

ABSTRACT

Title of Dissertation: ATOMICALLY PRECISE SILICON DEVICES
FOR ANALOG QUANTUM SIMULATION AND
QUANTUM INFORMATION PROCESSING

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This thesis explores silicon as a platform for dopant-based quantum computation and analog quantum simulation, employing scanning tunneling microscope (STM) lithography to achieve atomically precise device structures. Beginning with a comprehensive review of the device fabrication process and a theoretical introduction to transport in dopant-based nanostructures, this thesis establishes a framework for constructing dopant-based devices where both spin and charge degrees of freedom can be harnessed for quantum information processing. To address the challenge of scalability, automated STM patterning workflows are developed. Algorithms inspired by electronic design automation (EDA) are introduced to accelerate the creation of both atomically precise quantum structures and large-area electrical leads. The experimental chapters present device architectures for spin readout and analog quantum simulation. Charge sensing and energy-selective spin readout are demonstrated using a donor-dot single electron transistor (SET). Spin relaxation times (T_1) are measured across varying magnetic fields showing relaxation occurs mainly through charge noise enhanced spin-orbital coupling. These results provide a foundation for implementing spin manipulation

in the next stage of development. Works on analog quantum simulation include the experimental realization of the two-dimensional Hubbard model using dopant arrays, supported by numerical simulations based on an extended Fermi-Hubbard model. Spin filling in these arrays is further investigated through magnetotransport measurements, revealing a “Hund’s rule” like behavior in electron configurations. In addition, a 32×32 quantum dot array was fabricated to extend the study beyond small systems, enabling the simulation of transport through localized electronic states and the exploration of disorder-induced conduction phenomena.

Finally, I present results on optimized RF reflectometry circuits for charge sensing in a donor-dot SET, achieving a minimum integration time of 600 ns to resolve charge states on a donor cluster. Applied to a 3×3 quantum dot array, these techniques identify site-resolved charge addition lines through distinct capacitive couplings to the leads, enabling unambiguous assignment of electron occupation across the lattice. These studies demonstrate the versatility of atomically precise dopant systems in probing strongly correlated electron physics and advancing silicon-based quantum information processing.

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SIMULATION AND QUANTUM INFORMATION PROCESSING

by

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Summary of Contributions

Chapter 5 presents unpublished results on attempting to achieve high-fidelity single-shot spin readout using a donor-dot SET device. The device was fabricated by Xiqiao Wang. I performed all low-temperature measurements, data analysis, and interpretation.

Chapter 6 contains a combination of published, in-preparation, and unpublished work.

- **Section 6.3** is partially reproduced from *Wang, X., Khatami, E., Fei, F., et al. Experimental realization of an extended Fermi–Hubbard model using a 2D lattice of dopant-based quantum dots. Nature Communications 13, 6824 (2022)*. My contributions include theoretical interpretation of the experimental data and electrical transport measurements.
- **Section 6.3** also presents unpublished results on the spin-filling sequence of the strongly coupled 3×3 array. The device was fabricated by Xiqiao Wang. I carried out the measurements, performed all data analysis, and conducted the numerical simulations.
- **Section 6.4** includes work in preparation (*Fei, F., et al., Transport from Disorder-Induced Localization in a 32×32 Dopant Quantum Dot Array*). I fabricated the device, acquired the low-temperature transport data, and led the interpretation of the results.

Chapter 7 is reproduced from completed work intended for submission to *Physical Review Applied: Fei, F., et al., Optimizing RF-Reflectometry Measurements for Large-Impedance Silicon Quantum Devices*. I designed the experiment, performed the measurements, analyzed the data, and wrote the manuscript.

Chapter 8 is reproduced from completed work intended for submission to *ACS Nano: Fei, F., et al., RF-Reflectometry Measurements of Charge Configuration in a Si:P Quantum Dot Array*. The device was fabricated by Xiqiao Wang. I designed and executed the experiment, performed all data analysis, and wrote the manuscript.

List of Abbreviations

2DEG	Two-dimensional electron gas
AI	Artificial intelligence
a.u.	Arbitrary unit
AWG	Arbitrary wavefunction generator
AQS	Analog quantum simulation
CBM	Conduction band minimum
DOS	Density of states
EMT	Effective mass theory
ESR	Electron Spin Resonance
DFT	Density functional theory
FCL	Feedback controlled lithography
FET	Field effect transistor
FWHM	Full width half maximum
ICT	Interdot charge transition
LGT	Lattice gauge theory
LLM	Large language model
MBE	Molecular beam epitaxy
MCP	Model context protocol
NMR	Nuclear magnetic resonance
PSB	Pauli spin blockade
QPC	Quantum point contact
SEM	Scanning electron microscopy
SET	Single electron transistor

Si:P	Silicon-phosphorus
SIMS	Secondary ion mass spectrometry
STM	Scanning tunneling microscope
SUSI	Si sublimation source
RF	Radio frequency
RTA	Rapid thermal anneal
TB	Tight binding
TEM	Transmission electron microscopy
UHV	Ultrahigh vacuum
UNSW	University of New South Wales

Chapter 1: Introduction

1.1 Context and motivation

Over the past half century, advances in classical computing have transformed nearly every aspect of society. The exponential scaling of transistor density, codified by Moore’s law ¹, has powered the rise of personal computers, the internet, and more recently, artificial intelligence systems with billions of parameters by integrating more transistors. Yet as these systems continue to expand in scope and ambition, classical computing faces fundamental limitations. Shrinking transistor dimensions to the atomic scale introduces variability, leakage currents, and quantum effects that degrade performance. Although advanced semiconductor manufacturing foundries have been pushing for 2 nm or 1.4 nm node process, switching from FinFET ² technology to more scalable gate-all-around (GAA) ³ designs, the marginal improvements on performance are still expected to be limited. This can be seen as most personal electronic devices purchased a few years ago remain competitive to the newest hardware today. At the same time, supercomputers composed of thousands of CPUs and GPUs consume enormous power while still failing to address certain classes of problems, such as strongly correlated quantum systems ⁴ or large-scale combinatorial optimization ⁵.

Quantum computing emerges as a new alternative paradigm that leverages the principles of quantum mechanics with superposition and entanglement to perform computations in ways fundamentally distinct from classical systems. Rather than being an incremental continuation of Moore’s law, quantum computing represents a disruptive approach that has the potential to solve problems intractable for any foreseeable classical machine. Applications span from simulating the chemical properties of molecules and novel materials ⁶, optimizing logistics networks ⁷, to developing secure communication protocols resistant to quantum attacks ⁸. Recent milestones, such as the demonstration of quantum supremacy ⁹ by Google in 2019, advances in quantum error correction ¹⁰, and the scaling of platforms beyond 100 qubits ¹¹, signal the rapid progress and growing maturity of the field. At the same time, potential benefits from combining

quantum computing with artificial intelligence has attracted substantial industrial investment, accelerating research and development toward their eventual convergence, which could drive a paradigm shift in the entire computational science and technology ^{12,13}.

1.2 Basics of quantum computing

The fundamental unit of quantum information is the quantum bit, or qubit made by a two level quantum system. Unlike a classical bit that takes a value of 0 or 1, a qubit exists in a coherent superposition of both states, expressed as:

$$|\psi\rangle = a |0\rangle + b |1\rangle \quad (1.1)$$

where a and b are complex amplitudes satisfying $|a|^2 + |b|^2 = 1$. The relative phase between a and b encodes additional information, and the state can be visualized as a point on the Bloch sphere ¹⁴. Single-qubit operations correspond to rotations of this point, for example, the X, Y, Z gates represent a π rotation around the x, y and z axes of the Bloch sphere. As additional qubits are introduced, the dimension of the Hilbert space grows exponentially, providing the fundamental resource for quantum advantage. Two-qubit gates are essential as they generate entanglement, enabling correlations that have no classical analogue and allowing quantum information to be encoded in the vastly larger Hilbert space of multi-qubit systems. A simple yet profound example is the Bell state ¹⁵, $|\Phi^+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$, where the measurement outcome of one qubit is perfectly correlated with the other regardless of physical separation. Such entangled states form the foundation for executing quantum algorithms.

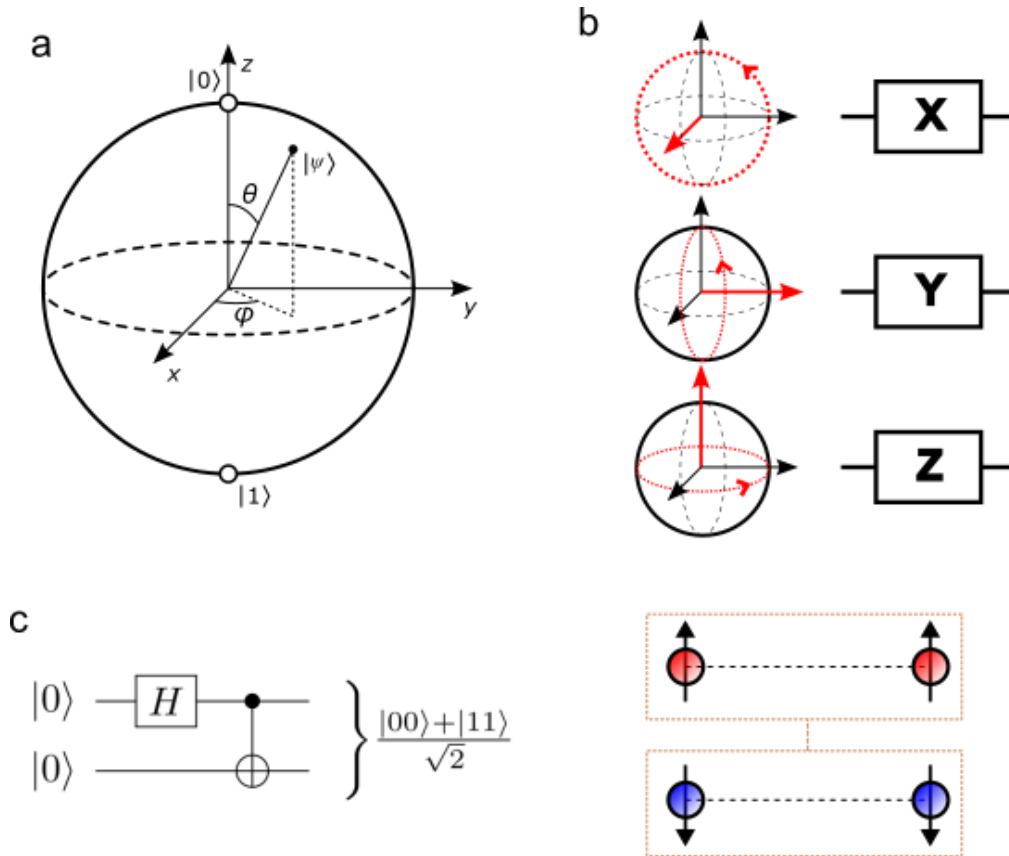


Figure 1.1 Qubit: The fundamental building block of a quantum computer. (a) Bloch sphere representation of a single qubit. The $|0\rangle$ and $|1\rangle$ states correspond to the north and south poles of the Z-axis. Unlike a classical bit, which can only be 0 or 1, a qubit state can occupy any point on the sphere's surface. (b) Single-qubit gates rotate the state vector on the Bloch sphere; for example, the X, Y, and Z gates correspond to π rotations about the respective axes. (c) Two-qubit gates generate entanglement between coupled qubits, enabling quantum information to be encoded in the much larger Hilbert space of multi-qubit systems. A Bell state, $|\Phi_+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$, can be created by applying a Hadamard gate followed by a controlled-NOT (CNOT) gate, resulting in two qubits that are maximally entangled—measurement of one qubit immediately determines the state of the other. Together, single- and multi-qubit gates form a universal gate set that enables the implementation of quantum algorithms.

For a quantum computer to be useful, it is generally agreed upon that the quantum hardware should meet the DiVincenzo criteria ¹⁶: (1) a scalable physical system with well-characterized qubits, (2) the ability to

initialize qubits into a known state, (3) coherence times long compared to gate operations, (4) a universal set of quantum gates, and (5) qubit-specific readout. Meeting these requirements simultaneously is technically demanding, leading to a diversity of hardware platforms being actively pursued.

A physical qubit is inherently fragile: it interacts with its environment even in the absence of intentional operations. Such unwanted interactions perturb the quantum state and lead to relaxation and decoherence. The relaxation time T_1 ¹⁴, describes the characteristic decay time from the excited state $|1\rangle$ to the ground state $|0\rangle$, while the decoherence time T_2 ^{14,17}, quantifies the loss of phase coherence due to the accumulation of small perturbations. The performance of a qubit platform is typically benchmarked by its gate fidelities, and achieving fidelities above the 99 % threshold required for quantum error correction¹⁸, is essential for constructing better logical qubits from more physical qubits and for scaling up qubit numbers to the level needed for practical algorithms. A viable quantum computing platform therefore needs to address all these challenges.

1.3 Quantum hardware platforms

Multiple physical implementations of qubits are under active development today, each with distinct advantages and challenges. Here we list a few major platforms:

- **Superconducting qubits:** Superconducting qubits such as the transmon qubit¹⁹, are fabricated using Josephson junctions²⁰ embedded in microwave resonator circuits. They offer nanosecond-scale gate times, compatibility with existing lithographic processes, and well-developed microwave control techniques. Companies like IBM and Google have scaled devices to over 100 qubits and demonstrated basic quantum algorithms. The main challenges include relatively short coherence times (tens to hundreds of microseconds) and significant overhead required for quantum error correction.
- **Trapped ions:** Individual ions are confined using electromagnetic fields in Paul or Penning traps^{21,22}, with qubits encoded in electronic states of each ion. Laser pulses are used to implement high-fidelity single- and multi-qubit gates, often exceeding 99.9 % fidelity. Coherence times in trapped ion qubits can

reach from seconds to minutes under optimized conditions, making them among the most reliable qubit platforms. However, scaling remains challenging due to the complexity of laser control systems and the difficulty of trapping and manipulating large ion arrays.

- Neutral atoms: Neutral atoms trapped by optical tweezers or optical lattices ²³ provide a highly reconfigurable platform for both digital quantum computing and analog simulation. Entanglement is generated using Rydberg interactions ²⁴, which are strong and tunable over micrometer ranges. Recent experiments have created defect-free arrays ²⁵ with hundreds of atoms, positioning neutral atoms as a leading candidate for large-scale quantum simulators. Challenges include achieving consistent high-fidelity gate operations at scale.
- Photonic qubits: Photons are natural carriers of quantum information, immune to decoherence during propagation. Photonic qubits ^{26,27} can be encoded in polarization, spatial modes, or time bins, and manipulated using beam splitters, phase shifters, and detectors. Companies like Xanadu and PsiQuantum aim to build scalable photonic processors integrated on silicon chips. The primary challenge is the probabilistic nature of gate operations, photon loss, and the lack of strong nonlinearities.
- Semiconductor qubits: Semiconductor qubits encompass a versatile family of implementations, including gate-defined quantum dots that confine single electrons electrostatically in CMOS-compatible silicon or III–V heterostructures, and dopant-based qubits that exploit the nuclear or electron spins of precisely positioned donor atoms in silicon. They benefit from long spin coherence times, compatibility with established semiconductor manufacturing, and the potential for dense integration. Recent milestones include demonstrations of high-fidelity single- and two-qubit gates ²⁸, scalable two-dimensional arrays ²⁹, and reliable electron shuttling across long distances ³⁰. Technical challenges include maintaining uniform device performance across large architectures and integrating fast, low-noise control and readout electronics.

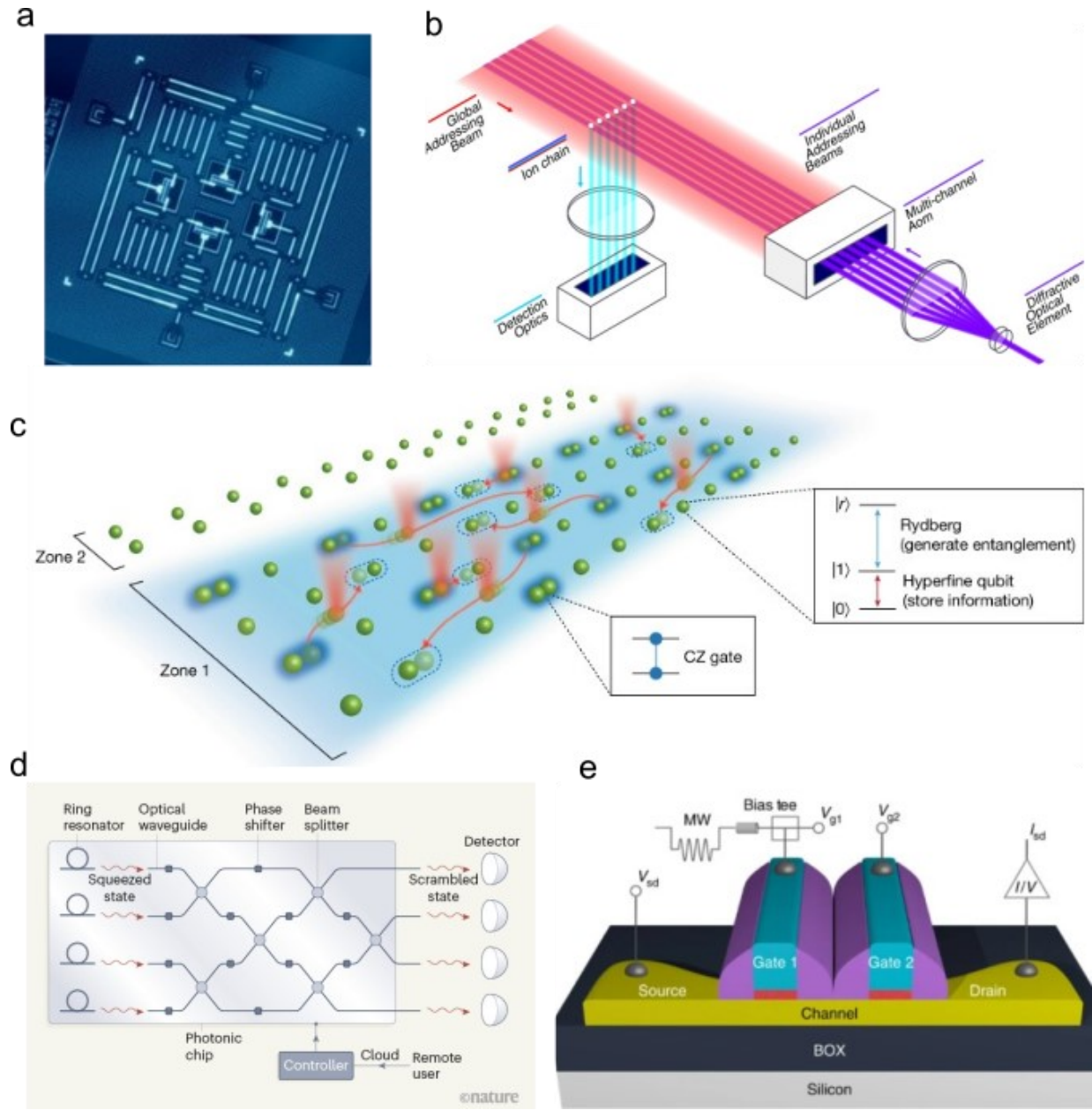


Figure 1.2 Illustrations of leading approaches to quantum computing: (a) Superconducting circuits, where Josephson junctions embedded in microwave resonators define transmon qubits. Image adapted from Gambetta et al.³¹ (b) Trapped ions, confined in electromagnetic traps and manipulated by laser pulses. Figure adapted from Wright et al.³² (c) Neutral atoms, arranged in reconfigurable optical tweezer arrays and entangled through Rydberg interactions. Figure adapted from Bluvstein et al.³³ (d) Photonic qubits, encoded in the polarization, path, or time-bin modes of single photons. Figure adapted from Andersen.³⁴ (e) Semiconductor qubits, where electron spins confined in quantum dots or bound to donor atoms define the qubit states. Figure adapted from Maurand et al.³⁵

Each of these platforms continues to advance along unique trajectories, reflecting diverse trade-offs between scalability, coherence, and control. While no single approach has yet emerged as dominant, semiconductor-based qubits are particularly compelling due to the prospect of leveraging mature silicon fabrication technologies for scalable quantum architectures, mirroring the success of Moore’s law in CMOS technology.

1.4 Semiconductor-based qubits

The research presented in this thesis lies within the semiconductor platform. The pioneer experimental milestones were achieved using gate-defined quantum dot architectures where metallic gates are patterned on the surface of a semiconductor heterostructure or quantum well, such as Si/SiGe or GaAs/AlGaAs ^{36,37}, to electrostatically confine single electrons whose spin states encode quantum information. Single-qubit control is implemented through electron spin resonance (ESR) or electric-dipole spin resonance (EDSR), while two-qubit operations are mediated by exchange interactions between neighboring dots. However, the atomic-scale abruptness of the confinement potential introduces inevitable variations between nominally identical quantum dots, compounding challenges such as crosstalk among densely packed control gates and the scaling of cryogenic control electronics. Although truly scalable architectures beyond 100 qubits have not yet been demonstrated, recent advances in fabrication uniformity ^{38,39} and the integration of cryo-CMOS control electronics ⁴⁰ have shed light on potential solutions to these bottlenecks.

Building on the successes of gate-defined systems, researchers have also considered the possibility of encoding quantum information directly into the nuclear or electron spins of individual dopant atoms embedded in silicon. This idea was first proposed in 1998 by Bruce Kane ⁴¹, who suggested using phosphorus donor nuclear spins in isotopically purified silicon as qubits. Silicon is a particularly appealing host material due to its abundance, its ability to be isotopically enriched to eliminate nuclear spin noise, and the direct compatibility with existing semiconductor technology. In Kane’s design, donor atoms are

positioned beneath the silicon surface with nanoscale precision, and metallic control gates on the surface manipulate the hyperfine interaction between each nuclear spin and its bound electron, enabling initialization, control, and readout. Neighboring qubits are coupled through exchange interactions mediated by the donor electrons.

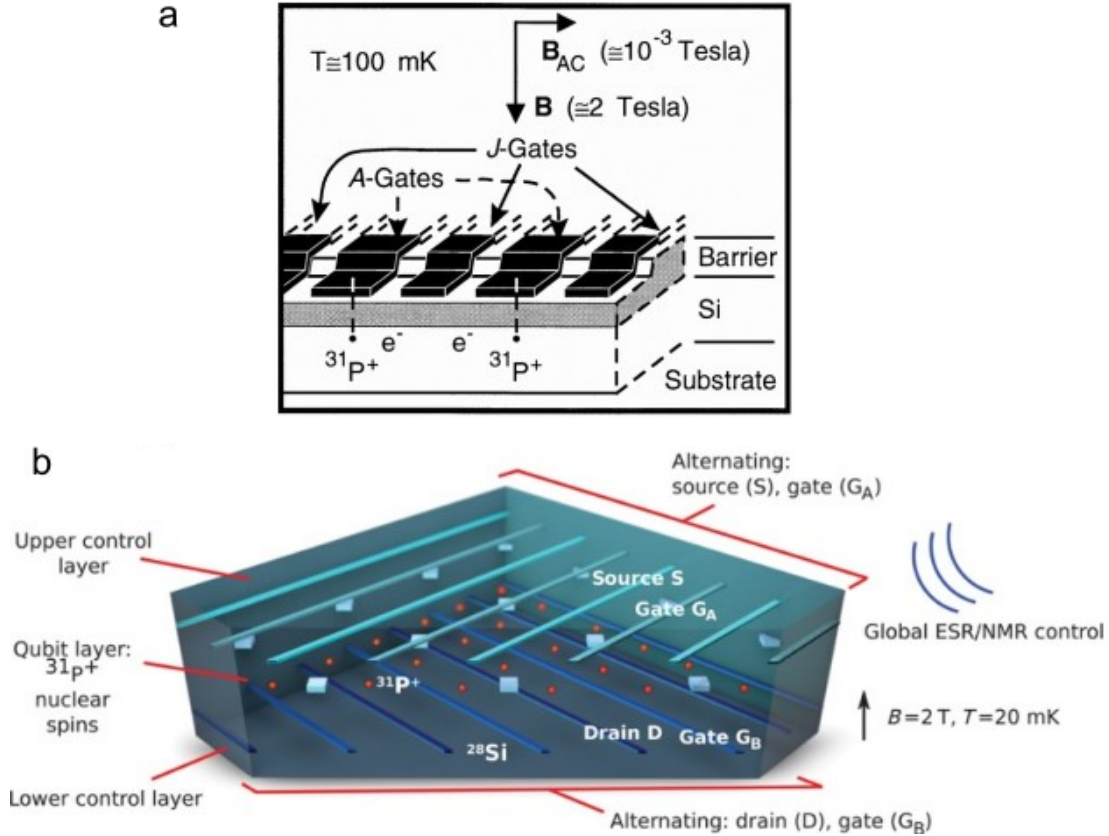


Figure 1.3 Schematic of Bruce Kane's quantum computer using individual dopant atoms in silicon as qubits. (a) Adapted from Kane's original proposal⁴¹. Quantum information is encoded in the nuclear spins of precisely positioned phosphorus atoms. A global AC magnetic field provides single-qubit control, while individual spins are addressed via the A-gates. Two-qubit operations are mediated by electron exchange interactions controlled by the J gates. (b) Donor-based surface code quantum computer, extending Kane's 1D array into a scalable architecture (adapted from Hill et al.⁴²). Shared-control lines enable parallel qubit manipulation, while readout is performed by nearby single-electron transistors (the square islands).

While Kane's architecture was not realized for a long time due to formidable fabrication challenges of placing individual donor atoms at precise locations and integrating the necessary gate structures, it inspired a broad research effort. An important breakthrough was the pioneering work of Joseph Lyding, William Shen, John Tucker ⁴³ who demonstrated hydrogen lithography on silicon surfaces using a scanning tunneling microscope (STM). Their technique employed the STM tip to selectively remove hydrogen atoms from a passivated Si (100) surface, creating atomically precise patterns at the single-dimer scale. which are now being enhanced to realize Kane's original blueprint. This allows dopants to be placed with single-atom precision onto the lithography defined patterns, forming donor-based quantum dots with unprecedented accuracy. Compared to ion implantation, STM lithography provides far better control over spatial control, enabling both digital qubits and analog quantum simulators based on engineered dopant arrays.

Building on this foundation, Michelle Simmons and her group at the University of New South Wales (UNSW) made pioneering advances in transforming hydrogen lithography into a practical tool for quantum device fabrication by demonstrating the deterministic placement of donor atoms and the encapsulation of atomic-scale structures into functional devices ^{44,45}. Additional milestones include the fabrication of single-atom transistors, spectroscopy measurement of few-donor quantum dots, and the first demonstrations of single and two (electron) qubit gate operations ⁴⁶ in STM-patterned quantum devices. In parallel, our group at NIST led by Richard Silver have developed complementary achievements such as the development of high-yield device contact technologies ⁴⁷ and the creation of artificial molecules ⁴⁸. All these results established that atomic precision fabrication could move beyond proof-of-principle surface patterning to fully encapsulated devices capable of coherent quantum operations, providing a pathway toward truly scalable dopant-based quantum computers. More recently, enhanced atomic-precision techniques have enabled tip-assisted dopant incorporation ⁴⁹, allowing the placement of an exact number of donors at each site with high yield and reducing the randomness inherent to stochastic thermal incorporation. Progress in multilayer three-dimensional device architecture ⁵⁰ has expanded the design space for more complex device layouts. With nuclear magnetic resonance (NMR) and addressability for individual nuclear spins, Kane's original proposal is finally brought close to experimental realization. The atomic discreteness that once

limited transistor scaling has now become a central resource: single- or few-dopant clusters can reliably encode quantum states, transforming the end of Moore’s law into a new opportunity for quantum information processing.

1.5 Outline of this thesis

This thesis focuses on the development and application of silicon-based donor devices fabricated through atomic-precision advanced manufacturing. The ultimate goal of this work is to advance the Si:P devices as a scalable platform toward practical quantum computing and analog quantum simulation. The structure of the thesis is outlined as follows:

- Chapter 2 details the fabrication process used in our lab to construct atomically precise Si:P devices. The procedure begins with wafer selection and wet chemical cleaning, followed by UHV surface preparation, hydrogen de-passivation lithography using an STM, dopant incorporation, and epitaxial encapsulation. Strategies for post-fabrication device relocation and the formation of low-resistance electrical contacts are also presented. The chapter also includes recent process improvements that address problems such as limited gate ranges and gate nonlinearities observed in earlier device iterations. By adopting an alternative flash-cleaning method or using intrinsic substrates effectively mitigates the small gate range issue. The second part of the chapter describes the cryogenic measurement setup used for most experiments in subsequent chapters, including the dilution refrigerator wiring, filtering strategies, and instrumentation control schemes that enable low-noise quantum transport and spin measurements.
- Chapter 3 introduces the basic theories necessary for understanding electron transport in Si:P quantum devices. It begins with an overview of the silicon band structure and the effective mass theory description of an electron wavefunction bound to a single phosphorus donor, emphasizing how localized dopant states, valley degeneracy, and tunnel coupling emerge within the silicon lattice. The discussion then

extends to δ -doped layers, which exhibit metallic behavior through the formation of impurity bands, and to the mechanisms of electron confinement in nanoscale islands that emerge as the doped regions are reduced in size. A detailed explanation of the operating principles and transport theory of single-electron transistors (SETs) is presented, introducing key concepts such as charging energy, Coulomb blockade, and Coulomb oscillations. The SET is typically used to assess the fabrication quality and serves as a highly sensitive charge sensor for detecting spin states in nearby donor clusters. The information in this chapter establishes the theoretical foundation for interpreting the device behavior and measurement results presented in the subsequent chapters.

- Chapter 4 presents automation algorithms developed to enhance the efficiency, precision, and reproducibility of STM-based hydrogen lithography. Manually writing device patterns at the atomic scale is both time-consuming and prone to human error; the automation framework introduced here functions as an electronic design automation (EDA) tool tailored for atomic fabrication. The system integrates image processing for feature recognition, optimized path-planning algorithms for tip control, and error correction procedures based on feedback loops, enabling reliable patterning across length scales ranging from individual quantum dots to large fan-out electrode regions. Two principal modes of operation are demonstrated: (1) atomic-precision patterning for small functional structures and quantum devices, and (2) high-throughput lithography for large-area outer contact pads. This work represents a practical step toward scalable, automated fabrication of atomically precise quantum devices.

- Chapter 5 presents the principles and experimental demonstration of spin readout in a donor–quantum dot single-electron transistor (SET). The chapter begins by introducing the device geometry and its charge stability diagram. The SET functions as a highly sensitive charge detector capable of resolving energy-selective tunneling events between itself and the donor dot. Measurements of the effective electron temperature confirm that the Zeeman splitting at $B=1.5$ T is sufficient to achieve spin-resolved regime. Single-shot spin readout experiments are demonstrated by loading and unloading an electron from the donor

dot with appropriate read position. Measurements of spin relaxation time (T_1) reveal a B^{-1} dependence on magnetic field strength, which is attributed to excess charge noise in the silicon environment. The chapter concludes with a discussion on future coherent spin manipulation experiments using integrated electron spin resonance (ESR) antennas to advance the donor dot to a fully functional qubit.

- Chapter 6 demonstrates the fabrication and characterization of small-scale quantum dot arrays as a prototype for dopant based analog quantum simulators. A 3×3 array of phosphorus atom clusters is constructed to emulate the two-dimensional Hubbard model. By tuning the lattice constant, the system exhibits a transition from a strongly tunnel-coupled regime to the atomic limit, where a Mott-like spectral gap emerges. Tracking the evolution of charge addition lines as a function of external magnetic field reveals a “Hund’s rule” like behavior, indicative of strong electron–electron correlations within the array. Beyond these few-site systems, the chapter also presents the fabrication and measurement of a larger 32×32 dopant array. Transport measurements indicate that the device operates in a regime dominated by localization and disorder-induced transport. Finally, the chapter ends with a discussion of the theoretical foundation and experimental feasibility of a new proposal to exploit phosphorus nuclear spins as a platform for lattice gauge theory simulations, expanding the potential of dopant-based quantum devices.

- Chapter 7 develops RF reflectometry techniques tailored for high-impedance Si:P quantum devices. A simple matching network based on a wire-wound chip inductor and parasitic capacitance is modeled using lumped-element and SPICE-based approaches to capture realistic losses and impedance transformation. A tunable varactor network is added to systematically characterize the circuit response to a quantum capacitance or conductance. Through both simulation and measurement, we demonstrate how quality factors and impedance-matching conditions determine the charge sensitivity of a resonator. Using the optimized RF circuitry, low-temperature measurements on a single-electron transistor demonstrate fast charge readouts with sub-microsecond integration time, limited primarily by amplifier noise. These results define the fundamental limits and optimization strategies of chip-based RF resonators for large-impedance

silicon devices and lay the groundwork for their application of charge sensing dopant-based arrays in the following chapter.

- Chapter 8 applies RF reflectometry to probe charge and spin configurations in a 3×3 STM-patterned Si:P quantum dot array. By monitoring site-dependent capacitive couplings, individual electron addition sites are identified and interdot transition signals are resolved, allowing direct extraction of Hubbard parameters such as tunnel couplings and Coulomb interactions. The chapter further investigates how input RF power influences effective electron temperature and establishes the optimal regime for spin-sensitive measurements. At finite magnetic field, Pauli spin blockade is observed between neighboring sites, and singlet–triplet relaxation times on the microsecond scale are measured. These results demonstrate RF reflectometry as a powerful technique for site-resolved charge sensing and spin-state detection in small dopant-based quantum dot arrays and its potential role in future analog quantum simulation devices.

- Chapter 9 summarizes the thesis and outlines several directions for future work, along with the associated challenges.

Chapter 2: Device Fabrication and Measurement Methods

Atomically precise silicon devices rely on a tightly integrated workflow that combines controlled thermal treatments, advanced nanofabrication techniques and high-quality molecular beam epitaxy. The functionality of a device also depends critically on maintaining pristine surface conditions throughout processing and achieving deterministic dopant placement within the silicon lattice.

Pioneering work by Michelle Simmons and her team at the University of New South Wales (UNSW) established the first complete fabrication scheme for atomically precise Si:P devices ^{44,45,51}, demonstrating their feasibility as a scalable platform for quantum technologies. Their achievements marked a milestone in atomic-scale device engineering, showcasing the controlled placement and activation of individual dopants ^{52,53} within a crystalline silicon lattice. However, reproducing devices of comparable structural and electrical quality remains highly challenging due to the complexity of the fabrication process and the sensitivity on silicon wafer selection.

This chapter presents a complete atomically precise fabrication scheme developed and used in Silver's laboratory ⁵⁴, in a transparent manner to promote reproducibility. Section 2.1 details the full fabrication workflow, starting from wafer selection and sample chemical cleaning, followed by UHV atomically flat Si (100) surface formation, STM-based hydrogen lithography and finally dopant incorporation and epitaxial encapsulation. Strategies for post UHV device relocation and electrical contact formation are also discussed. The higher level STM automation patterning techniques developed for this work are discussed separately in Chapter 4. In addition, we highlight recent process improvements that address limitations observed in earlier generations of devices, such as limited gate voltage ranges and nonlinear gate responses. Preliminary studies have shown promising results by adopting a modified flash annealing protocol or by using intrinsic silicon substrates, which significantly improved gate performance.

Section 2.2 introduces the cryogenic measurement setups used in this work, including wiring configurations, filtering strategies, and instrument control schemes that enable quantum transport measurements.

2.1 Device Fabrication Process

The fabrication of a functional Si:P device involves a sequence of carefully controlled processes and typically takes more than two weeks to complete before a device is ready for measurement. The procedure begins with wet chemical cleaning of diced silicon wafers, followed by preparation of atomically flat surfaces in an ultrahigh vacuum (UHV) environment. A hydrogen-terminated surface is then formed and serves as a resist layer for STM-based lithography, where selective desorption of hydrogen atoms using a STM tip exposes silicon dangling bonds. These reactive sites subsequently chemisorb phosphine (PH_3) molecules during the dosing stage, forming atomically precise patterned regions that can be engineered into quantum dots or donor islands for quantum information processing, while larger exposed areas define metallic contact leads. A rapid thermal anneal then drives the substitutional incorporation of phosphorus atoms into the silicon lattice, electrically activating the dopants. Finally, an epitaxial overgrowth step encapsulates the patterned structures within crystalline silicon, preserving both their spatial precision and electronic functionality. After UHV, the patterned devices are relocated relative to fiducial markers and connected by electrical contacts for low-temperature transport measurements. The following subsections describe each of these.

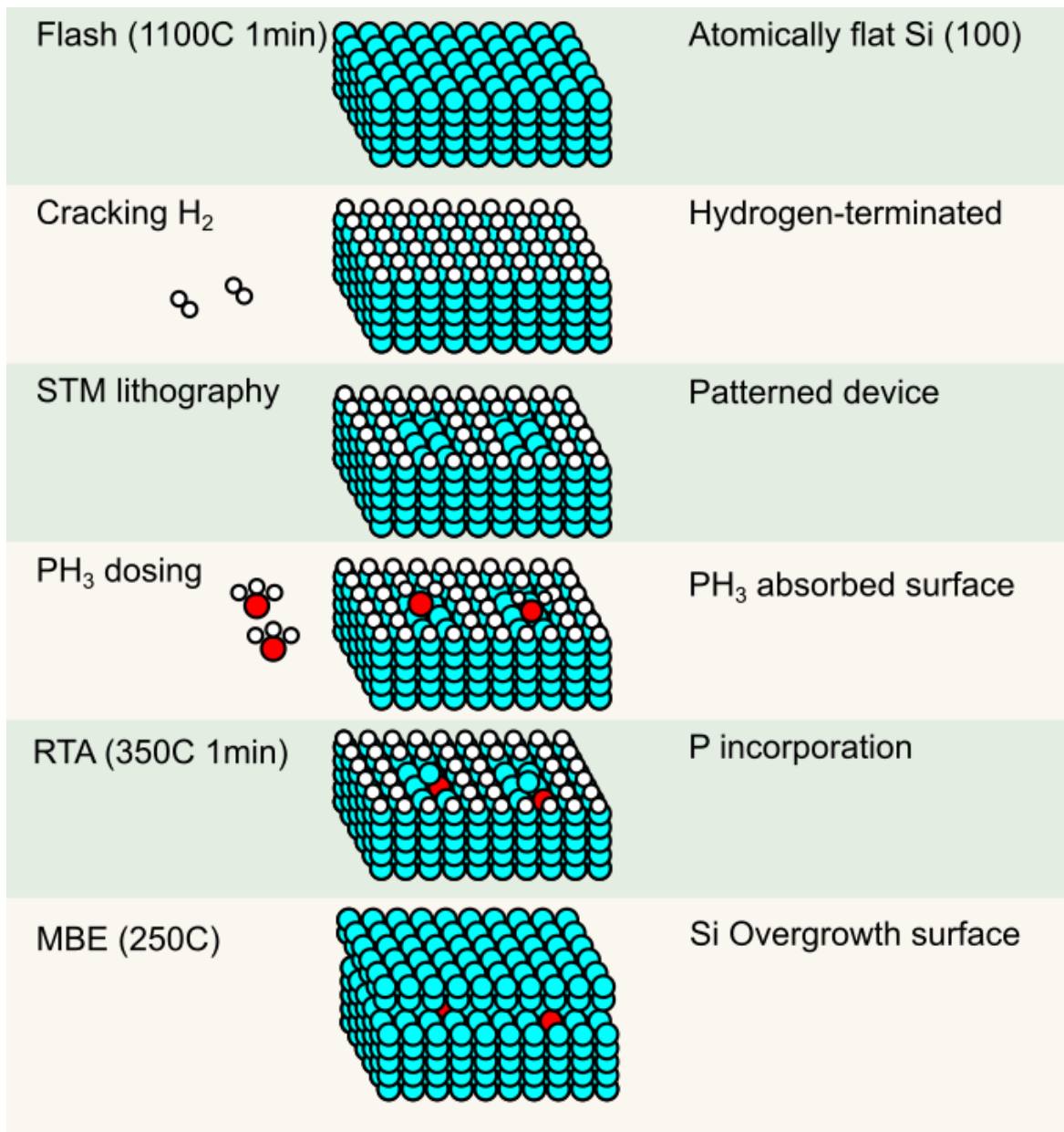


Figure 2.1 Overview of the UHV fabrication process for Si:P devices. The process proceeds from top to bottom sequentially with sample degassing and surface preparation, hydrogen termination, STM patterning, phosphine dosing, dopant incorporation, and epitaxial encapsulation. Silicon, hydrogen, and phosphorus atoms are depicted in aqua, white, and red color, respectively.

2.1.1 Pre-UHV Sample Preparation

The quality of the starting silicon wafer could significantly influence the performance and reliability of the final device. For a long time, we have been using float-zone (FZ)⁵⁵ [001]-oriented silicon wafers supplied by Virginia Semiconductor Inc. The float-zone growth method yields silicon with substantially lower impurity concentrations than the conventional Czochralski (CZ)⁵⁶ process. In FZ growth, a localized radio-frequency heating coil passes along the silicon rod, melting a narrow region that moves slowly from one end to the other. Impurities such as oxygen, carbon, and metallic elements segregate preferentially into the molten zone and are progressively swept toward one end of the ingot, leaving the remainder of the crystal with exceptionally low contamination levels. As a result, FZ wafers possess better purity and crystalline perfection suited for atomic-scale fabrication, minimizing defect-related charge noise and other potential artifacts that would otherwise degrade device performance.

The wafers are lightly boron-doped ($\sim 1 \times 10^{15}$ /cc) silicon with resistivities between 1 and 10 $\Omega \cdot \text{cm}$. This doping level is chosen primarily to ensure sufficient conductivity for resistive heating during high-temperature processing. A 4-inch wafer (300 μm thickness) after patterning registration marks is diced into individual chips measuring 10×2.5 mm in dimension, optimized for mechanical stability and compatibility with our UHV sample holders. These chips serve as the starting substrates that will be loaded into the UHV chambers for device fabrication.

