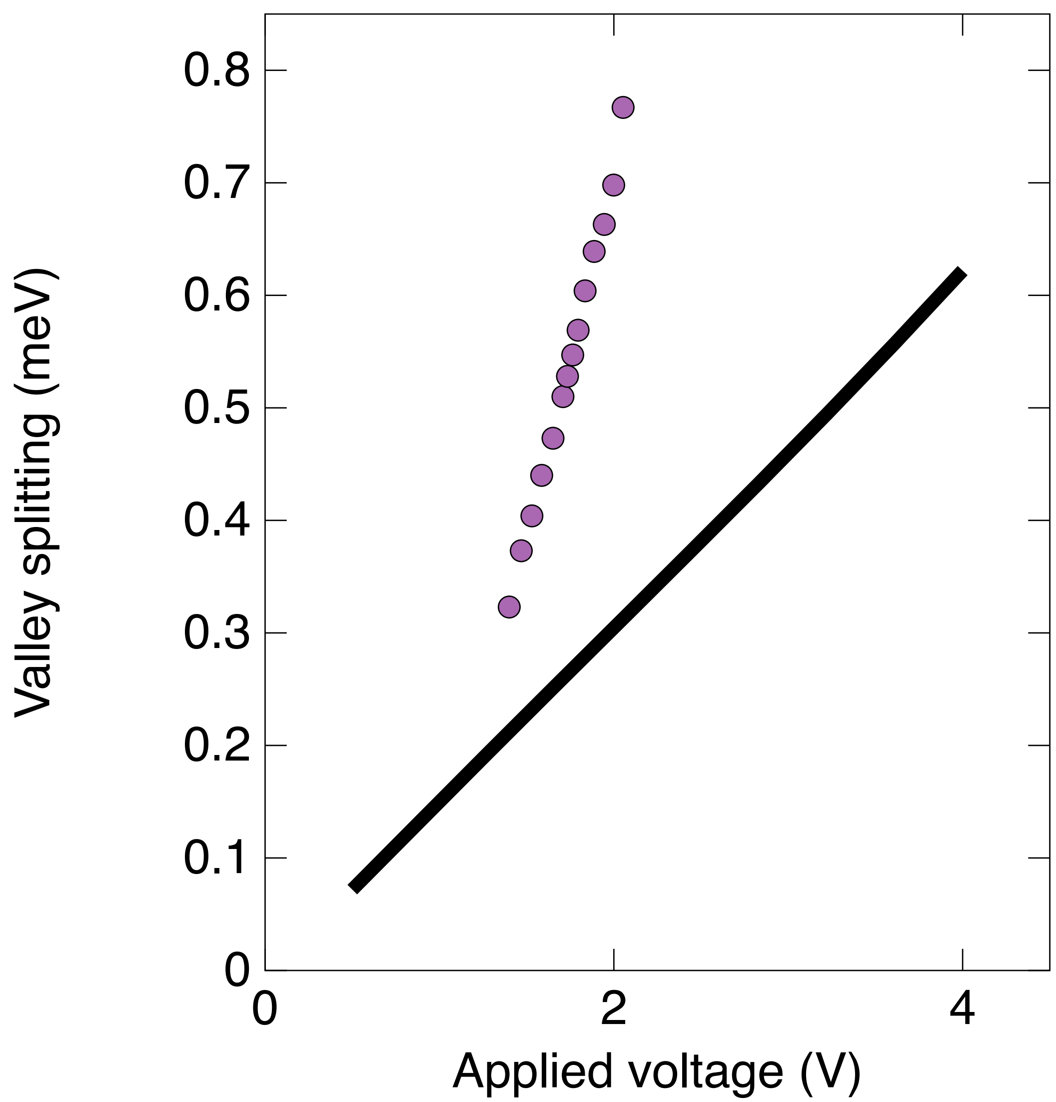


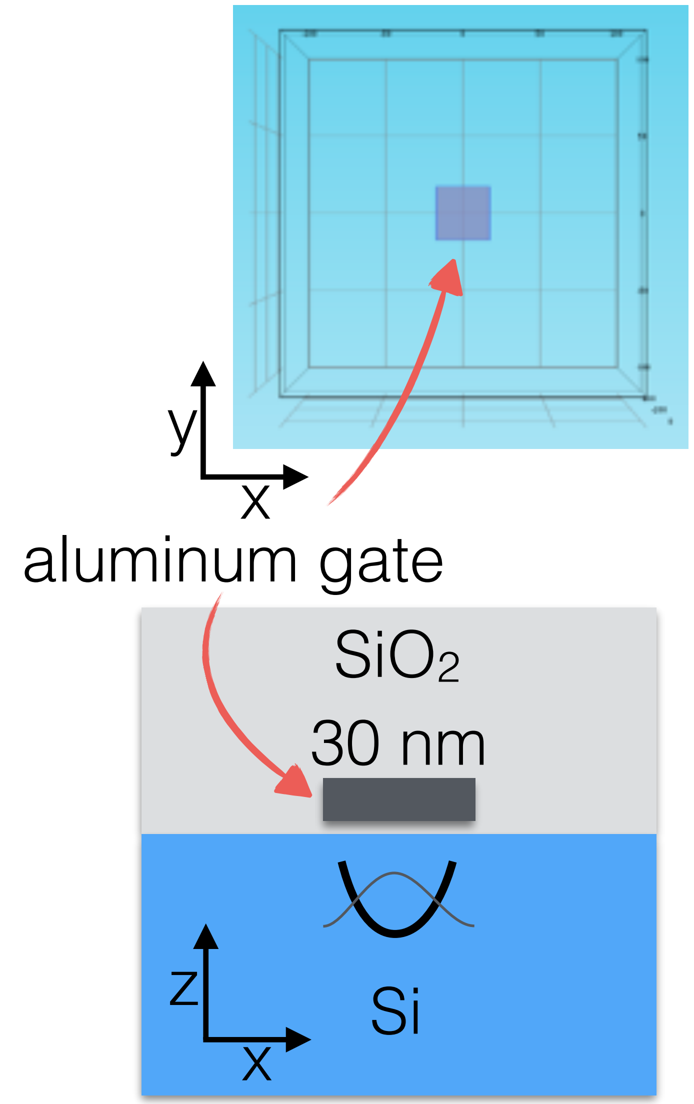


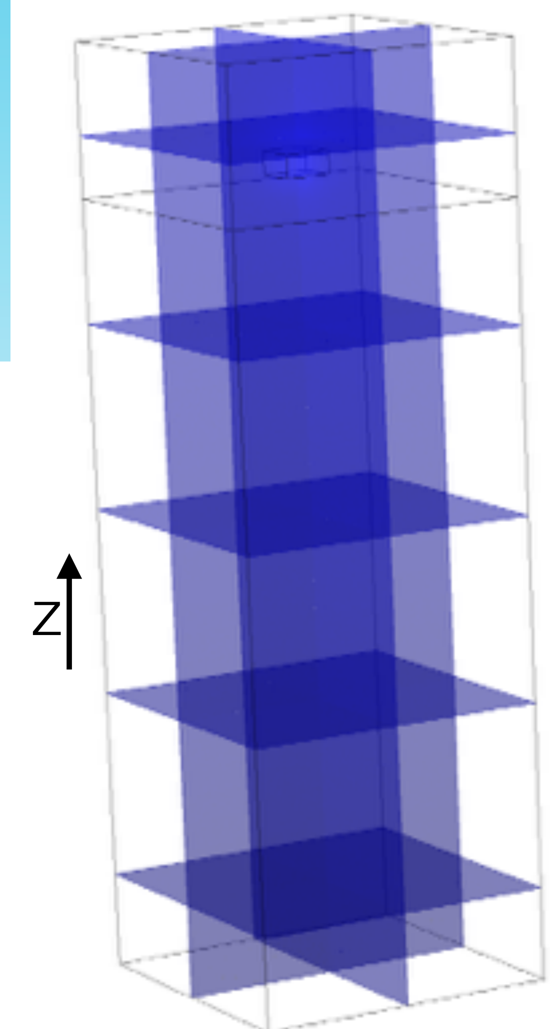
experiment: Yang et al.
Nature Comms. 4: 2069 (2013).

full Bloch functions

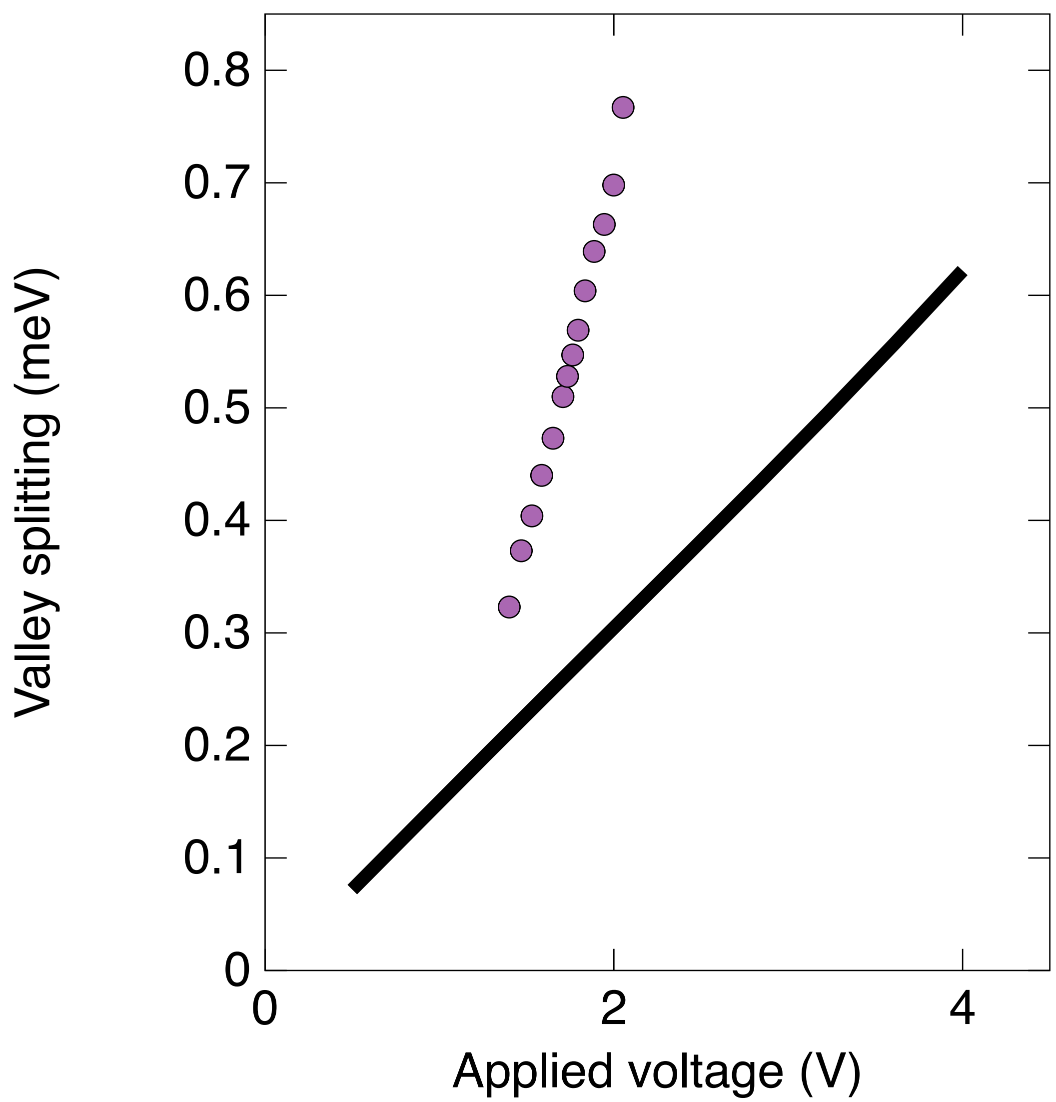
Valley splitting in silicon - full-scope approach

