# Calculation of carrier transport through quantum dot molecules

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**Abstract.** A detailed calculation is presented of the electronic structure and the ballistic current through a realistic InAs/InP open quantum dot molecule consisting of two vertically stacked InAs quantum dots. It is shown that a careful analysis of the experimental tunneling current allows one to extract a wealth of information about the energy levels, base widths, distance and lateral misalignment of the quantum dots in a quantum dot molecule.

## INTRODUCTION

In this paper we present a quantitative theoretical analysis of the ballistic current through a quantum dot molecule (QDM) based on two vertically stacked quantum dots (QDs) embedded within a resonant tunneling diode (RTD). In particular, we show that measurements of the resonant tunneling current provide a wealth of unique information about the size, geometry, and the energy levels of the QDM. Our calculations are based on a fully three-dimensional model of the RTD with realistically shaped QD structures. The local strain is calculated by minimizing the total elastic energy of the entire device. We solve the Poisson equation including the piezoelectric charges and subsequently calculate the ballistic current in terms of the contact block reduction method.[1] This scheme computes the quantum states of the open system with scattering boundary conditions rigorously. The quantum states themselves are evaluated in terms of the single-band Schrödinger equation for the conduction bands, taking into account spatially varying electron masses, band offsets, deformation potentials, and the electrostatic potential due to the piezoelectric charges. All calculations are carried out within the framework of next**nano**$^3$. [2]

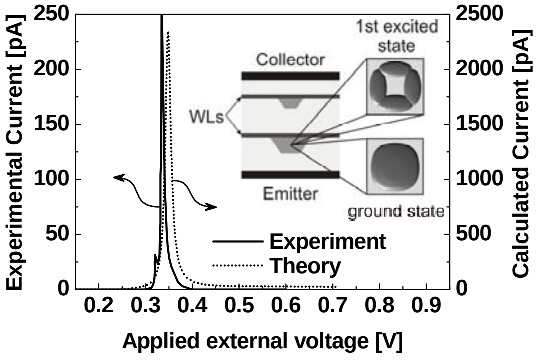

**FIGURE 1.** The experimental and calculated current through the InAs/InP QDM as a function of the applied bias. The inset shows the structure of the device, including the leads (black), WLs (dark gray), and the QDs (light gray), schematically. Furthermore, a top view of the 3D orbitals of the ground and first excited state of the large QD are plotted.

## RESULTS AND DISCUSSION

The RTD as depicted in the inset of Fig. 1 is composed of a 33 nm thick InP barrier with two embedded InAs QDs that are grown on 0.5 nm thick wetting layers (WLs). The distance between the WLs is 15 nm. This RTD was studied experimentally by Bryllert *et al.*[3,4] Upon applying a bias, pairs of bound states in the two adjacent QDs can be brought into resonance with one another, thereby increasing the electron transmission probability by several orders of magnitude.

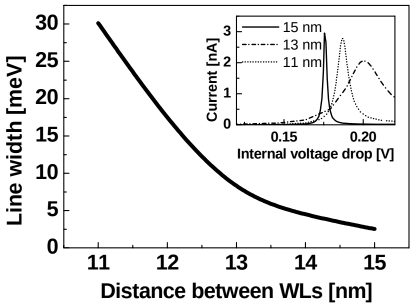

**Figure 2.** Calculated resonance line width as a function of the inter-dot distance. The inset shows the resonances for WL distances of 11, 13, and 15 nm, respectively. The peak current increases with increasing inter-dot distance, whereas the integrated current falls off exponentially.

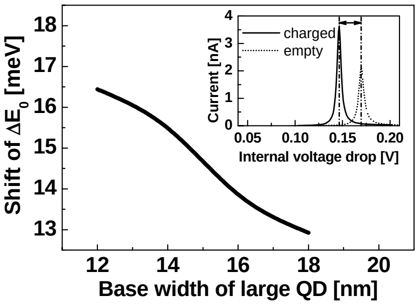

**FIGURE 4.** Change in the zero-bias energy difference $\Delta E_0$ between the two QD ground states due to charging of the large QD, plotted as a function of the base width. The inset shows the shift of the current resonance for the neutral and charged situation.

Fig. 1 shows the experimentally determined as well as the theoretically predicted current. The two QDs were modeled by truncated pyramids of 2.5 (5) nm height and 12 (16) nm base width, respectively. The difference $\Delta E_0$ of the zero bias ground state energies is 87 meV. The peak height and the line width of the current resonance depend strongly on the inter-dot distance and the lateral misalignment, which may explain the differences between theory and experiment. In fact, Fig. 2 shows the line width of the resonance to decrease exponentially with increasing QD distance which reflects the exponential decrease in the QD coupling. The inset shows the shape of several current resonances explicitly.

As depicted in the inset of Fig. 3, an additional resonance may occur if the excited state **1** in the large dot lies in resonance with the ground state **0’** of the small dot. Fig. 3 displays the ratio between the peak currents of the **1** → **0’** resonance and the **0** → **0’** resonance as a function of the relative lateral displacement of the two QDs.

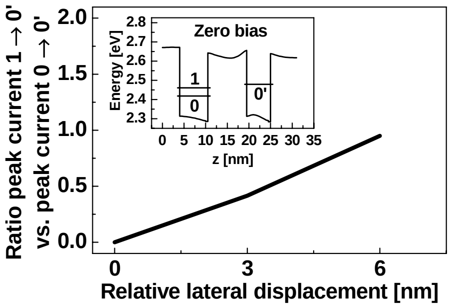

**FIGURE 3.** Ratio between the peak currents of the **1** → **0’** resonance and the **0** → **0’** resonance as a function of the relative lateral displacement of the two QDs. The inset shows the energies of the ground state **0** and excited state **1** in the large QD and of the ground state **0’** in the small QD.

The larger QD close to the emitter may be charged by emitter electrons. This charging decreases the energy difference $\Delta E_0$ and shifts the resonance bias as is illustrated in the inset of Fig. 4. This shift decreases for larger base width, as shown in Fig 4, and can therefore be used to estimate the lateral dimensions of the large QD.

The peak heights and positions, and the line widths of the tunneling resonances through ground and excited states yield quantitative information about the energy levels, base widths, distance and lateral alignment of the QDs in a quantum dot molecule.

## REFERENCES

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