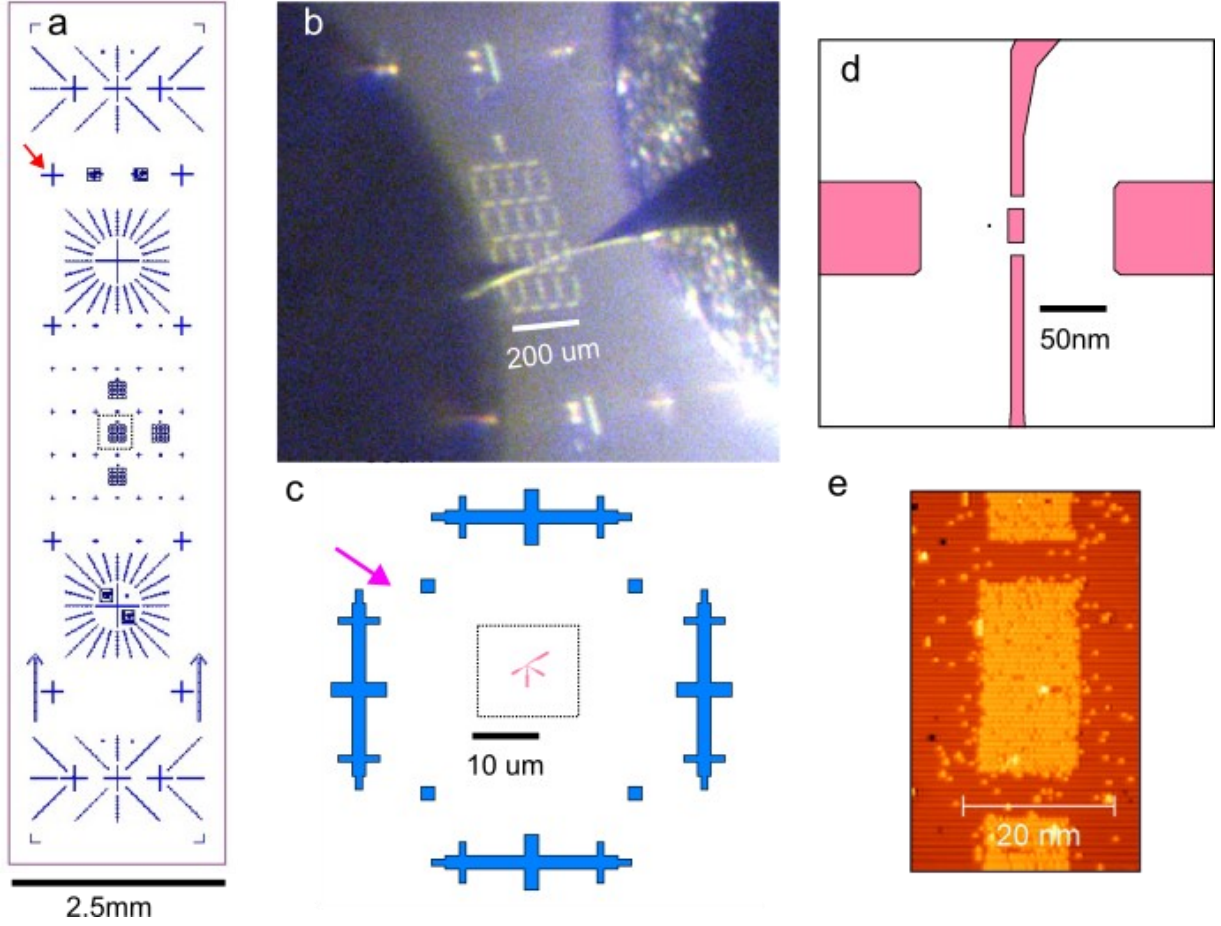


Figure 2.2 Hierarchical view of an atomically precise device. Each panel presents a progressively magnified region, transitioning from the macroscopic chip scale down to the nanometer scale features. Scale bars are shown at each level for reference. (a) Layout of the sample chip. Deep etched markers ($\sim 2 \mu\text{m}$, red arrow) provide coarse alignment during photolithography for electrical contact fabrication. (b) Optical image of a sample loaded on the STM stage. The STM tip can be deterministically landed onto a certain grid. (c) Typical size of a Si:P quantum device located within a $50 \times 50 \mu\text{m}^2$ shallow etched grid. The corner dots (purple arrow) serve as fiducial markers for both in situ relocation and e-beam alignment, enabling deterministic identification of the device position. (d) Central region of a donor-dot single-electron transistor device showing source, drain, and two tuning gates. (e) STM image of a patterned SET device, where individual dangling bonds (missing hydrogen atoms) and silicon dimers are visible.

To enable deterministic device relocation and electrical contact alignment, registration markers are patterned on each chip. A two-level marker design developed by our group is employed: (i) deep markers

($\sim 2\text{ }\mu\text{m}$) defined using a Bosch process ⁵⁷ , which serve as coarse alignment references during photolithography; and (ii) shallow markers forming $50 \times 50\text{ }\mu\text{m}^2$ grids etched by reactive ion etching (RIE), which provide fine fiducials for in situ STM positioning and post-fabrication relocation. Using an optical camera, the STM tip can be deterministically landed onto one of the sub grids for patterning a complete device which are typically $\sim 6 \times 6\text{ }\mu\text{m}^2$ in size. These markers are thermally stable under subsequent high-temperature processing and are used as robust alignment references during the device registration step. Before loading into UHV, samples first undergo a multi-step wet chemical cleaning sequence designed to remove organic residues, metal contaminants, and native oxides while leaving a particle-free silicon surface:

- Organic removal: Samples are first sonicated in PG remover followed by isopropanol (IPA) to dissolve photoresist residues and other organic films from dicing and handling.
- Piranha clean (10 min): A mixture of concentrated H_2SO_4 and H_2O_2 aggressively oxidizes the silicon surface and removes trace metals, carbonates, and organics. This step ensures that even strongly bound contaminants are broken down.
- HF dip (2%, 1 min): The chemical oxide formed during the Piranha clean is stripped with dilute hydrofluoric acid, leaving a hydrogen-terminated silicon surface. This step also smooths the topmost silicon layer by etching away surface roughness.
- RCA-1 ⁵⁸ clean ($\text{NH}_4\text{OH}/\text{H}_2\text{O}_2/\text{H}_2\text{O}$, 75–80 °C, 10 min): Removes residual organics and some metallic impurities, while re-oxidizing the surface. A brief 2% HF dip follows to strip the thin oxide layer, preventing oxygen contamination during subsequent steps.
- RCA-2 ⁵⁸ clean ($\text{HCl}/\text{H}_2\text{O}_2/\text{H}_2\text{O}$): Removes ionic and metallic contaminants such as Fe, Zn, and Cu, which can diffuse into silicon and degrade device quality.
- Final rinse and drying: The samples are thoroughly rinsed in DI water, or alternatively with a quick dip in IPA, and then blown dry with filtered nitrogen gas.

Each sample is then inspected under an optical microscope to verify surface cleanliness. Chips with visible particulate contamination or processing defects are discarded to avoid compromising subsequent UHV preparation.

2.1.2 UHV Sample Preparation

An ultrahigh vacuum (UHV) environment is essential for both STM lithography and the reliable operation of Si:P devices. Achieving atomic precision requires surfaces that are not only atomically flat but also chemically pristine. Even trace amounts of oxygen, carbon, or water molecules could potentially alter the silicon surface reconstruction, contaminate dopant sites, or disrupt the lithography process and ultimately compromising device performance⁵⁹. For this reason, maintaining a good quality of UHV environment and minimizing contamination to the lowest possible level is a constant priority.

Our vacuum system consists of four interconnected chambers namely load lock, transfer, process, and STM chambers isolated by gate valves to maintain separation pressures. Samples are first loaded into the load lock, where roughing and turbo pumps reduce the pressure to $\sim 10^{-8}$ Torr, followed by ion pumping down to below 1×10^{-9} Torr. The sample is then moved into the transfer chamber which serves as a buffer vacuum to the UHV chambers, minimizing the backflow of gas molecules such as water vapor and hydrocarbons. The process and STM chambers are maintained at a base pressure of $\sim 10^{-11}$ Torr, providing the true UHV environment necessary for atomic-scale fabrication. To sustain such conditions, the entire system undergoes routine bakeouts to remove residual adsorbates, especially water molecules, that accumulate from repeated sample exchanges.

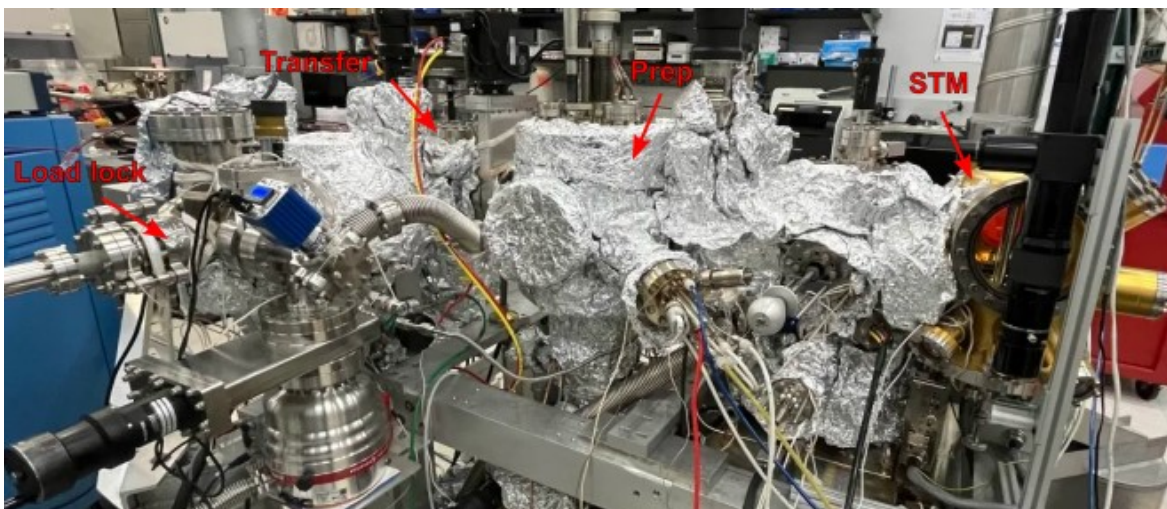


Figure 2.3 Photograph of the UHV system used for atomic-scale device fabrication. The system comprises four chambers: the load lock, transfer chamber, preparation (process) chamber, and STM chamber. High-temperature treatments and silicon epitaxial overgrowth are carried out in the preparation chamber. Hydrogen lithography is performed in the STM chamber using a Scienta Omicron VT-STM.

Inside the process chamber, samples are degassed overnight at $\sim 580^\circ\text{C}$ using a direct-current heater. This procedure drives off residual water vapor and other contaminants on the sample surface. A pyrolytic boron nitride (PBN) back heater is used parallel to degas the sample holder, ensuring that no secondary contaminants outgas during later high-temperature flash process.

The removal of the native silicon oxide is achieved by a series of rapid flash anneals to 1150°C , performed in short (~ 10 s) segments to prevent overheating of other chamber components. These flashes sublime the top surface layers, eliminating oxides and leaving behind a clean silicon lattice. A final 5 s flash, followed by a controlled cooldown⁶⁰, produces an atomically flat and well-reconstructed Si (100)- 2×1 surface. The presence of well-ordered dimer rows in this reconstruction is a prerequisite for hydrogen termination and for subsequent STM patterning with atomic precision.

The hydrogen resist layer is formed by introducing ultra-high-purity hydrogen gas into the chamber through a precision leak valve, with the pressure stabilized at approximately 10^{-6} Torr. A tungsten filament heated to $\sim 1800^\circ\text{C}$ dissociates the molecular hydrogen into atomic hydrogen, which reacts with the silicon surface.

The sample, maintained at ~ 280 °C and oriented toward the filament, is exposed to this atomic hydrogen flux for about 10 minutes, resulting in a uniform hydrogen-terminated Si (100)- 2×1 surface with minimal amount of residual dangling bonds. This chemically inert surface ⁶¹ not only serves as an ideal resist for subsequent STM lithography but also preserves surface cleanliness by preventing adsorption of residual gas molecules from the UHV chamber. Selective desorption of individual hydrogen atoms by the STM tip defines the active regions of the device forming the structural foundation for dopant-based quantum applications.

2.1.3 Scanning Tunneling Microscopy

The scanning tunneling microscope (STM) is the central instrument to enable this work, functioning both as an imaging tool with atomic resolution and as a lithographic platform for hydrogen de-passivation. Invented by Gerd Binnig and Heinrich Rohrer ⁶² in 1982, the STM revolutionized surface science by providing direct, real-space access to the atomic-scale structure of solid surfaces. Its unique capability arises from the quantum mechanical phenomenon of electron tunneling. When a sharp metallic tip is positioned within a few angstroms of a conductive surface and a bias voltage is applied, electrons tunnel across the vacuum barrier, generating a measurable current without physical contact. This tunneling current depends exponentially on the tip-sample separation, making it super sensitive to atomic-scale variations in height and enabling sub-angstrom vertical resolution.

A schematic illustration of the STM working principle is shown in Figure 2.4. The basic configuration consists of a conductive metal tip mounted on piezoelectric actuators that control its position with sub-nanometer precision in the x, y, and z directions. The sample is placed on a stage beneath the tip. When the tip is raster-scanned laterally across the surface in the x-y plane, a feedback loop continuously adjusts the vertical position (z) to maintain a constant tunneling current at a chosen current setpoint. The recorded z values are then mapped to produce a topographic image of the surface at atomic resolution. This is referred to as constant-current mode. An alternative mode is constant-height mode, in which the tip height is held

fixed while variations in the tunneling current are recorded. The latter is typically applied to small-area scans and is often combined with local I–V spectroscopy to probe local electronic properties. In this work, all lithography tasks are carried out in constant-current mode.

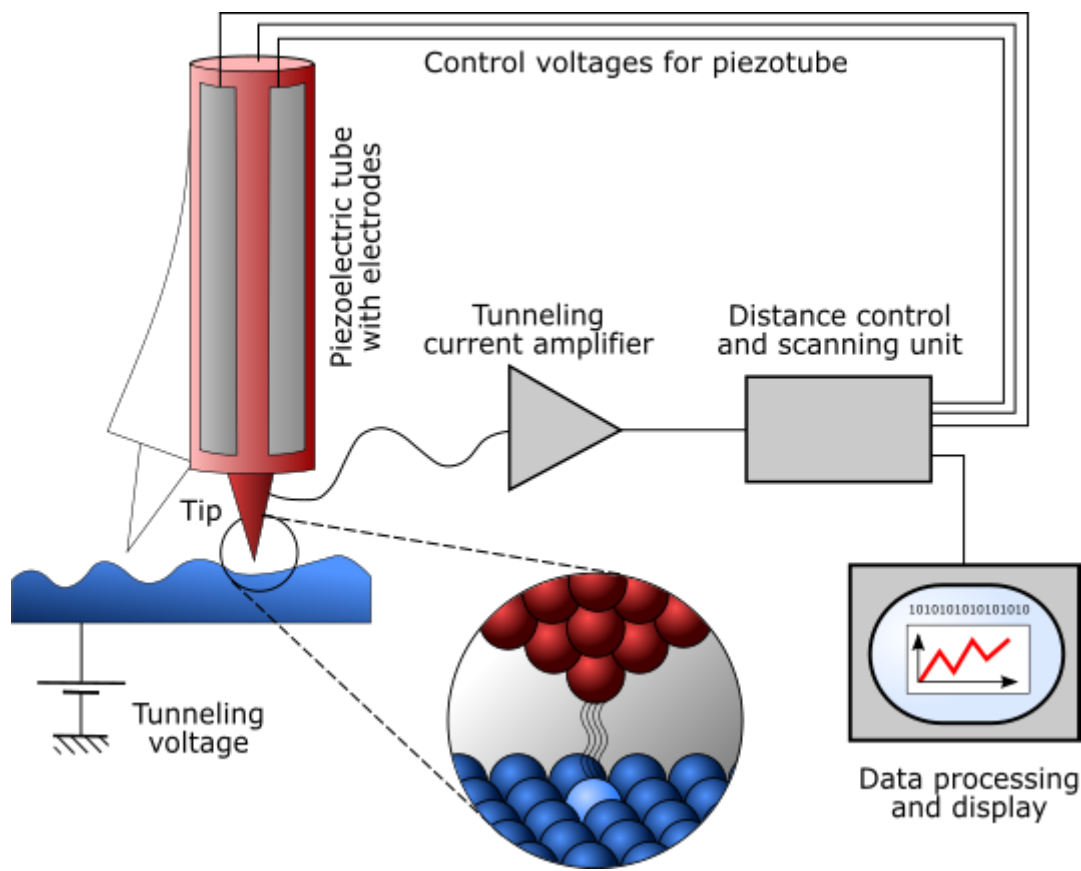


Figure 2.4 Schematic illustration of the working principle of a scanning tunneling microscope (STM). A sharp metallic tip is positioned within a few angstroms of a conductive sample. A voltage bias applied between tip and sample allows electrons to tunnel across the vacuum barrier, producing a current that depends exponentially on the tip–sample distance. A feedback loop regulates the z-position of the tip to maintain a constant current while raster scanning in the x–y plane, thereby generating an atomically resolved height map of the surface. This figure is adapted from the IAP/TU Wien STM Gallery ⁶³.

High-quality STM imaging depends on two essential prerequisites: (i) a chemically pristine and atomically flat sample surface, and (ii) an atomically sharp and mechanically stable tip. The clean Si (100)-2×1 reconstructed surface obtained through the UHV preparation satisfies the first requirement. For the second,

we are fabricated STM tips in-house by electrochemically etching a polycrystalline tungsten wire in a 1 M KOH solution under a DC bias of 3–5 V ^{64,65}. The etched tips are subsequently degassed at ~200 °C under UHV to remove adsorbed water and hydrocarbon species prior to mounting on the STM. This procedure routinely produces tips capable of achieving atomic-resolution imaging without the need for extensive in situ tip conditioning.

The atomic configuration of the tip apex, however, remains uncontrolled and varies between etching runs. Achieving a “good” tip with both high spatial resolution and long-term stability during lithography often depends on subtle factors such as the etch geometry and final rinse quality. Tips with asymmetric or multi-apex structures can produce image artifacts or degrade rapidly under repeated bias-switching writing conditions. To improve reproducibility, ongoing efforts in our laboratory focus on tip characterization and controlled apex preparation using field-ion microscopy (FIM) ⁶⁶ in a dedicated UHV system. This approach enables atomic-level visualization and conditioning of the tungsten apex, potentially leading to more consistent and durable tips for long-duration STM lithography tasks.

In our experiments, we employ a Scienta Omicron VT-STM equipped with its Matrix controller, which regulates the tunneling feedback loop, scan control, and signal acquisition. To minimize imaging distortions arising from piezoelectric creep, hysteresis, and thermal drift, all control signals are fed through a ZyVector controller ⁶⁷, which applies real-time corrections to the piezo voltages during both imaging and lithography. This configuration ensures improved positional stability over extended scans, a prerequisite for distortion free imaging and atomic-precision patterning.

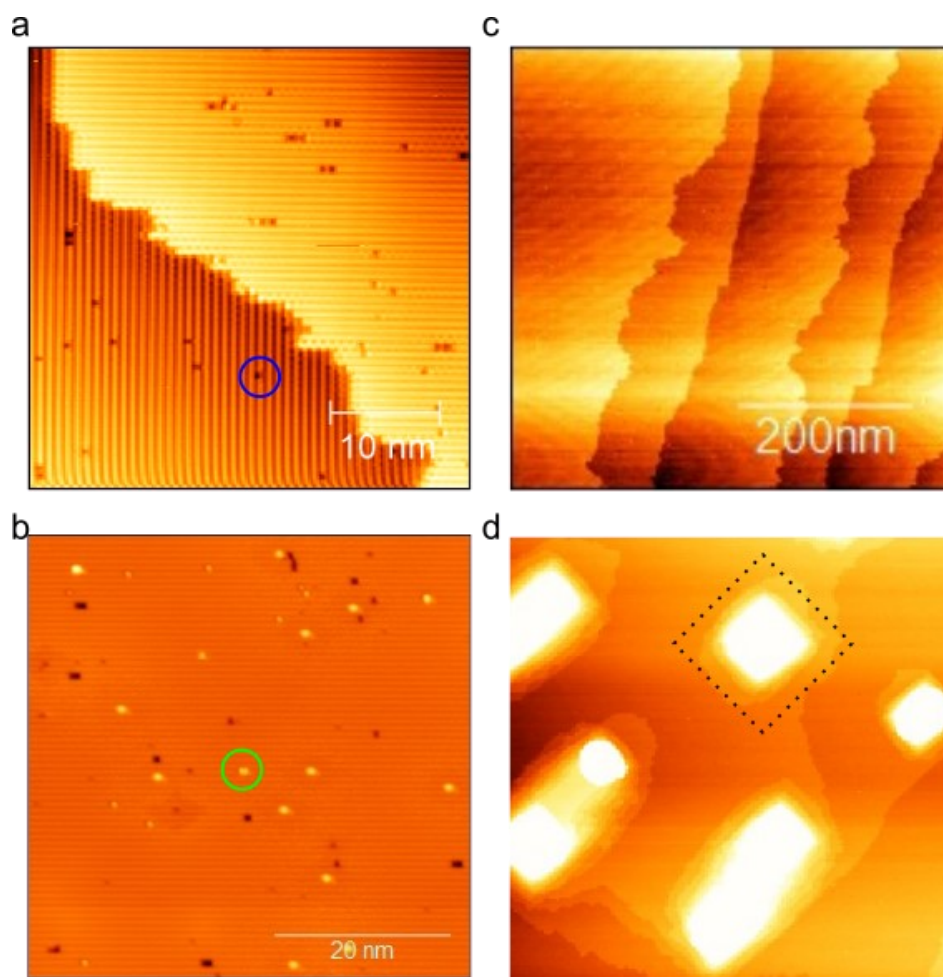


Figure 2.5 STM images of Si (100) surfaces. (a) Example of clean Si (100)-2 $\times$ 1 reconstructed surface after high-temperature flashing, showing well-ordered dimer rows. Minor defects appear as vacancies (missing surface silicon atoms) highlighted by the blue circle. (b) Hydrogen-terminated Si (100)-2 $\times$ 1 surface. Dark spots are silicon vacancies and bright spots are single dangling bonds (green circle). This surface quality, with low defect and contamination densities, is ideal for STM lithography. (c) Large-area (500 $\times$ 500 nm²) image of a properly prepared hydrogen-terminated surface, where atomic step edges flow smoothly. (d) Example of a bad surface after flashing. The pinning structures $\sim$ 10 nm in height (dashed square) are likely silicon carbide pyramids arising from carbon contamination prior to UHV loading. Such surfaces are unsuitable for device fabrication and can irreversibly damage otherwise well-prepared STM tips.

Figure 2.5 compares STM height images of Si (100) surfaces prepared under different conditions. All images are acquired in filled-state mode at $V_{\text{gap}} = -2.0$ V, $I_{\text{set}} = 0.1$ nA. High-quality bare and H-terminated silicon surfaces [Fig. 2.5(a, b)] exhibit well-ordered dimer rows and low defect densities, essential for

atomic-precision lithography. The most common defect features observed on the surface are silicon vacancies, which appear as dark depressions, and single dangling bonds, which appear as bright protrusions in the STM images. Figure 2.5(c) shows a larger-area STM image of a properly prepared Si (100) surface, where step edges flow smoothly and extended atomically flat regions without terraces are available. In contrast, Figure 2.5(d) shows an example of contaminated surface. The pinning structures, approximately 10 nm in height and over 100 nm in lateral size, are believed to be silicon carbide pyramids⁶⁸ formed due to carbon contamination. Surfaces like this are unsuitable for device fabrication and can easily cause damage to STM tips.

2.1.4 Atom manipulation and Hydrogen Lithography

Hydrogen de-passivation lithography (HDL) is a specialized form of atom manipulation in which individual hydrogen atoms are selectively removed from a passivated silicon surface to define device structures at the atomic scale. The broader field of STM-based atom manipulation, first popularized through landmark demonstrations such as the IBM “A Boy and His Atom”⁶⁹ movie (Figure 2.6), where CO molecules were moved across a copper surface to create atomic-scale images and animations. The same principles can be harnessed in a controlled manner to define functional quantum device architectures with atomic precision.

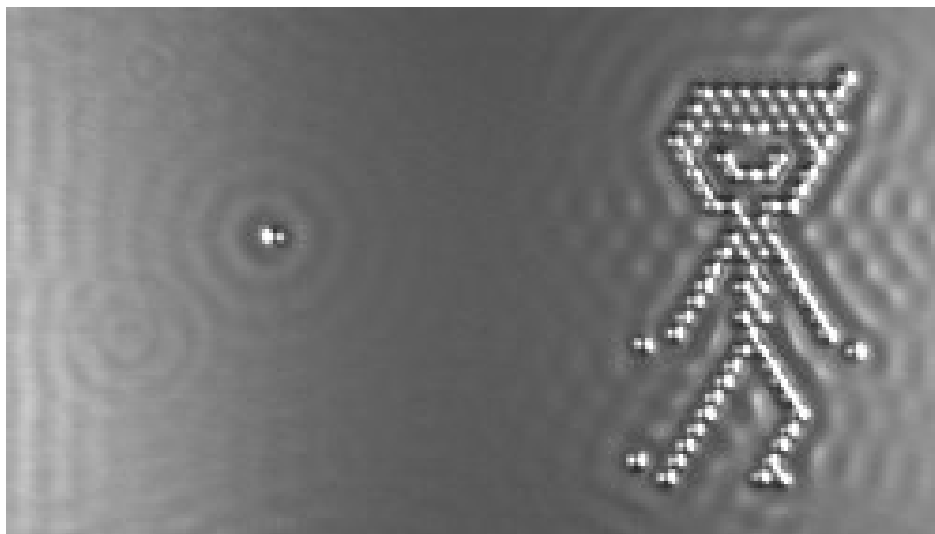


Figure 2.6 “A Boy and His Atom,” the world’s smallest movie created by IBM Research (2013). This stop-motion animation was produced by positioning individual carbon monoxide (CO) molecules on a copper surface using a scanning tunneling microscope (STM). Each white dot represents a single CO molecule manipulated atom-by-atom with sub-angstrom precision. The ripples arise from quantum interference between the surface-state electrons, reflecting variations in the local density of states. The demonstration illustrates the principle and capability of STM-based atom manipulation.

On a H-Si (100) surface, HDL is performed by applying a positive tip bias to inject electrons into the Si–H bond, breaking it and leaving behind a reactive silicon dangling bond ⁷⁰. The desorption dynamics vary between tips and can change over time even for the same tip, requiring careful calibration to achieve stable and reproducible writing conditions. These dangling bonds form the lithographic template for subsequent PH₃ dosing and dopant incorporation. The precision of the patterning process depends critically on several parameters, including the tip condition, bias voltage, tunneling current, and tip scanning speed. Here, we introduce the two distinct operational modes commonly used when patterning a device, illustrated in Figure 2.6.:

- Atomic Precision (AP) Mode: A low-bias, high-current setting (~4 V, 5 nA) that confines the electron beam size within a single dimer row directly beneath the tip apex. This enables the creation of atomically sharp features with nanometer-scale control but also places stringent requirements on maintaining an atomically sharp and stable tip apex. The typical writing speed is relatively slow

(~20 nm/s) to ensure complete de-passivation and to protect the tip. AP mode is used for patterning functional structures such as quantum dots, tunnel junctions, and donor chains, where exact positioning is essential.

- Field Emission (FE) Mode: A high-bias, low-current setting (~6 V, 2 nA) that produces a broader electron beam a few nanometers beyond the tip apex. This allows for rapid writing (>100 nm/s) of larger features, such as fanout leads and alignment pads, where atomic precision is not required. The only requirement is that the line pitch must be smaller than the effective beam diameter to ensure complete de-passivation of the patterned region. While unsuitable for quantum-confined features, FE mode greatly accelerates device fabrication by reducing the time spent on large-area patterning.

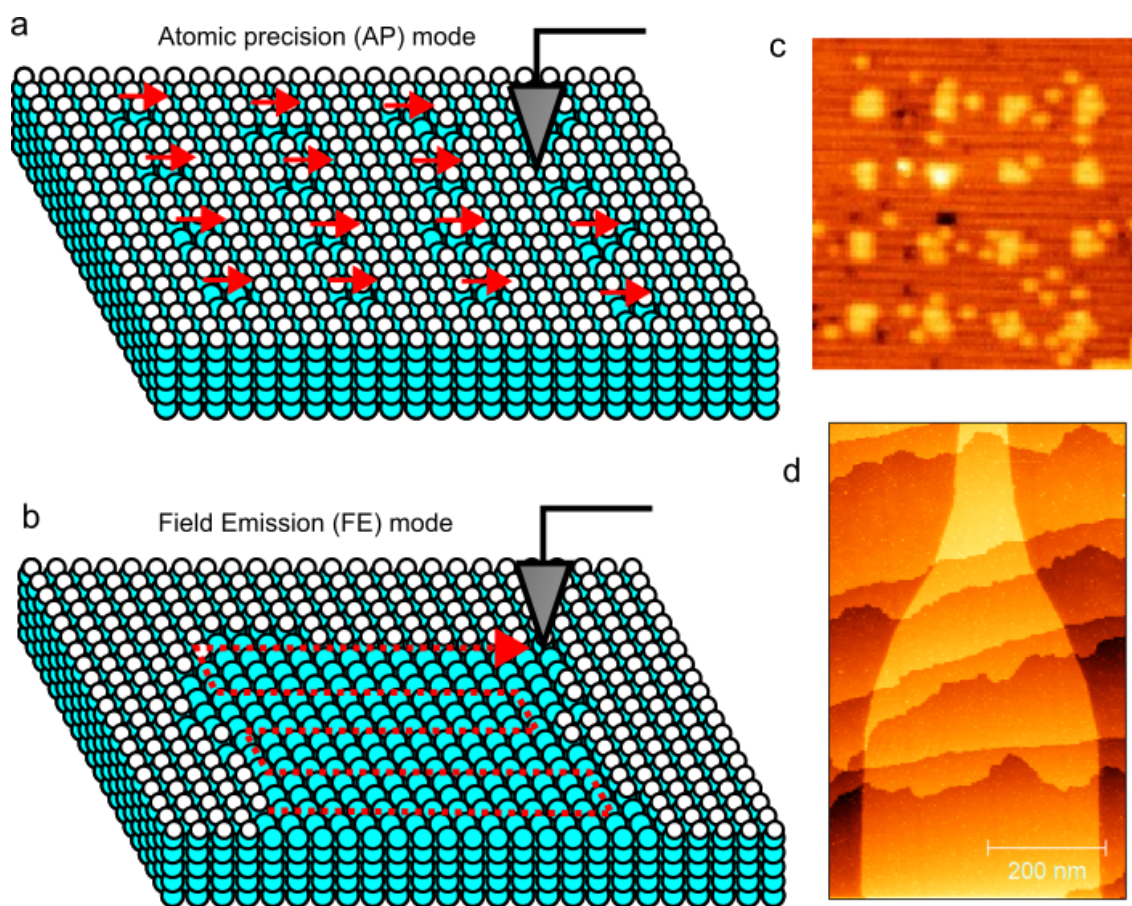


Figure 2.6 Hydrogen de-passivation lithography on H-Si (100) surfaces. (a) Schematic illustration of atomic precision (AP) mode, where low-bias, high-current conditions often confine desorption to within a single dimer row, enabling atomically sharp features. (b) Schematic illustration of field emission (FE) mode, where high-bias, low-current conditions generate a broader desorption footprint suitable for rapid large-area patterning. The path of the tip is labelled by red arrows. (c) STM image of a 4×4 dot array patterned using AP mode, demonstrating precise control over the location of individual dangling bonds. (d) STM image of a large fanout lead patterned using FE mode, where small-scale edge inaccuracy is acceptable.

The choice between AP and FE modes represents a trade-off between spatial precision and patterning efficiency. Together, they provide complementary capabilities that enable the fabrication of atomically precise device features alongside larger-scale contact structures.

2.1.5 Dopant Incorporation and Epitaxial Encapsulation

Once the lithographic pattern is complete, the exposed silicon dangling bonds become reactive sites for dopant precursor adsorption. To preserve the integrity of the patterned structures, this step must be performed promptly, as prolonged exposure risks contamination from residual gases in the STM chamber, which can also stick to the dangling bonds and degrade device performance. For this reason, phosphine (PH_3) dosing is typically carried out immediately after or even midway through the patterning process if the device contains a sensitive central region that requires early protection.

Phosphine gas is introduced into the STM chamber via a leak valve at a pressure of $\sim 3 \times 10^{-8}$ Torr for approximately 4 minutes. The PH_3 molecules chemisorb selectively^{71,72} onto the de-passivated sites, leaving passivated regions unaffected. An STM image of the surface after dosing (Fig 2.7(b)) shows the contrast between doped and undoped regions. The sample is then transferred back to the preparation chamber for thermal incorporation. A rapid anneal at $\sim 350\text{--}400$ °C for 1 minute is sufficient to break down the adsorbed phosphine molecules, allowing phosphorus atoms to incorporate substitutionally into the silicon lattice. STM imaging after this step (only for verification) reveals ejected silicon atoms, which appear as protrusions on the surface and signatures successful incorporation.

Following dopant incorporation, the device must be encapsulated and electrically isolated from the environment. This is achieved through epitaxial silicon overgrowth, which buries the dopant layer beneath a crystalline “cap” that protects the device and provides a bulk-like electronic environment. The goals of this encapsulation are threefold: (i) to fix the dopant atoms in place and prevent their diffusion, (ii) to restore a high-quality crystalline lattice with minimal defects, and (iii) to ensure sufficient depth ($\sim 30\text{--}40$ nm) to shield the buried device from surface states that would otherwise interfere with quantum information carried in the device layer.

In our lab, epitaxial encapsulation is performed using a silicon sublimation source (SUSI). A two-step growth process is employed to minimize dopant confinement and improve crystal quality. First, a thin locking layer⁷³ (~ 2 nm) is grown at room temperature at a rate of ~ 1.5 ML/min to suppress the dopant

segregation and diffusion by reducing surface mobility. A rapid thermal anneal (RTA) at ~ 350 °C is then applied to smooth the growth front. The sample temperature is subsequently raised to ~ 250 °C^{74,75}, and the overgrowth proceeds at ~ 1.0 ML/min until a total thickness of ~ 40 nm is achieved, typically requiring ~ 5 hours.

The quality of the overgrowth layer depends critically on both vacuum purity and growth conditions. To further reduce the chamber pressure beyond the base level with ion pumping, cryogenic panels are incorporated into our fabrication system. In one system (VT1), a liquid-nitrogen cooled copper shroud (~ 77 K) surrounds the SUSI source. In the other system (VT2), an ARS cold head (~ 20 K) equipped with copper plates is mounted near the growth region. Once cooled, these cryo-panels effectively condense residual gases such as water vapor and hydrocarbons that can be difficult to remove using ion pumps alone, significantly reducing the growth chamber pressure to the 10^{-12} Torr range.

Towards the end of the overgrowth, optional rapid thermal anneals (RTAs) at ~ 420 °C are performed to improve the surface morphology of the overgrown layer. These anneals help recover vacancy defects and reduce surface roughness without causing significant dopant diffusion. A comparison of sample surfaces at different stages, with and without post-growth RTAs is shown in Figure 2.7.

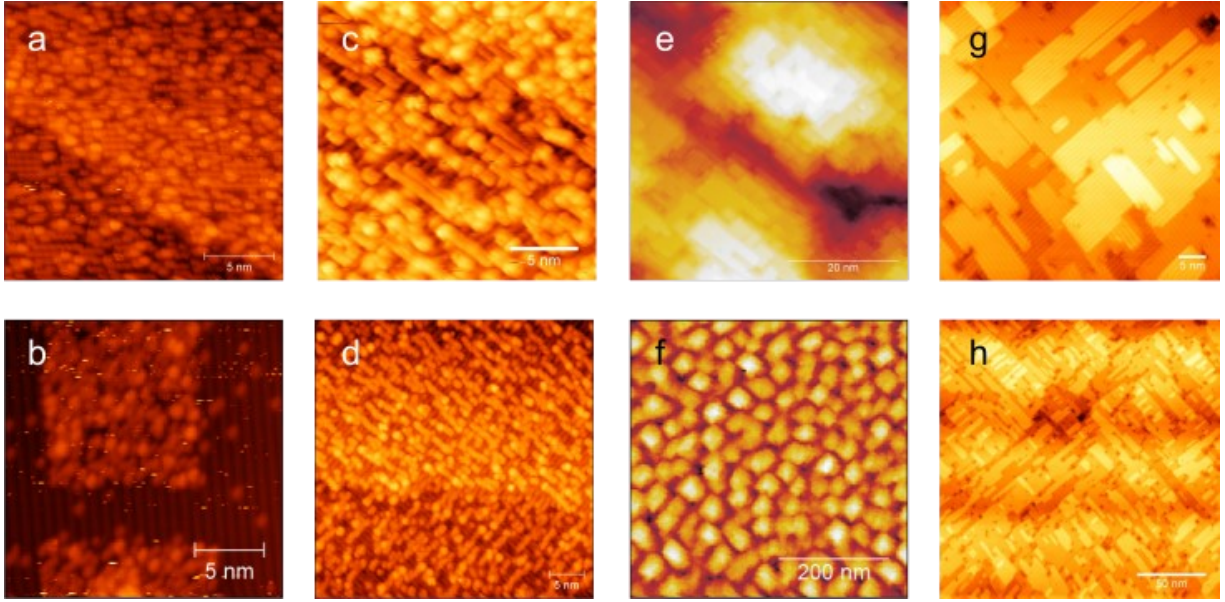


Figure 2.7 STM images of sample surfaces at different stages of dopant incorporation and epitaxial encapsulation, imaged at $V = -2.0$ V, $I = 50$ pA. (a) Bare Si (100) surface after PH_3 dosing. (b) Chemisorbed phosphine molecules selectively attach to de-passivated regions created by STM lithography, while the patterned boundaries remain atomically sharp. (c, d) Surface after thermal incorporation anneal, where ejected silicon atoms appear as bright protrusions, marking successful substitutional incorporation of phosphorus atoms. (e, f) Surface after epitaxial silicon overgrowth (~ 40 nm at 1.0 ML/min), which buries the doped region beneath a crystalline capping layer. The overgrowth retains same atomic order with the initial surface, but small growth islands form, resulting in a relatively high RMS roughness of 483 pm. (g, h) Surface after overgrowth followed by a rapid thermal anneal (RTA) at ~ 420 °C, showing improved surface smoothness (RMS roughness reduced to 128 pm) and lower defect density compared to (e, f). This level of flatness is sufficient for fabricating a second device layer.

Through this multi-step incorporation and encapsulation process, the dopants become embedded within the crystalline silicon lattice and are well isolated from the growth front by approximately 40 nm.

2.1.6 Device Relocation and Electrical Contacts

The buried Si:P device must be accurately relocated to enable electrical contact before any measurement can be made. Relocation can be performed in two complementary ways: in situ STM relocation and ex situ scanning probe microscopy.

In situ relocation is sometimes possible by returning the encapsulated sample to the STM chamber. Using a lock-in imaging mode, and sometimes just from topography, the buried device can be detected through subtle contrasts in the local density of states or surface roughness in the crystalline overgrowth. While this approach offers direct nanoscale confirmation of device placement and its relative position to the fiducial marks, it is time-consuming and not included for routine device processing.

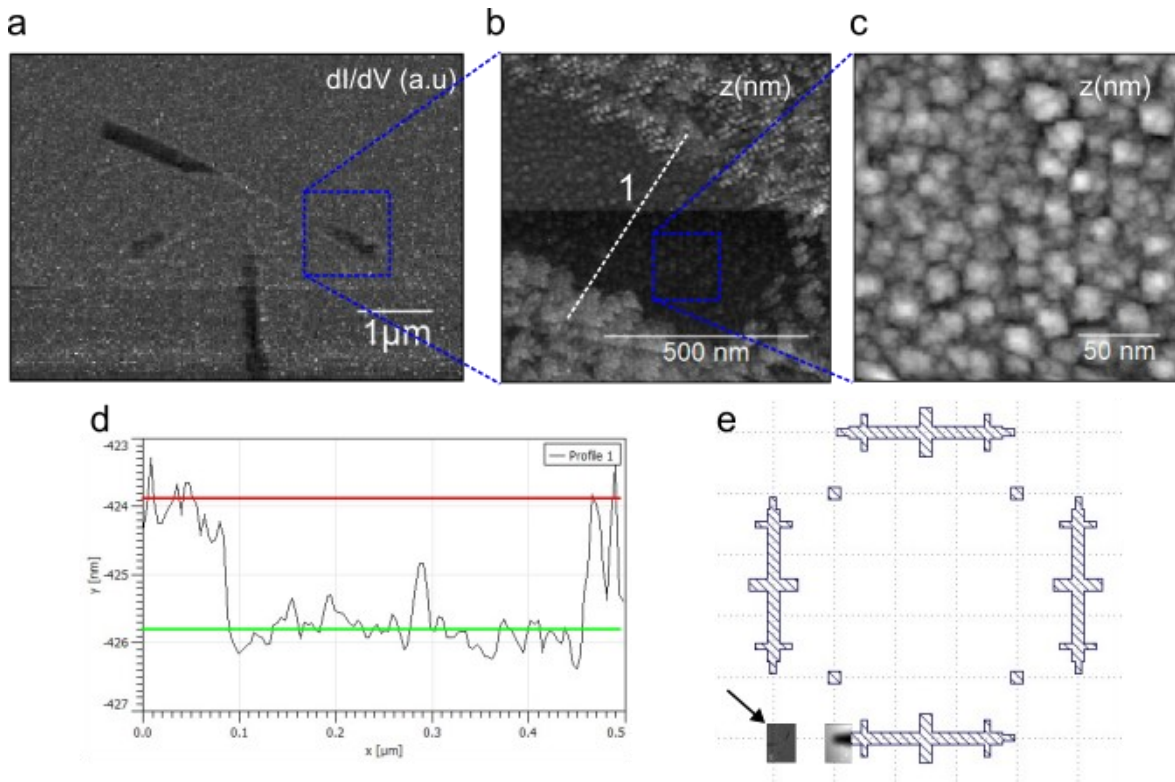


Figure 2.8 In situ device relocation after epitaxial overgrowth. (a) Lock-in dI/dV image of an entire patterned device acquired after encapsulation. (b) Topographic image (z) of a device lead, showing contrast in surface roughness between doped and undoped regions. (c) Higher-magnification view of (b), where individual silicon growth islands are visible. (d) Line profile along the dashed line in (b), revealing a $\sim 2\text{ nm}$ height difference between doped and undoped regions. (e) Fiducial markers from the predefined mask are

first identified, enabling the device to be located relative to them. Using this method, the absolute position of the buried device can be determined with an accuracy of $\sim 1\mu\text{m}$.