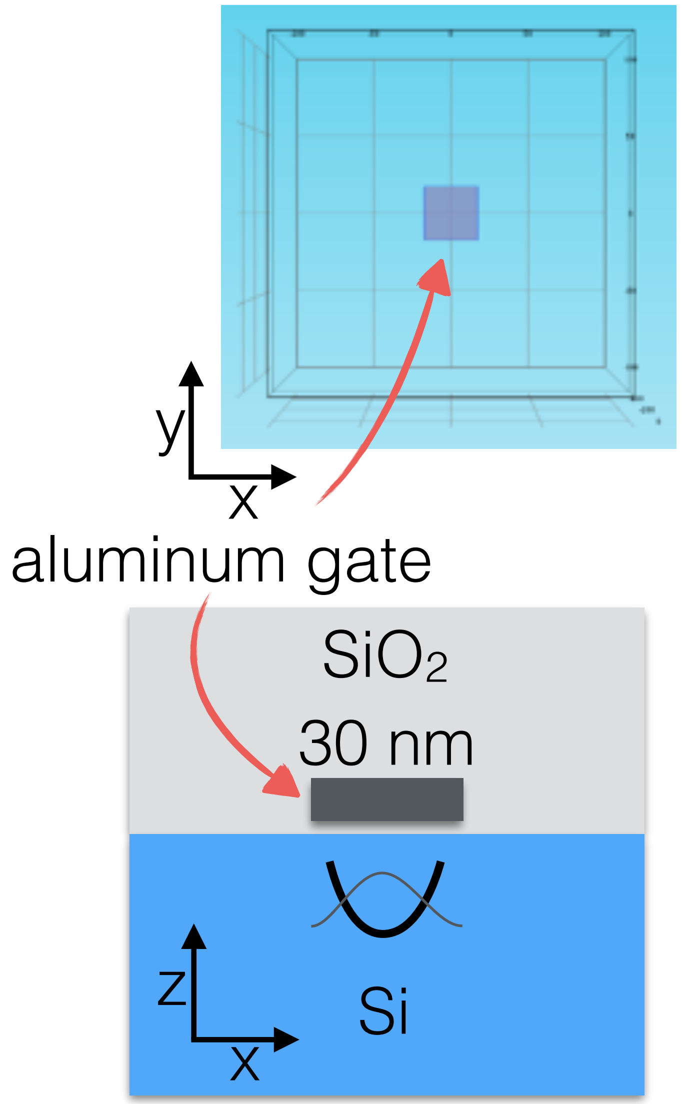


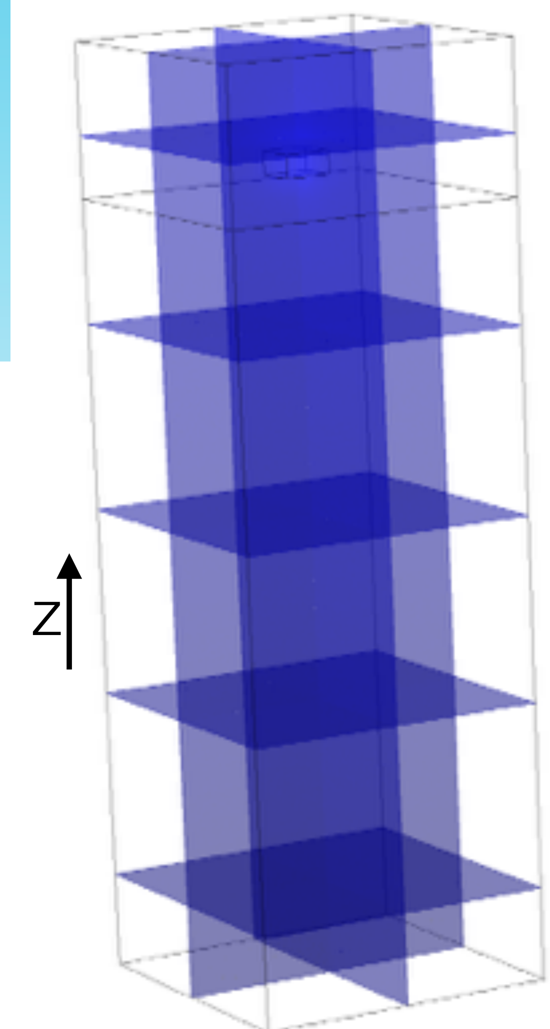




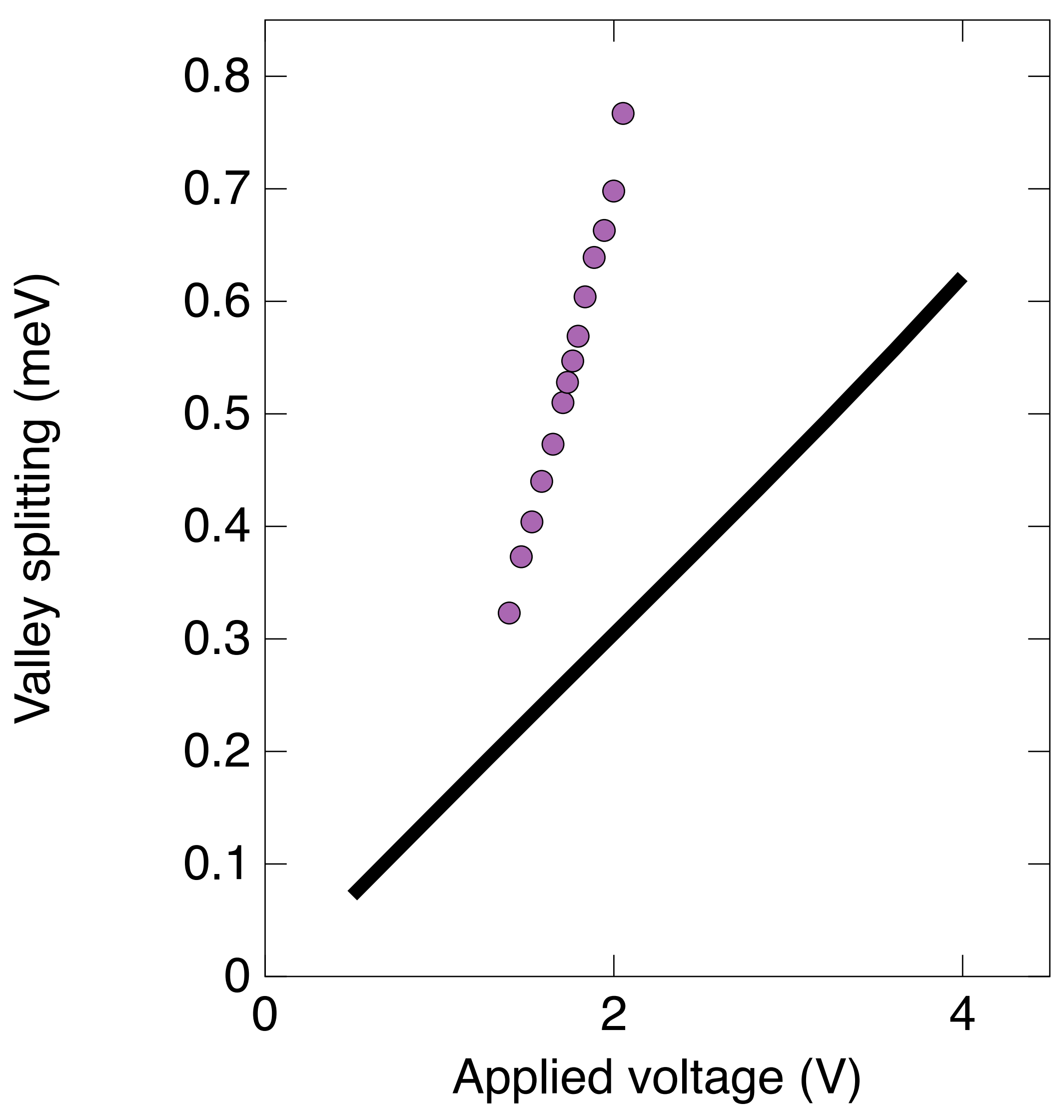
Valley splitting in silicon - full-scope approach

