## Atomistic Modeling of a Tunable Single-Electron Quantum Dot in

## Silicon using NEMO3D-peta

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I. Introduction II. Objective If the trend continues, Valley splitting (VS) — The energy seperation between The Scaling challenge 10 µn device will reach S. E. Thom the lowest two confined states atomic scale by 2030 Technology nod Large VS  $\rightarrow$  prevent loss of spin information  $\rightarrow$  good 1 µn size for spin aubit 130 nm Feature 90 nm Gate length 100 n →Quantum Computing Confinement Nanotechnology Potential could be next! Planar MOSFET limit 10 r [001] 1970 1980 1990 2000 2010 2020 Recent breakthrough: Experimental realization of Si 10101 MOS QD with low Si/SiO<sub>2</sub> Valley L1 (/m) 08 interface disorder -> operates Potential Splitting Si MOS Quantum Dot in the single electron regime ≁ Confinement created by electric field from gate bias **Project Goal:** clear "Coulomb <u>Advantage</u>: State-of-the-art Si MOS fabrication technology and liamond" at single a)Explore VS behavior in Si MOS QD: Industrial compatibility - What is the range of VS? A promising candidate Challenge: Si/SiO<sub>2</sub> interface What factors determines VS and how? disorder impedes single electron for "Spin Qubit"? b)Guide experimental design of VS for Si MOS QD occupancy III. Methodology **NEMO3D-peta Scaling Performance** V<sub>B</sub> NEMO3D-peta Simulation Structure Huge problem Size: Key assumptions: 8 million atoms •Only the QD region included , 10nm sp<sup>3</sup>d<sup>5</sup>s<sup>\*</sup> tight-binding model in calculating VS Top View Matrix size of 80 million Equilibrium throughout the 30nm entire device, E<sub>F</sub> set by source SEM Image n-type subst. and drain Almost perfect scaling! Low temperature ~ 100mK Electronic domain Side View 0nm •QD size varies: >30 x 60 x W<sub>c</sub> nm<sup>3</sup> Data 30nm Time (hours) -Fitted Slope type subs ≻W<sub>c</sub>= (30, 40, 50, 60) nm Ideal 10 Schrodinger Solver Reasonable cost: Self-Consistent Simulation  $(H+U)\psi=E\psi$ 2.2 hours @ 256 cpu Convergence check: Compare U(r) after elf-Consistent Ideal Slor 10<sup>0</sup> each iteration Potential Profile U(r) Charge Profile n(r) Loop Single electron in the QD: 10 10 10 >E must cross exactly the ground state NO. CPU Poisson Solve VS value changes little when simulation is NEMO3D-peta is capable of simulating  $\nabla(\varepsilon \nabla U) = q^2 n$ close to convergence atomistic structure of realistic size ! V<sub>B</sub> , V<sub>F</sub> V. Results and Conslusion VS Full Spectrum VS (ueV) VS vs. E-field VS vs. Barrier Height 500 500 500 0.88 30×30 (nm<sup>2</sup>) ♦ 30! 30 nm<sup>2</sup> 🔶 30! 30 nm 400 30! 40 nm<sup>2</sup> Á 30! 40 nm 0.86 400 30! 50 nm<sup>2</sup> 400 30! 50 nm (ueV) (ueV) 300 S 0.84 30×50 (nm<sup>2</sup>) 30×40 (nm<sup>2</sup>) splitting ( splitting ( 200 0.82 300 300 100 0.80 30×60 (nm<sup>2</sup>)  $1 \rightarrow 5$ Valley Valley 200 200 0.780 1.0 1.1 1.2 1.3 100 100 VP (V) VS range: 10 12  $\begin{array}{cccc} 10 & 20 & 30 & 40 & 5\\ \text{Barrier height from } E_{\text{F}}(\text{meV}) \end{array}$ 50 4 6 8 1 Electric Field (MV/m) This work: 95~470µeV; Experimental measurement: ~100µeV Regardless of QD size: ■Higher barrier → Larger VS Electron Conservation: V<sub>B</sub> and V<sub>P</sub> must "balance" Larger electric field → Larger VS Same barrier height: Larger V<sub>P</sub> pushes QD deeper → More electrons Smaller gate  $\rightarrow$  Stronger confinement  $\rightarrow$  Larger VS Smaller V<sub>B</sub> raises barrier height → Less electron Conclusion Simulated VS results matches well with experiment Small QD is preferred since it has larger VS A high potential barrier is preferred for large VS but hampers electron tunneling



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