For standard fabrication, we employ Kelvin probe force microscopy (KPFM)⁷⁶ to locate the buried doped regions. The phosphorus δ -doped layer, positioned $\sim 40\text{ nm}$ below the surface, significantly modifies the local surface potential, producing clear contrast in KPFM scans. By restricting the scan area to the $50 \times 50\mu\text{m}^2$ shallow fiducial grid where a device is patterned, the search time is minimized. Improved STM camera calibration and fiducial referencing further reduce uncertainty, allowing single shot relocation within a few microns.

Once the doped region is detected, its coordinates are determined relative to the pre-patterned fiducial markers by applying affine transformations that register the KPFM image to the original mask design. This alignment ensures that subsequent metal layers are deposited precisely on top of the patterned device features. Because the nanoscale leads of Si:P devices are far smaller than the resolution limit of conventional optical lithography, electron-beam lithography (EBL) is used to define fine metal traces that make direct contact with the buried doped regions.

For metallization, our group has developed a high-yield palladium (Pd) contact strategy⁴⁷. Pd is deposited and annealed at $\sim 250^\circ\text{C}$ for ~ 20 minutes. During annealing, Pd diffuses into the silicon substrate to form a uniform Pd silicide layer, which establishes ohmic contact to the buried phosphorus δ -layer. This process yields reproducible contact resistances on the order of a few $\text{k}\Omega$, with advantages including deterministic silicide formation, uniform metal diffusion, and compatibility with subsequent processing steps. Transmission electron microscopy (TEM) images of the Pd–Si interface (Figure 2.9(e)) confirm uniform silicidation and intimate contact with the δ -doped layer.

After the inner Pd contacts are made, larger fan-out electrodes are added using standard photolithography. Gold is deposited to connect the Pd leads to bond pads large enough for wire bonding. The final device thus integrates features spanning multiple length scales, allowing external instruments to directly interface with atomically defined structures. An SEM image (Figure 2.9(f)) shows this hierarchical contact architecture.

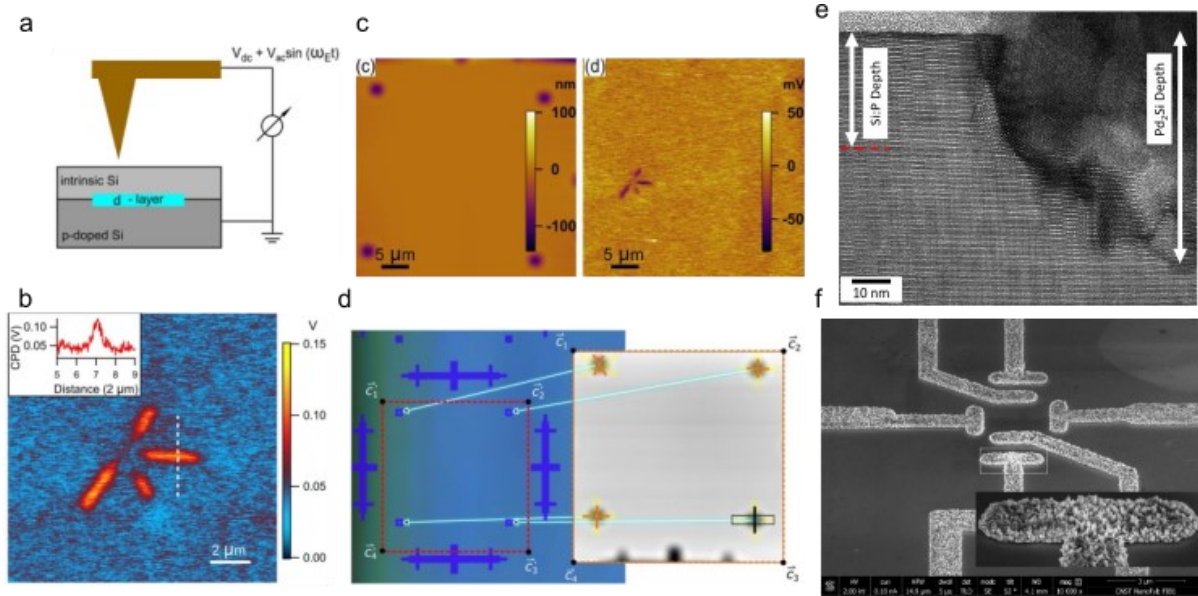


Figure 2.9 Device relocation and electrical contact. (a) Principle of Kelvin probe force microscopy (KPFM), which measures local variations in the surface work function. (b) Phosphorus δ -doped regions produce a clear surface potential contrast, readily detected by KPFM. (c) Combined AFM topography and KPFM potential maps used to locate the buried device. (d) Device coordinates determined from the positions of four corner fiducial dots. (a-d) are reproduced from Pradeep et al ⁷⁶. (e) TEM image of cross section of a Pd_2Si contact. (f) SEM image of the Pd contacts at 2.00kV. The buried device is faintly visible due to electron-surface interactions. Inset: magnified view of a contact pad, showing Pd silicide spikes.

2.2.7 Gate leakage test

For a Si:P device to operate effectively, one or more in-plane gates are typically required to tune the chemical potential of the quantum dots or donor islands of interest, thereby enabling controlled addition or removal of electrons to reach desired charge configurations. The maximum voltage that can be applied to a given gate electrode before a significant leakage current arises between gates (through the silicon substrate) defines the effective gate range of the device. Once leakage occurs, the resulting current not only obscures the small tunneling currents being measured but can also cause irreversible damage to the device.

Figure 2.10 shows an example of a single-electron transistor (SET) measurement where the tunnel current is limited by gate leakage.

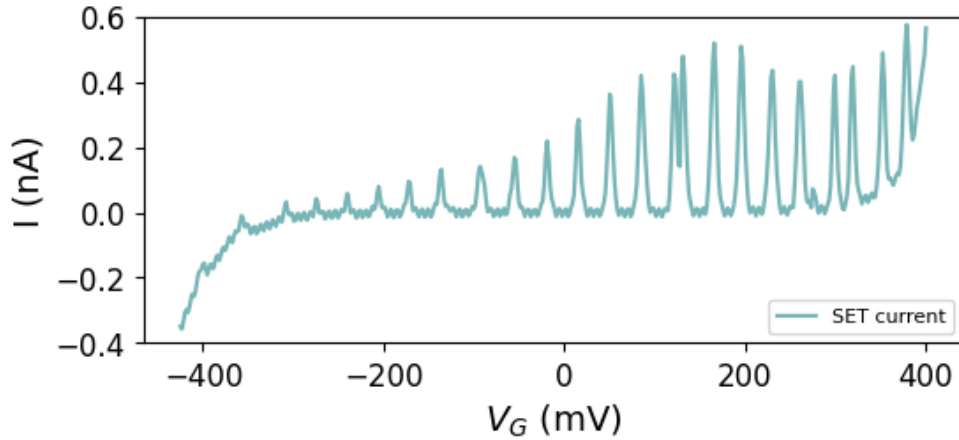


Figure 2.10 SET current measurement limited by gate range. The leakage current increases exponentially beyond approximately ± 400 mV, restricting the total number of observable SET charge transitions (Coulomb oscillation peaks) to 23.

The effective gate range defines the accessible configuration space of a device. For instance, a sufficiently negative gate voltage may be required to fully deplete a nearby donor cluster; a limited gate range would prevent this control, severely degrading device performance by eliminating access to the single-electron regime. Measurements of Si:P devices are performed at cryogenic temperatures, either in a 4 K cryoshroud or at even lower temperatures in a dilution refrigerator and the background boron dopants in the silicon substrate are fully frozen out. Although the precise mechanism of gate leakage at these temperatures remains unclear, it is believed to arise from the background dopants or unintentional charge traps that act as weakly coupled conduction pathways, allowing electrons to hop through.

Figure 2.11 shows the charge stability diagram of a typical single-electron transistor (SET) device fabricated in our group exhibiting a limited gate range of approximately ± 500 mV. In addition, the SET conductance lines in our devices show pronounced gate nonlinearity, complicating the accurate extraction

of gate lever arms and related parameters. We speculate that both the restricted gate range and the observed nonlinearity originate from excess contamination introduced during the UHV fabrication process.

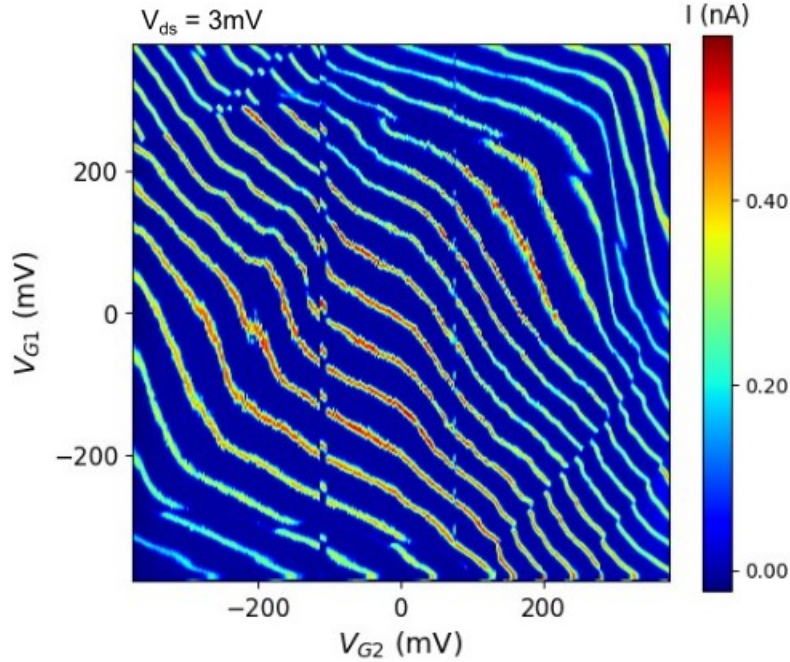


Figure 2.11 Charge stability diagram of a typical SET device fabricated in our group, where limited gate range and nonlinear conductance lines could be caused by impurity elements incorporated during the UHV steps.

To investigate the origin of the limited gate range, we designed a series of experiments to test devices fabricated under varying process conditions. Since the leakage current is believed to occur through the bulk silicon lattice, test samples were prepared without the STM patterning and PH_3 dosing steps. Instead, the silicon encapsulation layer was grown directly after achieving an atomically flat Si (100) surface. Following encapsulation, palladium silicide contacts were fabricated using the same procedure as patterned devices, with the nearest contact separations set to 600 nm, 1000 nm, and 1500 nm. Figure 2.12 shows optical images of these four-contact test structures. In a fully patterned device, these four terminals would typically serve as the source, drain, and two in-plane gates.

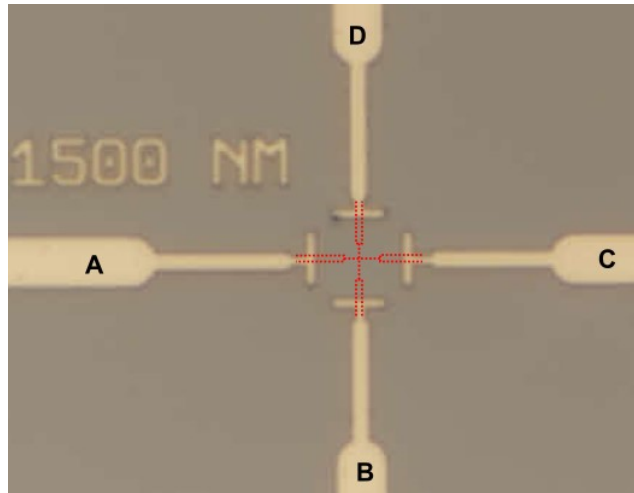


Figure 2.12 Test structures for characterizing leakage current. The four contacts are Palladium silicide with nearest neighbor separation of 1500 nm. The red dashed lines mark the scale of a possible STM patterned device.

We measured the leakage current between a pair of nearest-neighbor contacts A and B while keeping the other two contacts C and D electrically floating. Figure 2.13 compares the measured leakage currents for a control sample without processing and a sample fabricated using our standard procedure.

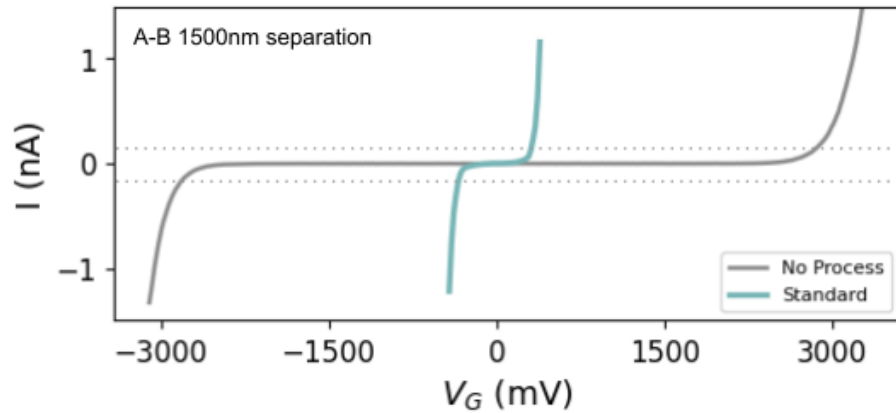


Figure 2.13 Gate range comparison between a no (UHV) process sample and a standard process sample with 30 nm of overgrowth. The standard process test sample shows a gate range of ± 400 mV similar to a STM patterned device, suggesting the leakage occurs through the bulk silicon.

The no-process sample, which was chemically cleaned but otherwise unprocessed, exhibited a significantly larger gate range of over ± 2 V, more than four times that of the standard process sample. This result indicates that the starting silicon wafer quality is sufficient and that the degradation of gate performance arises during the fabrication process. We have long speculated that the issue originates from the epitaxial overgrowth stage. At a vacuum pressure of $\sim 1 \times 10^{-10}$ Torr, significant residual gas molecules could be incorporated into the growing silicon lattice at a growth rate of ~ 1 monolayer per minute. This hypothesis is supported by secondary ion mass spectrometry (SIMS) measurements of the overgrowth layer, which reveal the elemental composition with nanometer-scale resolution. Figure 2.14 shows SIMS data from a delta-layer device with a 30 nm overgrowth thickness. The concentration of oxygen increases by almost two orders of magnitude from the substrate into the overgrown region, with similar trends observed for carbon and nitrogen. Additionally, aluminum impurities are detected at concentrations on the order of 10^{18} cm^{-3} , though their source remains unidentified. These findings motivated the implementation of internal cryogenic shrouds, described in the previous section, to further reduce the UHV base pressure and mitigate impurity incorporation during overgrowth.

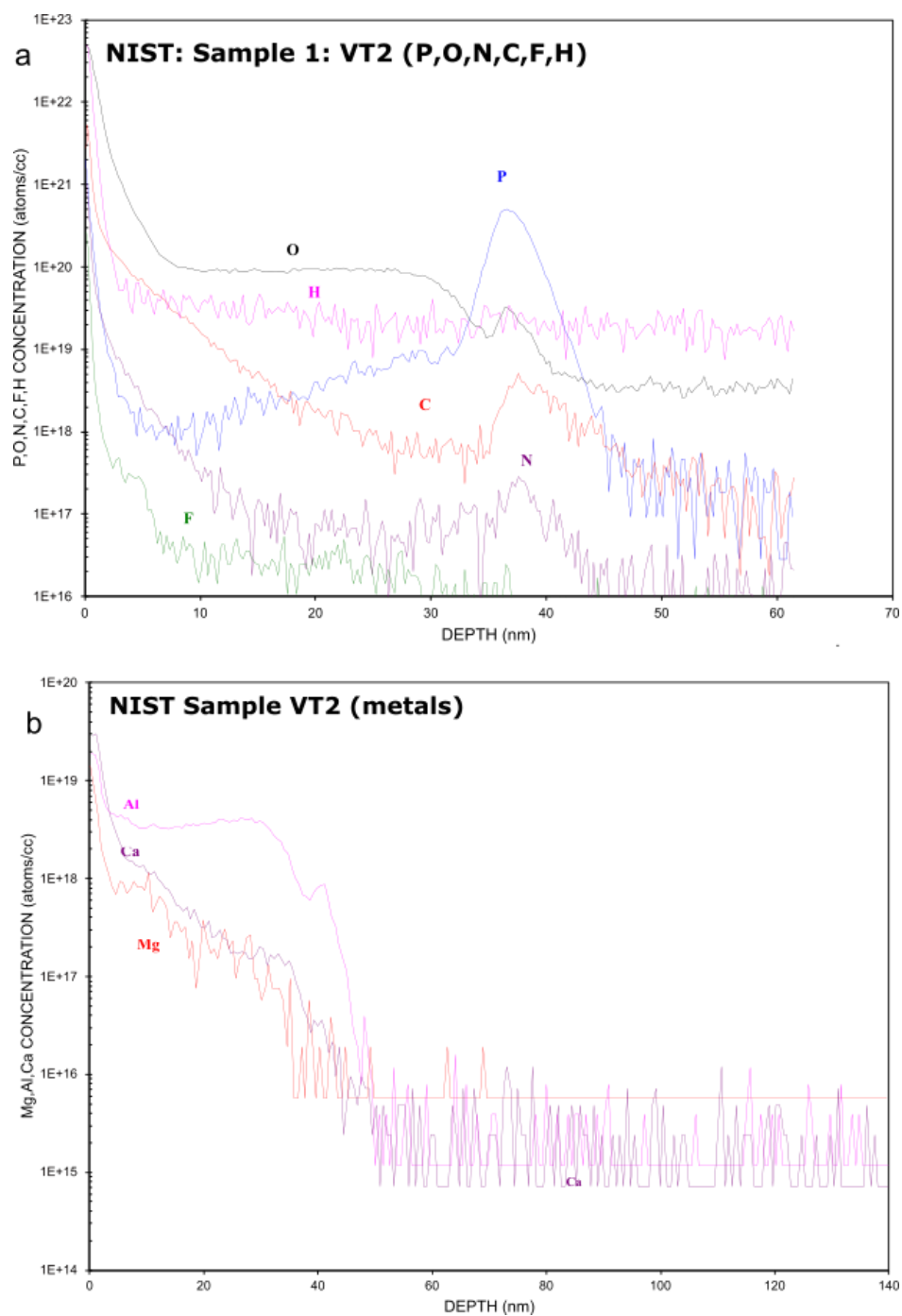


Figure 2.14 SIMS measurement result of a Phosphorus delta-layer device with standard overgrowth thickness of ~ 30 nm. (a) Oxygen concentration increases by almost two orders of magnitude from the substrate into the overgrown region. (b) $10^{18}/\text{cc}$ of Al is detected in the overgrowth layer. The data is taken by Eurofins EAG.

A test sample that underwent surface preparation but without epitaxial overgrowth provided new insight into this problem, showing a similarly reduced gate range to that of fully overgrown samples. This observation suggests that the overgrowth process itself may not be the root cause. Rather, changes introduced during the degassing or flash-cleaning steps could be altering the surface characteristics of the silicon wafer. To further investigate, we fabricated three test samples with varying wafer types and preparation conditions:

- Sample A: 10^{15} cm^{-3} boron-doped wafer; degassed for 3 hours at 470 °C; flashed six times for 10 s each plus a final 5 s flash at 1100 °C; followed by overgrowth at 250 °C.
- Sample B: 10^{15} cm^{-3} boron-doped wafer; degassed for 24 hours at 600 °C; total flash time of 5 minutes at 1250 °C; followed by overgrowth at 250 °C.
- Sample C: Intrinsic silicon wafer; degassed for 3 hours at 470 °C; flashed six times for 10 s each plus a final 5 s flash at 1100 °C; followed by overgrowth at 250 °C.

Figure 2.15 presents the results obtained from the three test samples. Sample A continued to exhibit a reduced gate range, whereas both Sample B and Sample C demonstrated satisfactory gate ranges exceeding $\pm 1.2 \text{ V}$. Each experiment was repeated multiple times, yielding consistent and reproducible results. The intrinsic wafer (Sample C) produced clean STM images and supported standard lithography parameters, although its high room-temperature resistance required a higher voltage to initiate heating. A similar phosphorus-doped sample processed under the same conditions as Sample A (not shown) displayed a comparably limited gate range.

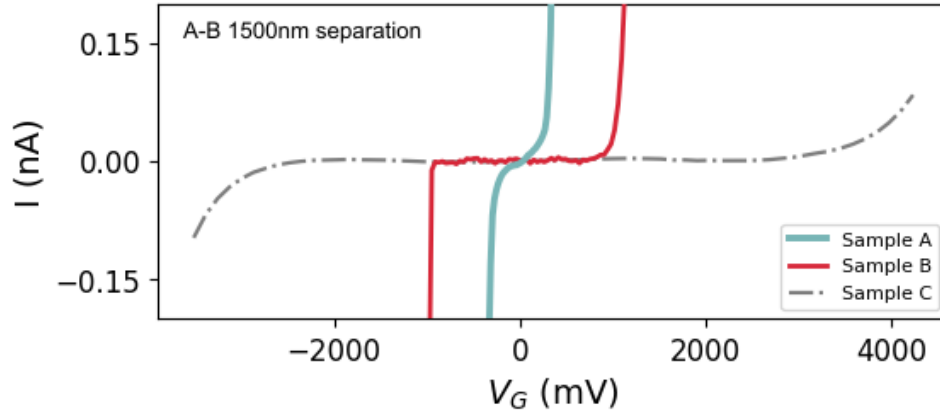


Figure 2.15 Gate range measurements for the three process variations. Both Sample B and Sample C exhibit a significantly increased gate range compared to the standard process, with Sample C showing an exceptionally large range of approximately ± 2.5 V. (Fan Fei fabricated Sample A, Jonathan Wyrick fabricated Sample B, Fan Fei and Utsav fabricated identical copies of sample C on two different systems, Brian Courts measured all three samples.)

The underlying mechanism responsible for these observations remains under investigation. We speculate that unintended boron accumulation occurs on the sample surface during UHV heating, leading to degraded electrical performance. In Sample B, the extended flashing time likely removed these surface boron contaminants, while Sample C inherently avoided this issue due to the absence of boron in the substrate. This hypothesis is supported by SIMS measurements (Figure 2.16) from a sample processed identically to Sample A with standard overgrowth, where a boron concentration peak is observed at the interface and decays gradually into the substrate.

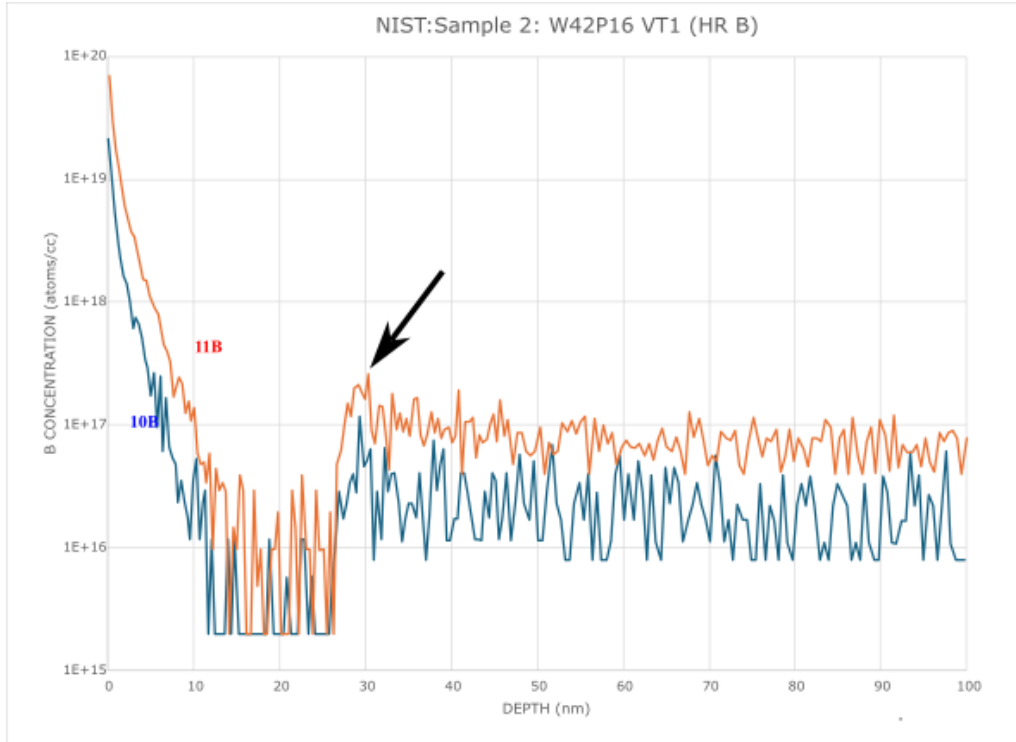


Figure 2.16 Boron profile of a test sample processed identically to sample A and with an overgrowth of ~ 30 nm thickness. A boron concentration peak is observed at the interface. This sample also shows a small gate range of ± 400 mV.

The two potential remedies identified in Samples B and C are now being implemented in STM-patterned devices, with the goal of resolving both the limited gate range and the gate nonlinearity issues that degrade device performance.

2.2 Low-Temperature Measurement Methods

Low-temperature electronic measurements of Si:P devices are performed using either a 4 K cryocooler (Advanced Research Systems, ARS) or a $^3\text{He}/^4\text{He}$ dilution refrigerator (BlueFors). Device samples are wire-bonded to custom-designed printed circuit boards (PCBs), which are then mounted onto the cold finger of a fridge.

The 4 K system has a compact sample space and can reach its base temperature of 4 K (or slightly below) within approximately two hours. This short cooldown time enables rapid characterization of test devices without the need for a prolonged thermal cycle. Wiring is implemented using continuous twisted-pair lines that extend from room temperature down to the cold finger, wrapped around the pulse-tube head to provide necessary thermal anchoring. No additional filtering or thermalization components are installed in this setup. As such, the 4 K cryostat is primarily used for preliminary electrical tests, including leakage current measurements and Coulomb oscillation scans, to determine whether a device is suitable for transferring to the dilution refrigerator for detailed low-temperature characterization.

A dilution refrigerator is used for high-sensitivity measurements presented in later chapters. It employs a helium-4 pulse tube to precool the system to 4 K, after which a closed-circuit $^3\text{He}/^4\text{He}$ mixture provides further cooling to millikelvin temperatures via continuous circulation managed by a dedicated gas-handling system. The refrigerator is equipped with a superconducting magnet capable of generating homogeneous magnetic fields up to 10 T, which is essential for spin readout and magnetotransport studies of Si:P devices. The mixing chamber typically achieves a base temperature of ~ 10 mK, as indicated by calibrated thermometers. However, the actual electron temperature within the device is often higher due to residual radiative heating and incomplete thermalization along the wiring lines. Here we describe the wiring configuration used in our laboratory and present corresponding electron temperature measurement results in Chapter 5.

2.2.1 Filters and Wirings

Figure 2.17 shows the schematic of the custom PCB used for all device measurements. The sample is mounted at the central slot of the board. Operation of a Si:P device requires not only low-frequency gate and bias voltages but also fast gate pulses with precise timing, radio-frequency (RF) signals for reflectometry readout, and microwave signals for spin manipulation. The custom PCB integrates all these

functionalities in an interleaved layout, providing maximum flexibility for a variety of device architectures. In total, the board includes 14 DC lines, each equipped with a two-stage RC low-pass filter with a cutoff frequency of 300 kHz; two RF lines for reflectometry measurements; and ten unfiltered lines that can be used for either DC biasing or high-speed gate pulsing. Additionally, microwave excitation is delivered via a coplanar waveguide (CPW) fed from two edge-launch connectors.

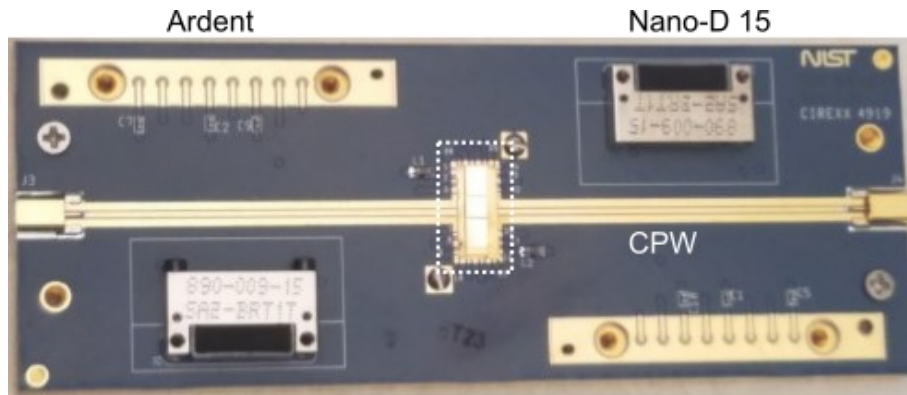


Figure 2.17 Photograph of the custom PCB used for cryogenic sample measurements. DC lines are connected via a Nano-D 15-pin connector to twisted-pair wiring, while AC lines are interfaced through an Ardent connector to SMA coaxial cables. Microwave excitation is delivered through a coplanar waveguide (CPW) ⁷⁷ integrated onto the PCB. This PCB is mainly designed by Alessandro Restelli with input from our group.

The DC wiring inside the dilution refrigerator consists of twisted pairs organized into looms terminated with 25-pin Micro-D connectors, with each stage thermally anchored using copper bobbins. In addition, the DC lines pass through a QDevil RF filter (65kHz low-pass) and a copper-powder filter box (~2 GHz low-pass) mounted at the mixing chamber to suppress high-frequency thermal radiation propagating from warmer stages. Installation of these copper-powder filters has been shown to reduce the effective electron temperature from approximately 600 mK to below 300 mK. Fast gate pulses are transmitted through semi-rigid SMA coaxial cables, which are thermally anchored at each stage using attenuators of varying values.

These SMA lines are also filtered by individual copper-powder filters before reaching the device or merging with DC lines via on-board bias tees. With this configuration, signals ranging from low-frequency DC control to nanosecond-scale gate pulses can be delivered reliably to the device with minimal thermal noise and signal distortion.

2.2.2 Instrumentation and Control

A range of electronic instruments are employed for different types of measurements, including DC transport, lock-in detection, high-frequency reflectometry, and pulsed-gate experiments. The key instruments used in this work are listed below:

- DC voltage sources: SIM928 (Stanford Research Systems, SRS) and SR860 (SRS) are used for supplying stable gate and bias voltages with microvolt-level resolution.
- Current amplifier: DLPCA-200 (Femto) provides low-noise current amplification with variable gain, essential for measuring picoampere-level tunneling currents.
- Lock-in amplifier: SR860 (SRS) is used for phase-sensitive detection and dI/dV measurements below 500 kHz.
- Arbitrary waveform generators (AWGs): NI6363 (National Instruments), DG5072 (Rigol), AWG5000 (Tektronix), and M3201A (Keysight) are used for generating gate pulses and custom voltage sequences with different levels of timing precision.
- Digitizers: DMM6500 (Keithley), NI6363 (National Instruments), and M3102A (Keysight) record time-domain signals such as current and I/Q values.
- Vector signal generators: DSG821 (Rigol) and N8267D (Keysight) provide continuous-wave or modulated microwave signals for spin resonance and reflectometry experiments.
- Vector network analyzer and spectrum analyzer: N5224B (Keysight) and N9000B (Keysight) are used for RF characterization, sideband detection and power calibration.

All instruments are integrated into an automated measurement environment using a custom Python-based control framework using the Virtual Instrument Software Architecture (VISA) interface.

Chapter 3: Low-Temperature Transport Theory of Si:P Devices

The operation of Si:P devices rely on a rich interplay between the electronic properties of silicon, the physics of dopant atoms, and the principles of quantum confinement. This chapter provides the theoretical foundation for understanding how such devices function at low temperatures, where quantum effects dominate.

We begin by reviewing the band structure of crystalline silicon, highlighting the six-fold valley degeneracy of its conduction band. We discuss the effective mass theory description of electrons bound to individual phosphorus donors, which form shallow impurity states located approximately 45 meV below the conduction band edge. Each phosphorus donor hosts both an electron spin ($S=1/2$) and a nuclear spin ($I=1/2$), coupled through the hyperfine interaction. These spin states can be coherently manipulated using a combination of magnetic resonance and electric-field control, with initialization and readout achieved via spin-dependent tunneling of an electron. The long coherence times of donor spins and electron spins in isotopically purified silicon make them exceptionally robust qubit candidates. Harnessing these spin degrees of freedom is central to donor-based quantum information processing. We then examine how tunnel coupling arises when two or more donors are placed in proximity, creating molecular-like hybridized states that can be harnessed to engineer dopant-based quantum dot arrays. The discussion extends to larger doped regions formed by delta doping, which act as metallic leads and gates essential for electrical control of the device. Using hydrogen lithography, arbitrary two-dimensional nanostructures can be precisely defined to confine or transport electrons, enabling a wide range of quantum phenomena. These dopant-based nanostructures provide the building blocks of functional Si:P quantum devices.

Building on this foundation, we review the transport theory of atomic scale Si:P devices, beginning with the operating principles of the single-electron transistor (SET). We review key concepts such as chemical potentials, charging energy, Coulomb blockade, and Coulomb oscillations within the framework of the constant-interaction model. These principles also apply to coupled quantum dots and arrays, which can be used to assemble an analog quantum simulator.

3.1 Silicon

Silicon is not only the backbone of the modern semiconductor industry but also the host material for donor-based quantum devices. The electronic properties of crystalline silicon offer a clean and stable environment for storing quantum information. In Si:P devices, phosphorus donors embedded in a single-crystal Si (100) substrate act as localized electron sites, while surrounding doped regions function as metallic leads and gates for electrical control. To develop a complete understanding of how these devices operate, it is essential to first examine the band structure of intrinsic silicon, the modifications introduced by individual donors, and the behavior of extended doped regions. These topics lay the foundation for the more complex nanostructures and quantum devices discussed later in this chapter.

3.1.1 Band Structure of Silicon and surface reconstruction

Silicon crystallizes in the diamond cubic structure with lattice constant $a = 0.357$ nm. Each atom forms four sp^3 hybridized covalent bonds with its neighbors, producing a tetrahedral lattice structure that extends throughout the crystal. This arrangement gives rise to a well-defined band structure, which forms the starting point for understanding electron transport in Si:P devices.

Intrinsic silicon is an indirect-gap semiconductor with a band gap of approximately 1.12 eV at 295 K. The conduction band minima (CBM) lie along the six equivalent directions near the X points of the Brillouin zone, giving rise to a six-fold valley degeneracy in bulk. At room temperature, the thermal energy (~ 25 meV) is far too small to excite a significant population of carriers across the band gap, making intrinsic silicon insulating. In practice, lightly doped substrates (in our case $1 \times 10^{15}/\text{cm}^3$ Boron doped) are used so that sufficient conductivity is maintained at room temperature for sample preparation, direct current heating, and STM imaging. At cryogenic temperatures, these background dopants freeze out, leaving the intrinsic band structure effectively unperturbed.

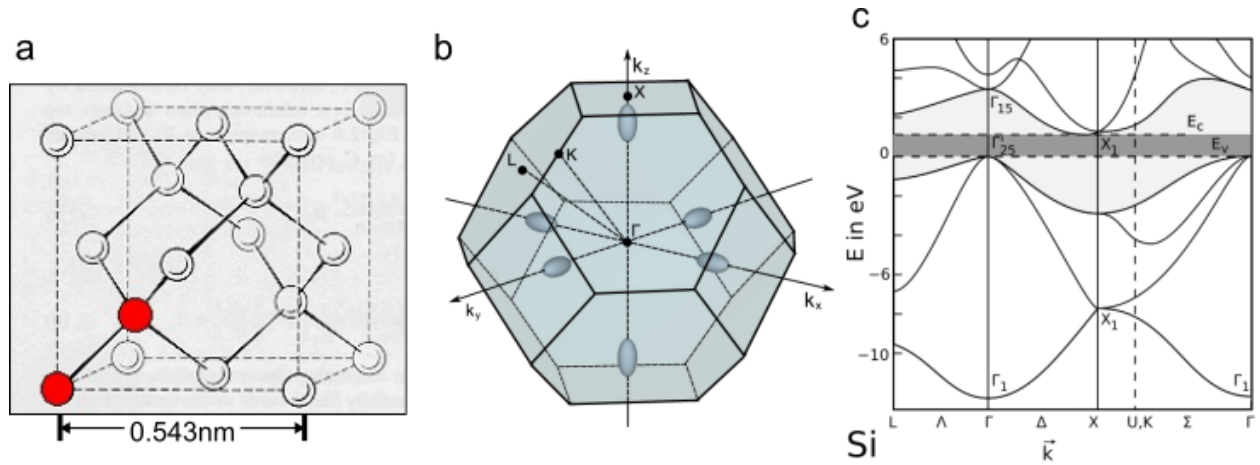


Figure 3.1 Crystal structure and electronic band structure of silicon. (a) Diamond cubic lattice of silicon with tetrahedral sp^3 bonding and lattice constant $a = 0.543 \text{ nm}$. This plot is taken from online resource.⁷⁸ (b) First Brillouin zone of silicon with the ellipsoids represents the six-fold valley degeneracy of the conduction band located at $k=0.85 \, 2\pi/a$ along the k axes. This plot is taken from Osintsev.⁷⁹ (c) Electronic band structure of intrinsic silicon, showing the indirect band gap of 1.12 eV (gray band) at room temperature. This plot is taken from Chelikowsky.⁸⁰

Figure 3.1 shows the crystal structure, first Brillouin zone and the band structure of pure crystal silicon. The conduction band minima are located at $k=0.85 \, 2\pi/a$ along the k axes in Figure 3.1(b), as the six degenerate ellipsoid blobs. Near an interface, the symmetry of the crystal is reduced, and the six-fold conduction band degeneracy is lifted into a lower-energy two-fold valley and a higher-energy four-fold valley. Within the effective mass approximation (EMA)^{81,82}, electrons near the conduction-band minima can be treated as quasi-free particles whose dynamics are governed by anisotropic effective masses: a longitudinal mass $m_{\parallel}$ and a transverse mass $m_{\perp}$, determined by the curvature of the energy bands near each valley minimum (the shape of the ellipsoids). The electron wavefunction can be expressed as a linear combination of valley Bloch states, each modulated by a slowly varying envelope function that satisfies the effective-mass Schrödinger equation under external or confining potentials. This multivalley EMA framework captures the essential physics of electrons in silicon and provides a simple yet precise approach

for analyzing donor-bound states, valley–orbit coupling, tunnel coupling, and quantum confinement effects in atomistic nanostructures.

The fabrication of Si:P devices take place at the silicon surface, where atomic reconstruction plays a crucial role in defining the structural and electronic properties. The clean Si (100) surface undergoes a characteristic 2×1 reconstruction^{83,84}, in which neighboring surface atoms pair to form dimers, thereby minimizing the number of dangling bonds and lowering the surface energy. In STM images, these dimers appear as parallel rows with a periodicity of $a = 0.768$ nm, providing a natural atomic grid for device patterning. Hydrogen passivation terminates the remaining dangling bond of each surface silicon atoms, while preserving the underlying dimer reconstruction. The surface also exhibits step edges⁸⁵, which are extended atomic terraces of single-layer height (~ 0.126 nm). These arise naturally from the substrate miscut angle and subsequent thermal processing. Across a step edge, the orientation of dimer rows rotates by 90° .

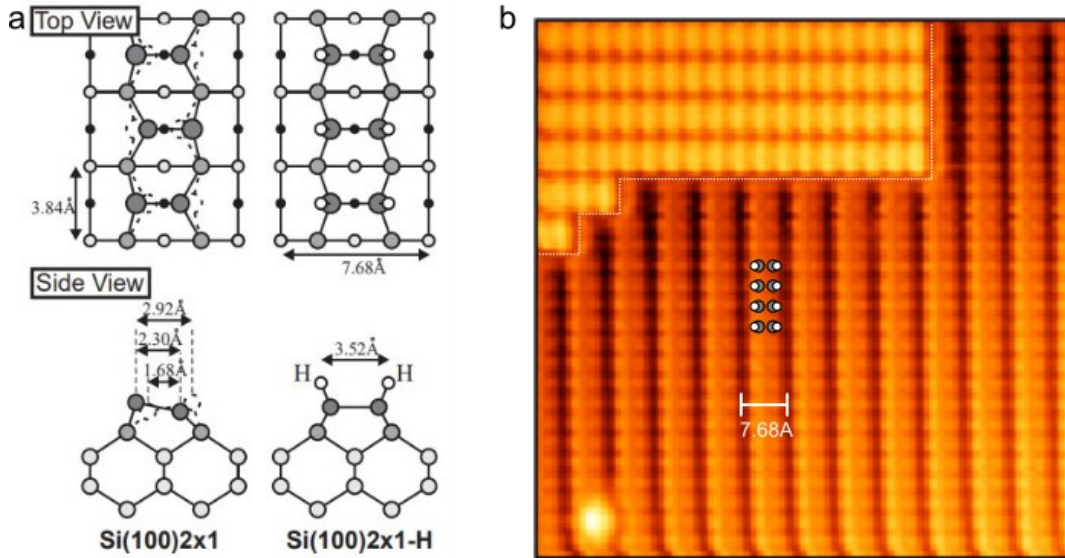


Figure 3.2 Si (100) surface reconstruction and STM imaging. (a) Schematic of the 2×1 reconstruction in which neighboring surface atoms pair to form dimers, reducing dangling-bond energy. This figure is taken from Yokoyama et al⁸⁶. (b) Close STM image of a H-Si (100) surface showing individual dimer rows with a periodicity of 0.768 nm. Across a step edge (white dashed line), the orientation of the dimer rows rotates by 90° , corresponding to atomic terraces one monolayer in height (~ 0.126 nm).