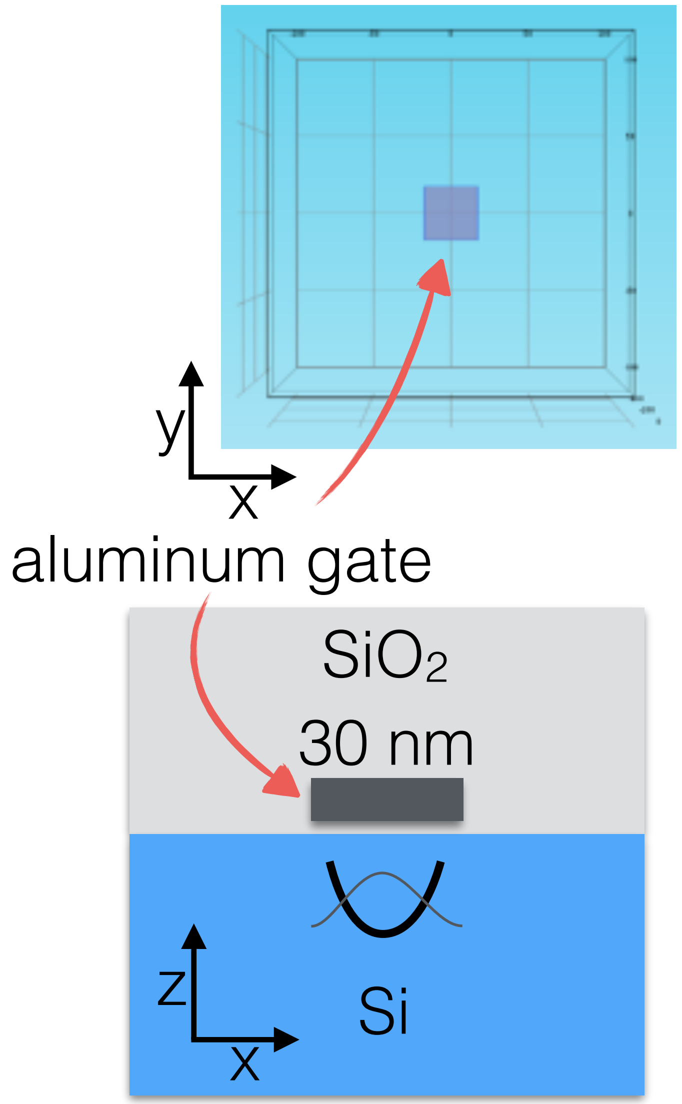


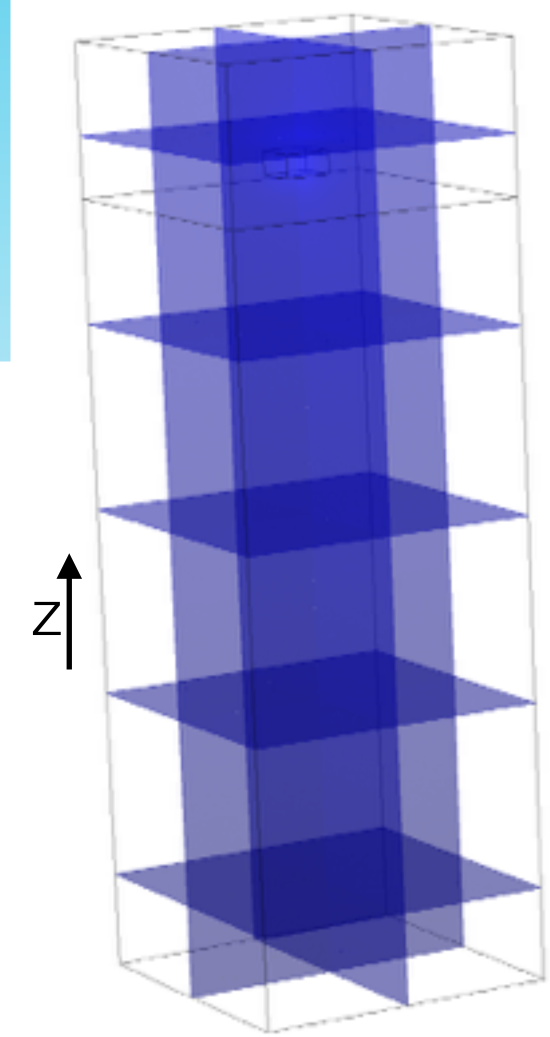




Valley splitting in silicon - full-scope approach



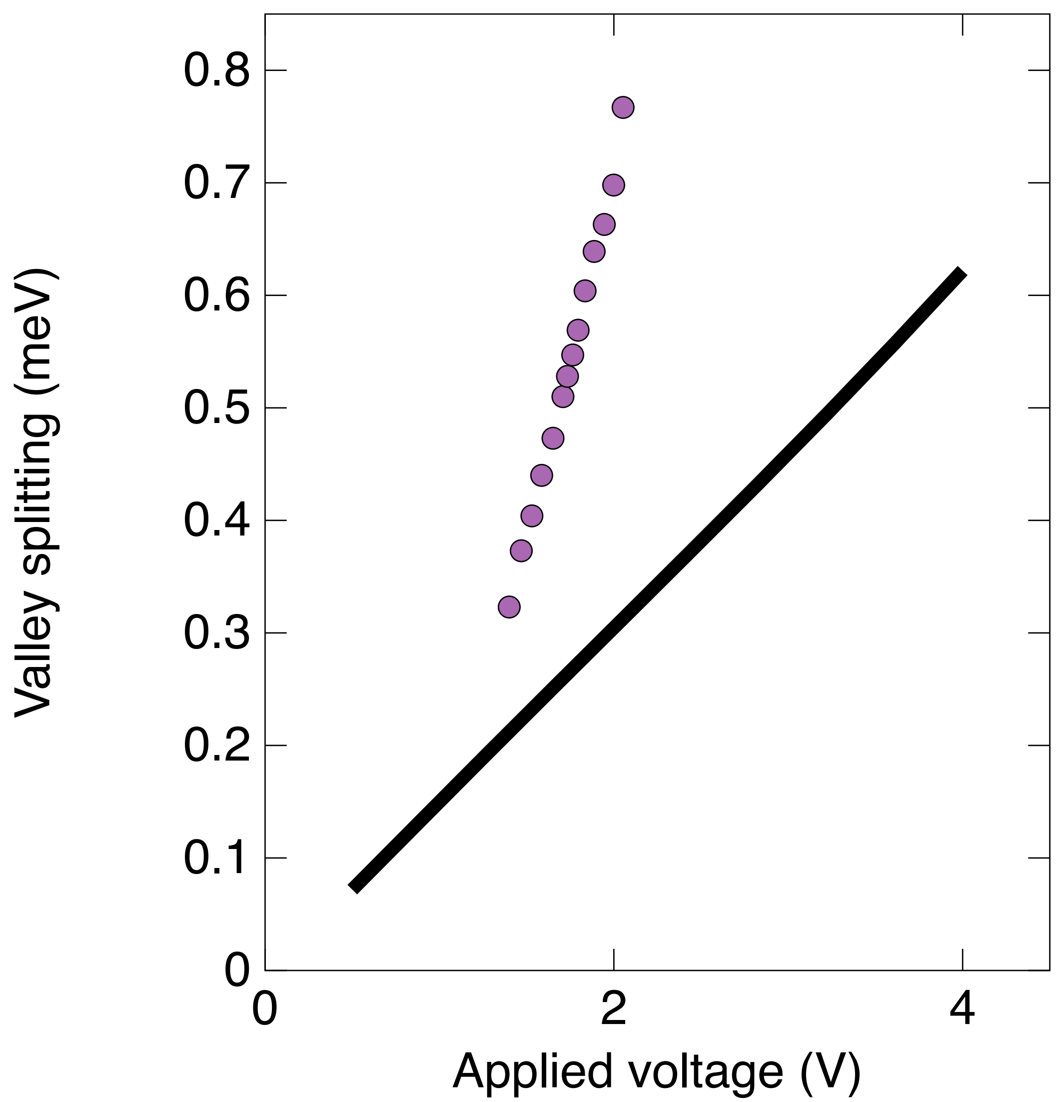


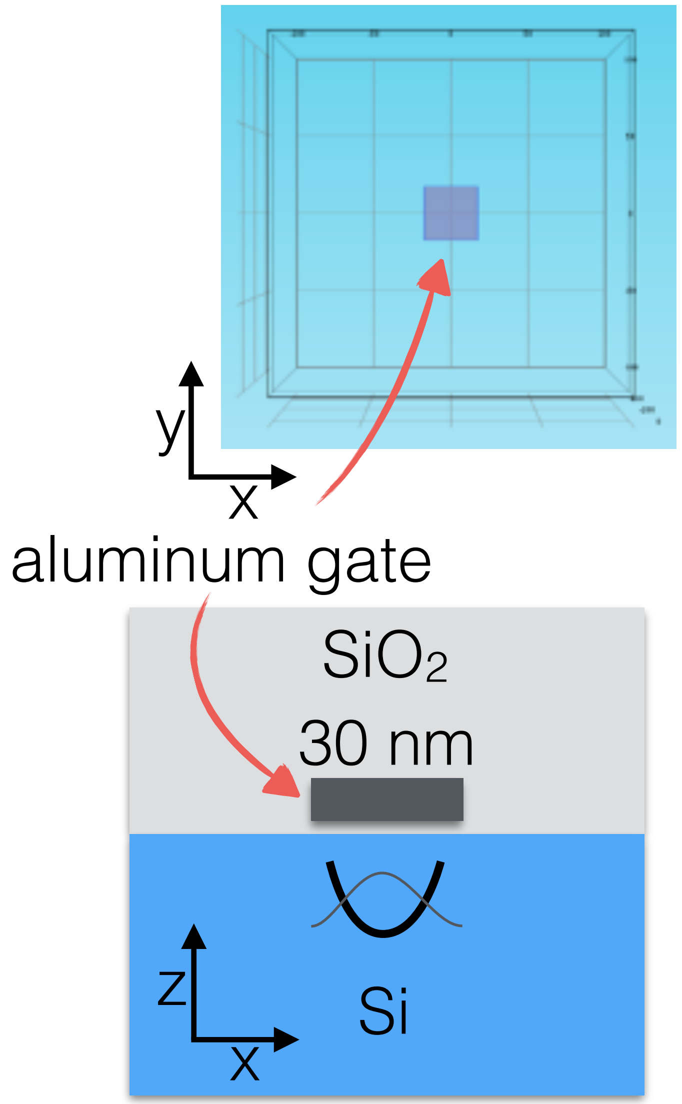


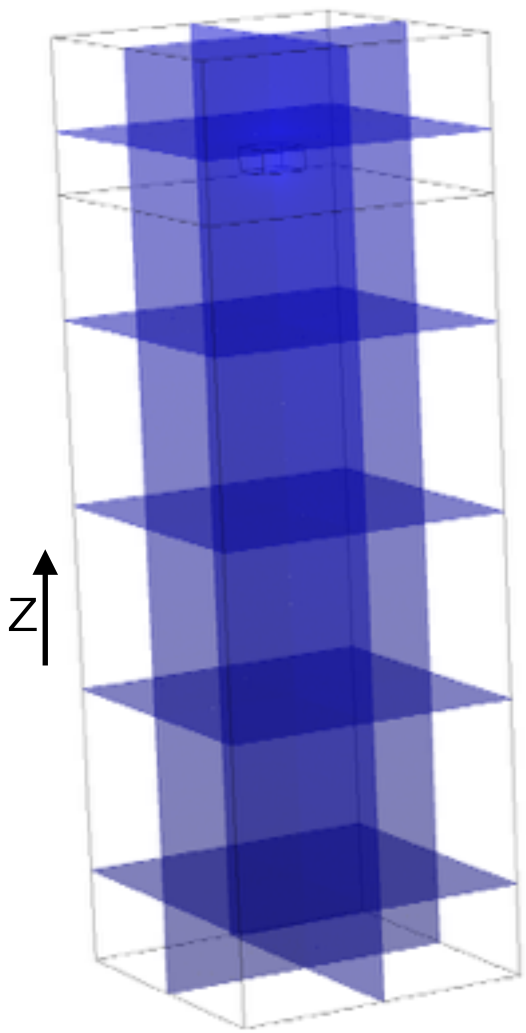
Used (6,6,60) grid of Gaussians with both z valleys + full Bloch functions.

