

Ab-initio method of designing artificial quantum bits

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Introduction

Nanocrystalline Si Quantum Dots (QDs) have widely been studied as fundamental building blocks for the bottom-up approach in order to construct nm-scale device structures. Strongly coupled Si QDs are particularly interested for quantum information device applications. The wave function interaction has been recently studied for double Si QDs, and the quasi molecular states, which are the bonding-like and anti-bonding-like states have been observed at 4.2K [1]. Theoretical analysis has also been recently reported on the stable structures for QDs with the size of under a few nanometers[2][3]. Upon these structures, the Icosahedral structure is hollow and distinctively different from bulk-like structures which can be scaled up to as large as 5nm[2]. Experimental studies have also been reported on the structures for extremely small Si QDs with diameter less than 2 nm [3][4]. In this paper we use the ab-initio method to demonstrate the electronic states of strongly coupled double Si QDs (Icosahedral structure) with diameter down to 1 nm. We analyze the formation of a two level system in an atomistic manner and discuss how the tunnel splitting between the two levels depends on the structural configuration of the double dots. The ultimate goal is to artificially design and control the two level system and use as a Quantum bit, the Qubit.

The Two Level System

Quantum computing requires a two level system constructed in a quantum manner. Fig.1 shows the maximum logic operations that can be executed as a function of the energy difference between the two level system. Although the number of times depend on the decoherence time of the system, a fairly large split will be required to accomplish the 10^6 times that will be needed to run actual quantum calculations.

In the present analysis we used the well tested SIESTA, which is the LCAO based DFT simulation package [5][6]. The Si bone-structure was terminated with hydrogen and relaxed with the classical molecular mechanics program. The SIESTA code has some distinctive features such as the DFT and pseudopotentials, and will minimize the free energy of the system to obtain wave functions, eigenvalues, optimal structures, etc. We have chosen the Icosahedral structure (Fig.2-d)[2] for the QD because of its very atomic like energy structure (Fig.2-c) and the scalability it possesses. Theoretical work for multiple QDs have not been accomplished so far, compared to the number of

researches done on isolated QDs. We first parted the Icosahedral QDs by vacuum and calculated the Total Density of States (TDOS) for the system. Figure 2 shows the splitting of each state, and the bonding and anti-bonding states can be observed. The normal subbands consist of a number of eigenvalues so the subbands will break into multiple states. However the normal LUMO state is composed of just one eigenstate and is fairly isolated from the other eigenstates. Therefore the LUMO states split into two states. The Localized Density of States (LDOS) are visualized in Figs.3,4 to observe the orbitals of these states. We have changed the orientation of the Icosahedral QDs and found that the orbitals can be classified into two categories. The conventional type of quasi molecular state (QMS) (Fig.3), and the quasi localized state (QLS) (Fig.4). The bonding- anti-bonding splitting is found 112 meV for QMS and 78 meV for QLS. Although the overall size of the LUMO split is found larger for QMS, the QLS can also form bonding and anti-bonding states.

Artificial Qubit Design Methods

As mentioned above, the relative position of the two quantum dots dominate the formation of the two level system. The distance between the dots are also important because they directly influence the wavefunction overlaps. To overcome this problem, we bridged the QDs via oxygen and SiO₂. By doing so, Fig.5 shows that the magnitude of the LUMO splitting is enhanced, and the relative positions are fixed.

Fig.6 shows the influence of an external electric field applied in the major axis. Dramatic increase in the LUMO splitting can be observed which may be used to modulate the resonance frequency of each qubit.

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References

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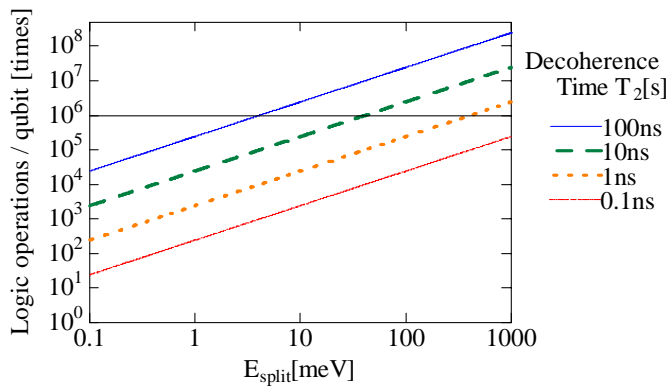


Fig.1: Maximum Logic Operations

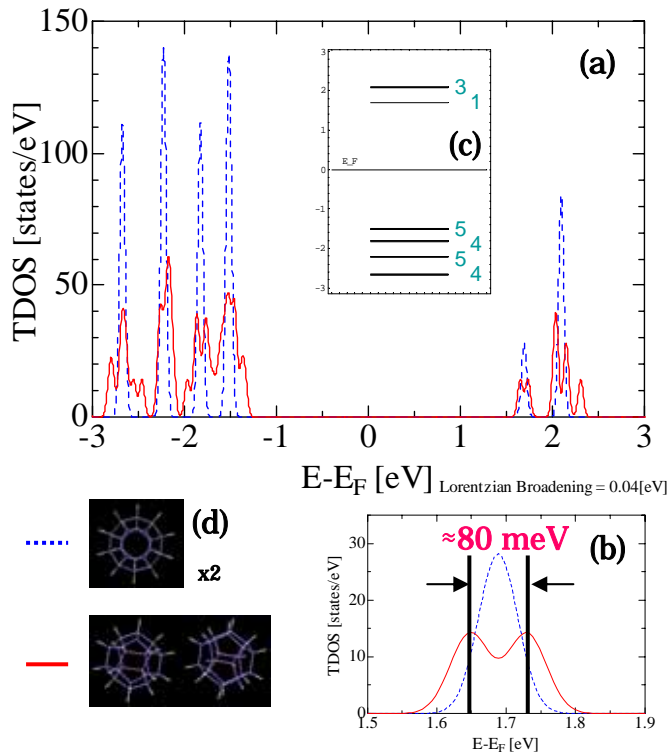


Fig.2: (a) Total Density of States (TDOS) (b)Close-up view of the split LUMO state (c)Bare eigenenergy spectra (d)Icosahedral Structure