3.1.2 Electronic Wavefunction of a Single Donor

When a silicon atom in the crystal lattice is substituted by a phosphorus atom (atomic number 15), the additional positive nuclear charge creates a confining potential, forming a shallow hydrogenic impurity state within the silicon band gap. The characteristics of this donor-bound electron, such as its binding energy, spatial extent, valley composition, and tunnel coupling to neighboring dopants, play a central role in determining the behavior of Si:P quantum devices and have been extensively studied in the literature. In the following, we briefly review the principal theoretical approaches used to describe such donor states in silicon, including density functional theory (DFT), tight-binding (TB) methods, and multivalley effective mass theory (EMT).

Atomistic Approaches: Tight-Binding and Density Functional Theory

The tight-binding (TB) method ^{87,88} provides an atomistic approach for modeling the electronic structure of donors in silicon. In this framework, the electronic wavefunction is expressed as a linear combination of localized atomic orbitals, typically including an extended basis set like $sp^3d^5s^*$ ⁸⁹ for silicon, to capture the essential characteristics of both the valence and conduction bands. Each atom contributes these orbital states, and the Hamiltonian is constructed from empirical or semi-empirical hopping parameters that describe interactions between neighboring orbitals. Because the method explicitly treats the atomic positions, strain fields, and dopant potentials, it naturally incorporates effects such as valley interference, central-cell corrections, and interface roughness. Modern TB simulations often include domains containing millions of atoms, allowing realistic modeling of donor wavefunctions in experimentally relevant device geometries, from few-donor clusters ^{90,91} to extended dopant leads ^{92,93}. The resulting electronic states can be visualized directly from the calculated amplitudes on individual atoms and orbitals, providing an intuitive, spatially resolved picture of the donor-bound electron and its interaction with nearby dopants or interfaces.

The density functional theory (DFT) approach offers a first-principles framework for calculating the electronic structure of donor impurities in silicon. In DFT, the many-electron problem is reduced to a set of self-consistent Kohn–Sham equations⁹⁴, where the electron density rather than the wavefunction serves as the fundamental variable. Unlike empirical models, DFT directly incorporates the donor potential and electron–electron interactions through exchange–correlation functionals, allowing accurate prediction of donor binding energies, valley–orbit splitting, and etc.⁹⁵ By using large supercells often containing several hundred to tens of thousands of atoms, DFT calculations can simulate the local relaxation of the silicon lattice and the central-cell effects surrounding the donor. The resulting donor wavefunctions can also be visualized in real space, showing both the hydrogenic envelope and the atomic-scale oscillations arising from the multivalley conduction band structure. Although computationally demanding, DFT provides benchmark results for calibrating more approximate models such as tight-binding and effective mass theory^{96,97}. The simulated surface electron densities are often compared with experimental spectroscopy and STM imaging, showing quantitative agreements^{98,99}.

Effective Mass Theory

Despite the power of atomistic methods, effective mass theory (EMT) remains a widely used and intuitive framework for analyzing donor states. Here, we follow the discussion from Wellard, et al¹⁰⁰ and Gamble, et al⁸². The donor-bound electron is described as a coherent superposition of the six conduction-band valley states, where each component consists of a Bloch function centered at a valley minimum and is modulated by a slowly varying envelope function:

$$\Psi(r) = \sum_{j=1}^6 F_j(r) u_j(r) e^{ik_j \cdot r} \quad (3.1)$$

where $u_j(r)$ is the periodic Bloch function at the j -th conduction band minimum, k_j is the corresponding k -vector at valley minimum, and $F_j(r)$ is the slowly varying envelope function analogous to the hydrogenic

orbital. The envelope functions $F_j(r)$ are obtained by solving an effective Schrödinger equation, originally formulated by Shindo and Nara¹⁰¹ accounting for the donor potential:

$$EF_l(r) = [T_l + U(r)]F_l(r) + \sum_{j \in \pm\{x,y,z\}} V_{lj}^{VO}(r) F_j(r) \quad (3.2)$$

where T_l is the kinetic energy operator of the l -th valley. $U(r)$ is the donor potential and $V_{lj}^{VO}(r)$ is the valley-orbital coupling between valleys l and j , $V_{lj}^{VO}(r) = \phi_l^*(r)U(r)\phi_j(r)$. A proper description therefore requires a reasonable knowledge of both the donor potential $U(r)$ and the form of the Bloch functions.

At long distances, the donor potential is well approximated by a bulk-screened Coulomb interaction,

$$U_c(r) \sim -\frac{e^2}{4\pi\epsilon_{Si}r} \quad (3.3)$$

Closer to the donor nucleus, however, this simple $1/r$ falloff fails due to reduced dielectric screening and reorganization of the local electronic structure. To account for these short-range effects, a central-cell correction (CCC)¹⁰² term $U_{cc}(r)$ is introduced, giving the total impurity potential

$$U(r) = U_c(r) + U_{cc}(r) \quad (3.4)$$

In practice, $U_{cc}(r)$ is modeled as a Gaussian centered at the donor site together with four equivalent Gaussians along the tetrahedral bonding directions,

$$U_{cc}(r) = A_0 e^{-\frac{r^2}{2a^2}} + A_l \sum_{i=1}^4 e^{-\frac{|r-bt_i|^2}{2c^2}} \quad (3.5)$$

The Bloch functions on the other hand, are taken from the DFT results on crystalline silicon. A variational approach is used to iteratively optimize the parameters of the central-cell correction and solve for the donor envelope functions, ensuring that the calculated spectrum reproduces the experimentally measured binding energies. For a single phosphorus donor, this procedure yields a singlet valley ground state A_1 at -45.6 meV below the conduction band edge. The envelope of its wavefunction is hydrogen-like $F_j(r) \sim e^{-r/2a_B}$, with an effective Bohr radius of approximately $a_B \sim 2$ nm.

The excited state spectra consist of a triply degenerate T_2 state and a doubly degenerate E state, consistent with the valley–orbit splitting observed in experiment. The energy spectrum, final donor potential and ground-state wavefunction are visualized in Figure 3.3 which captures both the hydrogenic-like decay at long distances and the central-cell corrections added to reproduce the measured donor spectrum.

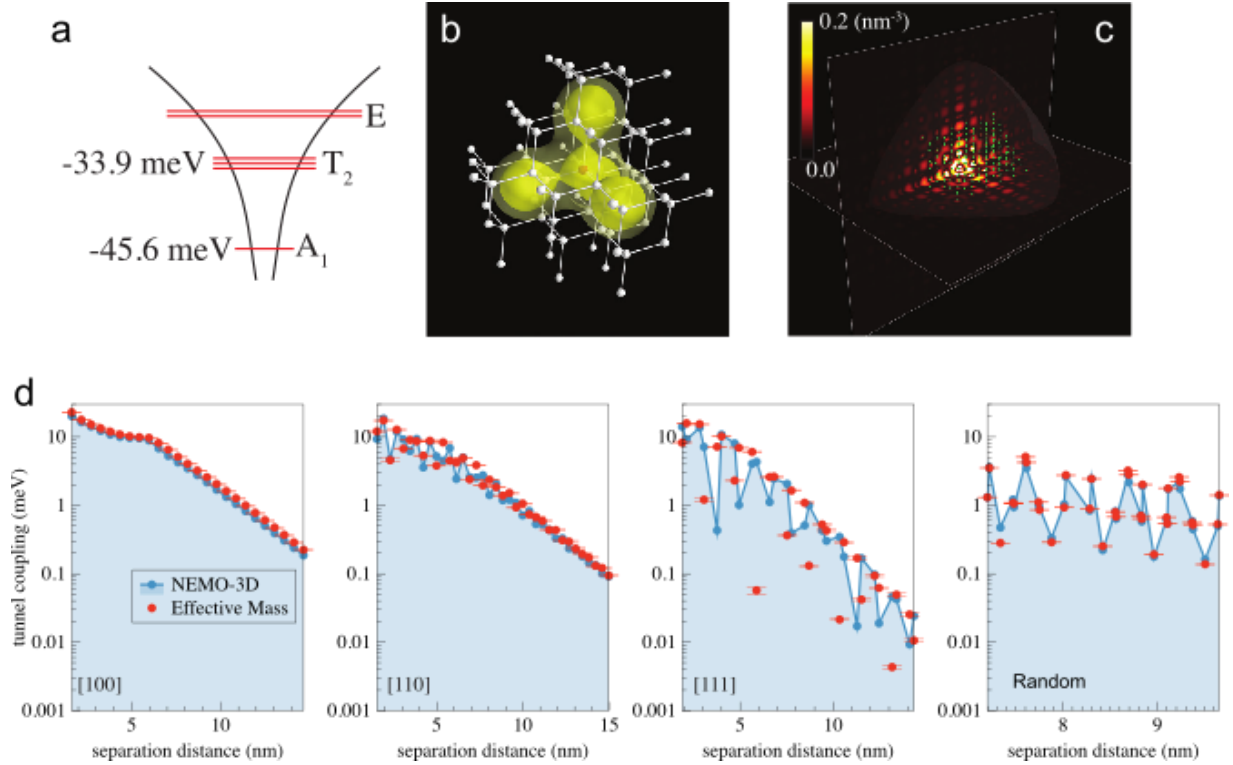


Figure 3.3 Electron wavefunction of a single phosphorus donor and tunnel coupling between two phosphorus donors in silicon calculated from EMT. (a) Energy spectrum of the single donor. (b) Equal potential surface of the converged donor potential. (c) wavefunction density of the A_1 ground state. (d) Tunnel coupling t as a function of donor separation along different crystallographic directions. Smooth decay is observed along [100], while strong oscillations appear along [110] and [111] due to valley interference. These figures are taken from Gamble et al ⁸².

The effective mass theory can also be extended to describe interactions between two closely spaced donors. When two phosphorus atoms are introduced within a few nanometers of each other, their donor-bound electron wavefunctions overlap and hybridize into molecular-like states. Within the multivalley EMT

framework, the tunnel coupling t is defined as the energy splitting between the bonding and antibonding one-electron states of the donor pair. A full configuration interaction (CI) ⁹⁶ method is employed to include electron–electron interactions, allowing accurate calculation of both the single-particle spectrum and the two-electron exchange energy.

The resulting tunnel coupling depends sensitively on both the donor separation and the crystallographic orientation of the pair. Along the [100] direction, the coupling decreases smoothly with increasing separation, consistent with the exponential decay expected from overlapping hydrogenic envelopes. In contrast, along the [110] and [111] directions, the tunnel coupling exhibits pronounced oscillations as a function of distance. These oscillations originate from valley interference, the constructive or destructive overlap of the six Bloch components that compose each donor wavefunction. This multi-valley interference is a signature of silicon’s conduction-band structure and has significant implications for the reproducibility and controllability of exchange interactions in donor-based qubits. Although the same full-configuration interaction method can, in principle, be extended to larger donor clusters, the computational cost increases exponentially with the number of donors and electrons, making such calculations rapidly intractable for large systems.

3.1.3 Delta Doping and 2D Conduction

When dopants are introduced into a semiconductor at sufficiently high density, the system undergoes a metal–insulator transition (MIT) ¹⁰³. At low concentrations, dopant electrons remain localized around individual impurity sites. As the dopant density increases, these localized states begin to overlap, creating extended states that can support metallic conduction. In silicon, the critical concentration for MIT is approximately $3.5 \times 10^{18} \text{ cm}^{-3}$. Above this threshold, impurity bands are formed below the conduction band, and the system exhibits finite conductivity even at cryogenic temperatures.

In STM-fabricated Si:P devices, dopants are introduced in a controlled manner by creating exposed regions in the hydrogen resist and incorporated into the silicon lattice. After encapsulation, these dopant atoms form

a two-dimensional sheet at the device layer, referred to as a delta-doped layer ⁷⁴ (dopant layer of only 1 monolayer thickness). The saturation doped density is approximately $2 \times 10^{14} \text{ cm}^{-2}$. Converting to bulk density, this value is well above the MIT threshold, resulting in metallic behavior. Density functional theory (DFT) calculations ⁹⁵ confirm that in such delta-doped structures, new sub bands within the silicon band gap are formed. As shown in Figure 3.4, the delta-doped layer produces two low-lying Γ bands (Γ_1, Γ_2) and four higher-energy Δ bands (Δ_1 to Δ_4). The Fermi level lies within these donor-induced sub bands, approximated 100 meV below the bulk conduction band edge, indicating that the delta layer remains metallic even at cryogenic temperatures.

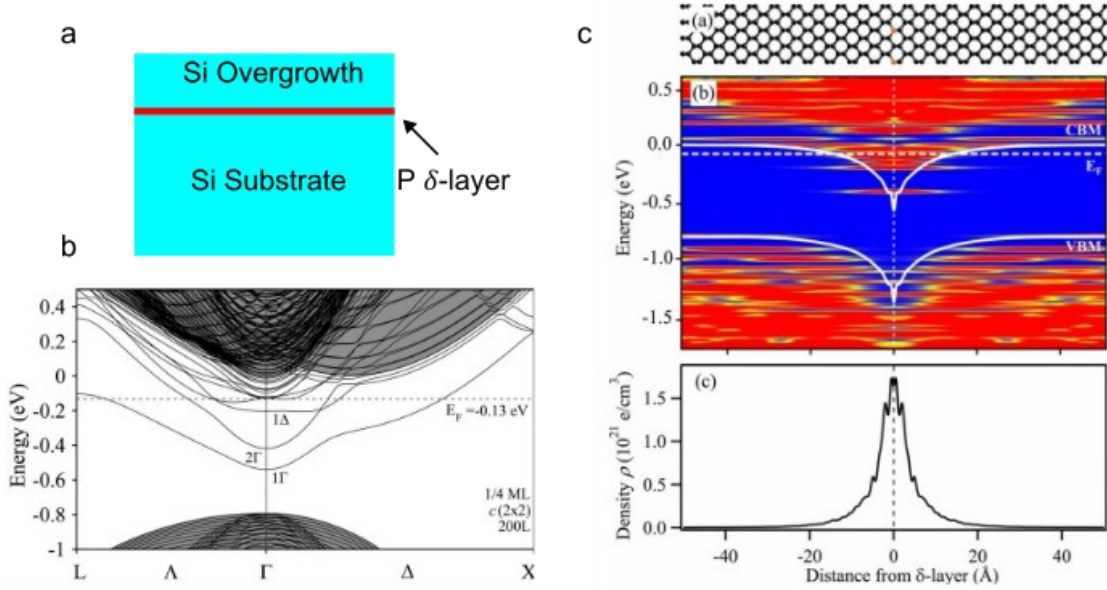


Figure 3.4 Delta-doped phosphorus layer in silicon. (a) Schematic of a delta-layer device formed by incorporating phosphorus atoms into a single atomic plane of the Si (100) lattice, subsequently encapsulated with $\sim 40 \text{ nm}$ of intrinsic silicon. Dopant segregation during encapsulation broadens the profile into a $\sim 2 \text{ nm}$ distribution. (b) DFT-calculated band structure of a saturation-doped phosphorus delta layer ($1/4 \text{ ML}$ coverage) in silicon, showing donor-derived sub bands within the band gap. (c) Atomic structure model, local density of states, and donor-electron distribution of a $1/4 \text{ ML}$ delta layer, plotted as a function of distance from the dopant plane. Panels (b) and (c) are adapted from Carter et al ⁹⁵.

3.2 Si:P Nanostructures

The flexibility of hydrogen lithography allows arbitrary 2D patches to be defined instead of just a uniform doped delta layer. These extended delta-doped regions can serve as metallic leads and gates in device architectures. Electrons in these regions form a two-dimensional electron gas (2DEG) system with a density of states (DOS) characteristic of two-dimensional systems:

$$g_{2D}(E) = \frac{m^*}{\pi \hbar^2} \quad (3.6)$$

This constant DOS is a useful property for defining stable electron reservoirs and electrostatic gates, as it allows for predictable capacitive coupling and screening effects.

When the delta-doped leads are further narrowed in order to interface with smaller nanostructures such as the quantum dots, the dimensionality of the system in terms of electrical properties changes. As the width approaches only a few nanometers, quantum confinement in the lateral direction lifts the continuous 2D spectrum into discrete sub bands which exhibit DOS more of one-dimensional characteristics:

$$g_{1D}(E) \propto \frac{1}{\sqrt{E - E_n}} \quad (3.7)$$

where E_n are the discrete sub band edges. This produces sharp peaks in the DOS corresponding to van Hove singularities⁸¹ that can be mistaken for features of the quantum dots under study if not carefully accounted for. For this reason, practical STM-fabricated devices are designed with lead widths greater than ~ 5 nm to ensure that DOS of the leads retain quasi continuous while providing reliable electrical contact and proper capacitive coupling to quantum dots.

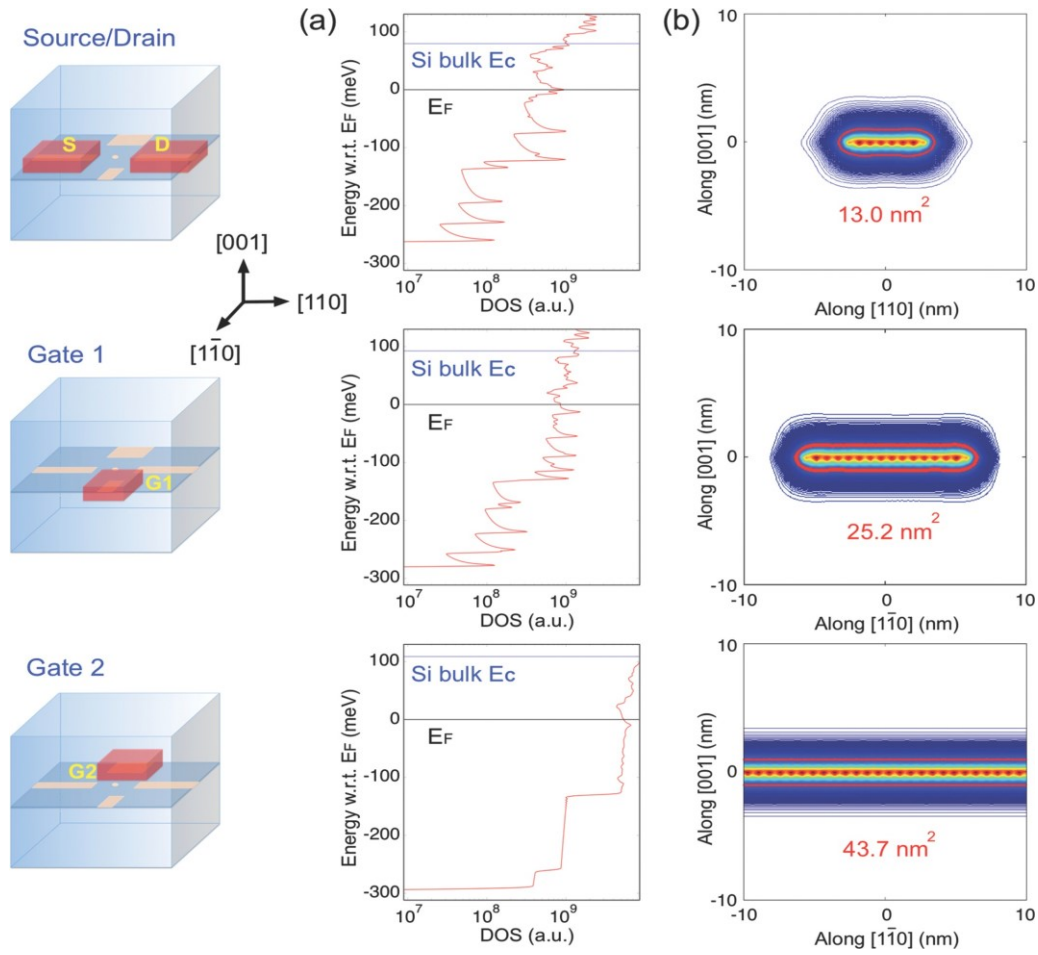


Figure 3.5 Simulated density of states (DOS) of phosphorus-doped leads with varying widths. Wide delta-doped leads (Gate 2) exhibit a nearly constant two-dimensional DOS. As the lead width is reduced to a few nanometers, quantum confinement lifts the 2D continuum into discrete 1D sub bands (Source/Drain and Gate 1), producing sharp van Hove singularities at the sub band edges. Such features can mimic quantum-dot resonances and therefore must be carefully distinguished in transport measurements. Figure adapted from Ryu et al ⁹².

3.2.1 Electron Confinement

As the lateral size of the two-dimensional electron gas (2DEG) continues to shrink, the system evolves toward a zero-dimensional (0D) island. In this regime, additional confinement effects emerge, giving rise to discrete electronic states and single electron charging phenomena. The behavior of such nanostructures is governed primarily by two key energy scales: the charging energy, associated with the electrostatic

energy of adding individual electrons, and the quantum confinement energy, arising from spatial quantization of the electronic wavefunctions.

Charging energy,

$$E_C = \frac{e^2}{C_\Sigma} \quad (3.8)$$

represents the cost of classical electrostatic energy for adding an extra electron onto the island, where C_Σ is the total capacitance of the island including contributions from nearby gates and the island's self-capacitance. This term is determined primarily by the island's size, geometry, and capacitive coupling to the leads. In the next subsection, we introduce the constant-interaction (CI) model to formalize how these capacitances and energies are calculated. Single electron charging events become observable¹⁰⁴ when the charging energy E_C exceed the thermal energy $k_B T$ and forms the basis of Coulomb blockade phenomena in single-electron transistors.

Quantum confinement energy arises from the finite lateral dimensions of the island, which form an effective two-dimensional potential well for the electrons. Within a simplified particle-in-a-box approximation, the allowed energy levels are given by

$$E_{m,n} = \frac{\hbar^2}{2m^*} \left[\left(\frac{m\pi}{L_x} \right)^2 + \left(\frac{n\pi}{L_y} \right)^2 \right] \quad (3.9)$$

where L_x and L_y are the lateral dimensions of the island, m^* is the electron effective mass, and m, n are integer quantum numbers defining the discrete modes. In larger islands, these confinement energies are small compared to the charging energy, resulting in nearly uniform electron addition spectra. As the island size decreases, the level spacing between successive states increases, and quantum confinement effects become more pronounced. When the island shrinks to only a few nanometers and comprises just a handful of phosphorus donors, the simple box model ceases to be valid. In this strongly confined regime, the discrete

atomic potential and electron–electron interactions dominate, requiring a full atomistic treatment of the energy spectrum using tight-binding or configuration-interaction methods.

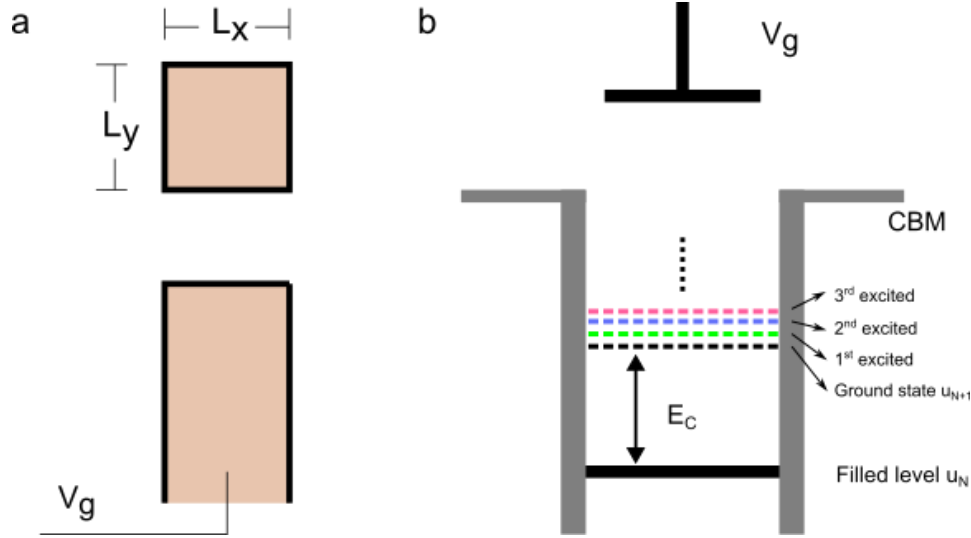


Figure 3.6 Electron confinement in a nanoscale dopant island. (a) Schematic of a dopant island coupled to a nearby gate with charging energy $E_C = \frac{e^2}{2C_S}$, where C_S is the total capacitance of the island. (b) Energy-level diagram of the island showing the relation between charging energy and quantum confinement energy.

The electron addition energy E_{add} of the island is the sum of these two terms,

$$E_{add} = E_C + E_{m,n} \quad (3.10)$$

In realistic Si:P devices, valley physics and electron–electron interactions add further complexity^{105,106} to this simple confinement picture by convoluting the two terms and creating valley-orbital states. Nonetheless the general trend remains that larger islands exhibit nearly uniform addition energies dominated by charging effects and a quasi-continuous density of states, whereas smaller islands display non-uniform addition spectra with pronounced quantum confinement features.

These principles serve as practical guidelines for engineering dopant-based quantum dots. By precisely controlling the island geometry and its capacitive coupling to surrounding gates, one can tune the charging and confinement energies to achieve regimes optimized for specific quantum applications.

3.2.2 Single-Electron Transistor (SET)

The simplest Si:P nanostructure that exhibits quantum tunneling behavior is a tunnel junction¹⁰⁷, where two phosphorus-doped leads are separated by a narrow undoped region of few nanometers. This barrier gap allows electrons to tunnel through. By placing two such junctions in series with a middle dopant island, a single-electron transistor (SET)^{104,108,109} is formed. In this geometry, the island acts as a central electron reservoir with a finite charging energy, while the source and drain leads serve as metallic contacts with quasi-continuous density of states.

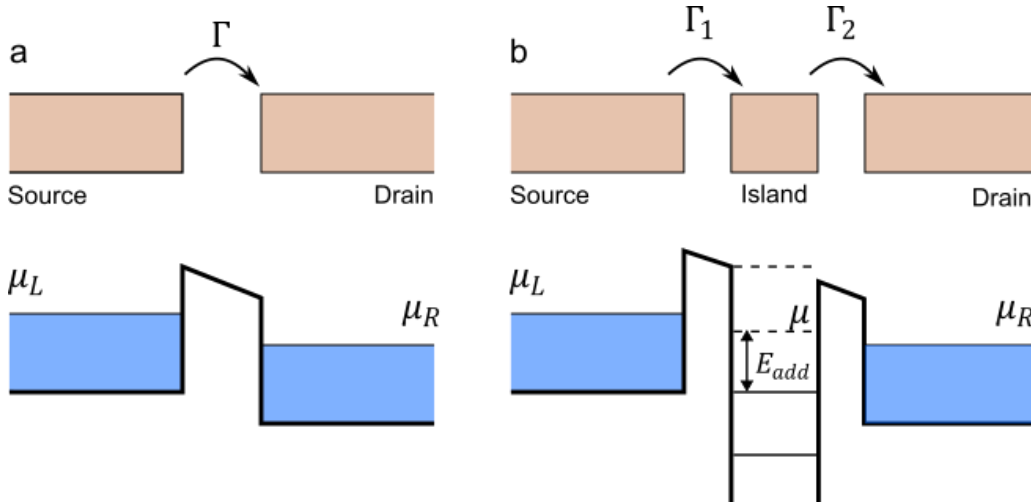


Figure 3.7 Schematic (upper panels) and energy diagrams (lower panels) of a tunnel junction and a single-electron transistor (SET). (a) In a tunnel junction, two metallic leads are separated by a single potential barrier, allowing electrons to tunnel through with a characteristic rate Γ when the chemical potentials satisfy $\mu_L > \mu_R$. Multiple electrons can tunnel at the same time. (b) In a SET, a small island is placed between the left and right leads, forming two tunnel barriers with rates Γ_1 and Γ_2 . The island supports discrete energy levels separated by the characteristic addition energy E_{add} . Once a level is occupied, Coulomb blockade prevents another electron from entering, ensuring that electrons can only tunnel one at a time from $\mu_L > \mu > \mu_R$.

Figure 3.7 illustrates the schematic and energy diagrams of a tunnel junction and a single-electron transistor (SET). The dopant regions are shown in orange, while the electron sea in the leads is depicted in blue. In a tunnel junction, many electrons can tunnel through the barrier simultaneously, resulting in a continuous current once a bias voltage is applied $\mu_L > \mu_R$. In contrast, the SET operates in the Coulomb blockade regime, where a finite charging energy restricts transport to one electron at a time.

Both tunnel junctions and SETs can, in principle, function as charge sensors for nearby quantum dots. However, in Si:P devices, the tunnel rate of a simple tunnel junction is only weakly affected by nearby charge rearrangements, unlike quantum point contacts (QPCs). In comparison, the electrochemical potential of the SET island is highly sensitive to nearby electrostatic changes, allowing the device to switch between conducting and blockaded states in response to a nearby charge transition. Therefore, a SET is used predominantly for charge sensing in the Si:P platform. In the following, we introduce the constant-interaction (CI) model ¹¹⁰ and explain the characteristic Coulomb oscillations observed in the SET conductance.

Within the framework of the CI model, all electrodes and quantum nanostructures are treated as metallic terminals, denoted by indices ij , that are capacitively coupled to one another. The electrostatic energy of the system is determined entirely by these capacitive couplings. For quantum dots, the internal single-particle energy levels are assumed to be independent of the external electrostatic environment. Furthermore, the capacitances between different terminals are taken to be constant and do not vary with applied voltages. Under these assumptions, the potential of floating nodes depends linearly on the applied voltages on the gates, with the proportionality called gate lever arms determined by the capacitance matrix C_{ij} . Although approximate, this model successfully captures the essential physics of SETs across a wide range of device geometries, from large metallic islands to single-donor systems. Figure 3.8 shows the schematic of the capacitance network representation of a SET device with two control gates.

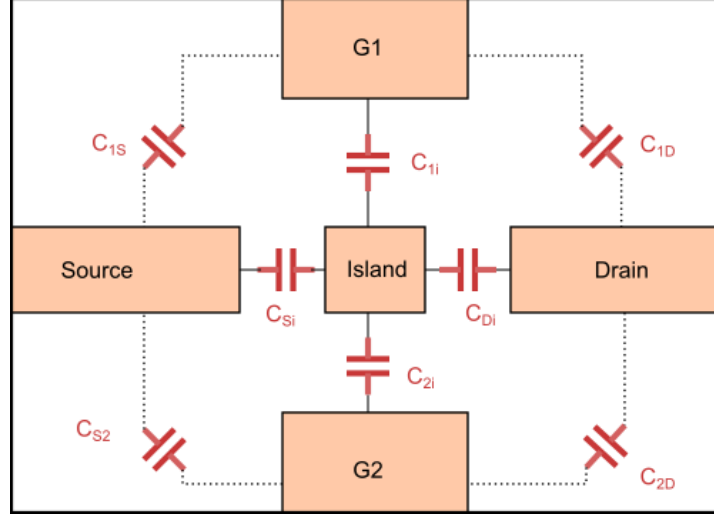


Figure 3.8 Capacitance network of a SET device with two control gates. All gates (source, drain, G1 and G2) are connected to a voltage source with fixed applied voltage. The central island is floating with its electrostatic potential determined by the gate voltages via the capacitance couplings. The mutual capacitances between different terminals are labelled in red.

To obtain the island potential at fixed gate voltages, we use the basic relation between voltages and charges, $Q=C \cdot V$ with C the symmetric Maxwell capacitance matrix, and V and Q the voltage and charge vectors:

$$\begin{pmatrix} Q_i \\ Q_1 \\ Q_2 \\ Q_S \\ Q_D \end{pmatrix} = \begin{bmatrix} C_{ii} & C_{i1} & C_{i2} & C_{iS} & C_{iD} \\ & C_{11} & & & \\ & & C_{22} & & \\ & & & C_{SS} & \\ & & & & C_{DD} \end{bmatrix} \begin{pmatrix} V_i \\ V_1 \\ V_2 \\ V_S \\ V_D \end{pmatrix} \quad (3.11)$$

Q_i and V_i are the total charge and electrostatic potential of the island. The empty elements in the upper right triangle correspond to capacitance between the leads and are not relevant for the present discussion. Since the gate voltages are fixed and we are not interested in the charges on the leads, the full 5×5 capacitance matrix can be reduced to an effective 1×1 form that describes the island:

$$Q_i = C_{ii} \cdot V_i + C_{i1} \cdot (V_i - V_1) + C_{i2} \cdot (V_i - V_2) + C_{iS} \cdot (V_i - V_S) + C_{iD} \cdot (V_i - V_D) \quad (3.12)$$

From which we obtain the island electrostatic potential:

$$V_i = \frac{1}{C_\Sigma} (Q_i + C_{i1}V_1 + C_{i2}V_2 + C_{iS}V_S + C_{iD}V_D) \quad (3.13)$$

where $C_\Sigma = C_{ii} + C_{i1} + C_{i2} + C_{iS} + C_{iD}$ is the total capacitance of the island. From this equation, the electrostatic potential of the island can be tuned linearly by the gate voltages, the corresponding coefficient is defined as the gate lever arm, for example, a 1V increase on gate 1 voltage raises the island potential by $\alpha_{i1} = C_{i1}/C_\Sigma$.

We now derive the charging energy of the island which gives Coulomb blockade. The total energy of the island can be written as

$$E(N) = \sum_{i=1}^N \epsilon_i + \frac{1}{2} C_\Sigma V_i^2 \quad (3.14)$$

where N is the number of excess electrons from charge neutrality related to the total charge by $Q_i = Ne - Q_0$, ϵ_i is the single-particle orbital energies equivalent to the quantum confinement energy $E_{m,n}$ defined in the 3.2.1. The chemical potential for adding the N+1 electron to the island is defined as:

$$\mu(N+1) = E(N+1) - E(N) \quad (3.15)$$

Written this expression explicitly gives,

$$\mu(N+1) = \frac{e^2}{2C_\Sigma} + \epsilon_{N+1} + e \frac{Ne - Q_0}{C_\Sigma} - e \sum_{\sigma} \alpha_{i\sigma} V_{\sigma} \quad (3.16)$$

where the first term is a constant, the second term represents the single-particle orbital energy of the added N+1 electron, the third term corresponds to the classical charging-energy, and the final term describes the gate-tunable contribution. The summation of σ is over all gate electrodes held at fixed voltages V_{σ} , and $\alpha_{i\sigma}$ represents the corresponding lever-arm coefficients. This gives the energy spectrum of the island as a ladder of single electron levels separated by its charging energy $E_c = \frac{e^2}{C_\Sigma}$. The island is filled with N electrons such that the chemical potential of the N+1 electron exceeds the Fermi-level of the source (μ_S) and drain (μ_D)

leads, that is, when $\mu(N + 1) > \mu_S, \mu_D > \mu(N)$. By varying the voltages on gates G1 and G2 (the plunger gates), one can easily add or remove electrons from the island.

For an electron to tunnel through the SET, the chemical potential of the next unfilled level, $\mu(N + 1)$, must lie within the source–drain bias window, satisfying the condition $\mu_S > \mu(N + 1) > \mu_D$. Under this alignment, an electron can sequentially tunnel onto the island from the source and then off to the drain, resulting in a measurable current. As the plunger gate voltages are continuously tuned, the electrochemical potential of the island shifts, periodically bringing new charge states into the bias window and producing a periodic modulation of the SET current known as Coulomb oscillations.

These oscillations manifest as a series of conductance peaks in the current–voltage characteristics of the SET and, in bias spectroscopy, give rise to the characteristic Coulomb diamond pattern shown in Figure 3.9. Each diamond represents an added electron onto the island. Within each diamond-shaped region, the current is suppressed due to Coulomb blockade, as no available island state lies within the bias window. When the applied source–drain bias exceeds the island’s charging energy, E_C , at least one energy level always remains accessible for tunneling, and the blockade vanishes, corresponding to the closure of the Coulomb diamonds.

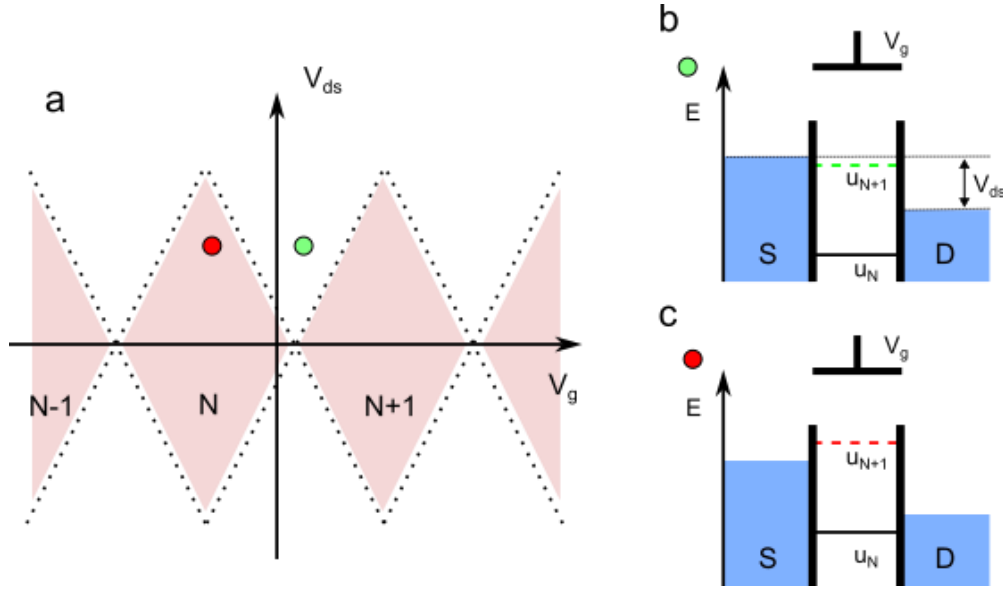


Figure 3.9 Coulomb oscillations in a single-electron transistor (SET). (a) Charge stability diagram showing the source–drain bias (vertical axis) versus gate voltage (horizontal axis). The shaded regions correspond to Coulomb diamonds, where electron tunneling through the SET is energetically forbidden. Each diamond represents an additional electron added to the island as the plunger gate lowers its energy levels. (b) and (c) Energy diagrams illustrating conditions outside (SET on) and inside (SET off) the Coulomb blockade region. When the source–drain bias exceeds the island’s addition energy, at least one level lies within the bias window, allowing continuous tunneling and closing of the diamonds.

Experimentally, the charging energy E_C is controlled by adjusting the size of the island, while the on-state tunneling current is determined by the width of the two tunnel barriers, which are precisely defined using STM lithography. The design principle is to achieve a sufficiently high on-state current for charge-sensing purpose, while maintaining strong electron confinement on the island.

3.2.3 Transport current through a SET

To quantitatively describe electron transport and estimate the steady-state current through a single-electron transistor, we employ a standard framework¹¹¹ in which tunneling rates are calculated using Fermi’s golden rule. In practice, one of the source-drain lead (here we choose the source) is grounded and connected to a

current amplifier. A bias voltage V_{DS} is applied on the drain to open a transport window. For current to transport through the SET, an island state must lie within the source–drain bias window $\mu_D = -eV_{DS} > \mu(N + 1) > \mu_S$ so that electrons can tunnel sequentially onto and off the island. The tunneling rates through the left and right barriers, Γ_L and Γ_R are determined by the overlapping of the electron wavefunctions across the corresponding junction and can be estimated under a low bias limit and assuming elastic tunneling ¹¹¹:

$$\Gamma_{L,R} = \frac{2\pi}{h} |A|^2 D_i D_f \frac{-\Delta F}{1 - \exp\left(\frac{\Delta F}{k_B T}\right)} \quad (3.17)$$

where A is the overlap matrix element, D_i, D_f are the initial and final density of states and ΔF is the change in Helmholtz's free energy due to the tunneling event, $\Delta F_L = \mu(N + 1) - \mu_D$, $\Delta F_R = \mu_S - \mu(N + 1)$. For a small ΔF , the density of states across the junction is approximately constant and the tunnel junction barrier therefore gives a symmetric and almost linear I-V characteristic.

To calculate the steady-state current, we use a rate-equation approach. For simplicity, consider only the charge states N and $N+1$ such that $P(N) + P(N + 1) = 1$. The probability $P(N)$ that the island contains N electrons evolves according to:

$$\frac{\partial P(N)}{\partial t} = \Gamma^{N,N+1} P(N + 1) - \Gamma^{N+1,N} P(N) \quad (3.18)$$

where $\Gamma^{N+1,N}$ is the rate for tunneling onto the island from the left/right lead, and $\Gamma^{N,N+1}$ is the rate for tunneling off the island. The steady state occupation probability can then be solved by setting $\frac{dP(N)}{dt} = 0$, and the steady-state current through the SET ¹¹²:

$$I_{DS}(N) = e \frac{\Gamma_L^{N,N+1} \Gamma_R^{N+1,N} - \Gamma_L^{N+1,N} \Gamma_R^{N,N+1}}{\Gamma_L^{N+1,N} + \Gamma_R^{N+1,N} + \Gamma_L^{N,N+1} + \Gamma_R^{N,N+1}} \quad (3.19)$$

In the zero-temperature limit ($\Delta F \gg kT$), the tunneling across the junction is directional such that $\Gamma \sim 0$ for $\Delta F > 0$. The above equation further simplifies to:

$$I_{DS}(N) = e \frac{\Gamma_L^{N,N+1} \Gamma_R^{N+1,N}}{\Gamma_L^{N,N+1} + \Gamma_R^{N+1,N}} = e \frac{\Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R} \quad (3.20)$$

This expression captures the essential dependence of the SET current on the tunneling rates (Γ_L and Γ_R) and the thermal broadening of the lead distributions when there is only one charge level within the source-drain bias. In addition, excited states of the island which appear as extra resonances in the differential conductance (dI/dV) spectrum can be modelled by adding more terms into the rate equation and manifest as line features running parallel to the main diamond edges.

In summary, the transport theory of the SET presented in this section integrates the electrostatic framework of the constant-interaction model with quantum tunneling dynamics to capture the full conductance behavior. In practical Si:P devices, the SET serves as a highly sensitive charge sensor, capable of detecting single-electron transitions in nearby quantum dots or donor sites.