Valley splitting in silicon - full-scope approach

Ramping the voltage leads to both increased confinement and increased valley splitting - not separable.







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Exploring two-dot tunneling with full valley physics

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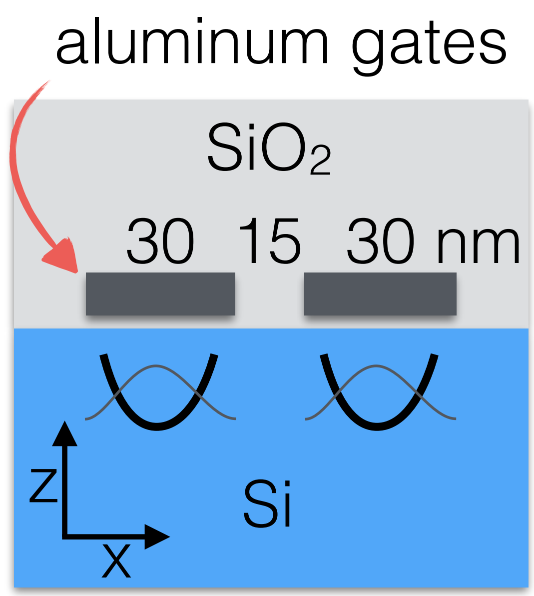
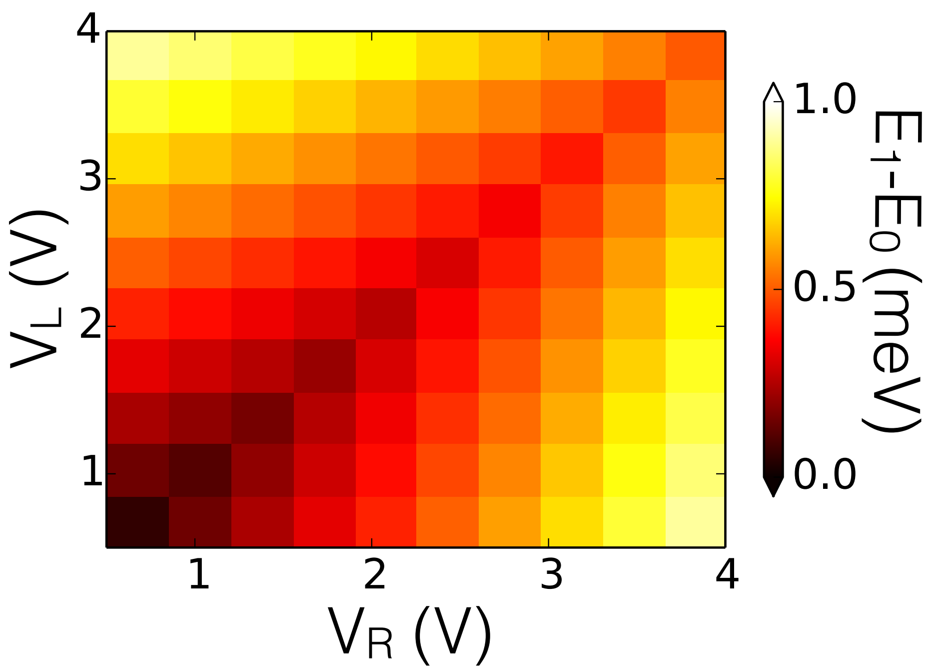
