DFT simulation of dynamic charge states in double silicon quantum dots

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Introduction

Quantum Computing has been motivated by the efficiency it may exhibit when handling some classes of problems that are classically infeasible [1]. Solid state implementations, which should be inevitable for large scale quantum circuits, have been realized through semiconductor based Double Quantum Dots (DQD) [2]. Isolated (leadless) silicon DQD has shown long coherence time up to 220 ns [3], which is a potential virtue for QIP applications.

In this work intensive study has been carried out to uncover the electronic structure of the isolated silicon DQD through an atomistic scale simulation. We have succeeded in combining *ab-initio* density functional theory (DFT) calculation with molecular dynamics to simulate the time dependant evolution of the quantum system. We have also compared it with the time evolution of an ideal two level system known as Larmor Precession.

Simulation model and Proposal for transient analysis

In the present analysis we used the well tested SIESTA, which is the LCAO based DFT simulation package [4] [5]. Fig. 1 shows the atom based DQD model, which can be seen as two individual dots bridged by a rod-like structure. The size scale of the DQD system should give an insight to the effect of scaling. Intentional asymmetry has been introduced in the DQD to slightly alter the electronic states of the left/right dot. The overall silicon bone structure is equivalent to the crystal structure of bulk silicon, and has been terminated with hydrogen to eliminate the dangling bonds on the surface.

By applying an electric field in the z direction, the effective potential on the left/right dot is shifted. Finite interaction through the 'bridge' leads to anti-crossing over the two dots which can be clearly observed in Fig. 2. The eigenstates denoted as 'WF663' corresponds to the anti-bonding state and 'WF662' to the bonding state, a two level system formed inside an artificial molecule with an energy gap ΔE of $\approx$3.16 meV.

We propose a time dependant simulation by combining DFT with molecular dynamics as a way to simulate time evolution of a quantum system. A simple picture is given in Fig.3 to understand the simulation procedure. Electric field E_z is applied to the DQD as a step function, forcing an arbitrary two level system into resonance (or slightly off-resonance). The electronic structure will be determined through DFT, and the forces on each atom will be calculated. Born-Oppenheimer approximation treats the nucleus as 'classical' particles, so the positions of the nucleus at time Δt can be derived from the classical equation of motion (Standard Velocity Verlet molecular dynamics method). Time interval Δt must be kept very short and 0.5 fs has been chosen to ensure qualitative accuracy. The wave functions will be extracted to examine time evolution.

Time dependant evolution of a two level system

The wave functions of WF661 to WF663 are visualized at two selected time domains in Fig.4. WF662 (bonding state) shows the wave function seeping into the right dot, as WF663 describes the opposite situation. On the other hand, WF661 does not change during this period, which emphasizes that the time evolution is not equivalent for each and every eigenstates.

For quantitative investigation the simulation cell has been simply divided into two identical boxes, and the DOS has been calculated for the whole region and left/right box for WF662. While the DOS for the unit cell stays constant, the DOS in the right box decreases and then increases accompanied with a much higher frequency fluctuation. The low frequency oscillation is thought to correspond to Larmor precession, while the higher frequency fluctuation is thought to arise from the Si-H and/or Si-Si bonds, which does not enter the picture when considering an ideal two level system.

Fig. 6 shows the E* (the energy difference between bonding and anti bonding states) for WF662 and WF663. The E_z for this particular simulation is off resonance, and the estimated Larmor precession period $T = \frac{h}{\sqrt{\varepsilon^2 + \Delta E^2}} \approx 450[fs]$ is longer than the simulated oscillation.

Acknowledgment

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References

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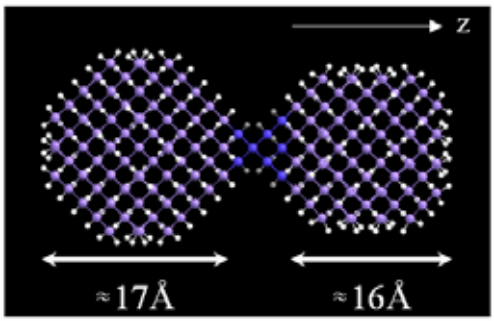

Total Atoms : 475 (Si:279, H:196)
Left Dot : 147 Si atoms
Right Dot : 123 Si atoms
Bridge : 4 layers (9 atoms)

Fig. 1: Simulation Model

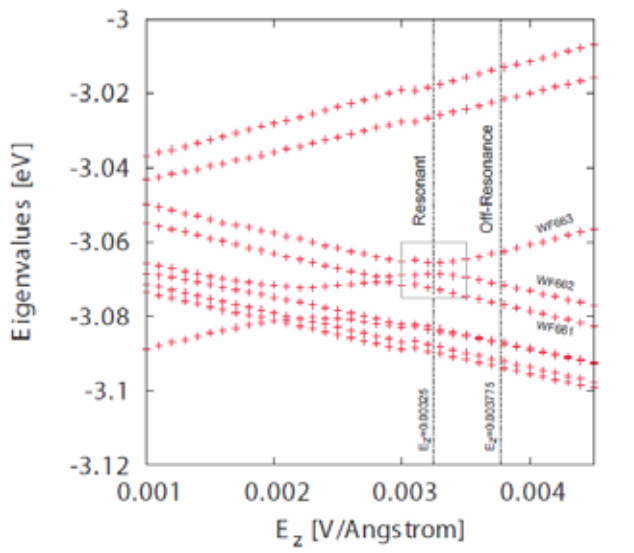

Fig. 2: Bare eigen-energy spectra (for unoccupied states) vs. Electric field in z direction

Discontinuity at Ez=0.003 [V/Å] is due to the finite accuracy for numerical calculations.