Chapter 4: STM Automation

4.1 Introduction and Motivation

Despite the extraordinary spatial resolution achievable with STM lithography, its throughput remains several orders of magnitude lower than that of conventional semiconductor patterning techniques. In traditional photolithography^{113,114}, including modern extreme-ultraviolet (EUV) systems, the entire device pattern is transferred in a single exposure step through a prefabricated mask, enabling wafer-scale processing at few nanometer precision and high yield. In contrast, STM lithography is a serial writing process^{53,115}: the tip removes hydrogen atoms line-by-line or site-by-site, which fundamentally limits the fabrication speed and makes the process highly sensitive to local variations in tip condition and slow drift of the sample surface, factors that are negligible in standard lithographic systems. Recent advances, such as EUV-induced hydrogen desorption¹¹⁶ have demonstrated promising routes toward one-pass large-area hydrogen lithography; however, the atomic-precision regions that define quantum dots, tunnel barriers, and dopant clusters must still be patterned using a STM tip. These constraints emphasize the necessity of developing robust STM workflows capable of maintaining atomic precision while improving throughput and reproducibility.

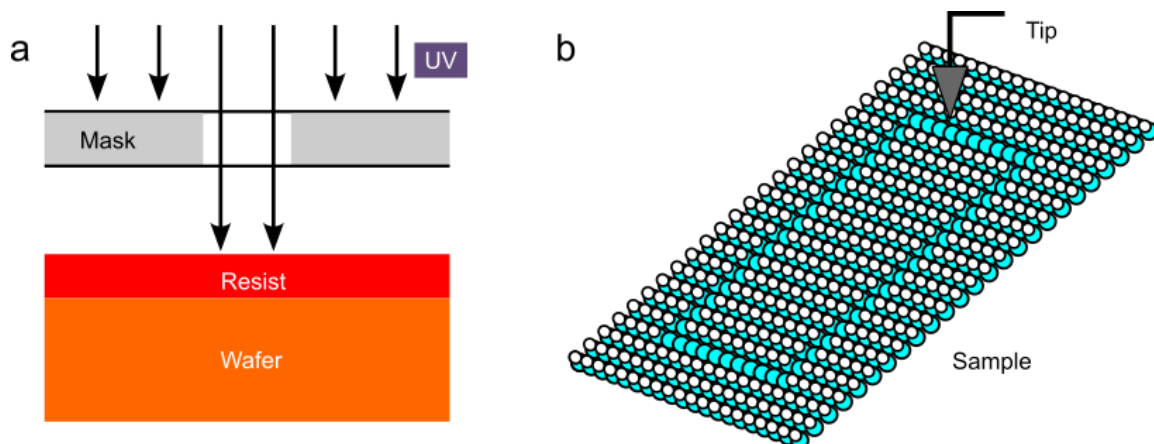


Figure 4.1 Comparison between traditional lithography and STM lithography. (a) Schematic illustration of conventional semiconductor lithography (optical, electron-beam, or EUV), where the entire pattern is defined in a single exposure through a prefabricated mask, enabling high-throughput, parallel fabrication. (b) STM hydrogen lithography, in which the STM tip removes hydrogen atoms sequentially along defined paths, forming patterns line-by-line. This serial process provides unparalleled atomic precision but is limited by slow writing speed, tip-condition variation, and sample drift. Automation strategies presented in this chapter aim to mitigate these limitations and improve the fabrication throughput.

The fabrication of atomically precise devices using STM lithography relies critically on the ability to pattern desired shapes or masks with high fidelity. In its current form, this process is often performed manually^{43,45}, requiring the operator to remove individual hydrogen atoms in carefully designed geometries patch by patch. While this approach has enabled the demonstration of proof-of-concept devices, it suffers from major limitations: patterning is extremely time-consuming, labor-intensive, and subject to operator variability. Even for experts, the patterning process of a single complex device can require many hours or days of effort.

To overcome these challenges, we have developed algorithms and workflows for automating STM patterning. The goal of this automation is analogous to that of electronic design automation (EDA) software in the semiconductor industry: to provide a framework where device layouts can be specified at a high level

and then automatically translated into well-defined STM instructions. By reducing manual intervention, these methods not only accelerate device fabrication but also improve reproducibility and open the path toward systematic prototyping of increasingly complex quantum architectures.

In this chapter, we address two complementary challenges in STM automation. The first is the patterning of atomic-precision structures, such as quantum dots and donor-dot arrays, where the number and position of hydrogen atoms removed must be controlled with nanometer accuracy. Such structures form the essential components for analog quantum simulators and spin-based qubits where the utility depends critically on precision. The second challenge is the fabrication of large fanout structures used to interface nanoscale devices with macroscopic electrodes. While these patterns are less demanding in terms of atomic accuracy, their large area makes them time consuming to produce manually. Automating both tasks establishes a consistent framework for STM-based device fabrication aiming for both precision and throughput.

4.2 Problem Definition

Automating STM lithography requires translating abstract device layouts into a sequence of low-level operations that the microscope can execute. Unlike conventional lithography, where the entire pattern is transferred in a single exposure, STM lithography proceeds sequentially, with the tip performing each operation individually. This process is conceptually similar to a graphic de-compiler that converts high-level geometric designs into a series of precise, executable tip movements, like a 3D printer. Such conversion or planning is often nontrivial and may be implemented through multiple strategies, each offering different trade-offs in efficiency and accuracy. Establishing a standardized and systematic translation framework is a critical step toward scalable and reproducible STM-based device fabrication. The major challenge to achieve this lies in fulfilling each planned step while conforming to constraints of the underlying fabrication process with many uncertainties. In the following, we propose a practical workflow for STM automation and define some of the key steps with an emphasize that every step can be executed in an unambiguous manner.

Transitional semiconductor node processes involve many different steps and layer stack ups^{117,118}. For STM lithography, only a single 2D layer of Hydrogen lithography mask needs to be created. The top-level key stages include:

- 1 Geometry specification – defining the device at a design level, for example as an array of quantum dots, an SET, or fanout structures. This stage specifies what needs to be fabricated and establishes the critical dimensions that must be maintained.
- 2 Pattern planning – decomposing the desired geometry into STM-compatible operations. For hydrogen lithography, these operations typically take two forms:
 - Line rasterization, in which the STM tip is scanned across a defined path while applying a lithographic voltage bias to remove hydrogen atoms along a continuous trajectory.
 - Point desorption, often done with feedback-controlled lithography, where voltage pulses at single locations selectively desorb hydrogen atoms with high spatial precision.
- 3 Instruction execution – converting planned patterns into sequences of voltage, current, and tip position commands that the STM control software can run precisely.
- 4 Verification and error correction – an optional imaging-based feedback loop used to confirm that the intended pattern has been accurately written and to apply corrective operations when significant deviations are detected. Traditionally, this verification has been performed manually, with the operator scanning the patterned region to ensure that all critical dimensions are met. In the automated workflow, an integrated error detection and correction algorithm compares post-lithography STM images with the original design file and automatically determines whether rework is required before proceeding to the next operation.

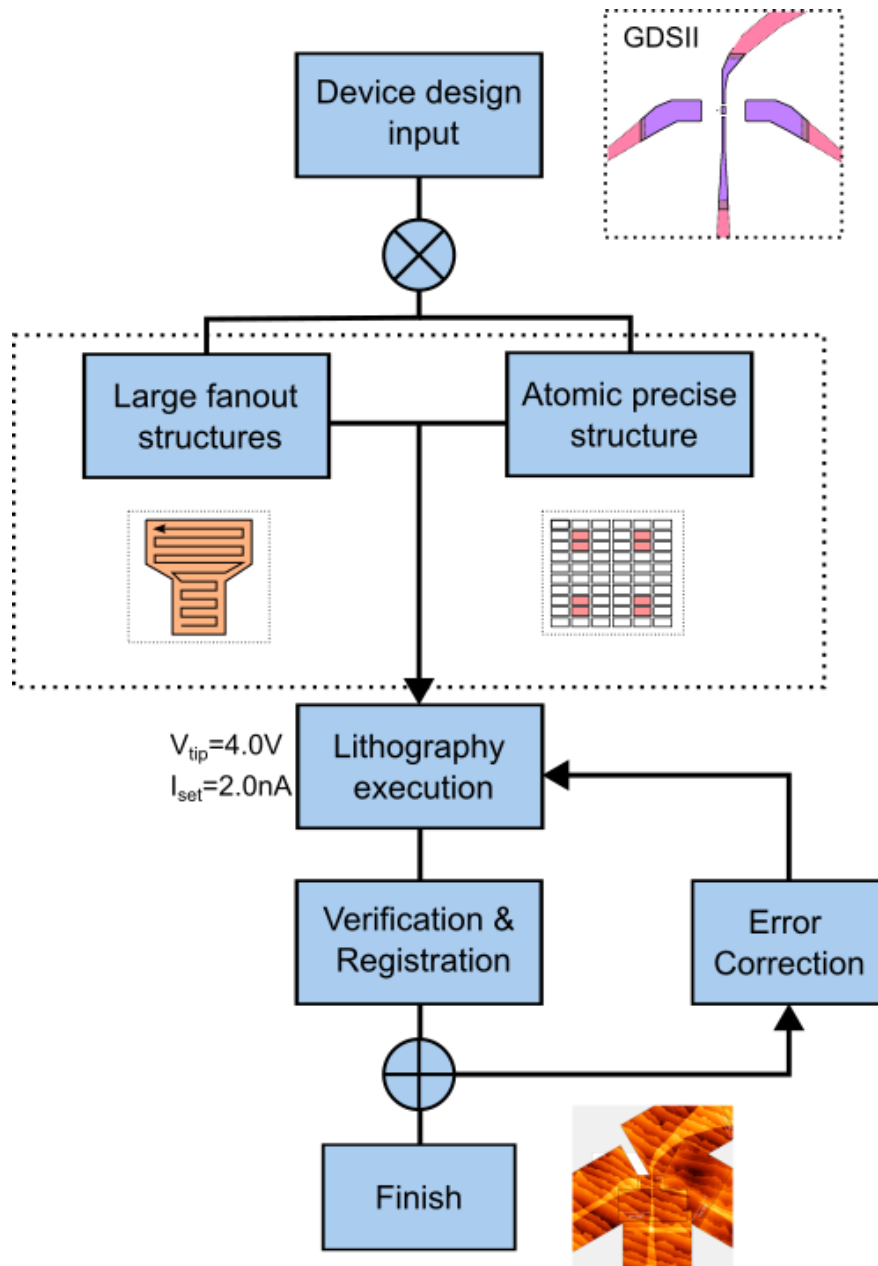


Figure 4.2 Flowchart for STM lithography automation. At the top level, high-level design intent, such as a geometric layout, a GDS file, or a natural-language request, is specified by the user. This design is passed to the pattern-planning layer, which translates the geometry into STM-compatible operations such as line rasterization or point desorption, accounting for lattice orientation and drift. The instruction-generation layer then converts these planned operations into low-level STM commands that define tip trajectories, tunneling bias, and current setpoints. Finally, the execution and feedback layer performs the lithography, acquires STM images for device verification and registration, and carries out optional corrections procedure

if necessary. This hierarchical workflow bridges high-level design intent with low-level tip control, forming the conceptual foundation of the STM automation framework developed in this chapter.

Within this proposed framework, STM automation is best understood not as a single algorithm, but as a hierarchical system of modules that can be combined to accomplish tasks with distinct accuracy and efficiency requirements. Small-scale structures such as quantum dots demand precise alignment and single-site hydrogen desorption, whereas large-scale fanout patterns prioritize writing speed and lithography completeness. The following sections examine each of these problems in detail, illustrating how the general framework adapts to their respective requirements.

4.3 Automated Patterning of Atomic-Precision Structures

Atomic-precision patterning lies at the core of STM-based fabrication because the functionality of a device is determined directly by the number and spatial configuration of dopant atoms. For example, in a few-dopant quantum dot, the binding energy and charging energy are highly sensitive not only to the exact dopant number but also to the arrangement of dopants within the cluster. Similarly, the tunnel coupling between neighboring quantum dots depends exponentially on their separation. A variation of even a single lattice site in spacing could shift the energy spectrum and alter exchange couplings significantly^{87,119}. These sensitivities mean that reliable qubit operation or analog quantum simulation requires patterning accuracy at the level of individual lattice sites.

To illustrate the automation process, we take an example pattern of a 4×4 staggered three-dimer patches. A ZyVector control unit operates in creep and hysteresis correction (CHC) mode to minimize the tip settling time after each tip movement. The atomic-scale automation workflow comprises a sequence of key sub-procedures aimed at achieving precise spatial control:

(i) Drift detection and correction.

The process begins by selecting a flat region of the surface with minimal dangling bonds and preferably no atomic step edges. Long STM patterning sequences are inherently susceptible to slow relative drift¹²⁰ between the tip and the sample, and when atomic precision is required, even the displacement of a single dimer should be avoided. To quantify and compensate for this effect, two images of the same region are acquired at a defined time interval, typically a few minutes apart. A phase-correlation algorithm^{121,122} is then applied to determine the relative offset between the two images and dividing this offset by the elapsed time yields the drift rate. This measured drift vector is subsequently incorporated into all patterning operations to dynamically correct the target positions, ensuring that each hydrogen desorption event remains accurately aligned with the intended atomic sites.

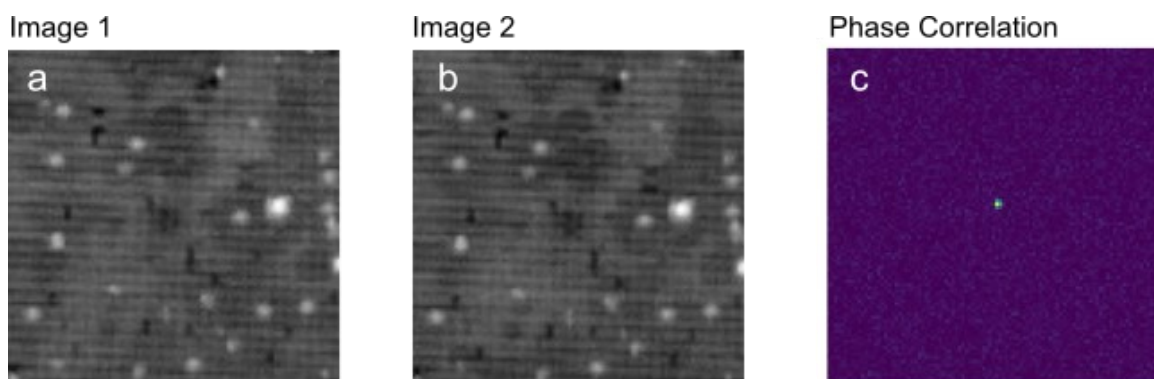


Figure 4.3 Drift detection using phase cross-correlation analysis. (a) and (b) STM images of a hydrogen-terminated Si (100) surface acquired with a 120 s time interval under imaging conditions of -2.0 V and 0.05 nA (100×100 pixels). (c) Phase cross-correlation amplitude map between the two scans. The map is obtained by first computing the two-dimensional Fourier transform of each image, forming the cross-power spectrum from the normalized product of the two Fourier spectra, and then applying an inverse FFT to generate the correlation map. The offset of the bright spot relative to the map center indicates the drift between the two scans. Dividing this offset by the total elapsed time (the sum of the waiting period 120 s and the scan time 34 s) yields a measured drift rate of approximately $(4, 0)$ pm /s.

(ii) Atomic order recognition.

The next step is to register the silicon lattice at atomic resolution. A high-resolution STM image of the target region is acquired, and its periodicity is extracted using Fourier transform to determine both the lattice orientation and lattice constant. Individual dimer rows and atomic sites are then registered and indexed within the image, providing a coordinate system tied to the crystal lattice. For larger fields of view, where tip drift and hysteresis distortions are non-negligible, the image is subdivided into smaller regions. Each subregion undergoes lattice identification independently, after which the results are stitched together to yield a consistent lattice map covering the full original scan.

(iii) Pixel definition and mapping to atomic sites.

Once the lattice is registered and drift is characterized, the desired lithographic pattern is mapped onto the surface as a collection of atomic “pixels”. In the current implementation, a pixel is defined as two hydrogen atoms on a single silicon dimer, reflecting the typical resolution of standard lithography methods. Future developments may extend this framework to “half pixels,” where a single hydrogen atom within a dimer is targeted, thereby enabling true single-atom precision. Each pixel corresponds to one or more lattice positions identified in step (ii).

(iv) Lithography execution.

Patterning is then performed by translating pixel definitions into STM tip trajectories. Two approaches are used: (1) line rasterization, where the tip is scanned between defined start and end points while applying a lithographic bias to desorb hydrogen along a continuous path, and (2) feedback-controlled lithography ⁵⁴, (developed by our group member Jonathan Wyrick), in which the hydrogen desorption process is monitored in real time through changes in tip height. The coordinates of each targeted pixel are corrected for drift based on the measured drift rate and elapsed time between imaging and patterning, minimizing positional errors during extended writing sessions.

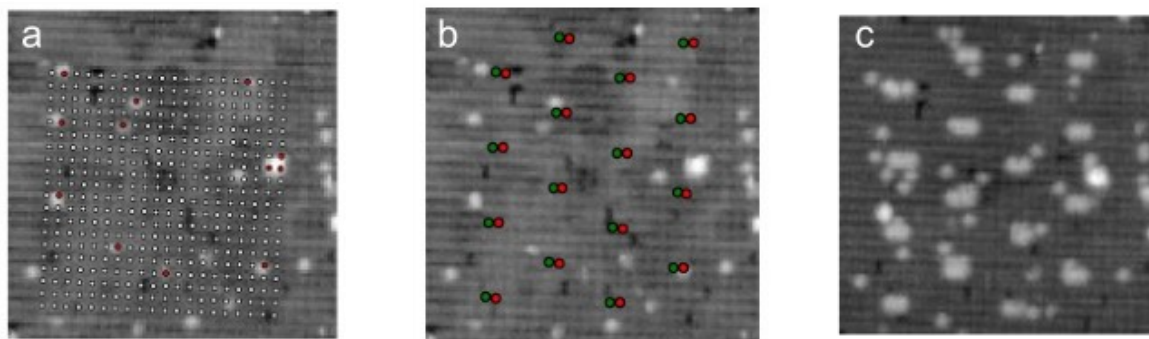


Figure 4.4 Atomic lattice registration and lithography execution. (a) The surface dimer k -vector (amplitude and orientation) is identified from the dominant peak in the Fourier transform of an STM image. An annular mask centered at the expected magnitude $|k| = 1/0.768 \text{ nm}^{-1}$ is applied to suppress low and high-frequency components and enhance the robustness of the lattice recognition. Once the k -vector is determined, individual dimer rows can be registered, and defects such as single dangling bonds or vacancies can be located with absolute atomic precision. (b) The target lithography mask (in this case a staggered 4×4 three dimer patch) is defined as either explicit spatial coordinates or bitmap representations in atomic-pixel units. Lithography is then performed using line rasterization or feedback-controlled desorption, with drift correction applied throughout to ensure accurate removal of the specified hydrogen atoms. (c) STM image of the surface after lithography, showing the patterned region corresponding to the predefined mask.

(v) Error detection and correction.

After patterning, an STM image is acquired to compare the actual device with the intended design. An error detection algorithm identifies discrepancies, such as missing desorption sites or unintended dangling bonds, and evaluates whether the mismatch exceeds a preset tolerance threshold. If necessary, error correction is attempted by either removing residual hydrogen atoms or capping unintended dangling bonds¹²³ by transferring a hydrogen atom from another location. This feedback-and-correction cycle continues until the error rate falls within the defined tolerance.

Together, these procedures combine into an automated pipeline capable of producing atomic-precision structures with improved reproducibility and throughput than manual tweaking. By combining lattice recognition, drift correction, pixel mapping, precision lithography, and error correction, the workflow

directly addresses the stringent requirements for patterning the critical parts of a Si:P quantum device. We note however that it is critical to start with a good tip with atomically sharp apex. In a good test case, the tip can perform well over a hundred atomically precise writes without requiring reconditioning. In a bad test case, the tip cannot maintain a single-dimer beam width, and attempted error-correction steps may introduce additional patterning errors rather than resolve them.

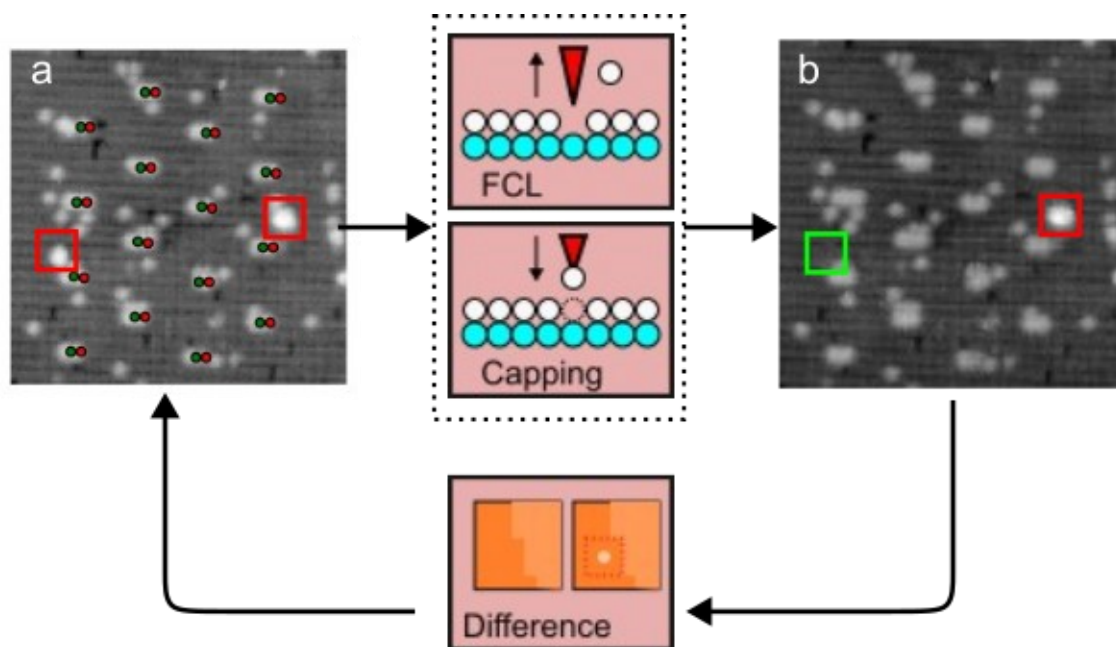


Figure 4.5 Error correction loop to restore lithography defects. (a) Designed lithography mask overlaid on an STM image of the patterned region. Two primary classes of defects can be observed. The first type is extra dangling bonds, which may preexist or be inadvertently created during lithography. Although isolated dangling bonds are generally benign, since they cannot adsorb PH_3 molecules. Larger defects (highlighted by red boxes) may contain multiple dangling bonds and incorporate unintended dopant atoms. The second type of defect arises from incomplete lithography, where hydrogen atoms that were intended to be desorbed remain on the surface. The defects are identified by comparing the experimental image with the ideal mask and are subsequently corrected either by feedback-controlled lithography to remove residual hydrogen atoms or by capping unwanted dangling bonds using a nearby hydrogen atom. (b) Example of a corrected region, where one defect (green box) has been successfully repaired while another (red box) remains after one correction loop. This feedback-driven correction process can be repeated iteratively until the defect density falls below a predefined threshold.

4.4 Automated Patterning of Large Fanout Structures

Large fanout structures bridge the atomically precise central device to macroscopic electrodes. In a donor-dot single-electron transistor (SET), for example, the central region consists of the SET island, a tunnel-coupled donor cluster, and the proximal segments of the source and drain leads. From these elements, multiple control leads (source, drain, and two or more plunger gates) “fan out” to enlarged contact pads. While atomic precision is not required over the full fanout, geometric continuity is non-negotiable. Any accidental gap within a lead or to the central region renders the device invalid.

To address this task, we developed an automated, step-by-step procedure for patterning large fanout structures. The workflow is designed to maximize throughput while preserving robust connectivity and alignment. [The following procedures have undergone preliminary test for the making of a two-lead device. Ongoing improvements aim to enhance the robustness of this workflow and extend its applicability to more complex device geometries.]

(i) Input layout and layer schema

The device layout is provided as a GDSII file containing two layers:

- Layer 1 (central region): includes the island, donor cluster, and immediately adjacent lead segments.
- Layer 2 (fanout network): contains extended leads and outer contact pads.

To guarantee electrical continuity, the two layers intentionally overlap at their boundary. This overlap region is patterned twice to avoid unintentional gaps.

(ii) Registration to the sample coordinate frame

The central region is patterned first, either manually or using the pipeline described in the last section and subsequently serves as a fiducial for registration when returning from the end of each lead. High-resolution

STM images of the central region are matched to the corresponding GDS geometry to compute an affine transform (scale, rotation, shear, and translation) that maps GDS coordinates to STM scan coordinates.

(iii) Patch-by-patch subdivision of each lead (stitch plan)

Because a single STM window cannot efficiently cover the high aspect ratios of long, narrow leads, each lead is decomposed into overlapping rectangular patches of reasonable size. Each patch includes an overlap with the previous patterned region, ensuring robust registration and continuity check when moving from one patch to the next.

(iv) Per-patch workflow

For each patch along a lead, the automation executes the following sequence:

- 1 Navigate and image. Move from the current position to the predicted location of next patch and acquire a topography and dI/dV scan under normal imaging conditions.
- 2 Overlap detection. Identify the overlap with the previously patterned region using a contrast-robust metric. dI/dV imaging is preferred as it provides clear contrast between hydrogen-desorbed and passivated regions while ignoring the step edges.
- 3 Local drift update. Compute the offset between expected and observed overlap via cross-correlation, then update the drift vector and refine the patch transform.
- 4 Fill-path generation. Rasterize the GDS polygons for this patch into STM tip paths using a scanline fill method inspired by the Boustrophedon algorithm. ¹²⁴
- 5 Lithography execution. Apply the lithographic bias and pattern the region according to the planned paths. Verification partial scans may be interleaved during long passes to periodically monitor litho quality and tip health.
- 6 Verification. After writing, acquire a fast dI/dV scan of the newly written region and its overlap. If continuity or coverage falls below threshold, a rewrite is invoked before proceeding. If no overlap is detected at all (rare case), the system assumes that the patch stride was too aggressive or that a

navigation error occurred. The scan window is then shifted backward by a fraction of a patch (e.g., 20%), re-imaged, and overlap detection is retried.

(v) Lead completion and safe return

Once a terminal contact pad is reached and verified, the system retraces the completed lead under imaging conditions. The central region is recognized by a pattern recognition algorithm, confirming successful return to the fiducial. The algorithm then anchors to the starting point of the next lead, checks transform consistency and repeats the patch cycle.

(vi) Error handling

- Tip-health monitoring: heuristics such as image roughness, and I–Z anomalies are used to assess the tip condition. If the score falls below threshold, the procedure requests tip re-conditioning.
- Checkpoints: after each patch is completed, scan window transformations and other metrics are stored, allowing the run to be resumed after interruptions.
- Abort conditions: repeated missing overlaps or poor lithography quality trigger a halt and request operator intervention (e.g., tip conditioning or parameter adjustment).

(vii) Overall connectivity assurance

After all leads are written, critical areas such as the Layer-1/Layer-2 overlap regions are re-imaged to confirm continuous connectivity. Optionally, the entire device can be re-imaged to check for any defects to ensure functionality.

The above describes a detailed, step-by-step workflow that translates a GDS layout into fully connected Si:P fanouts while preserving the integrity of the atomically precise central region. The procedure routinely patterns a complete lead without interruption when starting with a good tip. Tip deterioration during

lithography is detected by intermittent quality checks and trigger alarms for operator intervention. By reformulating the fanout task as a registered, overlapped, patch-and-stitch process with dI/dV-based continuity checks and drift compensation, this automation routine provides an effective solution for continuous large-area patterning and saves significant human time. Potential extensions of this workflow include in-situ tip restoration methods with re-qualification, adaptive segmentation that adjusts patch size and stride based on local geometry and drift rate to reduce unnecessary rewrites or relocations.

4.5 Conclusion and Outlook

In this chapter, we have introduced a framework for automating STM-based device fabrication that addresses both the need for atomic precision in quantum dot structures and the challenge of scaling to large-area fanout patterns. By developing algorithms that translate high-level device geometries into STM control instructions, we established a reproducible, efficient, and scalable approach to hydrogen lithography. The automated methods for atomic-precision patterning enable reliable fabrication of quantum dots, donor arrays, and other building blocks essential for qubit and quantum simulator architectures, while the large-area automation routines dramatically reduce human time required to construct extended fanout connections. These advances establish a comprehensive workflow that parallels the function of electronic design automation (EDA) in the semiconductor industry, but at the atomic scale.

It is important to note, however, that atomic-precision patterning is only the first step toward a fully functional device. The subsequent dopant incorporation process, where dopant atoms such as phosphorus are introduced into the exposed silicon sites, remains intrinsically stochastic. Variability in adsorption and incorporation rates can lead to nonuniform doping densities, which in turn influence device performance. Furthermore, after incorporation, dopants can diffuse or segregate^{75,125} during the silicon overgrowth stage, altering their intended spatial configuration. Addressing these challenges is essential for truly realizing reproducible, large-scale dopant-based systems for practical quantum applications.

Recent progress has begun to mitigate these issues through controlled chemical and thermal processes. Examples include tip-facilitated incorporation, in which the STM tip assists phosphine adsorption into engineered dangling bonds ⁴⁹, and elevated-temperature dosing strategies ¹²⁶ that improve incorporation efficiency and site selectivity. Extending automation into these stages, such as using machine learning to predict optimal dosing parameters or real-time incorporation outcomes ¹²⁷, represents a natural continuation of the automation framework introduced here.

By integrating these developments, future STM systems could expect end-to-end atomic device fabrication, from hydrogen lithography to dopant incorporation, entirely under automated control. Such progress would mark a key milestone toward the industrial realization of atomically precise semiconductor technology.

Chapter 5: Spin Readout in a Donor–Dot Single Electron Transistor

In the original proposal of the silicon-based phosphorus donor quantum computer, the nuclear spins of the donors were envisioned as qubits, while the bound electrons served as mediators for coupling via the exchange interaction. Although this architecture offers long coherence times and well-defined coupling mechanisms, it requires atomically precise dopant placement, an experimental challenge that remains beyond the current reach of fabrication capabilities.

As an intermediate step toward the original proposal, significant progress has been made using the donor-bound electron spins themselves as qubits. This approach relaxes the stringent requirements on dopant positioning while retaining the advantages of the donor-based platform. Pioneering work in this direction has been led by Morello’s group^{128,129} and Simmons’s group^{53,130} at the University of New South Wales (UNSW), employing ion implantation and scanning tunneling microscopy (STM) hydrogen lithography, respectively, to realize single-donor and few-donor qubits in silicon.

The advantages of using silicon as the host material for spin qubits were discussed in Chapter 1. Compared with other semiconductor systems, silicon possesses intrinsically weak spin–orbit coupling^{131,132}, thereby minimizing spin relaxation pathways, and benefits from a highly developed semiconductor fabrication infrastructure. In addition, the dominant source of decoherence for dopant spin qubits, the hyperfine interaction with naturally abundant ^{29}Si isotope, can be greatly suppressed through isotopic purification^{133,134}, down to the parts-per-million level, enabling exceptionally long electron spin relaxation (T_1) and coherence (T_2) times^{135,136}.

In this chapter, we present the donor–dot single-electron transistor (SET) device, which serves as a prototype single-qubit platform for demonstrating single-shot spin readout. In this architecture, the donor cluster hosts a bound electron that acts as the spin qubit, while the SET island functions both as an electron reservoir for the donor cluster and as a charge sensor capable of detecting spin-dependent tunneling events. We first describe the device geometry and electrostatic characteristics, followed by a discussion of its basic operation, including the processes of loading and unloading an electron from the donor cluster.

We then examine the critical role of electron temperature in achieving reliable spin readout. Because the electron spin states are Zeeman-split, the readout fidelity depends on maintaining a thermal energy well below the Zeeman energy. We determine the electron temperature in our device from low-bias transport measurements through the SET and confirm that the system operates within the spin-resolved regime at an applied magnetic field of approximately $B=1$ T.

Finally, we characterize the tunneling dynamics between the donor cluster and the SET island and demonstrate single-shot spin readout using the energy-selective tunneling approach. The spin relaxation time (T_1) is measured as a function of magnetic field, with the observed field dependence attributed to excess charge noise in the local environment. These results provide a foundation for future experiments integrating on-chip microwave antennas for electron spin resonance (ESR) control, enabling coherent spin manipulation and transforming the donor cluster into a fully functional spin qubit.

5.1 Introduction

The ability to accurately initialize and read out the state of a single qubit is one of the fundamental requirements for realizing any functional quantum computers. A well-defined state preparation and measurement (SPAM) protocol^{137,138} provides the essential physical interface for quantum-state manipulation in order to run higher-level quantum algorithms.

In silicon quantum-dot systems, the most common method for electron spin qubits is by energy selective readout through spin-to-charge conversion¹³⁹, where the electron spin state is mapped onto an observable change in the status of a charge sensor. This process can be realized through energy-selective tunneling or Pauli spin blockade mechanisms. In both cases, the detection of qubit spin state is performed by a nearby charge sensor, typically a quantum point contact (QPC) or a single electron transistor (SET). The status of the charge sensor is monitored to detect single-electron tunnel events which map into spin measurement results. An external magnetic field lifts the spin degeneracy via the Zeeman effect, splitting the spin-up and

spin-down energy levels by an amount $E_Z = g\mu_B B$ where g is the electron g -factor and μ_B is the Bohr magneton. When the electrochemical potential of the reservoir is tuned such that only the higher energy spin state lies above the Fermi level, tunneling occurs selectively for that spin orientation. By monitoring the SET (QPC) current in real time, one can infer the spin state of the electron based on whether a tunneling event occurs within a defined readout window. This single-shot measurement technique has become the standard for high-fidelity spin readout in both donor and gate-defined quantum-dot qubits. Figure 5.1 shows the original energy-selective spin readout scheme introduced by Elzerman et al.¹³⁹ in a GaAs/AlGaAs heterostructure device.

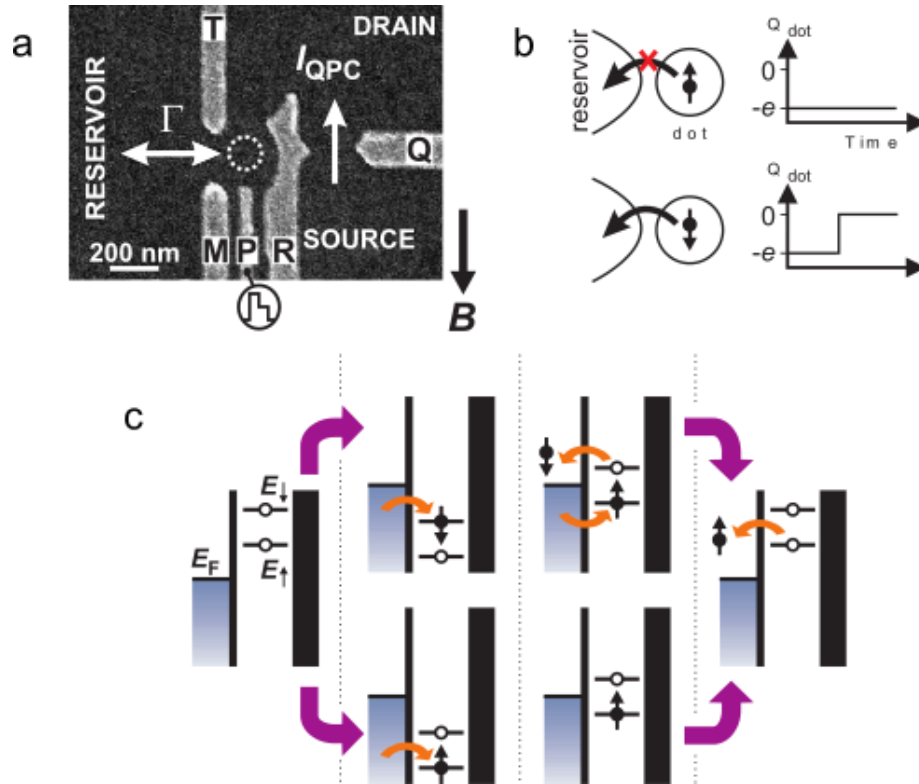


Figure 5.1 Schematic of the original energy-selective spin readout demonstration. (a) Micrograph of the experimental device, consisting of a quantum dot tunnel-coupled to an electron reservoir and monitored by a nearby quantum point contact (QPC) charge sensor. The QPC conductance is sensitive to single electron tunneling events between the dot and the reservoir. (b) Illustration of spin to charge conversion. The electron can tunnel to the reservoir only when its chemical potential lies above the reservoir Fermi level. The Zeeman splitting between the spin-up and spin-down states provides the energy selectivity

required for spin-dependent tunneling (c) Pulse sequence of the spin-readout protocol. Each cycle begins with loading a single electron with a random spin orientation, followed by tuning the dot potential to the readout position where only one spin state can tunnel out. The dot is then emptied to reset the system for the next measurement cycle. Figures are adapted from Elzerman et al ¹³⁹.

In this setup, a quantum dot hosting a single electron is defined electrostatically by surface gates in the two-dimensional electron gas (2DEG) of the heterostructure. The dot is tunnel-coupled to an electron reservoir with a tunnel rate of Γ , while a nearby quantum point contact (QPC) serves as the charge sensor. The source-drain current, I_{QPC} , depends sensitively on the dot's charge state through electrostatic coupling and is used to distinguish whether the dot is occupied or not. The spin degeneracy is lifted by the Zeeman energy into the spin-up and spin-down states with chemical potentials $E_{\uparrow}$ and $E_{\downarrow}$, respectively.

The spin readout process is demonstrated through a load–read–empty pulse sequence applied to the dot plunger gate (P). The sequence begins with the dot in an empty state. During the load phase, the dot potential is pulsed well below the reservoir Fermi level ($E_{\downarrow} \approx E_{\uparrow} \ll E_F$), allowing an electron of either spin to tunnel onto the dot. This load process occurs much faster than the characteristic spin relaxation time to ensure that a random spin is initialized. After an electron is loaded, I_{QPC} shifts from its “off” (dot empty) state to the “on” (dot occupied) state.

During the read phase, the dot's electrochemical potential is adjusted such that only the spin-up level lies above the reservoir Fermi energy ($E_{\downarrow} > E_F > E_{\uparrow}$). If the loaded electron is spin-up, it can tunnel out to the reservoir and subsequently a spin-down electron tunnels back in, causing I_{QPC} to transiently switch from “on” to “off” and back to “on.” If the loaded electron is spin-down, it remains in the dot and no current blip is observed. This transient signal—often called a “blip” in the time trace of I_{QPC} , provides a single-shot signature distinguishing the two spin states. By continuously monitoring I_{QPC} to detect the blip events during the read phase, single-shot spin readout can be achieved.

Finally, during the empty phase, the dot potential is raised to unload the electron and return the system to its initial state, preparing it for the next readout cycle. Statistical analysis of these time-domain signals

provides direct insight into the spin-dependent tunneling dynamics and confirms the two-level nature of the spin system.

Despite its conceptual simplicity, reliable spin readout imposes stringent requirements on both the device design and the measurement environment. Following the discussion by Mills et al ¹⁴⁰, the key conditions for achieving high-fidelity (>99%) spin readout in silicon qubits can be summarized as follows:

- The Zeeman splitting energy (E_Z) must be significantly larger than the electron thermal energy, ideally satisfying $E_Z > 13 k_B T_e$, to ensure well-resolved spin states.
- The tunnel-out time for the higher-energy spin state must be much shorter than the spin relaxation time (T_1), $T_1 > 100 t_{out}$, ensuring that the spin-selective tunneling event occurs before relaxation to the ground state.
- The sampling rate Γ_s of the readout electronics must be sufficiently fast to resolve the transient tunneling “blip” associated with a single-spin event, $\Gamma_s > 12/t_{in}$.

Beyond these universal criteria, dopant-based spin qubits impose additional requirements. The donor cluster must exhibit an even–odd electron filling sequence, providing a well-defined spin-up and spin-down pair that are degenerate at zero magnetic field. Furthermore, charge noise and local electrostatic fluctuations can lead to unintended tunneling events and readout errors, emphasizing the importance of maintaining a stable and low-noise electrostatic environment. In the following sections, we describe the architecture of the donor–dot SET device and evaluate how well these requirements are satisfied.

5.2 Donor-Dot SET as a single qubit device

Using STM hydrogen lithography, we define the donor-dot SET with a few-donor quantum dot tunnel-coupled to an SET island. The spin qubit will be realized by an electron bound to the donor dot. Figure 5.2 shows the STM images of the device. The SET operates in the Coulomb blockade regime, with the two in-plane gates (G1 and G2) controlling the chemical potential of the SET island and the donor dot. The tunnel

barriers between the SET island and the source–drain leads are engineered to be approximately 9.5 dimer rows wide, based on prior characterization of tunnel resistance R_T as a function of separation¹⁴¹. This value ensures sufficient electron confinement within the SET island while maintaining a high on-state current suitable for spin readout measurements.