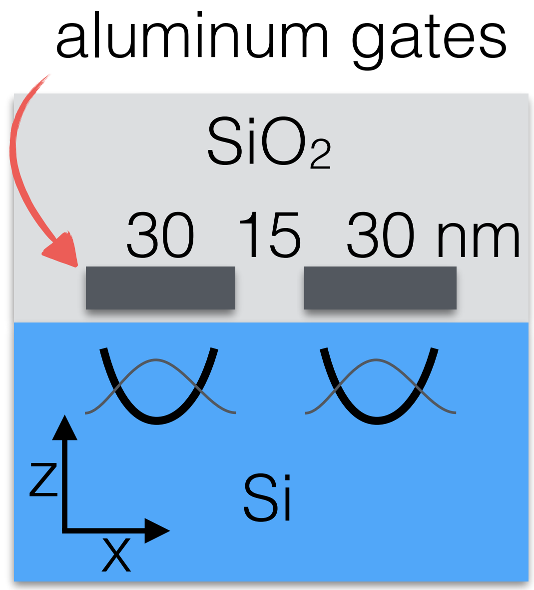


Exploring two-dot tunneling with full valley physics





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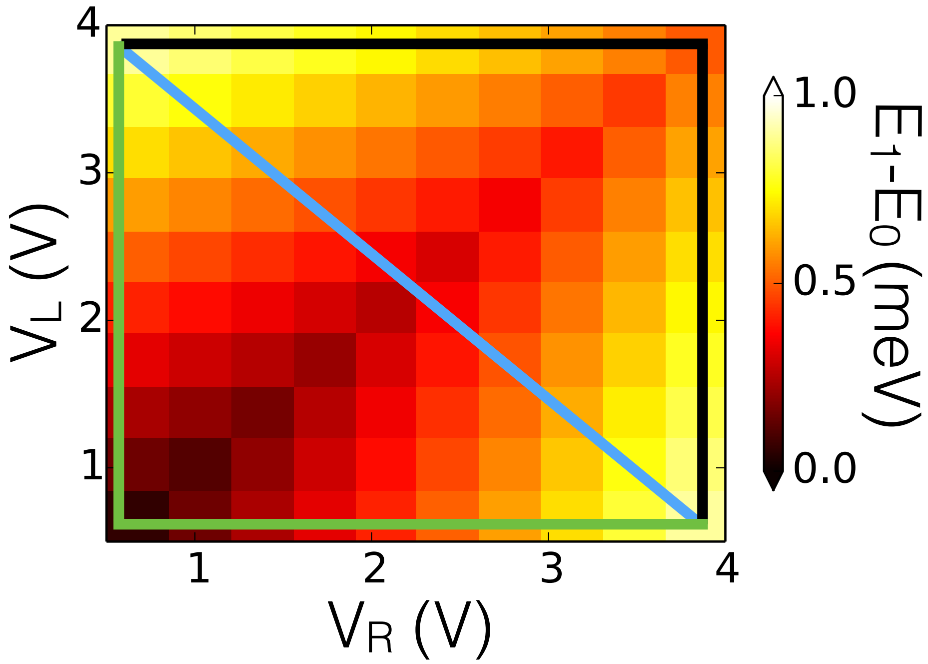
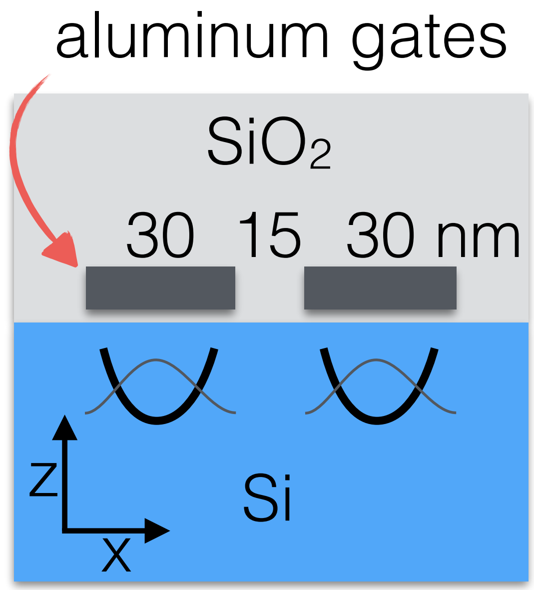
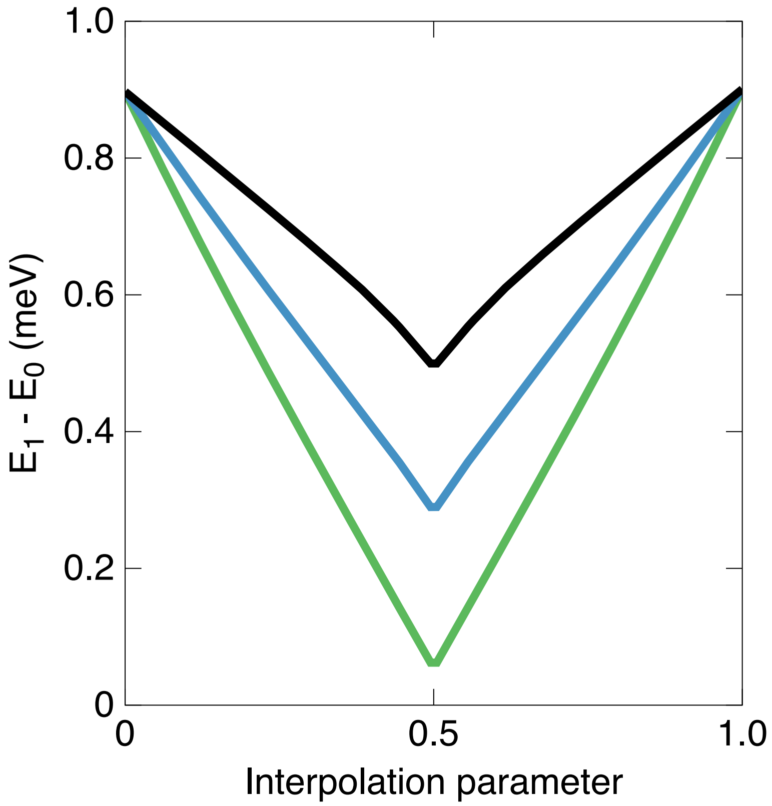
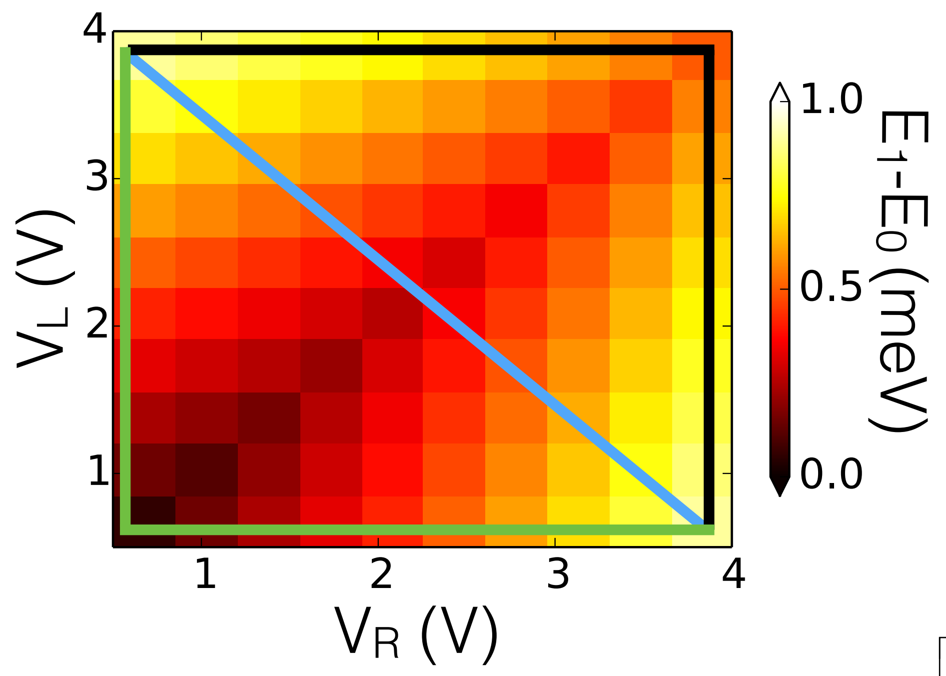
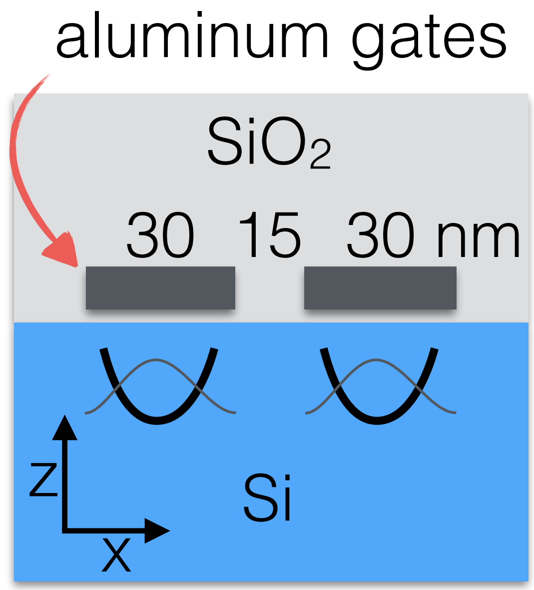


