Atomistic simulations of coherent tunneling adiabatic passage in an imperfect donor chain

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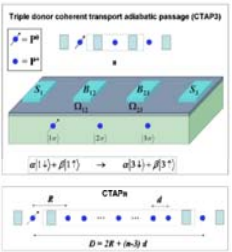
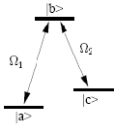
Coherent Tunneling Adiabatic Passage (CTAP)



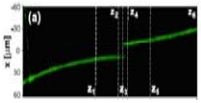
- Pathways in Eigen-space connecting end states
- Adiabatic modulation of tunnel barriers
- Minimal middle donor occupation
- Robustness
- Many donors, 4 gates
- Counter-intuitive pulsing

Greentree et al, PRB **70**, 235317 (2004).
Hollenberg et al, PRB 74, 045311 (2006).

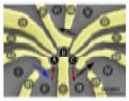
Quantum optics approx.
- analogue of STIRAP



Longhi et al 2007
(CTAP in triple waveguides)

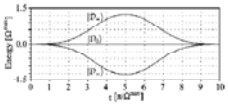


Schroer et al PRB 2007:
GaAs triple dots – test bed for CTAP



Effective 3 site CTAP Hamiltonian

$$H = \begin{bmatrix} E_1 & t_{12} & 0 \\ t_{12} & E_2 & t_{23} \\ 0 & t_{23} & E_3 \end{bmatrix}$$



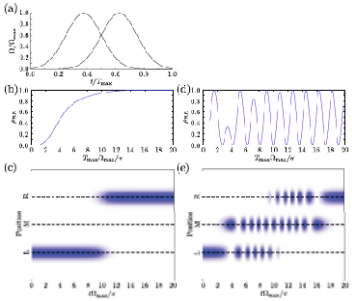
$$|\mathcal{D}_+\rangle = \sin\Theta_1 \sin\Theta_2 |1\rangle + \cos\Theta_2 |2\rangle + \cos\Theta_1 \sin\Theta_2 |3\rangle,$$

$$|\mathcal{D}_-\rangle = \sin\Theta_1 \cos\Theta_2 |1\rangle - \sin\Theta_2 |2\rangle + \cos\Theta_1 \cos\Theta_2 |3\rangle,$$

$$|\mathcal{D}_0\rangle = \cos\Theta_1 |1\rangle + 0|2\rangle - \sin\Theta_1 |3\rangle,$$

CTAP pulsing scheme

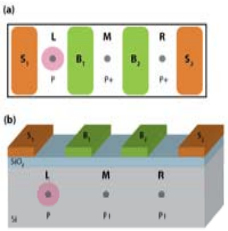
non-intuitive **intuitive**



Vanishing central density: signature of adiabatic transfer

Greentree et al, PRB **70**, 235317 (2004).
Rahman et al, arXiv, 1008.1494 (2010).

Atomistic simulations of CTAP (ideal donor placement)



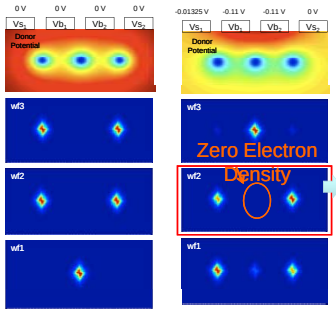
Objective:

- Investigate CTAP in realistic setting from atomistic Tight-binding (TB) in NEMO-3D.
- Include Si full band-structure, TCAD gates, interfaces, excited states, gate cross-talk.
- Find voltage sequence for the adiabatic path: 3 donor device.

About 3 million atoms (15 nm donor separation): 61 x 31 x 31nm^3 domain

Approach:

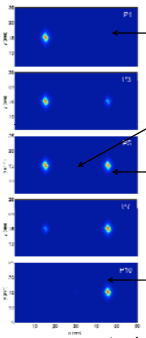
- TCAD gates coupled with a 3 donor TB Hamiltonian: molecular states in the solid state.
- Simulate 3-4 M atoms for a realistic device.
- Compute time of 4-5 hours on 40 procs for each voltage point.
- Fine tune gate voltages to explore the CTAP Regime.



CTAP Protocol (Desired Molecular States)

The 1st excited state under the specific voltage sequence without middle occupation

$|\Psi_2|^2$ at various voltages

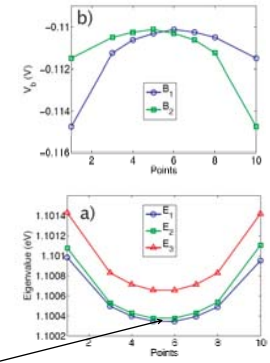


Left localized

Negligible population at center donor

Middle stage

Right localized

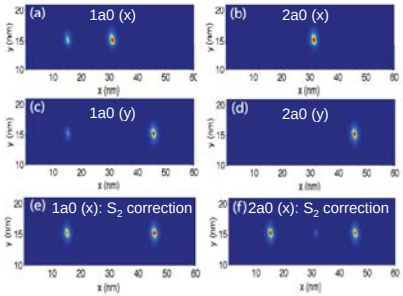


Anti-crossing gap => tunneling times

Rahman, Muller et al, PRB 80, 035302 (2009).

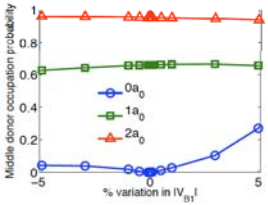
CTAP in an imperfect donor chain (donor straggle & gate voltage fluctuations)

- Effect of center donor misalignment on the adiabatic path
- Direct TB simulations.
- 1st excited symmetry
- Center donor density as a measure of the efficacy of CTAP



Displacements along the chain have the most detrimental effect, but gate voltages can be fine tuned to restore adiabatic path.

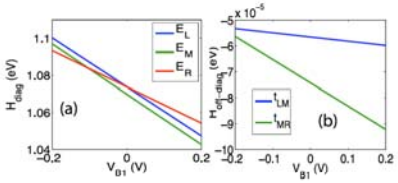
Sensitivity of the adiabatic path to Gate Bias



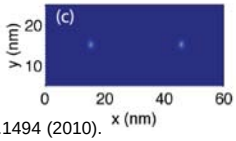
Extended effective 3x3 model based on TB wavefunctions

- Goal: Develop a small scale (3x3) model that encapsulates the atomistic TB information.
- Advantages: Optimal voltages can be obtained analytically from this parameterized model. Possible to simulate many configurations very fast to guide experiments.
- Approach: Use single donor TB wfs as basis for 3x3 model.
- Treat gate biases as perturbations & project full Hamiltonian on the single donor basis.
- Parameterize the matrix elements to characterize gate control.
- Find (V_{S1}, V_{B1}, V_{B2}, V_{S2}) that recovers original Hamiltonian

3x3 matrix elements with gate bias.



Verification of the model:
Ideal wf symmetry obtained using solutions of voltages from the parameterized 3x3 model.



Rahman, Muller et al, arXiv,1008.1494 (2010).

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