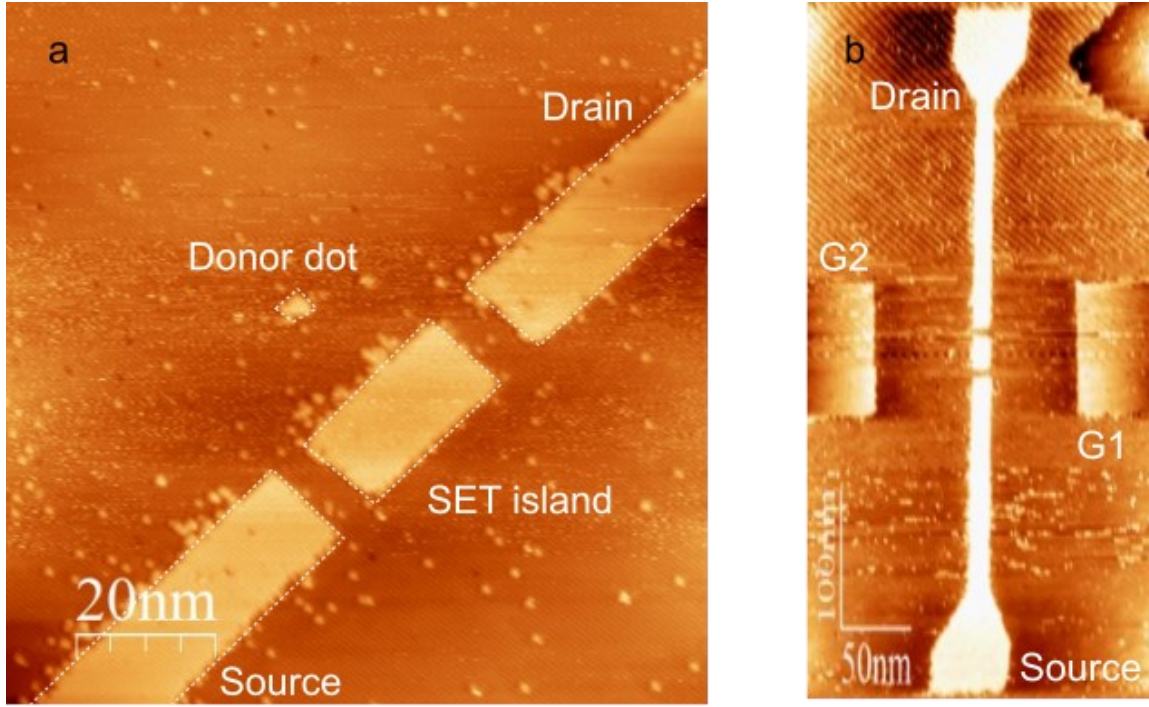


Figure 5.2 STM image of the donor–dot single-electron-transistor (SET) device used for spin readout experiments. (a) High-resolution STM image of the central device region, showing the donor dot containing approximately 3–5 phosphorus atoms and the adjacent SET island. The tunnel barriers between the SET island and the source/drain leads are approximately 9.5 dimer rows wide, providing sufficient confinement and measurable transport current. The donor dot and SET island are separated by about 14 nm, resulting in a weak tunnel coupling sufficient for resolving individual tunneling events. (b) Two in-plane gates (G1 and G2) are used to control the electrochemical potentials of both the donor dot and the SET island. Because the SET island is located near the midpoint between the gates, it exhibits roughly symmetric capacitive coupling to G1 and G2, whereas the donor dot is closer to G2 and is more strongly coupled to G2. This device is fabricated by Xiqiao Wang.

The donor dot is patterned roughly 14 nm from the edge of the SET island. This spacing provides a weak tunnel coupling between the donor and the SET. The resulting tunnel time t_{out} and t_{in} in the milli-seconds range, enables time-resolved observation of the spin-dependent tunneling events. Based on the lithographic

patch size, we estimate that the cluster contains three to five phosphorus donors. The exact energy spectrum of such a multi-donor cluster is considerably more complex than that of single-, double-, or triple-donor systems and lies beyond the scope of this work. For the purposes of this study, we assume that a well-defined spin orbital state is available on the donor dot for readout purposes.

The transport characteristics of the device are measured through its charge stability diagram. Figure 5.3 presents a gate–gate map showing the SET current as a function of the two in-plane gate voltages. The SET exhibits a series of parallel conductance lines corresponding to Coulomb blockade oscillations, with each line representing the addition of a single electron to the SET island. The line slopes reflect the expected equal capacitive coupling between the SET island and the two control gates G1 and G2 ($\alpha_1^I \approx \alpha_2^I$). The spacing between adjacent transition lines is proportional to the island’s charging energy E_C^{IS} , which can be quantitatively extracted from the heights of Coulomb diamonds in Fig 5.3(b).

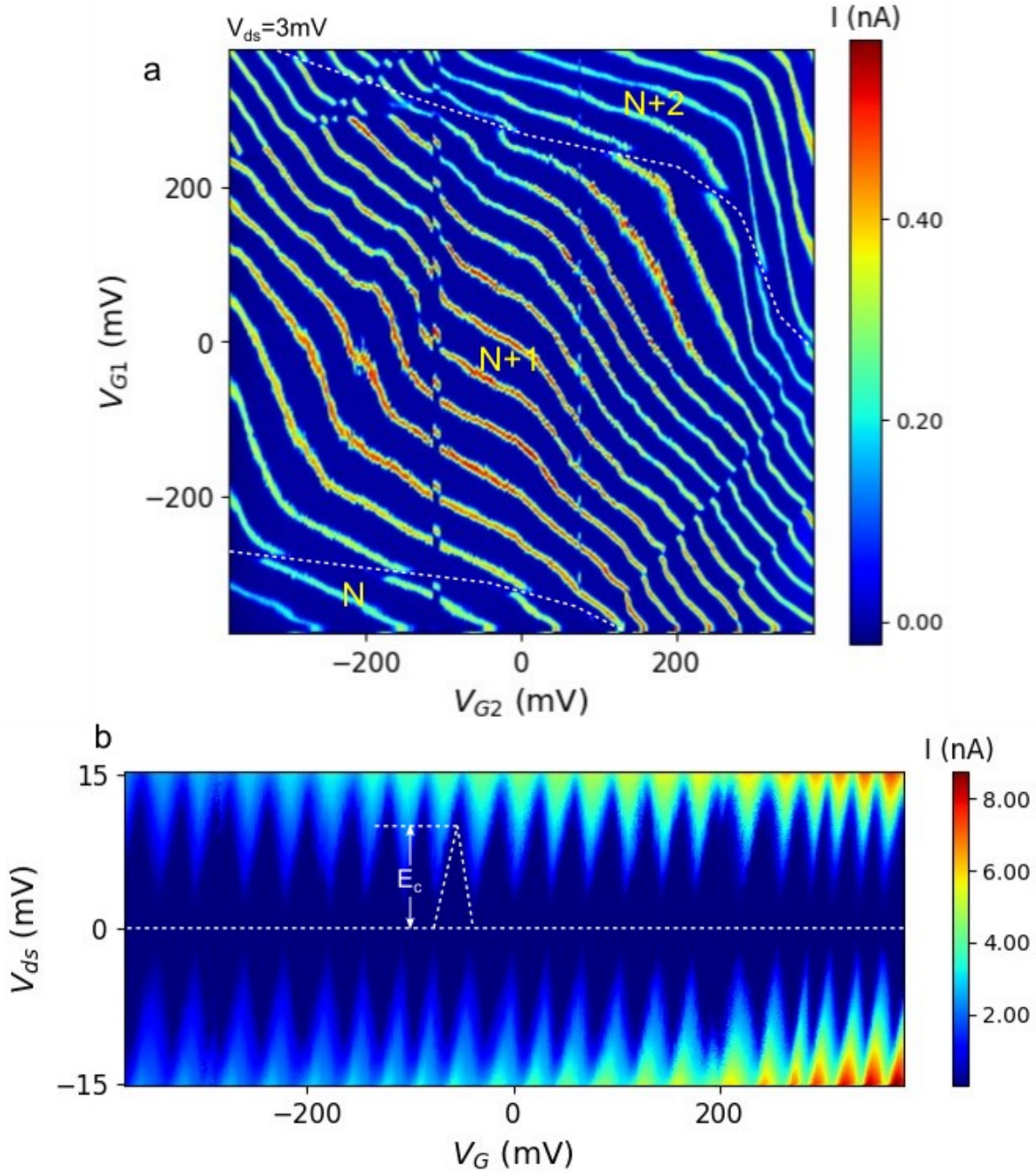


Figure 5.3 Transport measurement of the donor-dot SET device (sample W30 C14) in a dilution refrigerator with a base temperature of 10 mK. (a) Charge stability diagram measured at $V_{ds} = 3$ mV. The two charge transition lines associated with the donor dot are highlighted with white dashed lines, and the corresponding donor electron occupation numbers are labeled as N , $N+1$ and $N+2$ (b) Coulomb diamond measurement acquired along the diagonal direction of (a) with $V_{G1} = V_{G2}$. The charging energy of the SET island, extracted from the diamond height, is approximately $E_C^{IS} \sim 12$ meV. The combined gate lever

arm for G1 and G2 to the island is estimated as $\alpha = \frac{E_C}{\Delta V_G} \sim 0.32$, where ΔV_G is the width of the Coulomb diamond.

In contrast, the donor cluster is tunnel-coupled only to the SET island and not directly to the source or drain leads. As a result, its charge transitions do not appear as direct conductance lines but instead manifest as a series of discontinuities or breaks in the SET transition lines, highlighted by white dashed lines in the gate–gate map. These breaks arise from the mutual charging energy E_m between the donor dot and the SET island. Positioned closer to gate G2, the donor cluster exhibits a much stronger capacitive coupling to G2 compared with G1.

The charging energy of the donor dot E_C^{DD} is significantly larger than that of the SET island, since the dot confines only a few electrons. Consequently, the spacing between successive donor transitions is much wider, and within the accessible gate range, only two donor charge transitions are observed.

The charge configuration of the combined system is denoted as (m, N) , where m represents the number of electrons on the SET island and N the number on the donor dot. Each time a charge transition line is crossed while sweeping the gate voltage from lower to higher values, the corresponding electron number increases by one. Because full depletion of the island and donor dot cannot be reached within the available gate range, these electron numbers are understood as relative quantities rather than absolute counts.

Across the break in the SET conductance line, the donor-dot electron number changes by $\Delta N = 1$. The on or off state of the SET is therefore used to determine the occupancy of the donor dot, forming the basis for energy-selective spin readout. Figure 5.4 shows the charge stability diagram near such a degeneracy point where spin readout experiments are performed, along with a schematic defining the corresponding charge configurations and key notations used in the following analysis.

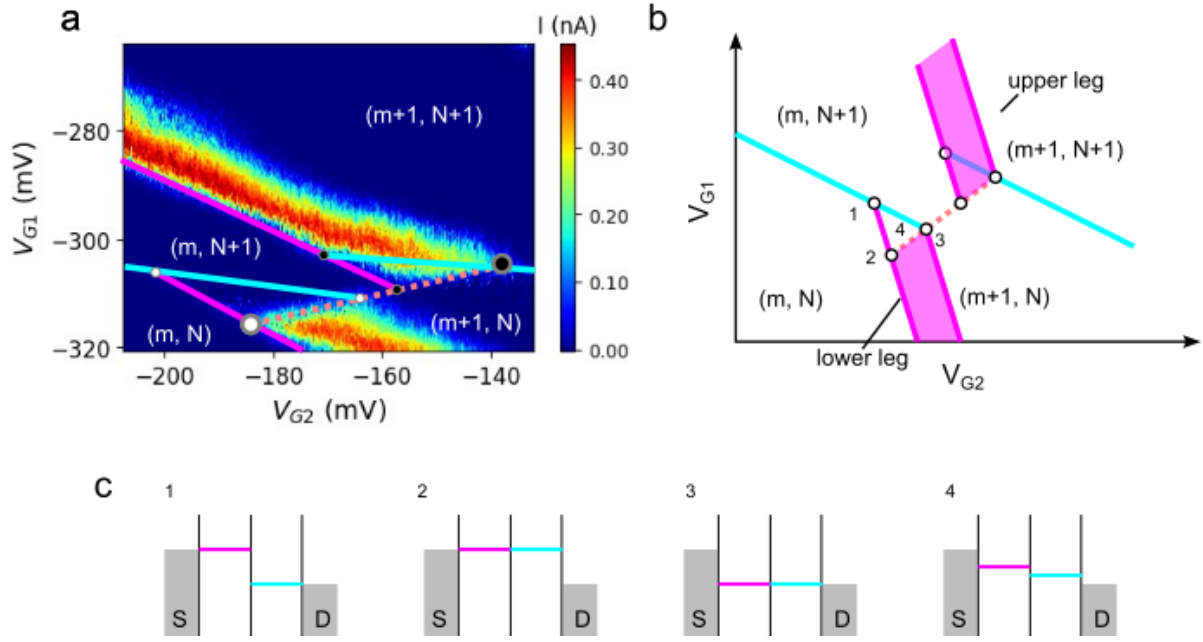


Figure 5.4 Charge degeneracy between the SET island and the donor dot. (a) Measured charge stability diagram at $V_{ds} = 3$ mV. A SET conductance line breaks into an upper leg and a lower leg due to the addition of a new electron onto the donor dot. (b) Schematic illustration of the charge configuration at the degeneracy point. Both the SET and donor transition lines are shifted by their mutual charging energy. The degeneracy line marks the boundary between the $(m, N + 1)$ and $(m + 1, N)$ charge configurations, where an electron can tunnel between the donor dot and the SET island. The orientation of the degeneracy line is determined by the lever arms of the dot and the island with respect to the two gates.

Since the slopes of the donor-dot and SET charge transition lines are quite similar at this particular charge degeneracy, some of the key features related to the readout process appear with high aspect ratios and are therefore difficult to visualize from the measured charge stability diagram. For clarity, these features are better illustrated in Figure 5.4(b), where the slope of the donor-dot transition (cyan) and that of the SET transition (magenta) are drawn more distinctly for visualization.

At finite source–drain bias, the charge-degeneracy region consists of a degeneracy line (pink dash line) and two bias triangles (upper and lower), whose sizes scale proportionally with the applied bias voltage. The

corresponding energy level relations of the donor dot (μ_{DD}) and SET island (μ_{IS}) at the three vertices (1, 2, 3) and an interior point (4) of the lower bias triangle are shown in Figure 5.4(c). The three triangle edges are defined by the following conditions:

- Edge 12: $\mu_{IS} = \mu_S$
- Edge 13: $\mu_{DD} = \mu_D$
- Edge 23: $\mu_{IS} = \mu_{DD}$

Within the lower bias triangle (point 4), both the donor-dot and SET energy levels lie within the bias window, satisfying $\mu_S > \mu_{IS} > \mu_{DD} > \mu_D$. When the donor-dot level becomes occupied, the mutual charging energy shifts the SET island level above the source–drain window, thereby blocking current flow. On the other hand, μ_{DD} remains above μ_{IS} within the upper bias triangle and therefore no blockade in current. Loading and unloading an electron from the donor dot are achieved by tuning the (G1, G2) gate voltages across the charge degeneracy line.

At zero source–drain bias, the two bias triangles collapse into two triple points, and the overall charge stability diagram reduces to the characteristic honeycomb pattern^{132,142,143} of a double quantum dot system.

According to the constant interaction model, which treats the dopant leads as metallic, both the SET island and the donor dot are expected to be capacitively coupled to the gates with constant lever arms, resulting in linear charge transition lines in the stability diagram. However, the experimentally observed curved SET conductance lines and curved donor transition lines, referred to here as the gate nonlinearity problem, deviate from this ideal behavior. We attribute this curvature to background charge inhomogeneities that can be modulated by the gate voltages, likely related to the limited gate operating range of the device. Nonetheless, near the degeneracy regions, the relative energy alignment and tunneling characteristics between the donor dot and the SET island, which are crucial for spin readout, remain mostly unaffected by

these artifacts. Therefore, the device remains capable of demonstrating single-shot spin readout despite the observed nonlinearities.

Figure 5.5 presents the charge stability diagrams measured at other donor–dot transition points. The SET conductance lines at these locations exhibit different slopes and shapes depending on their position in the gate-voltage space, a consequence of the gate nonlinearity problem. These data were acquired using a short integration time, and the graininess observed in the current signal arises from small potential fluctuations induced by environmental charge noise.

Given the irregularity of the transition patterns and their potential influence on data interpretation, we focus our analysis on the specific donor–dot charge transition shown in Figure 5.4, where the transition lines display a relatively regular and well-defined pattern, providing the most stable conditions for the spin readout measurements described in the following sections.

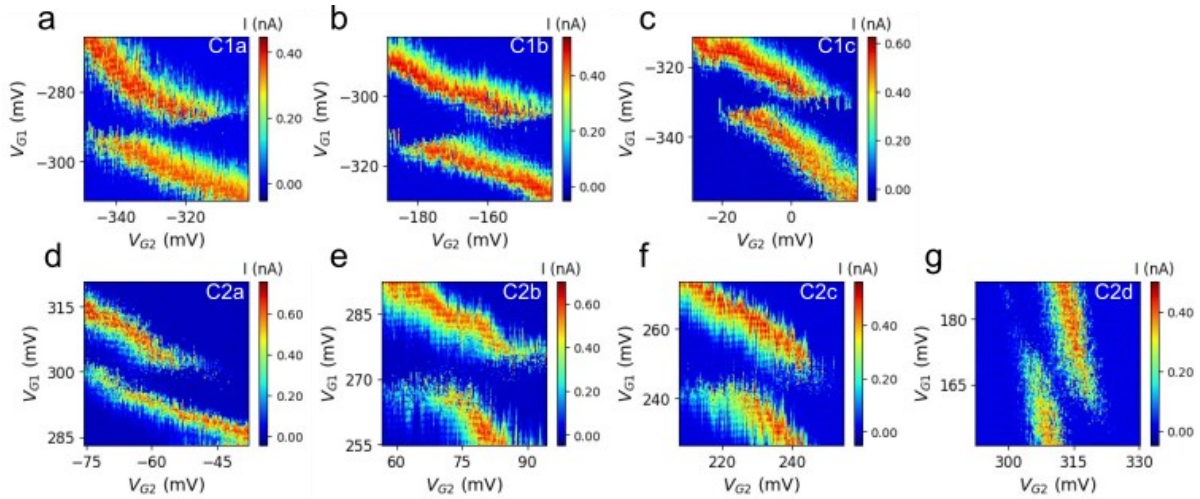


Figure 5.5 Other donor–dot transitions within the accessible gate range. The irregularities in the SET conductance lines and donor charge-transition patterns arise from the gate nonlinearity and the discrete density of states in the SET island. The graininess observed in the current signal is attributed to potential fluctuations caused by environmental charge noise¹⁴⁴.

5.3 Electron temperature

Before demonstrating energy-selective spin readout based on Zeeman splitting, it is essential to first characterize the electron temperature of the donor-dot SET system. The electron temperature can differ substantially from the base temperature of the dilution refrigerator's mixing chamber due to imperfect thermalization¹⁴⁵. Because the signal and control lines are directly connected to room-temperature electronics, thermal radiation over a broad frequency range can propagate down the wiring and elevate the effective electron temperature in the device.

To mitigate this, we implemented custom copper powder filter (CPF)¹⁴⁶ boxes designed to strongly attenuate high-frequency noise and absorb electromagnetic radiation above 2 GHz. These were combined with commercial QDevil RF filter modules, which provide well-characterized filtering with a low pass cutoff frequency of approximately 65 kHz. This setup significantly reduces high-frequency noise on all control and signal lines, allowing the device electron temperature to approach the cryogenic limit such that spin-resolved regime ($k_B T_e \ll E_Z$) can be achieved.

To estimate the improved electron temperature, we analyze the shape of the SET Coulomb peaks at the low-source drain bias ($V_{ds} \rightarrow 0$ V). In this regime, the peak broadening arises from two primary mechanisms:

(a) Lifetime broadening^{110,147}. This occurs when the tunnel rate between the SET island to the source drain lead becomes significant and the electron confinement on the island is reduced. The conductance broadening is signatured by a Lorentzian profile:

$$G = G_{max} \frac{(h\Gamma)^2}{e^2 \alpha_G^2 \Delta V_G^2 + \left(\frac{h\Gamma}{2}\right)^2} \quad (5.1)$$

where G_{max} is the peak conductance when a state on the island is aligned with the Fermi-level of the leads, Γ is the average tunnel rate of the two tunnel junctions and $\alpha_G \Delta V_G$ is the offset to the alignment position.

(b) Thermal broadening¹¹⁰. This effect arises from the temperature-dependent occupation probabilities of electronic states in the source and drain leads. Following the discussion in Section 3.2, the SET conductance at zero source–drain bias ($V_{ds} = 0$ mV) around a Coulomb peak exhibits a Gaussian profile:

$$G = G_{max} \cosh^{-2} \left(\frac{e\alpha_G \Delta V_G}{2.5k_B T_e} \right) \quad (5.2)$$

In an actual device, both lifetime and thermal broadening contribute to the overall shape of the Coulomb peaks. Typically, one of the mechanisms dominates and determines the resulting line shape: Lorentzian for lifetime broadening and Gaussian for thermal broadening. When the two mechanisms are comparable, the observed profile becomes a convolution of both. Figure 5.6 shows measured Coulomb peaks acquired at progressively smaller source–drain biases (V_{ds} approaching zero). The experimental line shapes fit well with a Gaussian function, indicating that in this device, the peak broadening is primarily governed by thermal effects ($k_B T_e \gg \hbar\Gamma$), and therefore indeed represents the electron temperature of the system.

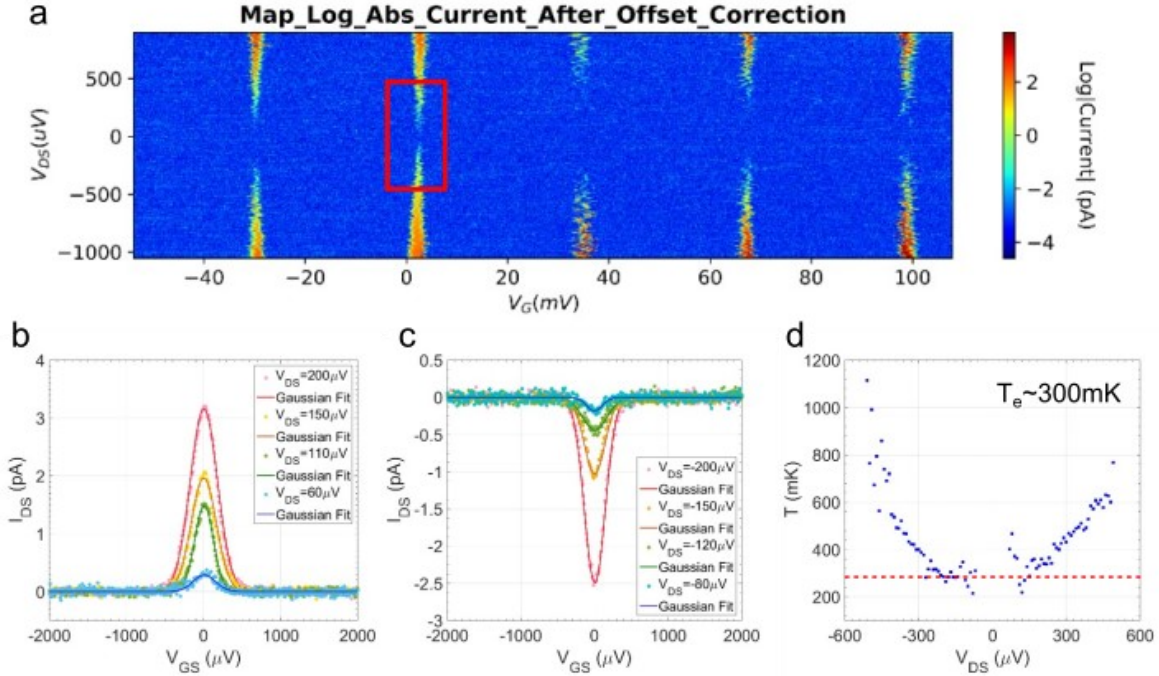


Figure 5.6 Electron temperature characterization of the donor–dot SET device. (a) Coulomb diamond map highlighting the tips of the Coulomb diamonds. Among the five visible peaks, the second from the left (red box) is selected for electron-temperature extraction, as it exhibits minimal charge noise. (b, c) Line

cuts (dots) across the selected Coulomb peak taken at positive and negative source–drain biases, respectively, together with Gaussian fits (solid lines) used to obtain the full width at half maximum (FWHM). (d) Extracted FWHM values from (b) and (c) converted to electron temperature. The linear trend reflecting bias broadening saturates around 300 mK, indicating an effective electron temperature of approximately 300 mK.

The electron temperature can then be obtained from the full width at half maximum (FWHM) of the conductance peak through $\text{FWHM} = 4.35 k_B T_e / \alpha$. The FWHM values extracted from Gaussian fits of the selected Coulomb peak at various positive and negative biases [Figures 5.6(b) and 5.6(c)] were converted into effective electron temperatures. As shown in Figure 5.6(d), the apparent electron temperature decreases with bias and saturates at approximately 300 mK, which is taken as the upper limit of the true electron temperature T_e in the device.

5.4 Single shot spin readout

5.4.1 Tunnel-Rate Characterization

Next, we characterized the tunneling rate between donor dot and the SET island to verify the second necessary condition for high-fidelity spin readout. We work at the upper leg of the one charge degeneracy shown in Fig 5.4 and measure the SET current along the charge degeneracy axis across the charge transition where the SET switches from the “on” to “off”. The resulting current profile exhibits a sigmoidal shape characteristic of a Fermi–Dirac distribution, reflecting the gradual change in electron occupation probability as the donor-dot chemical potential crosses the Fermi level of the SET island.

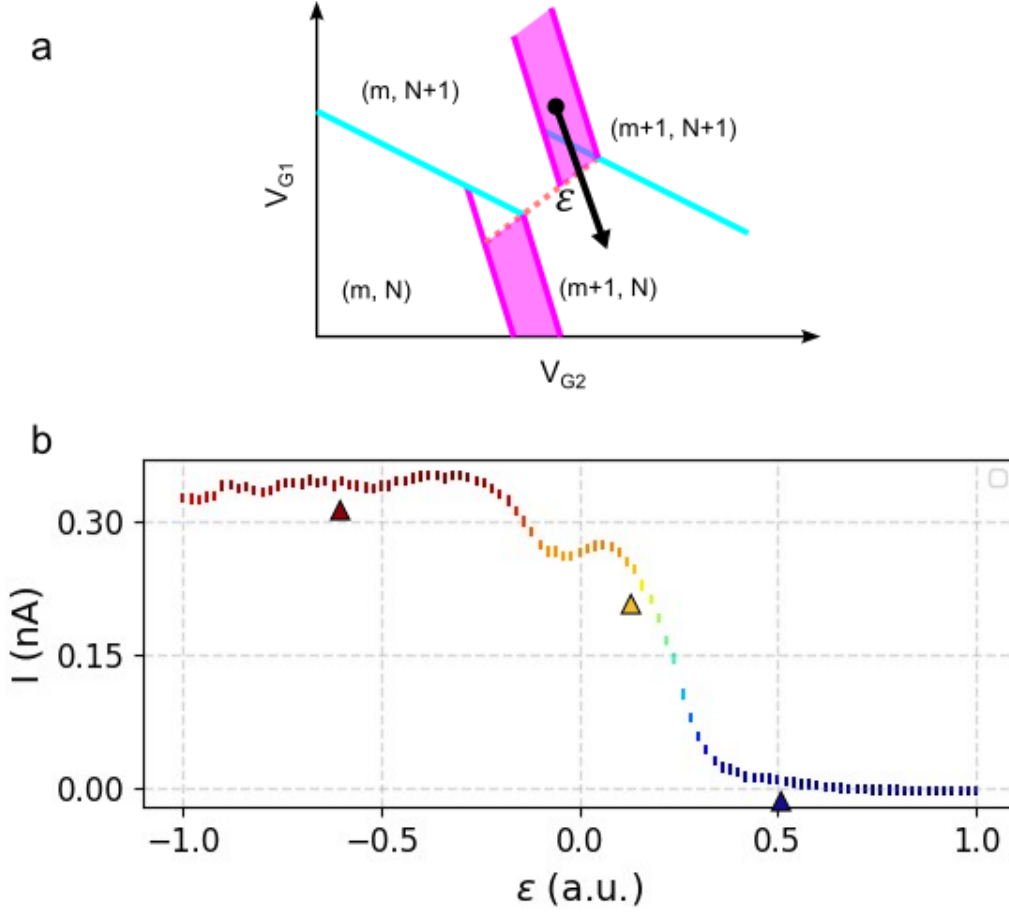


Figure 5.7 Definition of the charge detuning axis. (a) The charge detuning axis follows the SET conduction line and crosses the charge degeneracy line, as indicated by the black arrow on the upper leg. The direction points from the $(m, N + 1)$ configuration to the $(m + 1, N)$ configuration. When the detuning parameter $\epsilon < 0$, an electron is loaded onto the donor dot and the SET current is high (“on” state). (b) SET current measured along the detuning axis as ϵ is swept from negative to positive values. Each data point represents the average current over a 100 second integration window. Near the transition region ($\epsilon \approx 0$), electrons can tunnel back and forth between the donor dot and the SET island, producing random telegraph signals (RTS) in the SET current. The average current in this region therefore reflects the average dwell time of the donor dot in the loaded state.

Additional fine structures (an extra bump in I_{SET} at $\epsilon \sim 0$) are also observed within this transition interval, which we attribute to the discrete density of states (DOS) in the finite sized SET island¹⁴⁸.

Near the center of the degeneracy, where the chemical potentials of the donor dot and the SET island are nearly equal, the electron can tunnel back and forth between the two sites. This results in random telegraph signals (RTS) ¹⁴⁹ in the SET current corresponding to stochastic electron tunneling events.

The time-domain SET current traces measured at three different detuning values, as labeled in Figure 5.7(b), are shown in Figure 5.8. The alternating high and low current segments correspond to the occupied ($N + 1$) and empty (N) charge states of the donor dot, respectively. The cyan dashed lines represent the binary fit of the SET current traces to the on and off state. A transition from the SET “off” state to the “on” state indicates that an electron has tunneled from the SET island onto the donor dot, and the reverse transition corresponds to the electron tunneling back to the island.

The duration for which the SET remains in the “on” state, t_{on} , represents the dwell time before the electron tunnels out of the donor dot, i.e., $t_{\text{out}} = t_{\text{on}}$. Similarly, the dwell time of the “off” state corresponds to the electron tunneling into the donor dot, $t_{\text{in}} = t_{\text{off}}$. The characteristic tunnel-in and tunnel-out rates, Γ_{in} and Γ_{out} , are obtained by statistically analyzing the dwell-time distributions of the high and low current segments. These tunnel rates are defined as the inverse of the average dwell time,

$$\tau_{\text{in}} = \frac{1}{\Gamma_{\text{in}}}, \tau_{\text{out}} = \frac{1}{\Gamma_{\text{out}}} \quad (5.3)$$

Both the tunnel-in and tunnel-out rates depend sensitively on the detuning and can vary by orders of magnitude across the charge degeneracy point. In Figure 5.8(a), where $\mu_{\text{IS}} < \mu_{\text{DD}}$, the donor-dot level lies above the SET island, and the dot remains mostly unoccupied. Occasional thermal excitations allow an electron to tunnel onto the dot, leading to $\Gamma_{\text{out}} \gg \Gamma_{\text{in}}$. In Figure 5.8(b), the chemical potentials of the SET island and donor dot become nearly aligned ($\mu_{\text{IS}} \approx \mu_{\text{DD}}$) around $\epsilon \approx 0$, resulting in frequent tunneling events in both directions, where $\Gamma_{\text{out}} \approx \Gamma_{\text{in}}$. Finally, in Figure 5.8(c), when $\mu_{\text{IS}} > \mu_{\text{DD}}$, the donor-dot level lies below that of the SET, and the dot remains mostly occupied, giving $\Gamma_{\text{out}} \ll \Gamma_{\text{in}}$.

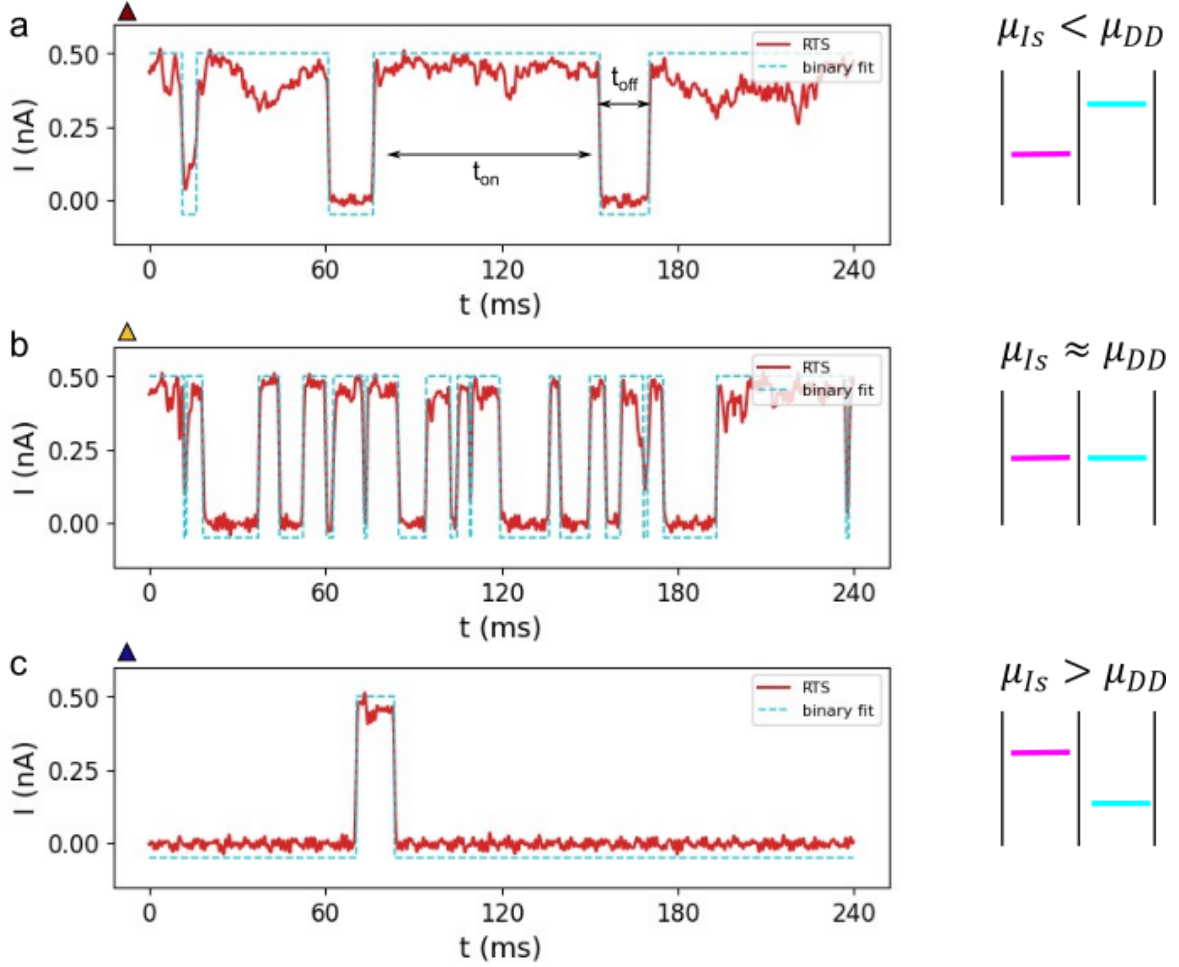


Figure 5.8 Selected random telegraph signal (RTS) traces of the SET current measured within a 240-ms time window at three different detuning values. (a) When the donor-dot level lies well above the SET island ($\epsilon < 0$), the dot remains mostly unoccupied, and the tunnel-in rate Γ_{in} is much smaller than the tunnel-out rate Γ_{out} . (b) Near the charge degeneracy point ($\epsilon \approx 0$), the donor and SET levels are nearly aligned, allowing electrons to tunnel back and forth frequently with $\Gamma_{in} \approx \Gamma_{out}$. (c) At large positive detuning ($\epsilon > 0$), the donor-dot level lies below the SET island, and the dot remains mostly occupied, resulting in a small Γ_{out} and only a few tunneling events observed within the measurement window.

To quantify the tunneling rates relevant for the spin readout experiments, we focus on the zero-detuning point of the upper leg, corresponding to the region near the second marker in Figure 5.7(b). The reason why spin-dependent statistics are observed only on the upper leg, and not on the lower leg, will be discussed later in this chapter. An external magnetic field is applied to lift the spin degeneracy of the donor-dot state,

enabling energy-selective tunneling. Following the approach of Gorman et al.¹⁵⁰, we analyze the statistics of the tunneling events at $B = 1.5$ T, corresponding to a Zeeman splitting of $E_Z = 173 \mu\text{eV}$ (assuming $g = 2$). This energy separation is more than six times larger than the thermal energy, $k_B T_e = 25.8 \mu\text{eV}$, corresponding to the measured electron temperature of 300 mK.

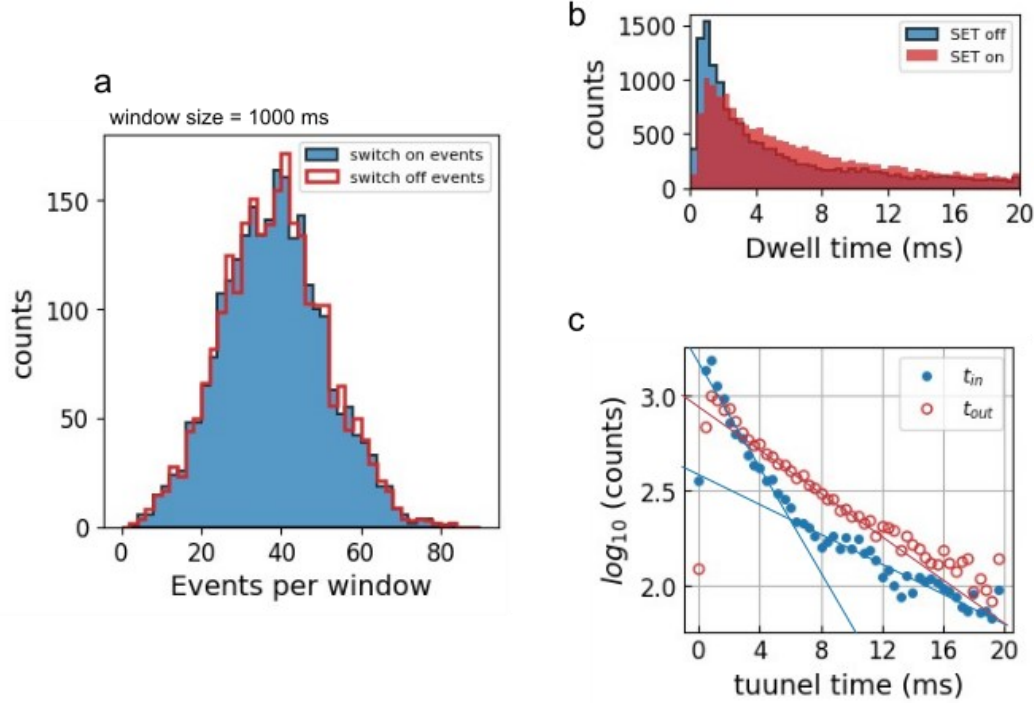


Figure 5.9 Tunneling statistics near zero detuning ($\epsilon \approx 0$) at the upper leg, measured at $B = 1.5$ T with a sampling rate of 5 kSa/s. (a) Histogram of the total number of switching events recorded within fixed 1000-ms time windows. The distribution exhibits a Gaussian-like profile with a mean of $\mu \approx 40$, a standard deviation of $\sigma \approx 30$, and a slight positive skew. (b) Histogram of the dwell times for the SET “on” states (red) and “off” states (blue), corresponding to the tunnel-out time (t_{out}) and tunnel-in time (t_{in}), respectively. The bin size is 0.4 ms. Both distributions exhibit Poisson-like statistics, consistent with stochastic tunneling processes. (c) The same histograms plotted on a logarithmic y-axis. The tunnel-out events follow a single-exponential decay, while the tunnel-in events show a double-exponential behavior, suggesting the presence of two distinct tunneling rates contributing to the overall process.

Continuous RTS signals are recorded at $\epsilon \sim 0$ with a sampling rate of 5 kSa/s and a total acquisition time of 500 seconds. Figure 5.9(a) shows the histogram of the total number of switching events (both on to off and off to on) counted within successive 1000-ms time windows (200-ms overlap). The distribution follows an approximately Gaussian profile centered around a mean of $\mu \approx 40$, indicating that the tunneling process is random but statistically stationary over the acquisition time.

The dwell-time histograms for the SET “on” (occupied) and “off” (empty) states are shown in Figure 5.9(b). The dwell time also corresponds to the tunnel-out and tunnel-in times, respectively. Both types of events exhibit Poisson-like distributions^{151,152}, consistent with stochastic single-electron tunneling governed by the corresponding characteristic tunnel time. When plotted on a logarithmic scale [Figure 5.9(c)], the tunnel-out events follow a clear single-exponential decay, reflecting a single dominant tunneling rate Γ_{out} . In contrast, the tunnel-in events display a double-exponential decay, suggesting that the process involves two distinct tunneling pathways Γ_a, Γ_b . These results strongly indicate that the donor–dot charge transition under investigation corresponds not to the $D^+ \rightarrow D^0 (0 \text{ e} \rightarrow 1 \text{ e})$ type transition, but rather to a $D^0 \rightarrow D^- (1 \text{ e} \rightarrow 2 \text{ e})$ type transition, similar to that discussed by Watson et al.¹⁵³. In this regime, when the system is tuned to negative detuning, two electrons occupy the outer shell of the donor dot ($N = 2$), forming a singlet state. As the detuning is increased toward zero, one of the two electrons can tunnel out to the SET island, and the tunnel-out rate is given by the sum of both spins,

$$\Gamma_{out} = \Gamma_{out}^{\uparrow} + \Gamma_{out}^{\downarrow} \quad (5.4)$$

In contrast, the tunnel-in process involves two distinct tunneling channels, $\Gamma_{in}^{\uparrow}$ and $\Gamma_{in}^{\downarrow}$ ($\Gamma_{in}^{\downarrow} \gg \Gamma_{in}^{\uparrow}$), corresponding to the refilling of the donor dot with a spin-up or spin-down electron from the reservoir forming the basis for energy selective readout. From the double-exponential decay observed in the tunnel-in time, we extract $\Gamma_{in}^{\downarrow} = 345 \text{ Hz}$ and $\Gamma_{in}^{\uparrow} = 92 \text{ Hz}$ at this detuning level.

5.4.2 Readout Pulse Sequence

After characterizing the tunneling dynamics, we implement the energy-selective spin readout process using a three-phase pulse sequence applied to the two gate electrodes similar to the original Elzerman readout setup at $B=1.5$ T. For $D^+ \rightarrow D^0$ type donor dot charge transition, the pulse sequence consists of the load, read, and empty phases, each corresponding to a distinct electrochemical configuration of the donor dot relative to the SET reservoir.