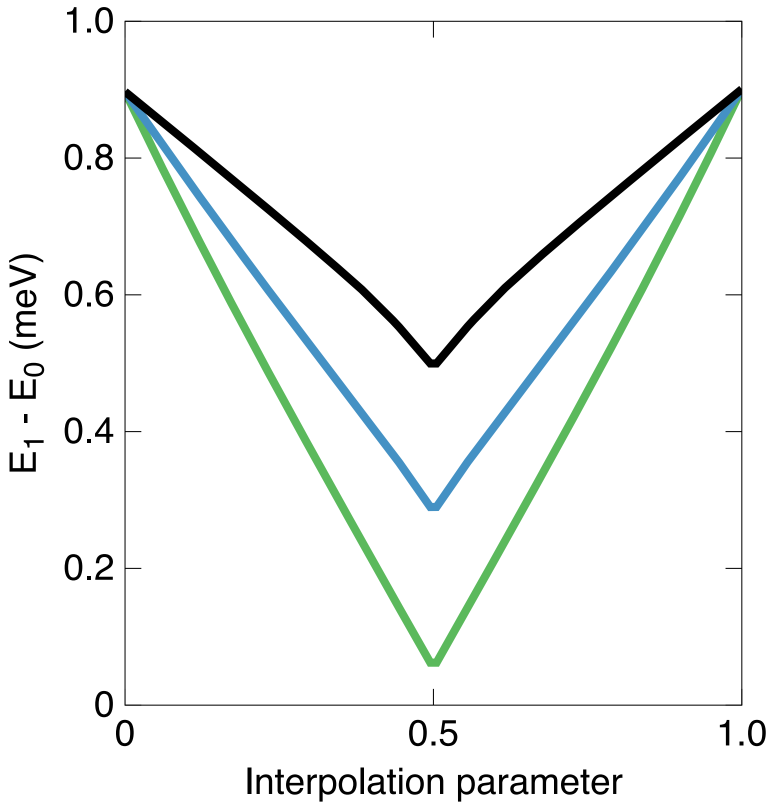


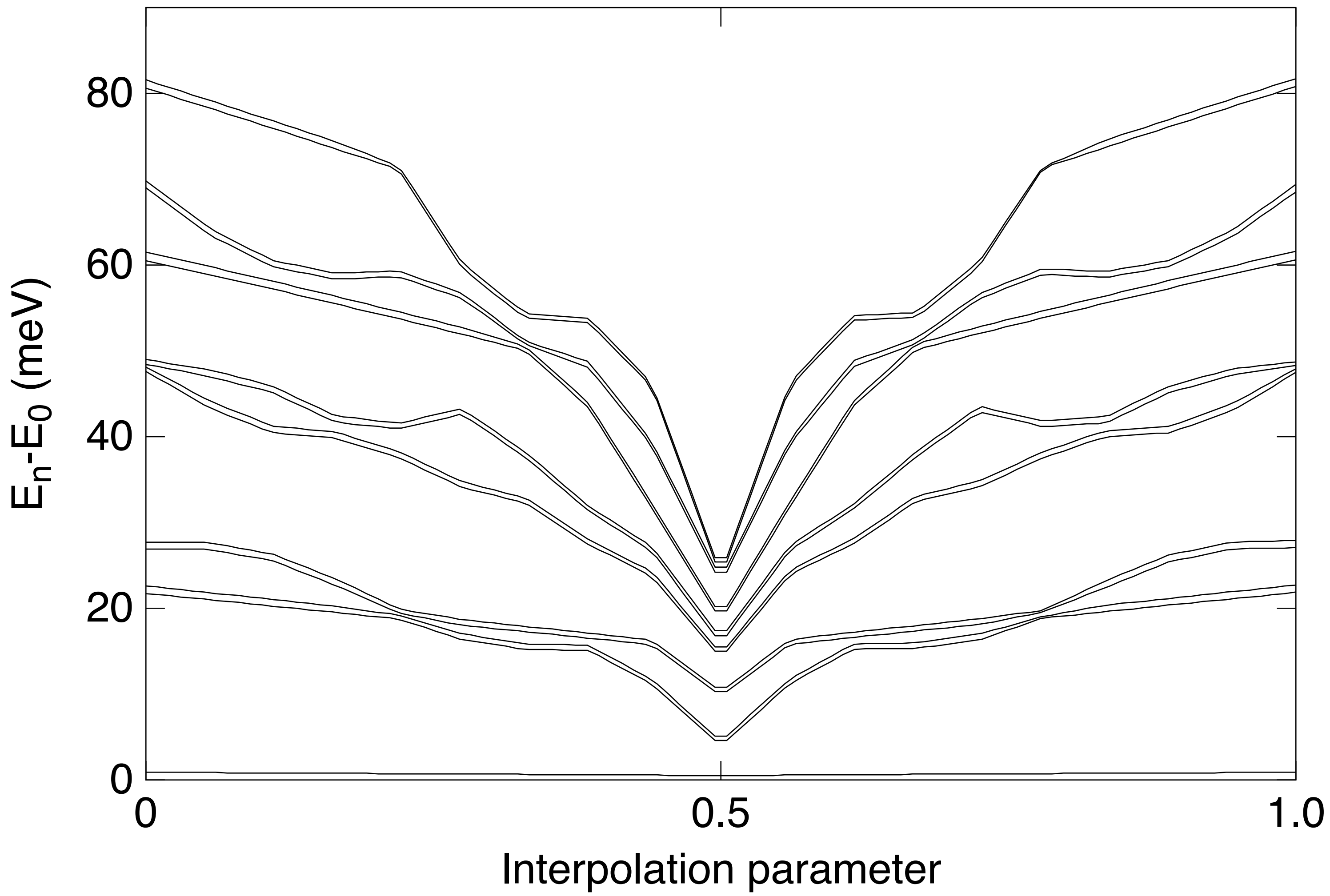


Exploring two-dot tunneling with full valley physics

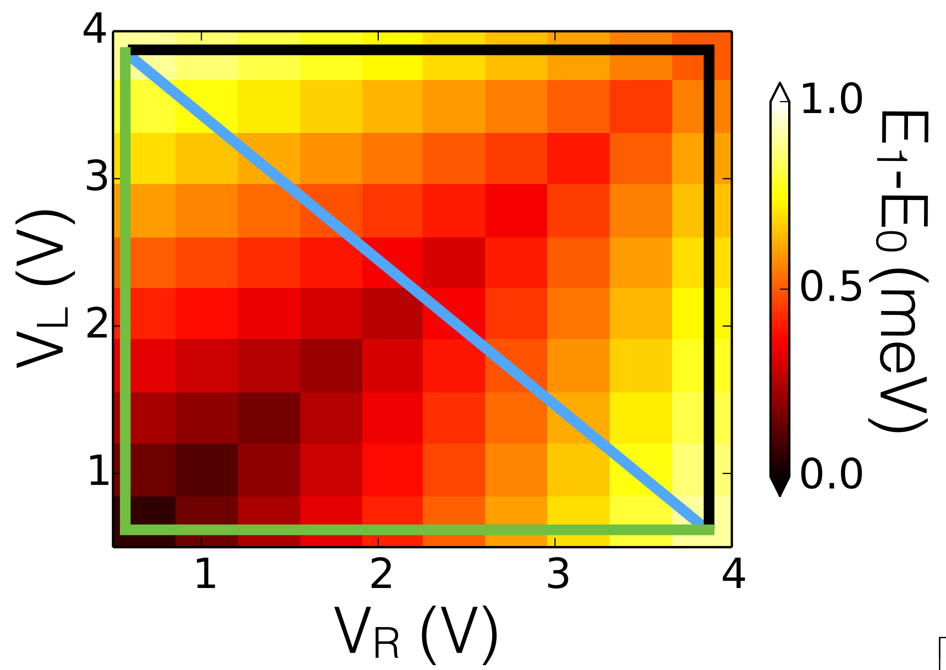


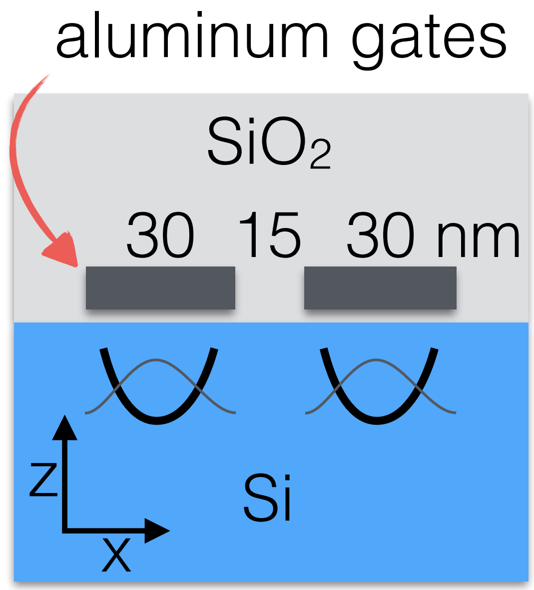


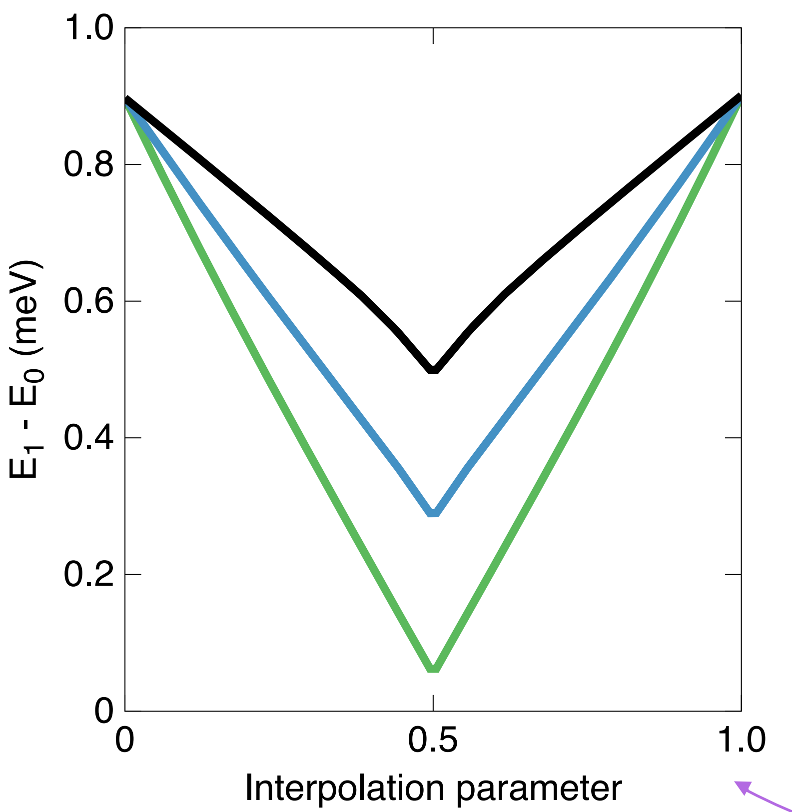


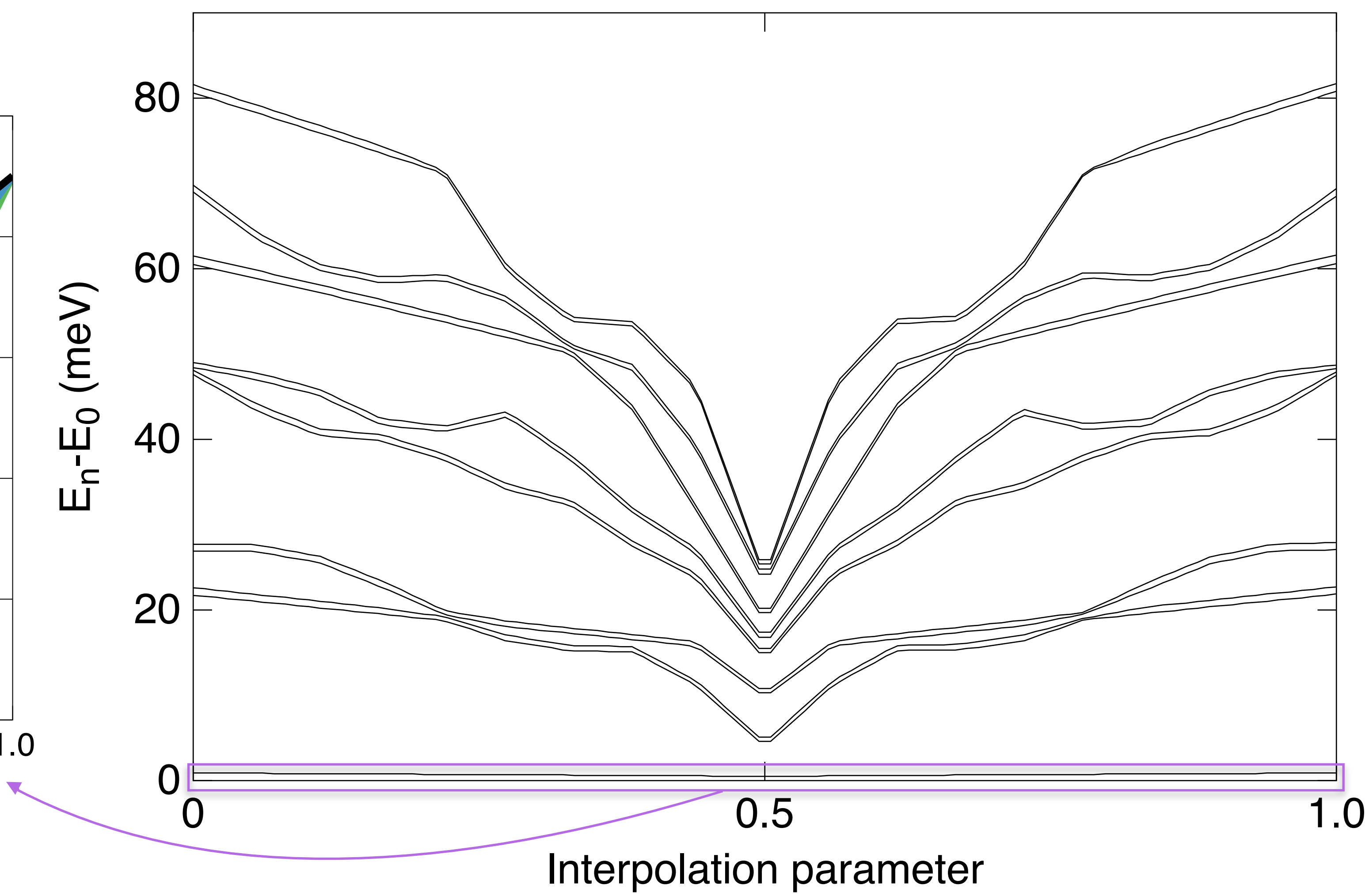