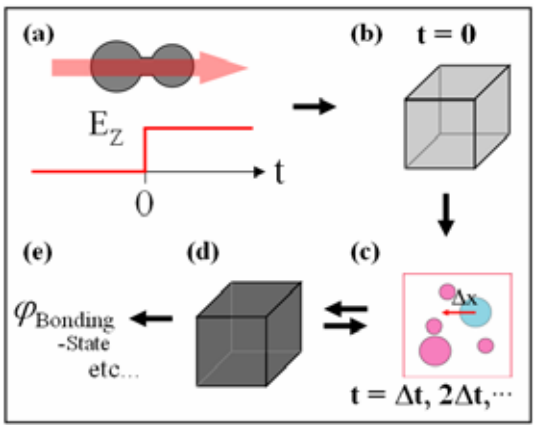

Fig. 3: Simulation Method

(a) The 'step function' at t=0 is taken into account by using initial parameters converged at E_z=0 (time independent analysis). (b), (d) DFT calculation (c) Positions of nucleus updated according to Velocity Verlet Algorithm (e) Wave functions are projected to a 3D finite grid.

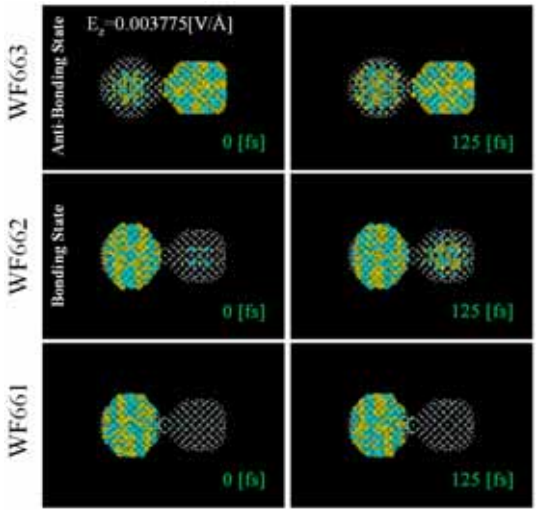

Fig. 4: Wave functions visualized for specific states

WF661 represents eigenstates at Energy=-3.077[eV] @ Ez=0.003775 [V/Å]. WF662, WF663 are denoted similarly.

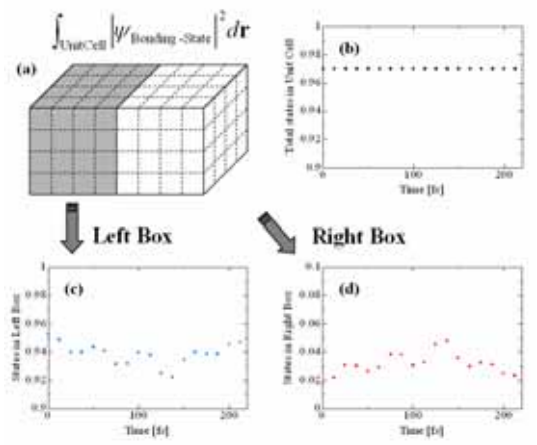

Fig. 5 Quantitative evaluation of DOS in Left/Right and Unit Cell

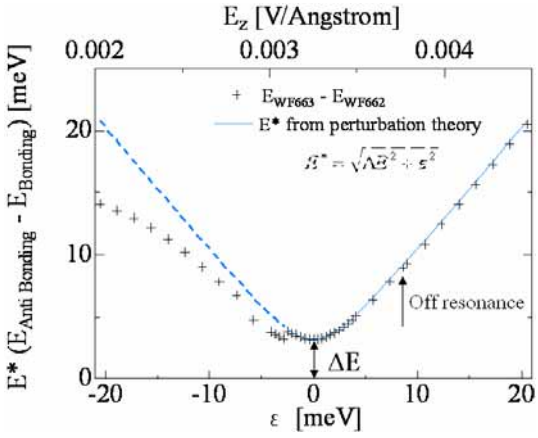

Fig. 6 E* for WF662 and WF663

ε stands for the energy difference between the uncoupled charged states. The discontinuity at Ez=0.003 [V/Å] is due to finite accuracy, and the gap between simulation and theory at negative ε corresponds to the existence of other resonant states.