- **Load phase:** The donor-dot potential is pulsed below the Fermi level of the SET, allowing an electron with random spin orientation to tunnel onto the donor dot.
- **Read phase:** The dot potential is raised such that only the spin-up state lies above the SET Fermi level ($\mu^\uparrow > \mu_R > \mu^\downarrow$). A spin-up electron can therefore tunnel out, followed by a spin-down electron tunneling back in, producing a transient blip in the SET current. If a spin-down electron was initially loaded, no tunneling occurs, and the current remains constant.
- **Empty phase:** The dot potential is further raised above the reservoir Fermi level to eject the electron, resetting the system for the next measurement cycle.

For a $D^0 \rightarrow D^-$ type donor-dot charge transition, the same pulse sequence is applied with a modified charge configuration corresponding to the unload, read, and refill phases shown in Figure 5.10. During the unload phase, the donor-dot potential is pulsed above the Fermi level of the SET island, allowing one electron with a random spin orientation to tunnel out. In the read phase, the donor potential is brought back to the charge-degeneracy point, where spin-dependent tunneling events can be detected as transient blips in the SET current. Finally, during the refill phase, the donor-dot potential is returned to its initial position, enabling an electron to tunnel back in and reset the system for the next measurement cycle.

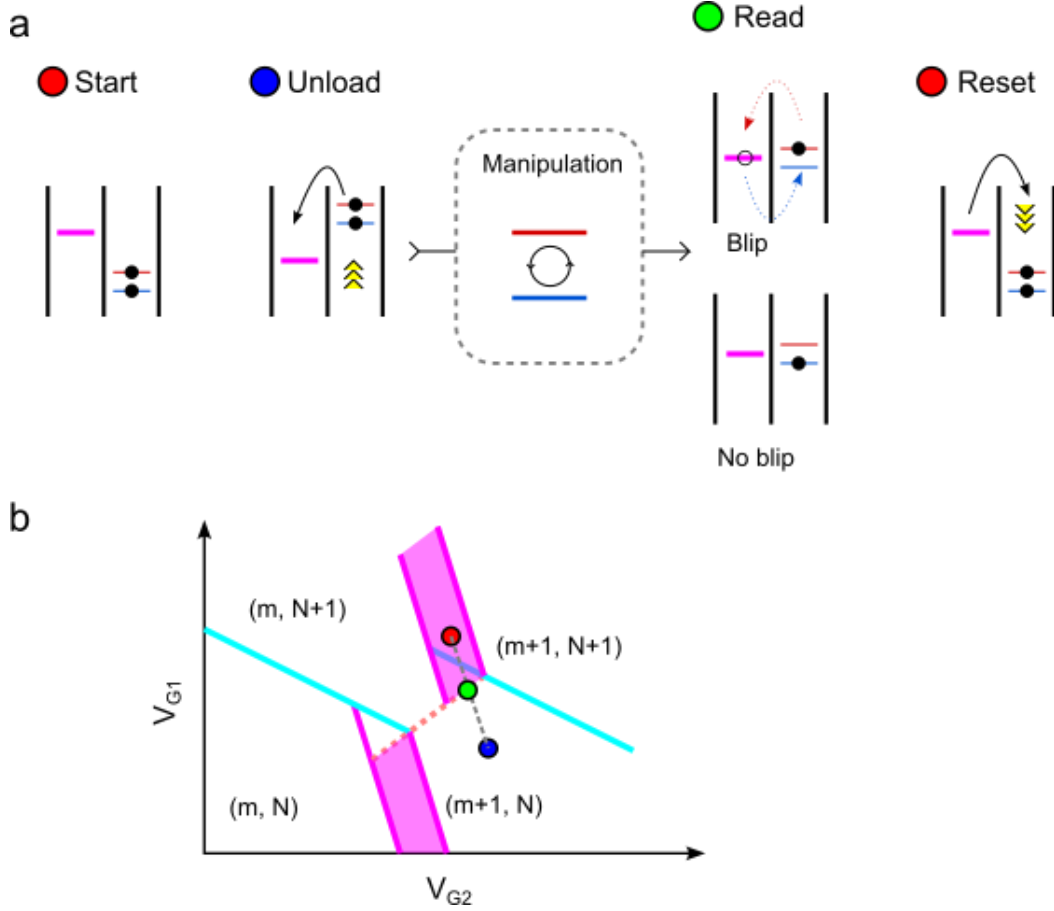


Figure 5.10 Spin readout pulse sequence for the $D^0 \rightarrow D^-$ style donor-dot charge transition. (a) Energy-level schematic illustrating the unload, read, and reset (refill) phases. During the unload phase, an electron with a random spin orientation is removed from the donor dot, turning the SET current off. In the read phase, if the remaining electron on the donor is spin-up, a spin-down electron from the SET island can tunnel in to form a singlet, followed by the spin-up electron tunneling out producing a characteristic blip in the SET current. If the remaining electron is spin-down, no tunneling occurs. During the reset phase, the donor-dot potential is returned to its initial value, allowing an electron to tunnel back in and reinitialize the system for the next readout cycle. (b) Pulse sequence overlaid on the schematic charge stability diagram, showing the voltage levels corresponding to each phase. The voltage pulses applied to gates G1 and G2 are synchronized such that the pulse trajectory lies entirely along the charge-detuning axis, ensuring consistent electrostatic tuning during the sequence.

5.4.3 Statistical spin tail

To observe spin-dependent tunneling events, we apply the three-level gate pulse sequence with each phase defined by an appropriate gate voltage. The reset (start) and unload phases are chosen to be approximately symmetric about the charge degeneracy line separated by a pulse vector of $(\Delta V_{G1}, \Delta V_{G2}) = (-13.2 \text{ mV}, 24.5 \text{ mV})$ corresponding to a detuning range of $\Delta\epsilon=2.4 \text{ meV}$. The read level is then set near the midpoint of this vector, with a proportionality factor of $r \approx 0.5$ to the pulse vector. The duration of each phase must also be optimized so that the unload phase is sufficiently long for the donor dot to fully unload, yet short enough to avoid spin relaxation. In the present experiment, the pulse cycle has a total period of 250 ms, with the unload, read, and reset phases beginning at $t = 25 \text{ ms}$, $t = 100 \text{ ms}$, and $t = 225 \text{ ms}$, respectively. The rise time between each phase is $\sim 50 \text{ }\mu\text{s}$, which is much shorter than the characteristic tunnel time. The SET current is sampled at 5 kSa/s.

Figure 5.11(a) shows representative single-shot traces of the SET current corresponding to spin-up (red) and spin-down (blue) electrons, over the full cycle. A trace is counted as spin up if a blip is observed within the duration of the read phase according to the spin readout protocol. However, when examining the full time traces, numerous RTS fluctuations are observed during the 125 ms read phase, rather than the ideal single-blip versus no-blip behavior. This behavior arises from excess charge noise present in the nominally clean silicon vacuum environment, which is also evident from the graininess seen in the charge stability diagrams. The presence of such charge noise significantly degrades readout fidelity, as charge-noise-induced tunneling events can be misidentified as spin-up blips. One practical mitigation strategy is to restrict the effective readout window to only a few multiples of the characteristic tunneling time, thereby reducing the likelihood of false events. A detailed analysis of the optimal readout-time and blip threshold selection can be found in Buchs et al ¹³⁰.

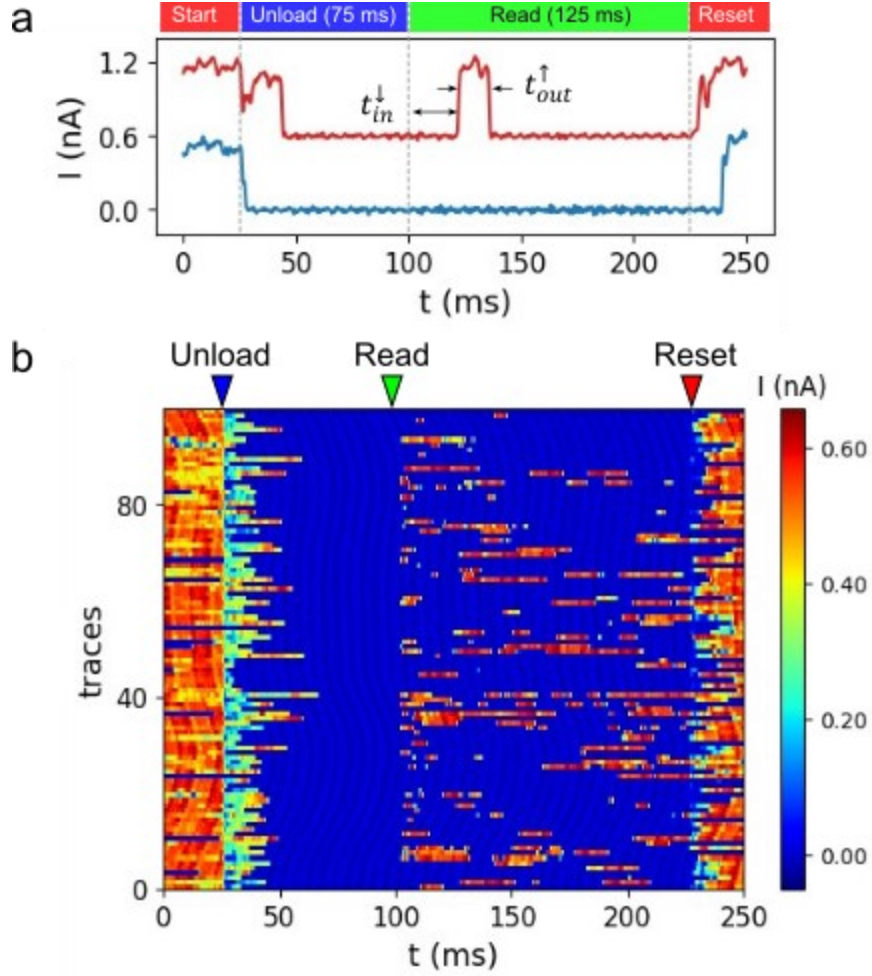


Figure 5.11 Single-shot spin readout traces of SET current within the correct readout window. $B=1.5$ T
(a) Example traces showing a spin-up electron (blip observed from $t = 120$ ms to $t = 135$ ms) and a spin-down electron (no blip). The dashed line marks the beginning of the read phase at $t = 100$ ms. (b) Full cycle SET current data from 100 randomly selected traces. The unload, read, and reset phases begin at $t = 25$ ms, $t = 100$ ms, and $t = 225$ ms, respectively, with a total cycle period of $T = 250$ ms. Frequent back-and-forth tunneling events are observed during the read phase, in contrast to the ideal single-blip behavior. These events are attributed to excess charge noise in the environment, which constitutes the primary factor limiting readout fidelity in this device.

However, the two-level spin system of the donor-dot state can still be recovered statistically by collecting a large number of traces while varying the read-level position. By averaging many such traces, the resulting

data reveal the characteristic “spin-tail” feature^{128,153,154} that is otherwise obscured in individual traces by charge-noise-induced tunneling events.

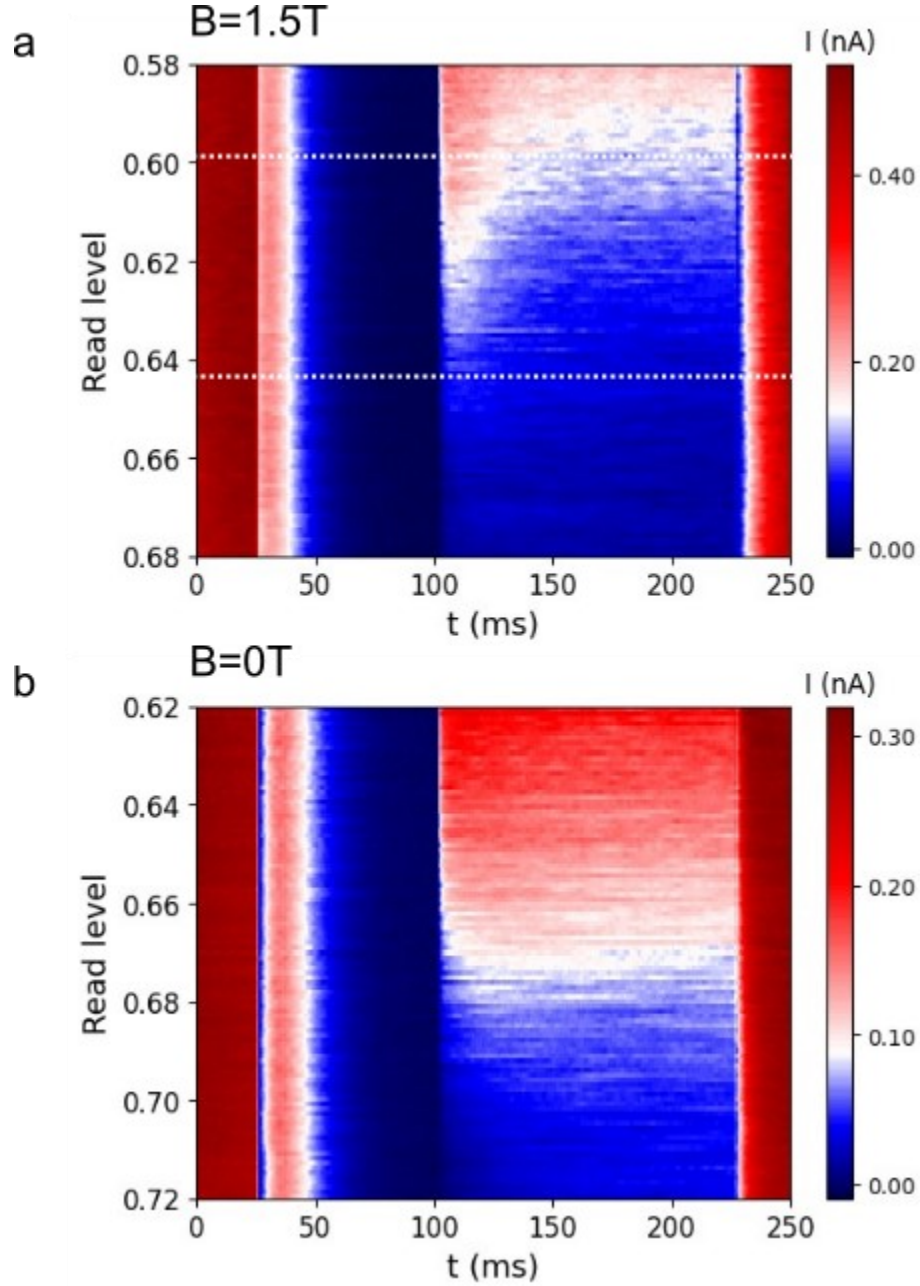


Figure 5.12. Statistical averaging of single-trace current data showing the spin-tail feature. The reset and unload levels are fixed and separated by a voltage pulse vector of $(\Delta V_{G1}, \Delta V_{G2}) = (-13.2 \text{ mV}, +24.4 \text{ mV})$. The read level is varied along the y-axis to identify the optimal read window. The y-axis values represent the ratio r of the read position relative to the pulse vector. Each read level is averaged over 1000 cycles of

identical readout pulse sequences. (a) At $B = 1.5$ T, a distinct spin-tail feature emerges between $r = 0.60$ and $r = 0.64$ at the beginning of the read phase corresponding to a Zeeman split energy of $E_Z = 173$ μ eV. This feature represents the statistical average of spin-up blip events associated with energy-selective tunneling, while the background current arises from charge-noise-induced tunneling events. An alternative colormap is used to highlight the tail shape. (b) At $B = 0$ T, using the same voltage pulse sequence, no tail-like structure is observed, confirming the magnetic-field dependence of the spin-selective signal.

In Figure 5.12, we performed repeated single-shot measurements while systematically varying the read-level position. The reset and unload levels were held constant, defined by the voltage pulse vector $(\Delta V_{G1}, \Delta V_{G2}) = (-13.2$ mV, $+24.4$ mV), while the read level was incrementally shifted along the detuning direction by its ratio to the pulse vector. For each read-level, 1000 identical pulse cycles were executed, and the resulting SET current traces were averaged to obtain a two-dimensional map of current intensity as a function of read-level ratio (r) and time within the read phase. This statistical averaging suppresses uncorrelated charge-noise-induced fluctuations, allowing the spin-dependent tunneling events to emerge as a characteristic spin-tail feature. At $B=1.5$ T (Figure 5.12(a)), the correct readout window spans from $r=0.60$ to $r=0.64$ corresponding to a Zeeman split energy of $E_Z = 173$ μ eV. The tail broadens toward the upper end of the readout window (around $r \approx 0.60$) because the spin-up electron level approaches the SET island level, resulting in an increased tunnel-out time $\tau_{out}^\uparrow$. To confirm that the spin-tail is indeed produced by the magnetic field, we apply the same measurements at $B = 0$ T (Figure 5.12(b)), where spin degeneracy is restored and no tail is observed.

5.4.4 Spin Relaxation Time (T1) Measurement

As no on-chip ESR antenna is integrated into this device to drive electron Rabi oscillations, the only available form of “manipulation” is by waiting. In Figure 5.13, the same readout voltage pulse sequence is applied while measuring the average SET current at a fixed read level of $r = 0.60$ and $B = 1.5$ T as a function of the wait time t_{wait} , defined as the duration of the unload phase. This experiment effectively measures

the spin relaxation time (T_1), since a spin-up electron begins to relax toward the spin-down ground state once the spin-down electron has been unloaded.

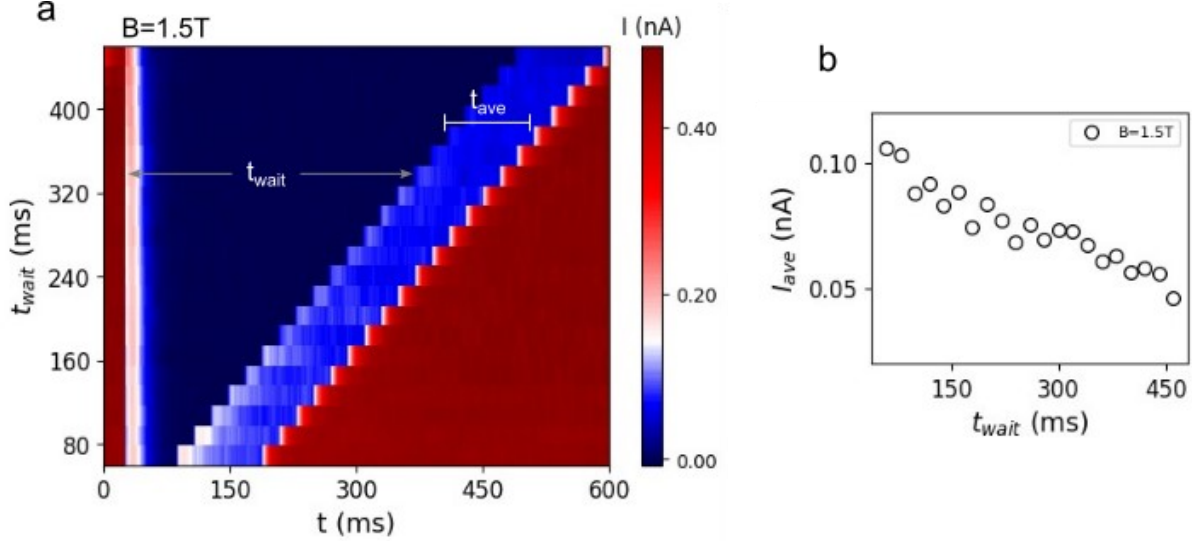


Figure 5.13. Pulse sequence and measurement result for T_1 time characterization at $B=1.5T$. (a) The same readout voltage pulse sequence is applied but with varying t_{wait} (duration of the unload phase) at $r=0.60$. The highlights at the beginning of each read phase correspond to spin-selective blips and gradually decreases at longer t_{wait} due to spin relaxation. (b) Average current over the read interval t_{ave} as a function of t_{wait} . The average current can be modelled as the sum of two contributions: spin-selective tunneling events and charge-noise-induced random telegraph signals such that $I_{ave} = I_{blip} + I_{RTS}$.

However, due to frequent random tunneling events induced by charge noise, counting individual spin-up and spin-down blips is less unreliable (low fidelity). Instead, we calculate the average current I_{ave} measured over a read interval of $t_{ave} = 100$ ms. This average current consists of two components: the spin-selective tunneling contribution I_{blip} , which decays exponentially by the spin relaxation time (T_1), and the charge-noise-induced random telegraph signal I_{RTS} , which forms a constant background after averaging. By fitting the average current to $I_{ave}(t) = a e^{-t/T_1} + b$, we extract a spin relaxation time of $T_1 = 220$ ms at $B = 1.5$ T.

The same measurement on T_1 time is repeated at different magnetic fields and shown in Figure 5.14.

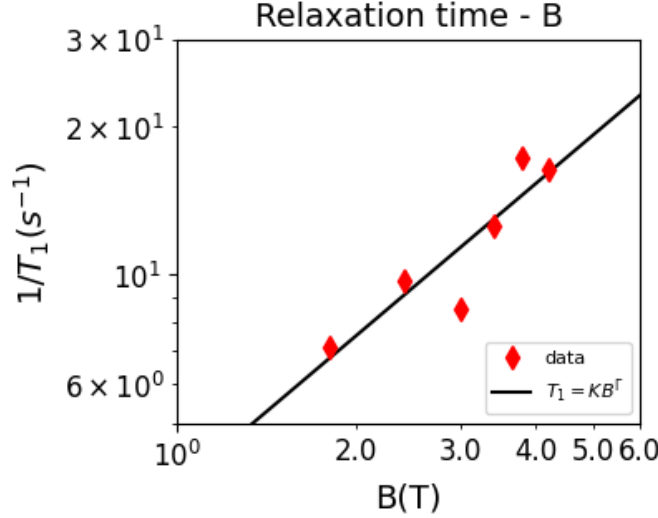


Figure 5.14. Spin relaxation time (T_1) as a function of magnetic field. Measurements were performed at $B = 1.8$ T, 2.4 T, 3.0 T, 3.4 T, 3.8 T, and 4.2 T. The solid black line represents a fit to the power-law relation $T_1 = KB^\Gamma$, yielding $K = 0.76$ and $\Gamma = -1.02$.

In silicon donor-based devices, spin relaxation exhibits several distinct mechanisms each with characteristic magnetic-field dependencies. For example, phonon-mediated spin-orbit relaxation typically yields a rate scaling as $1/T_1 \propto B^5$ at high fields, while at intermediate fields phono-mediated Hyperfine relaxation give a lower exponent $1/T_1 \propto B^3$. In contrast, mechanisms driven by electric-field fluctuations or charge noise can produce a different dependence, such as $1/T_1 \propto B^1$ under certain conditions¹⁵⁵. In our measurements the extracted dependence of $T_1 = KB^\Gamma$ with $\Gamma \approx -1.02$ strongly indicates that excess charge noise dominates the relaxation process in this device regime. In this case the charge fluctuations modulate the donor or SET potential and thereby drive spin flips via residual spin-orbit coupling, this channel becomes dominant when the device environment is noisy. Consequently, the B^{-1} dependence on T_1 we observe is consistent with a charge-noise-limited relaxation framework rather than the higher-order B^{-3} or B^{-5} laws expected for phonon assisted Hyperfine or spin-orbit interactions.^{156,157} The relatively short T_1

time measured in this device underscores the critical importance of minimizing charge noise to achieve longer spin lifetimes and higher readout fidelity.

5.5 Summary

This chapter demonstrates single-shot spin readout in a donor-dot single electron transistor (SET) device, an essential step toward achieving full spin control in donor-based silicon quantum architectures. The results show that spin-dependent tunneling between the donor cluster and the SET island can be detected in real time, enabling energy-selective readout for the Si:P qubit platform.

The study also identifies the primary factors limiting readout fidelity. Excess charge noise in the device environment induces fluctuations in the local electrostatic potential, reducing the stability of the energy-selective tunneling and contributing to spin relaxation. Additionally, the signal-to-noise ratio (SNR) in the direct-current (DC) transport measurement of the SET current constrains the temporal resolution of single-shot detection. Some of the faster tunneling events appear as a single data point in the current trace and cannot be properly characterized.

Future improvements will focus on improving device gate linearity, reducing charge noise, integrating on-chip microwave antennas to enable coherent spin manipulation through electron spin resonance (ESR) and nuclear magnetic resonance (NMR), as well as exploring two-qubit coupling via the exchange interaction between adjacent donor clusters. By incorporating high-bandwidth charge sensing methods such as RF reflectometry and implementing more scalable device layouts, further enhanced readout speed can be achieved. Together, these next steps will provide the foundation for realizing high-fidelity control and readout for donor-based spin qubits.

Chapter 6: Analog quantum simulation using quantum dot arrays in Si:P

The central concept of analog quantum simulation ¹⁵⁸ is to engineer a controllable quantum system whose native degrees of freedom, interactions, and geometry directly map onto a target Hamiltonian. Rather than calculating eigenstates on a classical computer, one physically constructs the Hamiltonian in a hardware platform and probes it experimentally to access regimes of strong correlation ^{159,160}, nonequilibrium dynamics ^{161,162} within large Hilbert spaces ¹⁶³ that are otherwise intractable. Modern analog simulators are programmable to varying degrees and serve as a valuable complement to digital, gate-based quantum computers, which typically rely on Hamiltonian trotterization ^{163,164} to decompose continuous dynamics into discrete gate operations. The analog approaches often offer the advantage of enabling direct measurement of physical quantities without requiring extensive computational post-processing. However, this comes at the cost of needing the simulator's intrinsic physics to closely mirror that of the target Hamiltonian.

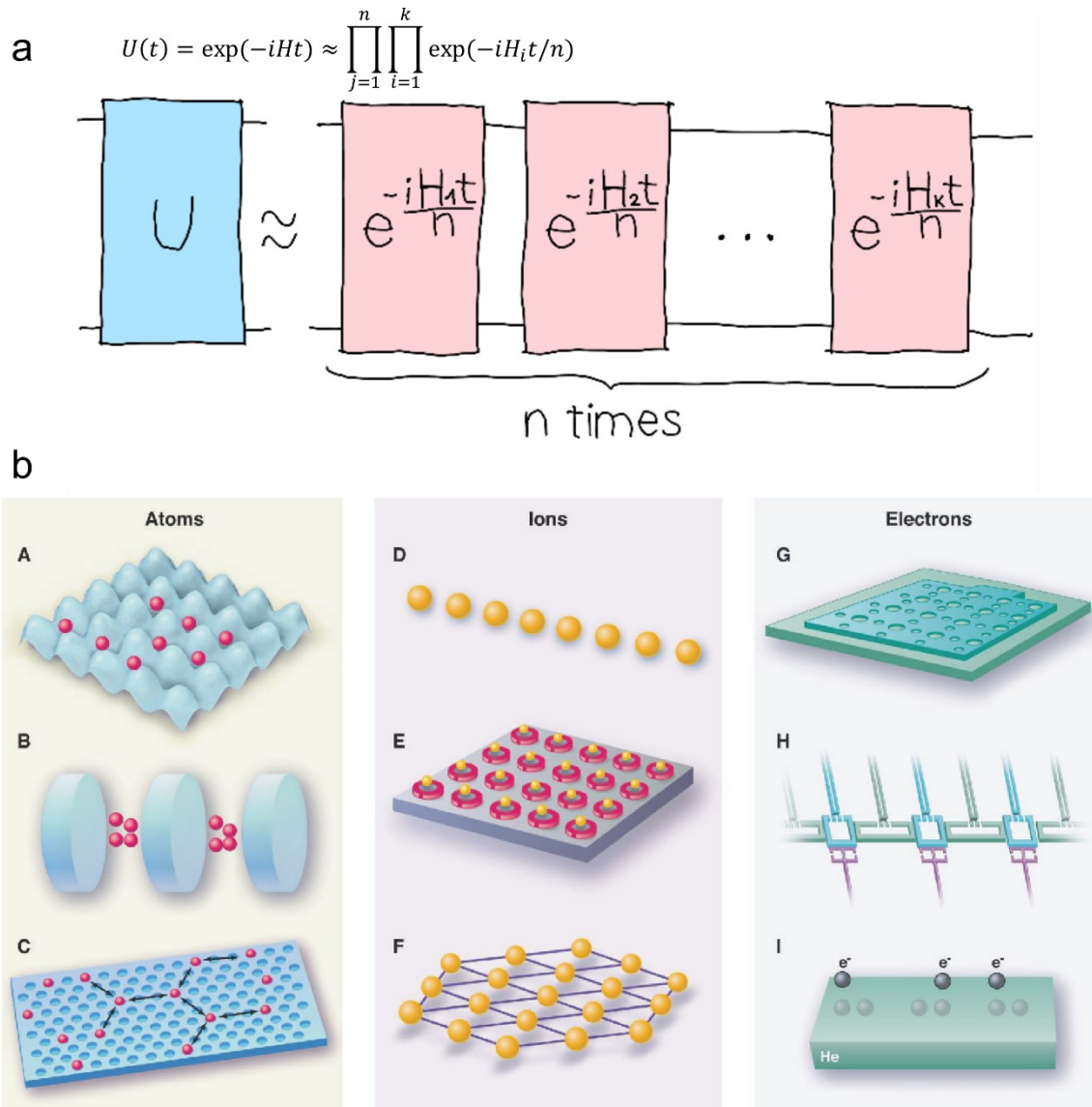


Figure 6.1 Digital versus analog quantum simulation. (a) In digital quantum simulation, the time evolution of a quantum system is decomposed into small time steps and Hamiltonian components, each mapped onto a sequence of qubit gate operations. Figure is taken from online resource.¹⁶⁵ (b) In analog quantum simulation, a physical system consists of atoms, ions, or electrons is directly engineered to realize the target Hamiltonian. Figure adapted from Georgescu et al.¹⁵⁸

We briefly review several prominent analog quantum simulation platforms, outlining their respective advantages and limitations, before introducing the type of simulator that can be realized in the Si:P dopant-based platform.

6.1 Analog quantum simulators

A wide variety of physical systems have been developed to realize analog quantum simulators, each exploiting distinct mechanisms for confinement, interaction, and control. Ultracold atoms in optical lattices^{166,167} provide decent realizations of the Bose- and Fermi-Hubbard models, with lattice geometry and interaction strength tuned by laser intensities and magnetic fields. Arrays of trapped ions^{168,169} are an excellent playground for programmable spin models and many-body physics, offering flexible connectivity and exquisite single-particle control. In parallel, condensed-matter-based platforms such as moiré superlattices¹⁷⁰, gate-defined semiconductor quantum dots¹⁷¹, and dopant-based quantum dots¹⁷² in silicon bring analog simulation into a solid-state setting where strong Coulomb interactions and direct transport measurements are naturally available. Each platform occupies a distinct region of the trade-off space between quantum coherence, scalability, and Hamiltonian flexibility, enabling diverse experimental routes to study many-body quantum phenomena in an analog framework.

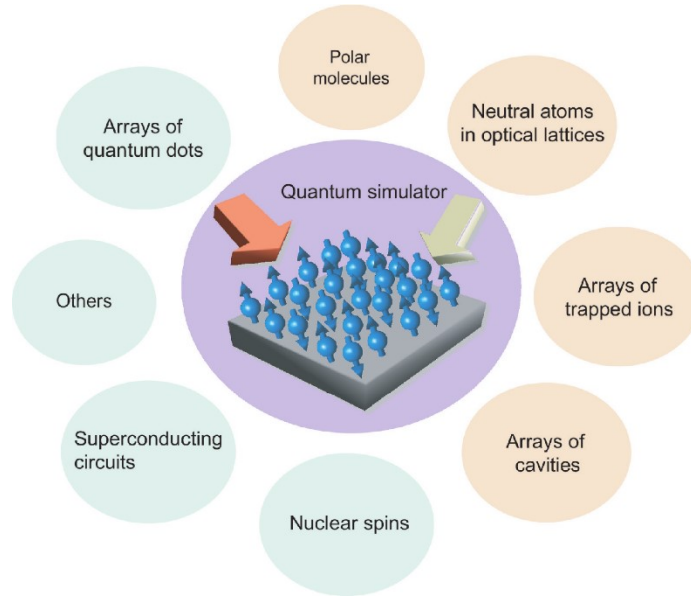


Figure 6.2 Various experimental platforms for constructing specialized quantum simulators aimed at exploring problems in condensed-matter physics. This figure is taken from Georgescu et al.¹⁵⁸

Optical lattices with ultracold atoms

Ultracold atoms trapped in optical lattices represent one of the most mature platforms for Hubbard model simulation. The atoms are cooled to near absolute zero temperatures¹⁷³ and confined in periodic potential formed by interfering laser beams. These systems benefit from nearly perfect periodicity, high tunability, and the ability to realize a wide range of lattice geometries. Site-resolved imaging techniques such as quantum gas microscopy have enabled direct observation of Mott insulating states and antiferromagnetic correlations. Long-range Coulomb interactions are usually absent in neutral atom systems and must be engineered indirectly, while destructive measurement techniques can make dynamical studies difficult. Shao, et al¹⁷⁴ have succeeded in demonstrating an antiferromagnetic phase transition in a three-dimensional Fermi–Hubbard system, providing a milestone toward accessing strongly correlated magnetic phases with ultracold matter.

Moiré superlattices in two-dimensional materials

Moiré superlattices realized by stacking two or more atomically thin layers with slight twist or lattice mismatch have emerged as a promising platform for emulating strong correlation physics in two dimensions. In such systems, the interference between adjacent layers generates a moiré potential that can dramatically alter the electronic bands and the effect of Coulomb interactions.

A compelling demonstration of correlated behavior is from a moiré superlattice in WSe₂/WS₂ bilayer heterostructure, where Xu et al¹⁷⁵ observed nearly two dozen correlated insulating states at fractional moiré fillings. The key strength of moiré-based simulators lies in their direct connection to itinerant electrons and the ability to electrostatically tune filling factors, displacement fields, and twist angles. This tunability allows one to sweep across regimes of weak to strong correlations, and to probe emergent phases such as correlated insulators, superconductivity, and topological orders. Because the moiré unit cell is much larger than atomic lattice constants, effective hopping parameters are naturally reduced, placing the system deep in the correlated regime.

Gate defined semiconductor quantum dot arrays

Gate-defined quantum dots formed within a two-dimensional electron gas (2DEG) in semiconductor quantum wells provide another route for constructing Hubbard simulators. By precisely engineering barrier and accumulation gates, these quantum dots can be coupled into ordered arrays that emulate small Hubbard clusters, allowing controlled exploration of strongly correlated electronic states. The principal advantage of this platform lies in its high degree of electrical tunability: gate electrodes enable independent control of site potentials, tunneling amplitudes, and overall filling factors, while transport measurements and microwave-based techniques provide direct access to both charge and spin degrees of freedom. A demonstration of this approach is the observation of Nagaoka ferromagnetism in a four-site quantum dot plaquette¹⁷⁶. In this work, a square array of four GaAs quantum dots was tuned to the regime of a single hole away from half-filling. The system exhibited a maximally spin-polarized ground state, consistent with Nagaoka's theorem for the Hubbard model, which predicts ferromagnetism under these conditions. This experiment provided one of the first direct realizations of a correlated magnetic phase within a solid-state artificial lattice, highlighting how even small quantum dot arrays can capture essential many-body physics predicted by the Hubbard model.

However, scaling semiconductor quantum dot arrays beyond a few sites remains challenging, as each dot requires individual tuning, leading to a line-crowding problem^{177,178} similar to that faced when increasing the number of qubits in quantum processors. In addition, maintaining coherent control over large arrays is difficult because decoherence effects typically increase with the number of coupled neighbors.

Dopant-based quantum dots in silicon

Among semiconductor-based approaches, arrays of dopant-based quantum dots, such as phosphorus donors in silicon, offer a particularly distinctive route to quantum simulation of the Fermi–Hubbard model. Unlike gate-defined dots, electrons bound to donor clusters naturally map onto Hubbard sites and inherit atomic-scale features, including ion cores, nuclear spins, and strong long-range Coulomb interactions. The key Hubbard parameters, such as site potential, inter-site spacing, and tunnel coupling, can be defined directly

by the lithographic pattern, which achieves sub-nanometer placement precision through STM hydrogen lithography. These capabilities make dopant arrays an attractive platform for exploring strongly correlated two-dimensional electron systems.

Despite the diverse implementation, all analog quantum simulation platforms share the common objectives. Each aims to achieve a clear and precise mapping between hardware controls, such as lattice depth, site spacing, coupling strength and the parameters of the target Hamiltonian, which corresponds to on-site interaction U , hopping amplitude t , long-range couplings, and external fields. Equally important is the ability to perform precise diagnostics: from transport measurements to quantum gas microscopy. These techniques provide direct access to correlations and many body observables that numerical methods would fail to give reasonable results. In the next section, we focus on the Fermi–Hubbard model and present the experimental realization of a 3×3 phosphorus dopant array that, for the first time, achieves a tunable two-dimensional extended Fermi–Hubbard system in silicon with atomically precise geometry and intrinsically strong interactions.

6.2 Fermi-Hubbard Model

The Hubbard model, originally formulated by John Hubbard, provides a minimal yet powerful framework for describing interacting particles in a periodic potential. It includes both fermionic and bosonic variants: the Bose–Hubbard model captures the interplay between tunneling and on-site interactions in systems of interacting bosons, while the Fermi–Hubbard model describes electrons in a crystalline lattice where spin, Pauli exclusion, and Coulomb repulsion give rise to rich correlation effects. Despite its apparent simplicity, the Hubbard model is widely believed to encapsulate the essential physics underlying many strongly correlated phenomena, including Mott insulating behavior, magnetism, and unconventional superconductivity.

6.2.1 Basic formulation

In its simplest form, the Fermi-Hubbard model¹⁷⁹ represents the system as a set of discrete lattice sites, each hosting a localized orbital where a fermionic particle like an electron may reside. Particle motion between sites is described by a kinetic term, while electron–electron interactions are captured by a potential term. Written in second quantization, the minimal Fermi–Hubbard Hamiltonian is

$$H = \sum_{\langle i,j \rangle, \sigma} (-tc_{i\sigma}^\dagger c_{j,\sigma} + h.c.) + \sum_{\langle i \rangle} U n_{i\uparrow} n_{i\downarrow} \quad (6.1)$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) a fermion of spin σ at site i , and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the number operator.

The first term parameterized by t describes electron hopping between neighboring sites, while the second term with strength U accounts for on-site Coulomb repulsion.

When $U = 0$, the model reduces to the tight-binding Hamiltonian, capturing the single-particle band structure of a periodic lattice. However, with finite interactions, the model exhibits behaviors entirely absent from the single-particle picture. For example, at half-filling and large U/t , the ground state becomes a Mott insulator^{180,181}, a material that is insulating due to strong repulsion between electrons, despite band theory predicting metallic behavior.

To describe real physical systems more faithfully, the extended Fermi–Hubbard model^{182,183} introduces additional terms: site-dependent chemical potentials and long-range Coulomb interactions. The Hamiltonian becomes:

$$H = \sum_{\langle i, \sigma \rangle} \mu_i n_{i\sigma} + \sum_{\langle i,j \rangle, \sigma} (-tc_{i\sigma}^\dagger c_{j,\sigma} + h.c.) + \sum_{\langle i \rangle} U n_{i\uparrow} n_{i\downarrow} + \sum_{\langle i \neq j \rangle} U_{ij} n_i n_j \quad (6.2)$$

where μ_i is the chemical potential on site i which includes contributions from binding energies and gate-controlled potentials, and U_{ij} represents long-range Coulomb interactions. This extended formulation is particularly relevant to dopant-based silicon devices, where inter-site Coulomb coupling play critical roles in determining electron behavior.

6.2.2 Solutions and challenges

Solving the Hubbard model precisely is extremely challenging beyond one dimension ¹⁸⁴. The difficulty arises from the exponential growth of the Hilbert space with the number of sites, which quickly out resource any classical computers when n is ~ 50 .

A key concept for understanding these correlated systems is the single-particle Green's function, which encodes how an electron propagates through the interacting many-body background. From it, one can derive physical observables such as conductivity, correlation lengths, and spin or charge susceptibility. The imaginary part of the Green's function defines the spectral function ¹⁸⁵, which is essentially the density of states of a non-interacting system. In a finite system, the spectral function appears as a set of discrete peaks corresponding to allowed excitations. In the thermodynamic and large system limit, these broaden into continuous bands, resulting in non-trivial material properties.

However, computing the Green's function is often difficult: exact evaluation requires knowledge of all many-body eigenstates, which is only possible for very small systems. For this reason, a wide variety of numerical approaches have been developed. Exact diagonalization (ED) ^{186,187} provides exact spectra for small clusters; Quantum Monte Carlo (QMC) ^{188,189} stochastically samples imaginary-time Green's functions but faces the fermionic sign problem; Dynamical Mean-Field Theory (DMFT) ¹⁶⁰ approximates the lattice by a self-consistent impurity model that captures local, but not non-local, correlations. Other techniques including tensor networks ⁴ and renormalization group ¹⁹⁰ approaches, succeed in some parameter regimes but fail in others.

This unsatisfactory result from numerical methods again emphasizes why analog quantum simulation is so compelling. By mapping the Hubbard Hamiltonian into a controllable physical system, one can directly probe Green's functions and spectral properties that are otherwise inaccessible to classical computation provided that some methods of reading the state of the system are available. The dopant-based quantum dot arrays studied in this thesis serve precisely this role, providing a platform where the interplay of hopping, strong on-site repulsion, and long-range Coulomb interactions can be explored experimentally.

6.3 Experimental realization of an extended Hubbard model by dopant-based quantum dots

Building on the unique advantages provided by STM lithography, we now focus on our group’s realization of extended Hubbard physics using dopant-based quantum dots¹⁷². While earlier studies established dopant-based devices as candidates for qubits and one-dimensional model systems¹⁹¹, the challenge has been to scale these techniques to two dimensions and to probe many-body phenomena. Our work demonstrates that such systems can be fabricated, tuned, and characterized using low-temperature quantum transport. The results represent one of the first demonstrations of a tunable two-dimensional extended Fermi–Hubbard model in a solid-state system, where hopping amplitudes, on-site repulsions, and long-range Coulomb interactions can be engineered through device design. The ability to define two-dimensional arrays with atomic precision opens new opportunities for exploring correlated quantum phenomena beyond the reach of other simulators. However, stochastic variations in dopant number and clustering introduce disorder, limiting the device’s ability to emulate an ideal disorder-free system. Overcoming these challenges through improved dopant incorporation and atomic manipulation techniques presents as the next crucial step toward realizing more complex and tunable physics in dopant-based arrays.