Exploring two-dot tunneling with full valley physics

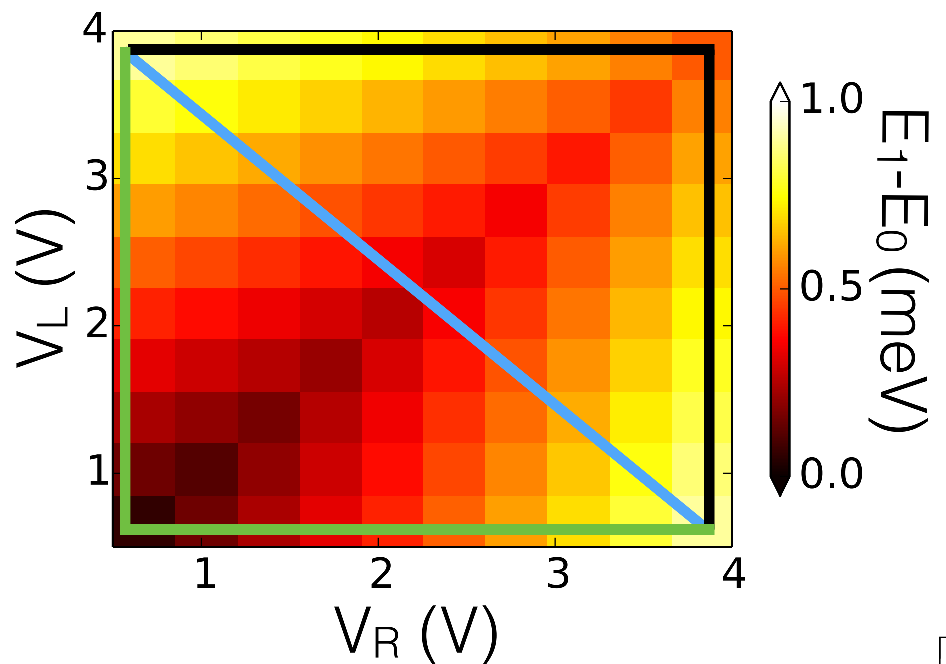


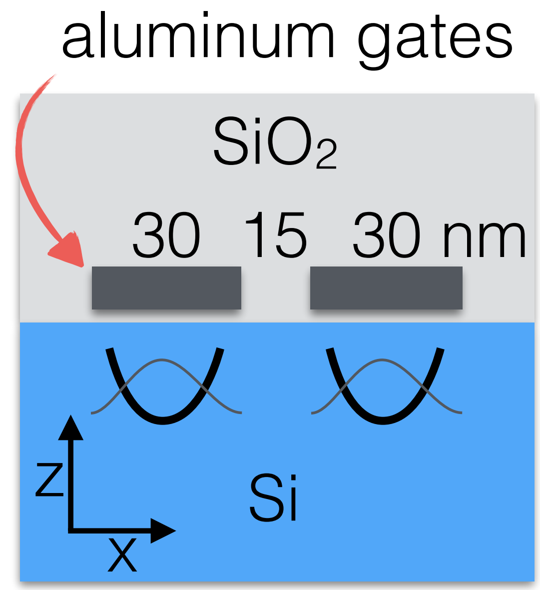


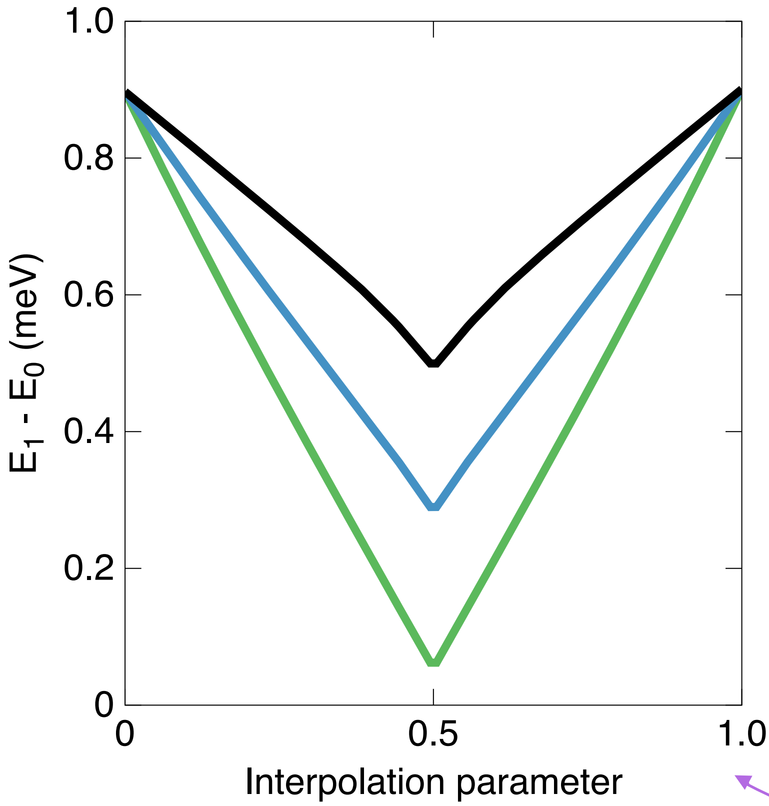


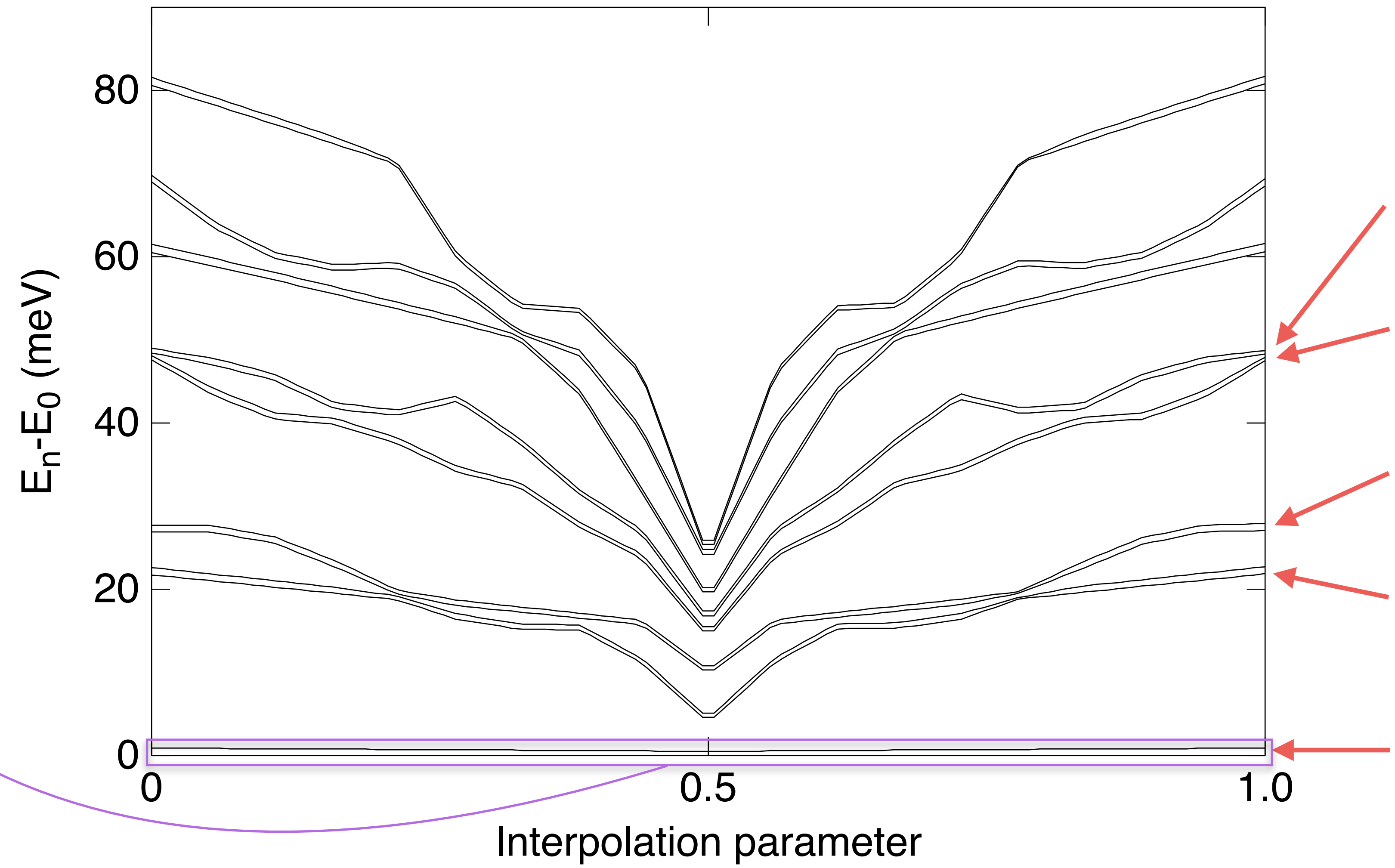


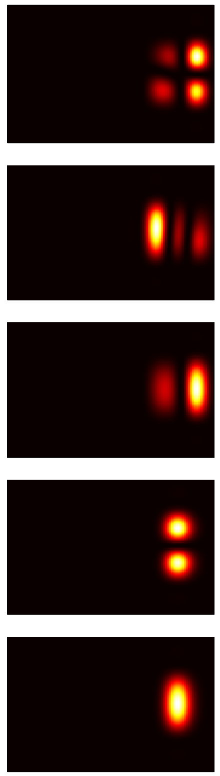
Exploring two-dot tunneling with full valley physics