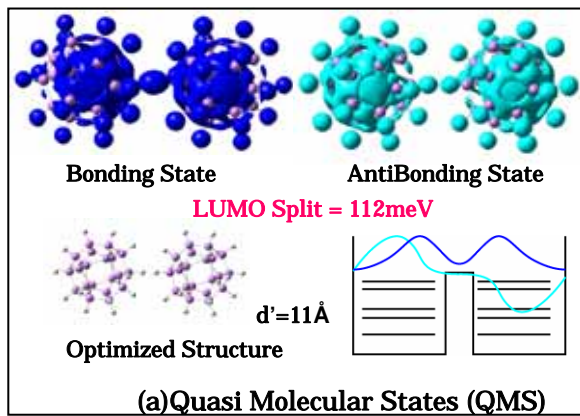


Fig.3: Visualization of the Local Density of States (LDOS) for QMS

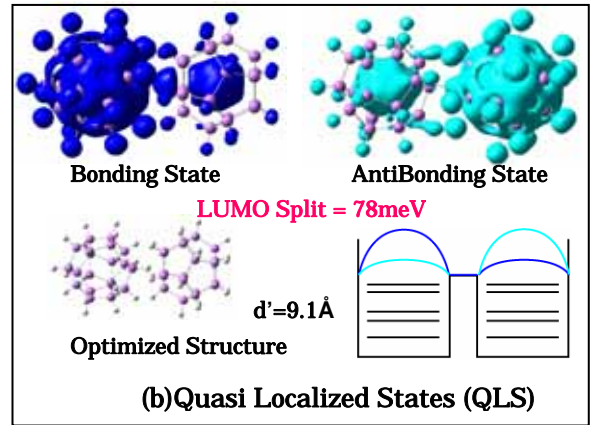


Fig.4: Visualization of the Local Density of States (LDOS) for QLS

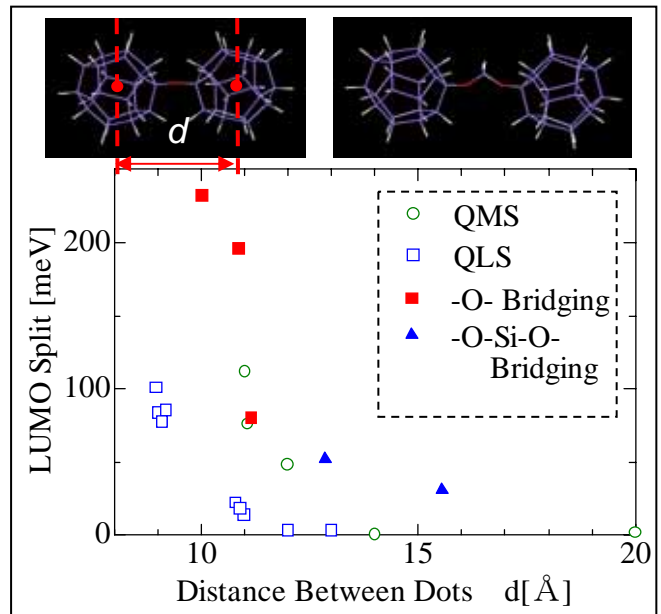


Fig.5 Bridged Structures

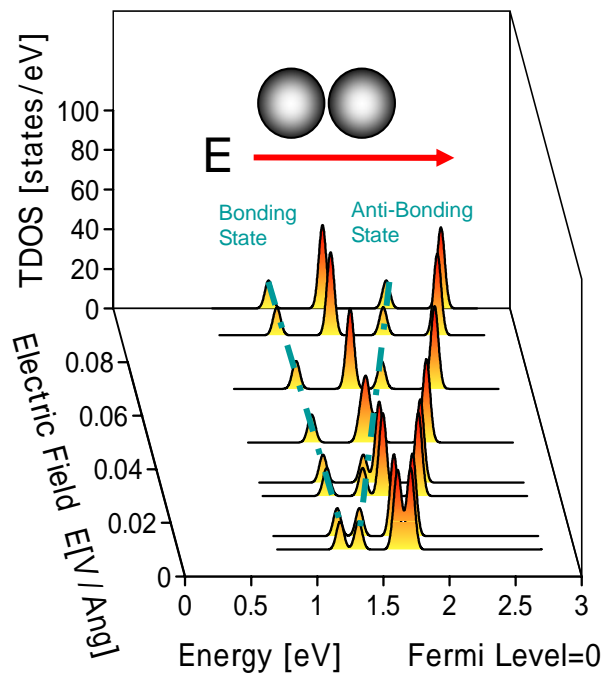


Fig.6 Split change due to External Electric Field