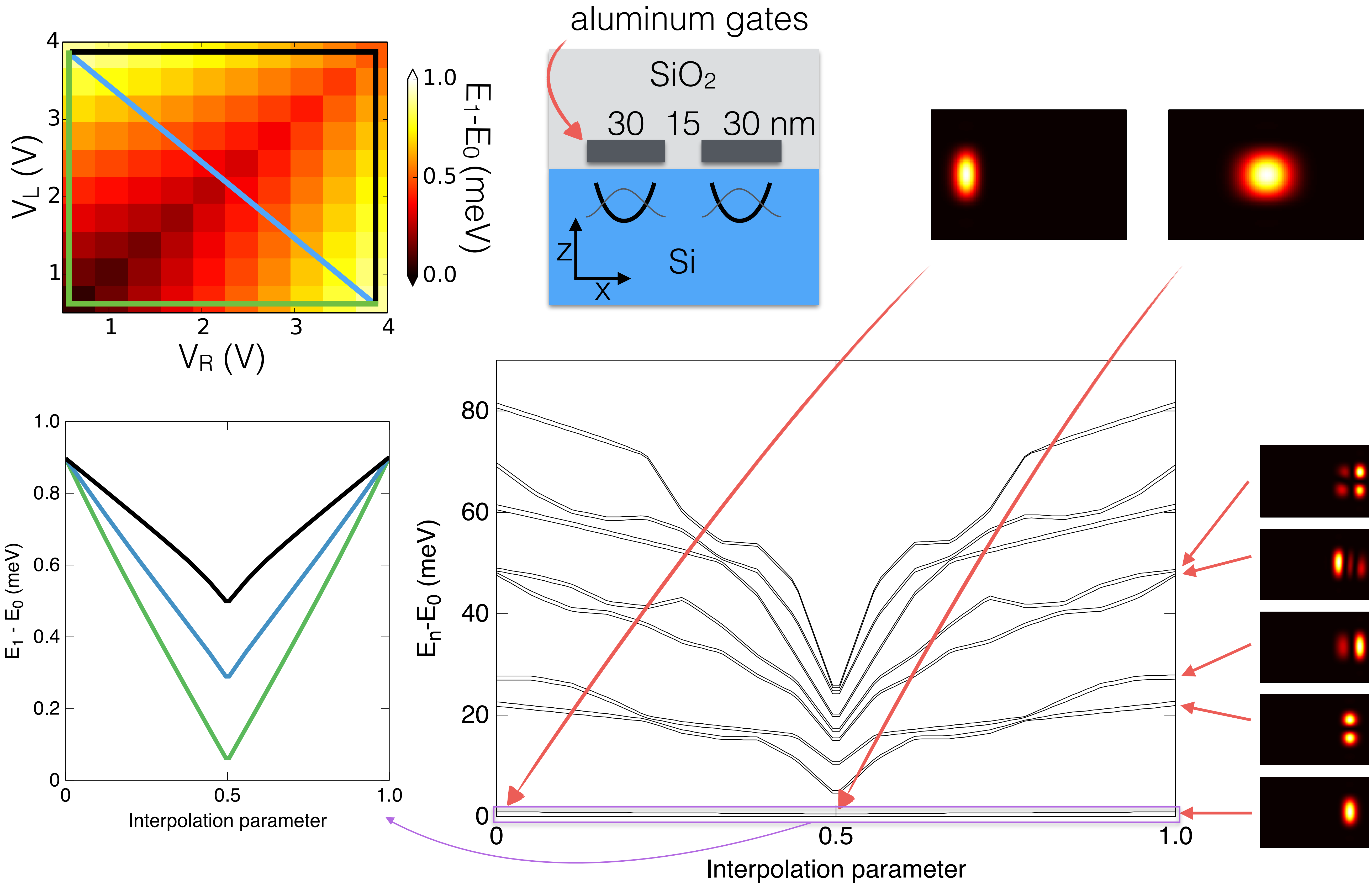








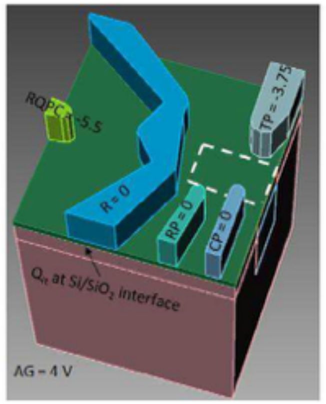
Exploring two-dot tunneling with full valley physics



Summary & future work

Summary & future work

Full scope modeling



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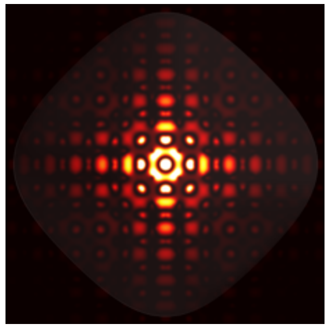

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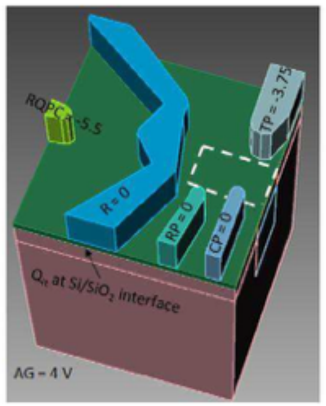
Full scope modeling



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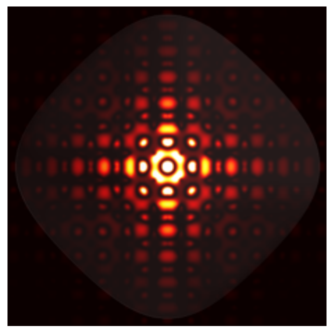
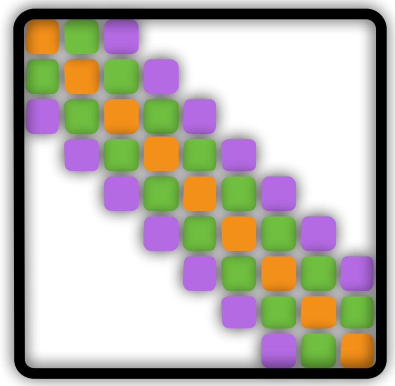


→

gaussian grid



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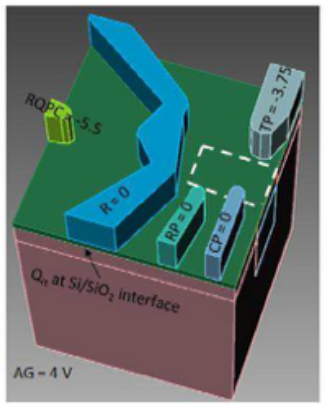

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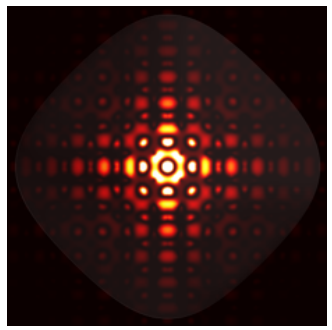

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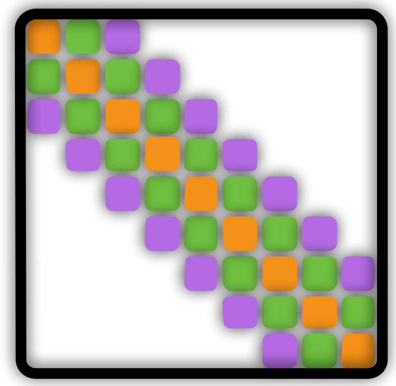
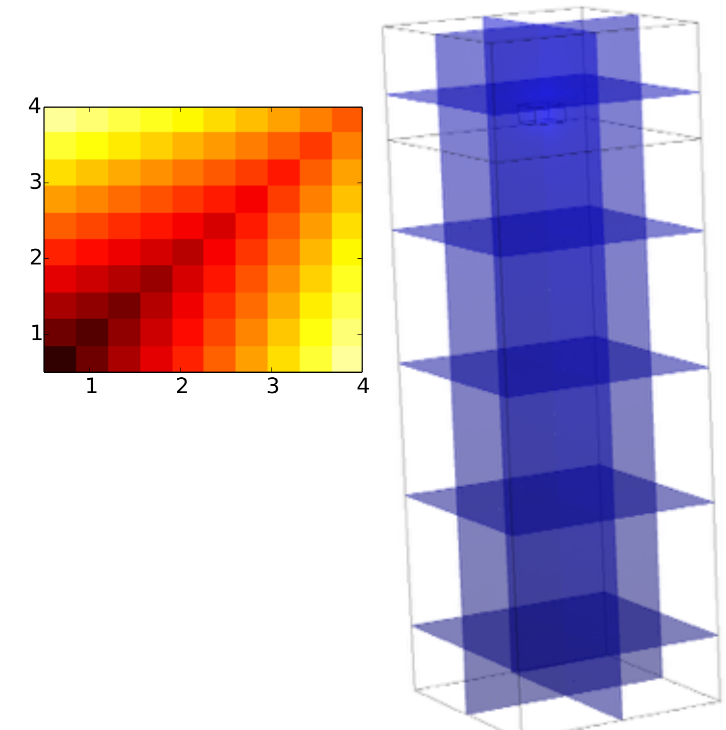


device-level simulation with full valley physics



Summary & future work

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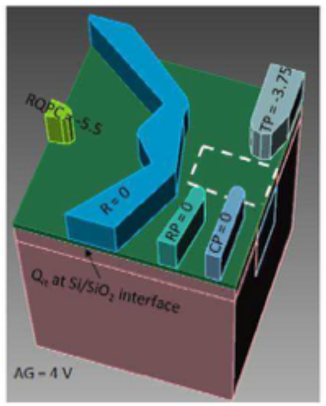

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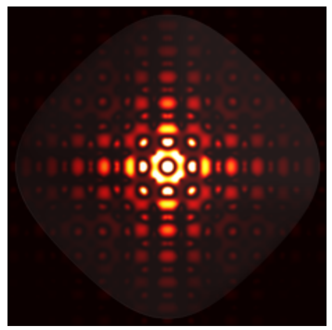
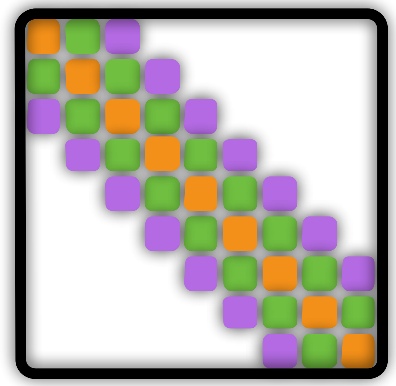


gaussian grid



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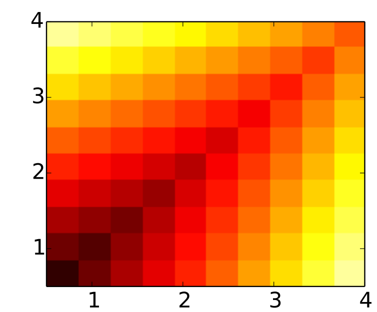

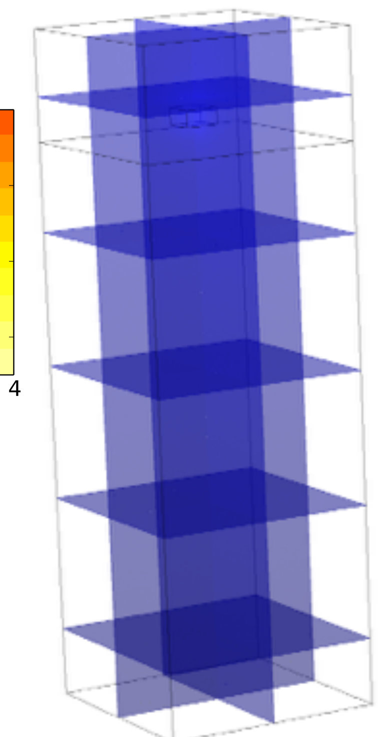

- Multiple electrons
- More realistic structures (including disorder)
- Dynamical modeling (optimal control?)
- Spin physics

Thanks!

Collaborators:

Andrew D. Baczewski

W37.00008 - Device-Level Models Using Multi-Valley Effective Mass

N. Tobias Jacobson

W37.00009 - Multi-valley effective mass theory for device-level modeling of open quantum dynamics

Adam Frees

W37.00010 - Multi-valley effective mass treatment of donor-dot tunneling in silicon

Inès Montaño

Erik Nielsen

Richard P. Muller