In the following, I describe in detail the device geometry, mapping of physical device attributes to Hamiltonian parameters, transport measurements that illustrate the tuning of hopping and long-range interactions and finally numerical simulations that connect experiment to theory.

6.3.1 Device design and fabrication

To experimentally realize a two-dimensional Hubbard system, we created a series of 3×3 square arrays of phosphorus dopant clusters by removing a small patch of (~ 10 to ~ 20) adjacent hydrogen atoms. The size of this minimal two-dimensional array is chosen that it is large enough to capture nontrivial many-body correlations yet still small enough to be solved by exact diagonalization. Despite the presence of inevitable

disorder arising from dopant incorporation, these arrays exhibit clear signatures of extended Hubbard physics as we explain.

Each lattice site consisted of a lithographic patch targeted to incorporate two to three phosphorus atoms, forming a few-dopant quantum dot. These dots were weakly tunnel-coupled to source and drain leads, which were saturation-doped to ensure quasi-metallic conduction. Two in-plane gates were placed on either side of the array to capacitively tune the chemical potential landscape and thereby control electron filling across the entire lattice.

To investigate how inter-site spacing influences correlated behavior, the three arrays are designed with varying lattice constants of approximately 4.1 nm (Array #1), 6.6 nm (Array #2), and 10.7 nm (Array #3). This progression spans the regime from strong tunneling at small separations to interaction-dominated physics at larger distances. The STM images of these arrays are shown in Figure 6.3, highlighting the variation in lattice constant used for accessing different coupling regimes, while maintaining a consistent tunnel gap to the source and drain leads.

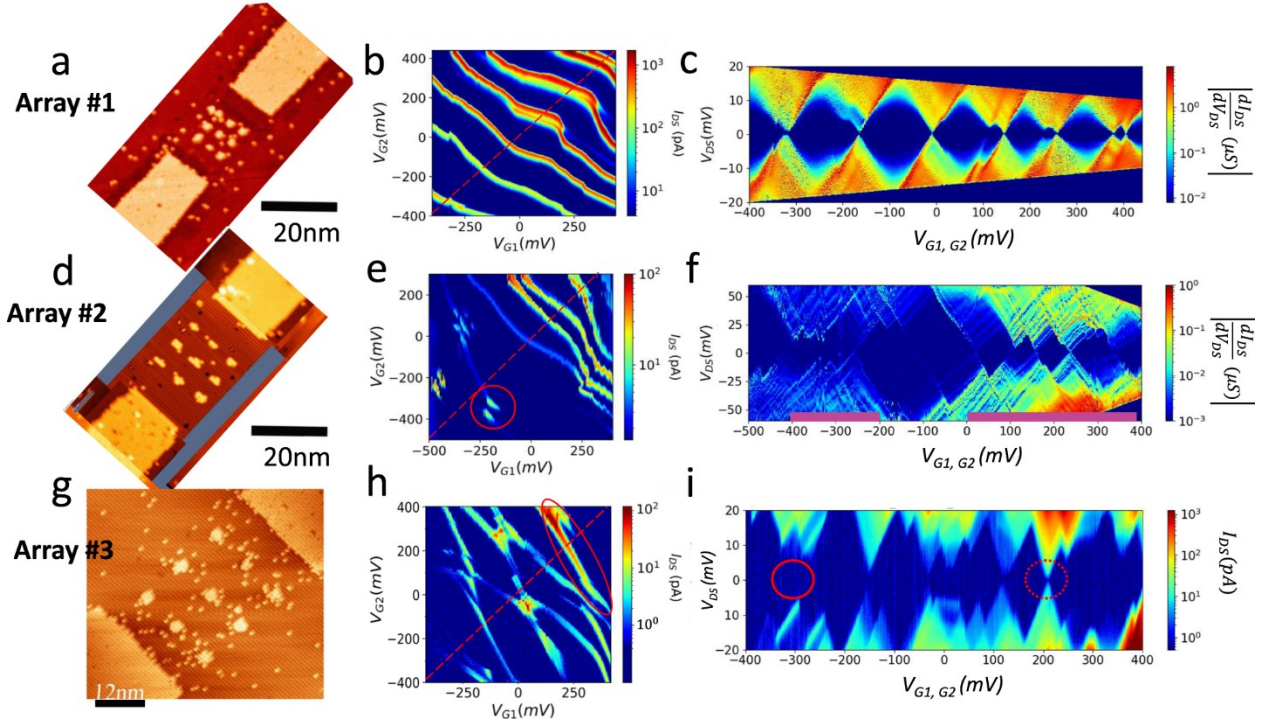


Figure 6.3 Transition from metallic behavior to the Coulomb blockade regime with increasing lattice constant. (a, d, g) STM images of three 3×3 dopant arrays with lattice constants of $a_1 = 4.1 \pm 0.3$ nm, $a_2 = 6.6 \pm 0.3$ nm, and $a_3 = 10.7 \pm 0.3$ nm, respectively. (b, e, h) Experimentally measured DC conductance charge stability diagrams for the three arrays, obtained at a bias voltage of $V_{\text{bias}} = 2$ mV for Array #1 and $V_{\text{bias}} = 4$ mV for Arrays #2 and #3, at the base temperature of the dilution refrigerator ($T = 10$ mK). (c, f, i) Differential conductance Coulomb blockade diagrams for Arrays #1 and #2, and a DC conductance Coulomb blockade diagram for Array #3, measured along the dashed lines indicated in panels (b, e, h). Solid and dashed circles in (i) highlight examples of open and closed Coulomb diamonds, respectively. This figure is taken from Wang et al.¹⁷²

6.3.2 Observation of a Finite-Size Analogue of the Metal–Mott Insulator Transition

The measured charge stability diagrams for the three arrays, obtained at a base temperature of approximately $T \sim 10$ mK (electron temperature ~ 300 mK), are shown in Figure 6.3 (b, e, h). In the first array, the charge addition boundaries run largely parallel across the gate–gate plane, resembling the stability diagram of a single metallic island in a single-electron transistor (SET). When comparing the charge stability diagrams of the three arrays, a key observation is that the third array exhibits boundaries composed

of straight segments with distinct negative slopes and characteristic bias triangles at avoided crossings. In contrast, the second array displays addition lines that intersect primarily at negative gate voltages and evolve into smoother curves at more positive voltages.

These features are further clarified by examining the differential conductance bias spectra of the first and second arrays, shown in Figure 6.3 (c, f) measured along the dashed lines indicated in Figure 6.3 (b, e), respectively. In the first array, the Coulomb diamonds are well defined, closing at small bias and exhibiting similar diamond heights, consistent with the conventional Coulomb blockade behavior of a metallic SET. Despite this overall metallic character, small discontinuities appear in the high-voltage range, likely arising from nearby charge instabilities.

In contrast, the Coulomb diamonds of the second array are irregularly shaped, reflecting the influence of intrinsic disorder, yet the bias spectrum still reveals distinct structure. Two groups of smaller Coulomb diamonds, highlighted by magenta bars, correspond to the upper and lower Hubbard bands, separated by a region of large, irregular Coulomb diamonds that represent the finite-size analogue of a Mott gap¹⁸⁰ as U/t increases. The separation between the two Hubbard bands, characterized by the addition energy of the diamonds at the gap (~ 50 meV), agrees well with the addition energies¹¹⁹ expected for few-dopant (1–3 P atoms) quantum dots. Moreover, a qualitative difference emerges in the bias conductance spectra. In the second array, lines of enhanced differential conductance run parallel to the edges of the Coulomb diamonds, indicating a discrete eigenstate spectrum, whereas in the first array no such structure is visible, signifying a quasi-continuous, metallic-like density of states where individual addition levels cannot be resolved at the measurement temperature.

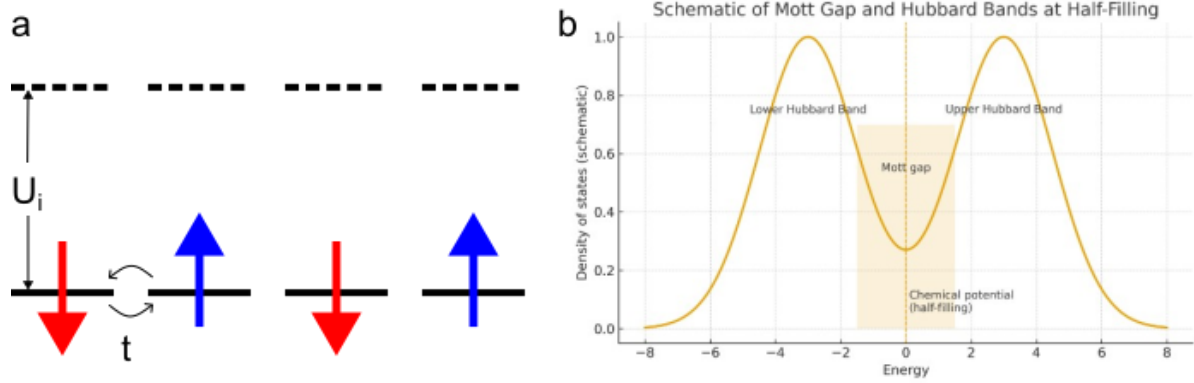


Figure 6.4 Schematic of the Mott gap and Hubbard bands at half-filling. (a) Spin and charge configuration in a half-filled Mott insulator. The large on-site repulsion U_i suppresses double occupancy, while the residual exchange interaction aligns neighboring spins in an antiferromagnetic configuration. (b) The interacting density of states splits into lower and upper Hubbard bands when the on-site repulsion U_i dominates over the tunneling amplitude. At half-filling, the chemical potential lies within the interaction-induced Mott gap, suppressing charge transport that would otherwise occur in a half-filled, non-interacting band. This schematic highlights the qualitative features relevant to the gap observed in the second 3×3 dopant array.

To summarize, by tuning the lattice constant, we can effectively control the hopping amplitude and therefore the interaction ratio U/t , enabling a continuous evolution from a strongly tunneling, metallic regime to a Mott-like insulating state and ultimately to the atomic limit. Interpreting each artificial lattice site as an “impurity” atom in silicon, the lattice constants of the first, second, and third arrays correspond to equivalent bulk doping densities of approximately $1.5 \times 10^{19} \text{ cm}^{-3}$, $3.5 \times 10^{18} \text{ cm}^{-3}$ and $8 \times 10^{19} \text{ cm}^{-3}$ respectively, spanning from above to below the critical density for the metal–insulator transition in phosphorus-doped bulk silicon. This tunability demonstrates that dopant-based arrays can access a wide range of correlated electronic phases of the extended Fermi–Hubbard model. In the following subsections, we describe the mapping between the physical device and the corresponding Hubbard parameters, followed by a qualitative simulation of the charge distributions and energy spectra of the dopant arrays.

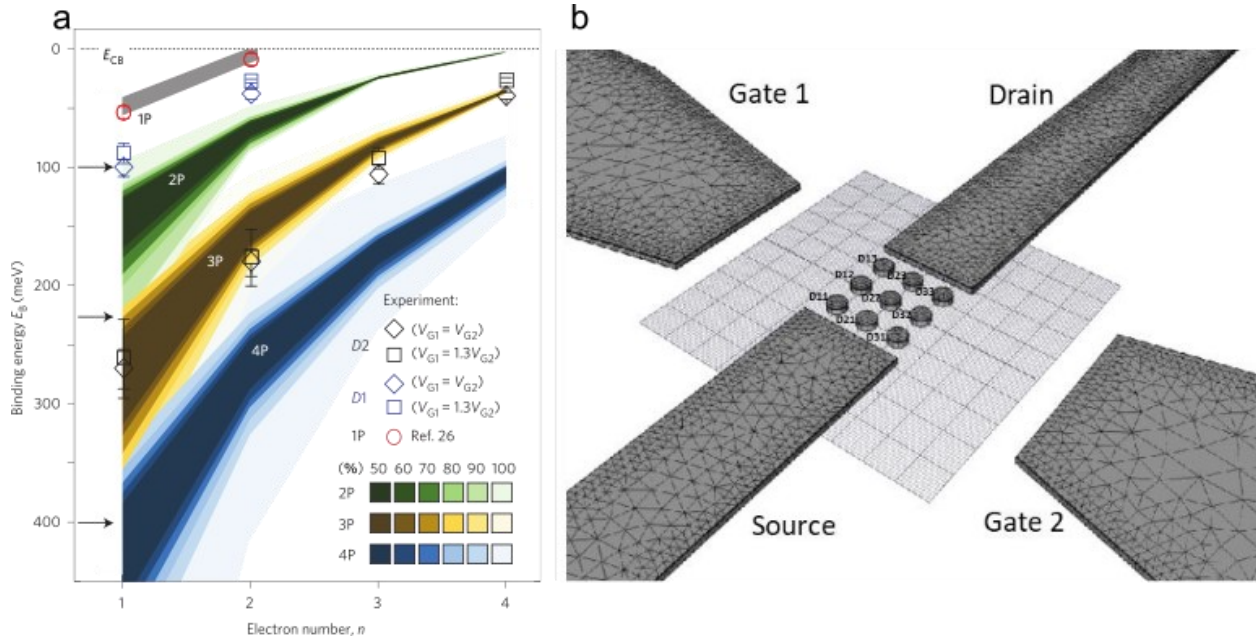
6.3.3 Mapping device geometry to Hubbard Hamiltonian parameters

One of the key advantages of the dopant-based platform is that each term of the Hamiltonian maps directly onto a physical feature of the system, making the correspondence between model and device particularly intuitive. In other words, the artificial lattice we fabricate is itself an experimental realization of the extended Fermi–Hubbard model and the mapping from device geometry to Hamiltonian parameters proceeds in a straightforward way.

The size of the lithographic patch determines the number of phosphorus atoms incorporated at each site, which determines the binding energy and hence the local on-site repulsion U_i . The separation between sites controls both the hopping amplitude t , which decays exponentially with distance, and the long-range Coulomb interaction U_{ij} , which scales approximately as $1/a$. The chemical potential of each site μ_i is the summation of local binding energy E_{bi} , Coulomb interactions with ion cores at neighboring ion cores $\sum V_{ij}$ and a tunable contribution p_i from the capacitive coupling to the gates. After fabrication, the only parameter that can be dynamically adjusted is p_i , controlled by the gate voltages V_{G1}, V_{G2} and the source-drain bias V_{ds} .

However, determining the exact numerical values of these Hubbard parameters remains challenging due to disorder and the many possible configurations in which dopants can arrange within a single cluster¹¹⁹. To address this, we propose a protocol for obtaining reliable estimates of all relevant parameters based on spectroscopic characterization of few-dopant quantum dots (E_{bi}, U_i, t) combined with electrostatic simulations (U_{ij}, V_{ij}). From STM images, we estimate that each site contains approximately 2 ± 1 dopants, corresponding to an average addition energy $U_i \sim 45 \text{ meV}$ according to tight binding calculations shown in Figure 6.5. The three lattice constants correspond to estimated average hopping amplitudes ranging from $t \approx 8 \text{ meV}$ at a spacing of 4.1 nm to $t \approx 0.5 \text{ meV}$ at 10.7 nm, reflecting an exponential reduction of inter-site coupling with increasing distance. In practice, the pairwise hopping amplitude depends not only on the physical separation between sites but also on the spatial form of the electron wavefunction. For electrons

bound to few-donor clusters, the wavefunctions are less sensitive to Bloch-phase oscillations or crystallographic orientation compared with single-donor systems (see section 3.1), resulting in smoother and more predictable variations of t across the array. The long-range interactions U_{ij} are estimated based on capacitance simulation of the devices which fall in the few milli eV range. The V_{ij} describing the electron-ion Coulomb interactions, is approximated using a point-charge approximation $V_{ij} = -\frac{V_0}{|R_i - R_j|}$ where $V_0 = \frac{e^2}{4\pi\epsilon_r\epsilon_0} = 123 \text{ meV} \cdot \text{nm}$ in silicon. In a finite 3×3 array, this term shifts the local chemical potentials unevenly. The central site, surrounded by eight neighbors, experiences the largest cumulative offset, producing a “sagging couch” effect in the potential landscape. Taken together, we estimate that the three arrays span interaction-to-hopping ratios U_{ii}/t from ~ 6 to ~ 90 , ranging from a metallic regime in the smallest array to the atomic limit in the largest array.



binding energy E_{bi} and interaction term U_i are extracted from the transition between the charge-neutral and negatively charged states near the Fermi level for the corresponding donor numbers. (b) Electrostatic simulation of the device potential landscape using a finite element software package, FasterCAP¹⁹², Lever arms α_i and mutual charging energies U_{ij} are derived from the simulated capacitance matrix using the constant-interaction model. The ratio of gate lever arms determines the slope of the conduction lines observed in the charge stability diagrams.

With the key parameters determined, we simulated the charge configuration and transport behavior of the arrays within the extended Fermi–Hubbard framework to visualize how gate voltages tune charge distributions and to compare qualitatively with experiment. Here we focus on Array #3, which lies near the atomic limit ($U/t \gg 1$), where tunneling between sites is weak and transport occurs in the Coulomb blockade regime, consistent with the zero-conductance regions observed experimentally at finite bias. The blockade can be lifted by applying plunger gate voltages that align an available energy level of the array with the Fermi level of the source and drain, allowing single-electron tunneling events that produce finite conductance.

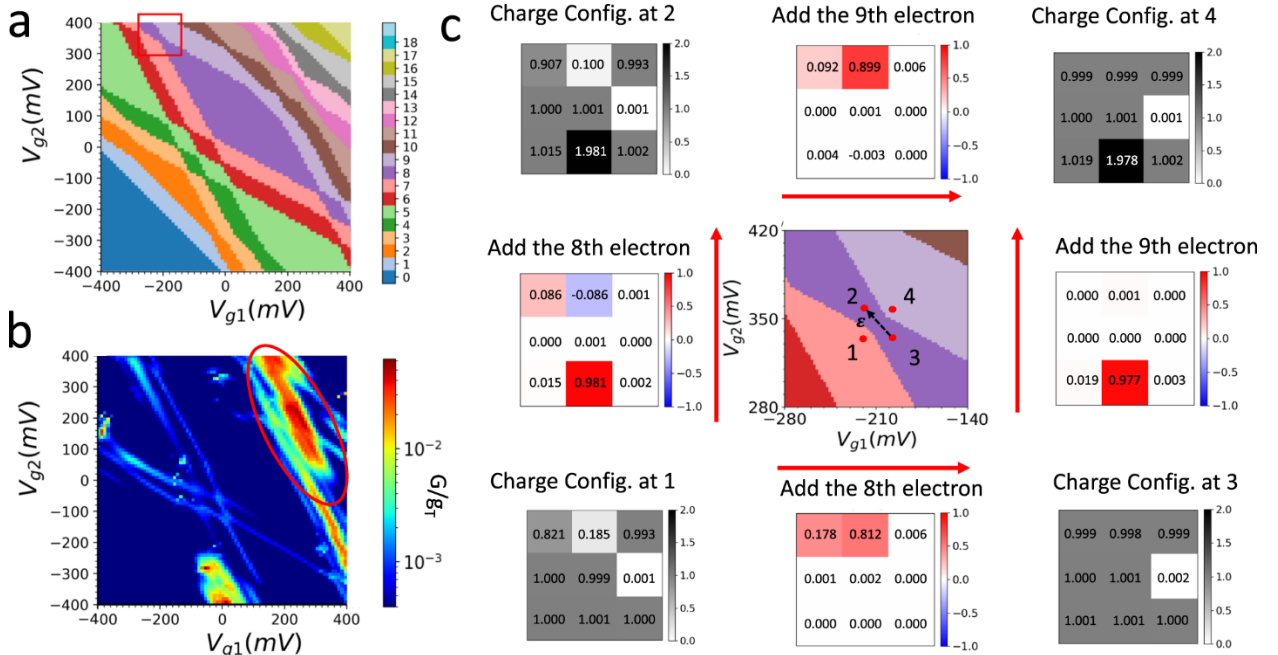


Figure 6.6 Simulated charge addition and resonant tunneling in Array #3. (a) Numerically simulated charge stability diagram of the 3x3 array ground state with hopping amplitude $t = 0.5$ meV. (b) Simulated resonant conductance map including a finite bias window, modeled by setting $k_B T = 1$ meV. (c)

Schematic charge configurations corresponding to the region highlighted by the red box in panel (a). Black–white color maps show the ground-state charge occupation, while red–blue maps indicate changes in occupation upon crossing a charge-addition boundary. Numbers overlaid on each panel denote the site occupation of the ground and charge-added states. This figure is taken from Wang et al.¹⁷²

Figure 6.6 (a, b) shows the numerically simulated charge stability diagram and corresponding conductance map for Array #3. Within each color domain, the total number of excess electrons N remains constant, corresponding to Coulomb-blockaded regions in transport. Sweeping the gate voltages along the 45° diagonal direction tunes the total electron number, while sweeping along the negative 45° direction mainly tilts the chemical potential landscape, redistributing charge among sites without substantially altering the overall filling. Because of disorder, the largest charging energy in the simulation occurs at $N = 8$ ($\approx 11\%$ hole doping) rather than the half-filling state expected for an ideal uniform lattice.

Charge stability boundaries correspond to conductance lines in the simulated transport map, though not all boundaries appear with equal visibility. Both the simulated and measured conductance maps exhibit enhanced conductance along specific lines of negative slope at positive gate voltages. The non-closing Coulomb diamonds and asymmetric shapes of the stability diagrams arise primarily from non-uniformities of dopant-number variations across sites, which distort the potential landscape and affect transport. Secondary effects include small asymmetries in gate coupling and atomic-scale variations in hopping amplitudes.

Figure 6.6 (c) illustrates the ground-state charge and charge-addition distributions near an avoided crossing around $N = 8$. The simulations confirm that electron addition occurs predominantly at individual sites, reflecting the localized nature of charge in this regime. The ratio of lever arms from the upper (Gate 1) and lower (Gate 2) gates to each dot depends on their relative distances, giving rise to three distinct slopes in the addition lines corresponding to the upper, middle, and lower rows of the array.

6.3.4 Details of numerical simulation

We model the dopant arrays using an extended Hubbard Hamiltonian restricted to a single spinful orbital per site near the Fermi level, allowing up to 18 valence electrons in the system. At each gate–gate voltage point, the many-body Hamiltonian is solved by exact diagonalization in the Fock basis to obtain ground and excited states. The hopping amplitudes are set to $t = 8$ meV, 2 meV, and 0.5 meV for the first, second, and third arrays, respectively. The Hamiltonian is block-diagonalized in subspaces of fixed electron number n_e and spin projection S^z . For each subspace, basis states are constructed as binary strings denoting site occupancies of spin-up and spin-down electrons, e.g., $|01010\rangle \otimes |00000\rangle$ represents one spin up on dot 2 and one spin up on dot 4 for a five-dot system. Matrix elements are computed using fermionic anti-commutation relations, and efficient state indexing is handled through a Lin lookup table¹⁹³. For (n_u, n_d) electrons in on N sites where $n_u(n_d)$ is the number of spin up (down), the possible configuration number of all arrangement or the dimension of the Hilbert space is $d = C_N^{n_u} \times C_N^{n_d}$ where $C_N^{n_u}, C_N^{n_d}$ are the total combination factor of the spin up, spin down section.

The basis states are indexed according to their binary representation. For instance, $|00011\rangle$ is assigned index 0 as the first state, whereas $|11000\rangle$ corresponds to index 9 as the last state within the $n_u = 2$ sector. The Hamiltonian matrix elements are evaluated by sandwiching the relevant operators between the bra and ket states, which can be expressed in the general form $c_{i\sigma}^\dagger c_{j\sigma}^\dagger \dots |0\rangle$ and its Hermitian conjugate. The fermionic anti-commutation relation $[c_{i\sigma}^\dagger, c_{j\sigma}] = \delta_{i,j}$ is preserved during evaluation, yielding a sign inversion (multiplication by -1) each time creation and annihilation operators are permuted across distinct sites or spin indices. Diagonal contributions, such as on-site and long-range Coulomb interactions, are obtained directly from the electron occupation numbers of the state vector. Off-diagonal hopping terms are computed by utilizing the binary representation of the basis states and referencing their indices from the lookup table to identify the corresponding matrix elements. Each subspace labeled by (n_e, n_u) is subsequently diagonalized to solve for eigenenergies and eigenvectors.

Spin sectors with dimensions smaller than 2000 are solved by full diagonalization; larger subspaces are treated with a custom Lanczos¹⁹⁴ routine that iteratively converges to the lowest ≈ 40 eigenstates within a prescribed tolerance. This hybrid scheme preserves accuracy for transport-relevant states ($\Delta E < k_B T$) while reducing computation time. By comparing ground-state energies across charge sectors, charge-transition boundaries and stability diagrams are obtained as functions of gate voltages.

To simulate transport, the coupling between the array and metallic leads is introduced as perturbative terms H_{tun} . The Hamiltonian of the full system is:

$$H = H_{array} + H_{leads} + H_{tun} \quad (6.3)$$

The first term is the extended Fermi-Hubbard Hamiltonian of the array, the second term describes the non-interacting modes in the source and drain:

$$H_{leads} = \sum_{k\sigma} (\epsilon_{k\sigma}^R + \epsilon_{k\sigma}^L) d_{k\sigma}^\dagger d_{k\sigma} \quad (6.4)$$

$$H_{tun} = \sum_{kj,\sigma} V_{kj,\sigma} (d_{k\sigma}^\dagger c_{j\sigma} + h.c.) \quad (6.5)$$

Two complementary approaches (one simpler and the other more sophisticated) are used to derive the conductance.

Rate-equation model

Under small bias, the tunneling processes between leads and localized states can be approximated by a master-equation approach¹⁹⁵. Transition rates are computed from the solved many-body wave functions $\Psi_\alpha^{n\uparrow, n\downarrow}$ with energy $E_\alpha^{n\uparrow, n\downarrow}$ where α denoted the state index in the same spin sector. The tunneling rate $\Gamma_{\alpha,\beta,\sigma}^{(L)}$ of an electron entering from the left lead to the array can be obtained using the Fermi's golden rules through the overlap between a pair of many body wavefunction with $\Delta N = 1$ (assuming identical tunnel rate $t_{kj} = \gamma$)

$$\Gamma_{\alpha,\beta,\sigma}^{(L), n_\sigma, n_{\sigma'}} = 2\pi |\gamma|^2 M_{\alpha,\beta,\sigma}^{(L), n_\sigma, n_{\sigma'}} \quad (6.6)$$

$$M_{\alpha,\beta,\sigma}^{(L),n_\sigma,n_{\sigma'}} = \sum_j \left| \langle \Psi_\alpha^{n_\sigma,n_{\sigma'}} | c_{j\sigma}^\dagger | \Psi_\beta^{n_{\sigma-1},n_{\sigma'}} \rangle \right|^2 \quad (6.7)$$

The summation over j includes all edge sites with nonzero tunnel coupling (t_{kj}) to the left lead. The tunneling rate for the reverse process, as well as for tunneling from the right lead, can be expressed in an analogous form. Electron transport through the array can be interpreted as a steady-state process in which electrons enter from one lead and exit through the other, under the condition that the tunneling rates at both boundaries are nonzero. This corresponds to a finite addition electron density at both the left and right edges of the array. Therefore, localization of electronic states leads to suppression in the tunneling current at low source-drain bias as is the case for array # 3. Within the rate-equation formalism, and accounting for the thermal occupation of states at finite electron temperature, the linear-response conductance is given by:

$$G = g_T \sum_{n_\sigma, n_{\sigma'}} \sum_{\alpha, \beta, \sigma} \frac{M_{\alpha, \beta, \sigma}^{(L), n_\sigma, n_{\sigma'}} M_{\alpha, \beta, \sigma}^{(R), n_\sigma, n_{\sigma'}}}{M_{\alpha, \beta, \sigma}^{(L), n_\sigma, n_{\sigma'}} + M_{\alpha, \beta, \sigma}^{(R), n_\sigma, n_{\sigma'}}} \times P_\alpha^{n_\sigma, n_{\sigma'}} \left[1 - f_{FD} \left(E_\alpha^{n_\sigma, n_{\sigma'}} - E_\beta^{n_{\sigma-1}, n_{\sigma'}} - \mu \right) \right] \quad (6.8)$$

where $g_T = e^2 \Gamma / (\hbar k T)$ and

$$P_\alpha^{n_\sigma, n_{\sigma'}} = \frac{\exp \left[- \left(\frac{1}{kT} \right) (E_\alpha^{n_\sigma, n_{\sigma'}} - n\mu) \right]}{\sum_{n_\sigma, n_{\sigma'}, \alpha} \exp \left[- \left(\frac{1}{kT} \right) (E_\alpha^{n_\sigma, n_{\sigma'}} - n\mu) \right]} \quad (6.9)$$

is the grand canonical ensemble probability that the array is in state $\Psi_\alpha^{n_\sigma, n_{\sigma'}}$ and f_{FD} is the Fermi-Dirac distribution function. This rate-equation approach is valid in the weak-coupling regime such that the physics of the array is not disturbed by the existence of the leads. Another relevant energy scale is the thermal energy $k_B T$. In the low-temperature limit ($k_B T \ll \Delta E$) transport is dominated by transitions involving only the few lowest-energy states. At elevated temperatures, a larger number of excited states become thermally accessible, increasing the computational complexity of the conductance calculation. It should be noted that evaluating the conductance G requires a double summation over all many-body states differing by $\Delta n = 1$, which constitutes the most computationally intensive part of the simulation, significantly exceeding the

time used for exact diagonalization. The simulated conductance shown in Figure 6.6(b) was calculated using this approach.

Meir-Wingreen formula

For comparison, we also evaluate conductance using the non-equilibrium Green's-function (NEGF) approach formulated by Meir and Wingreen¹⁹⁶ which extend beyond the zero source-drain bias limit. The Meir-Wingreen formula describes the electric current through an arbitrary mesoscopic system by NEGF in the Keldysh formalism¹⁹⁷. It is a standard tool for calculating the current for systems such as molecular junctions, coupled quantum dots and nanoscale devices. The total Hamiltonian includes the interacting region, non-interacting leads, and tunneling matrix between the two. The tunneling current can be written as the expectation value of the tunnel operator:

$$J = \frac{ie}{h} \Sigma (V_{k\alpha,n} \langle c_{k\alpha}^\dagger d_n \rangle - V_{k\alpha,n}^* \langle d_n^\dagger c_{k\alpha} \rangle)$$

where $V_{k\alpha,n}$ are the tunneling matrix elements. Using the definition of the Keldysh Green's function, the current can be expressed solely in terms of the Green's functions of the interacting region (the array), under the assumption that the lead-array tunneling acts as a perturbation.

$$J = \frac{ie}{h} \int d\varepsilon \text{Tr} \{ [f_L \Gamma^L - f_R \Gamma^R] (G^r - G^a) + (\Gamma^L - \Gamma^R) G^< \} \quad (6.11)$$

where G^r, G^a and $G^<$ are the retarded, advanced, and lesser Green's functions of the interacting region (the array), $\Gamma^{L(R)}$ is the tunneling matrix at the left (right) lead. In the non-interacting limit, this expression reduces to the Landauer formula¹⁹⁸. Despite its concise formulation and intuitive interpretation, the numerical calculation of the current is still limited by the system size of the interacting regions as the knowledge of its Green's function requires the solution of the full Hamiltonian. Figure 6.7 presents an example from Gaw lczyk et al¹⁹⁹, where finite-bias transport through a disordered 3×3 dopant array was calculated using physical parameters comparable to those of our device.

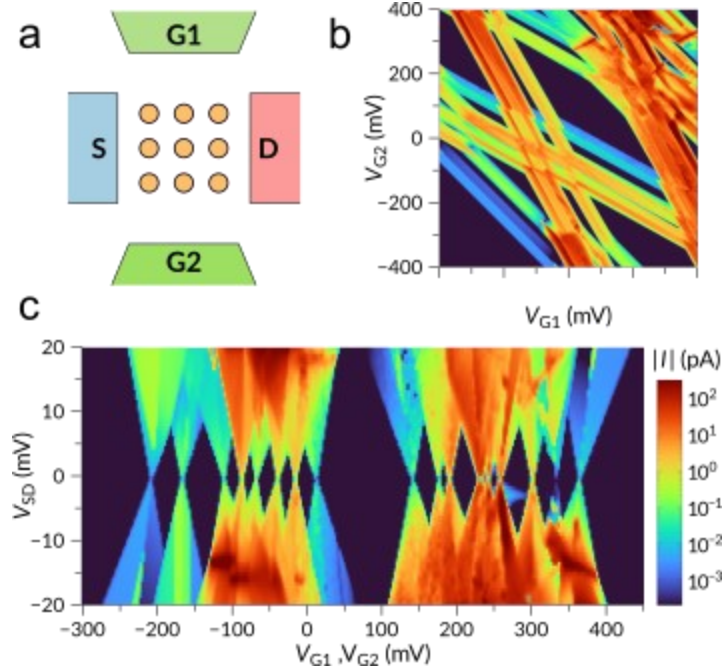


Figure 6.7 Transport simulation beyond zero bias using non-equilibrium Green's functions. (a) Device configuration. (b) Stability diagram at 8mV of source-drain bias and (c) Coulomb blockade diagram simulated for the weakly tunnel coupled array. Figure adapted from Gawelczyk et al.¹⁹⁹

6.3.5 Spin filling sequence and magnetotransport measurement

So far, we have only discussed the charge configuration and transport characteristics. Understanding how electrons occupy spin states in quantum-confined systems provides deeper insight into their underlying level structure and interactions. Foundational works^{200–202} from Dzurak's group on silicon metal–oxide–semiconductor (MOS) quantum dots established the use of magnetotransport spectroscopy to determine spin filling sequences by analyzing the slopes of charge transition lines in the stability diagram. In such measurements, the slope of a charge transition line with magnetic field reflects the change in total spin of the dot upon adding one electron, following

$$\frac{\partial \mu_N}{\partial B} = -g\mu_B \Delta S_{\text{tot}}(N) \quad (6.12)$$

where μ_N is the electrochemical potential of the N th electron, g is the electron g-factor, μ_B is the Bohr magneton and $\Delta S_{tot}(N)$ is the change in total spin of the dot after adding the N th electron. Assuming the newly added electron does not alter the spin configuration of the already filled electrons, $\Delta S_{tot}(N)$ can only take the value of $\pm 1/2$. A positive slope ($+1/2g\mu_B$) indicates the addition of a spin-up electron, while a negative slope ($-1/2g\mu_B$) corresponds to adding a spin-down electron. By tracking how consecutive Coulomb peak positions shift with magnetic field, the spin filling sequence can be deduced. Figure 6.8 shows the Si MOS device schematic and the magnetotransport measurement used in Lim et al.²⁰²

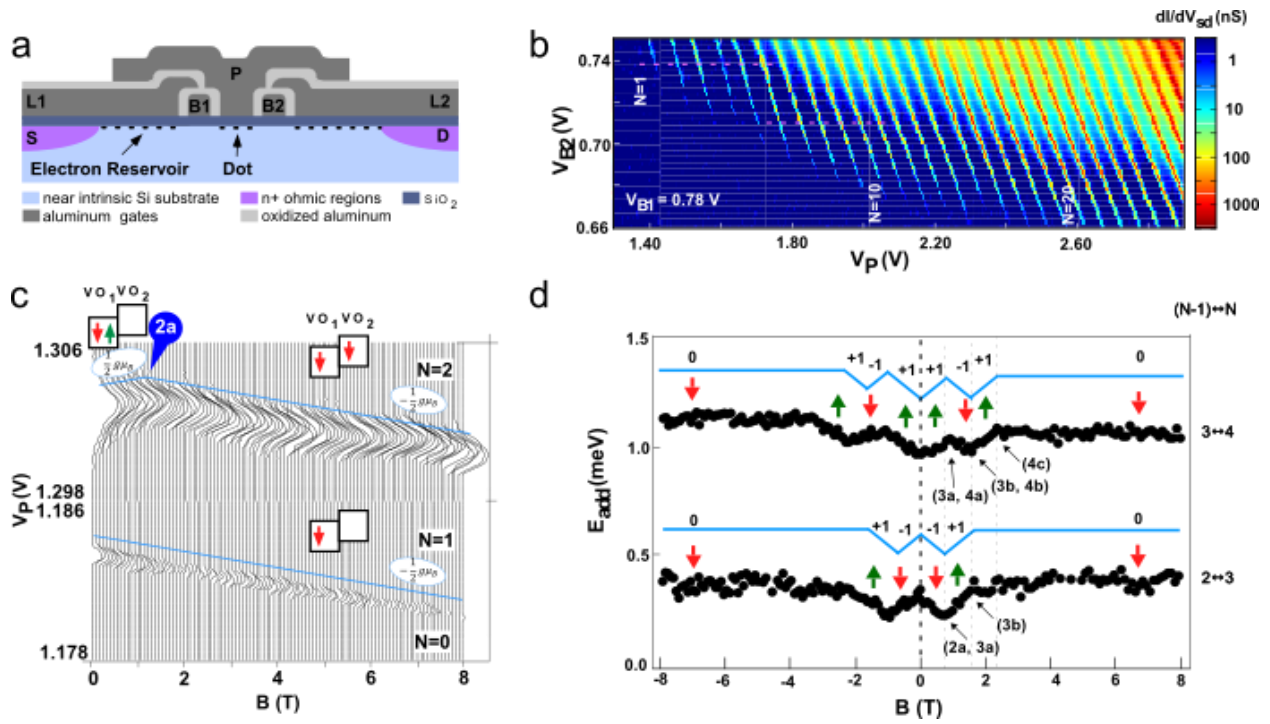


Figure 6.8 Magnetotransport spectroscopy of a gate-defined silicon MOS quantum dot (adapted from W. H. Lim et al.²⁰²). (a) Schematic cross-section of the Si-MOS quantum dot device. The source, dot, and drain form a single-electron transistor (SET) controlled by the plunger gate P and barrier gates B1 and B2. (b) Differential conductance plotted as a function of barrier-gate and plunger-gate voltages, showing the Coulomb blockade regions. (c) Magnetospectroscopy of the first two electrons entering the quantum dot. VO_1 and VO_2 denote the two lowest valley-orbital states. At $B > 0.86$ T, the Zeeman energy exceeds the valley-orbital splitting, and the second electron occupies a spin-down state in VO_2 instead of a spin-up state in VO_1 , producing a characteristic kink in the current-field trace. (d) Addition energies of the third

and fourth electrons as a function of magnetic field, showing additional kinks corresponding to the filling of higher valley–orbital states.

Importantly, kinks in the Coulomb peak trajectories appear when a spin-up state crosses a spin-down state as the magnetic field increases. This level crossing occurs when the Zeeman energy compensates for the orbital or valley splitting between opposite-spin states. At these points, the ground-state configuration of the added electron switches, for example, from a lower valley–orbital spin-up state to a higher-orbital spin-down state, thereby reversing the sign of $\frac{\partial \mu_N}{\partial B}$.

At low magnetic fields, the first four electrons follow an even–odd spin-filling sequence, forming the 1s shell of the two-dimensional quantum dot. At higher occupancies, however, the observed spin-filling pattern deviates from this simple alternation due to more complex valley–orbital coupling. The resulting spin–valley shell structure manifests as a sequence of spin transitions and a characteristic addition-energy spectrum, analogous to the shell filling of a two-dimensional artificial atom.

While the spin-filling sequence in a single gate defined quantum dot is primarily governed by valley–orbital coupling, in multi-site systems such as the 3×3 dopant array, the underlying mechanism is qualitatively different. In natural atoms, Hund’s rule²⁰³ arises from the competition between the exchange interaction J and Coulomb interaction U of electrons occupying degenerate orbitals, favoring parallel spin alignment to minimize the total energy.

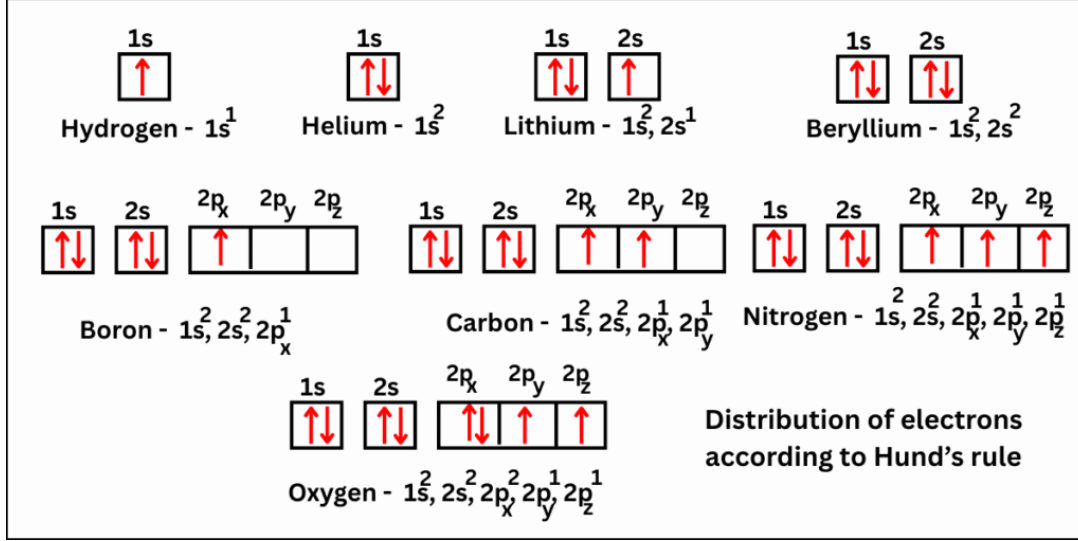


Figure 6.9 Electron spin configurations from hydrogen to oxygen atoms, figure taken from online resource ²⁰⁴. The filling sequence of the 2p orbitals follows Hund's rule, whereby the p_x , p_y , and p_z orbitals are each singly occupied before any orbital becomes doubly filled. This occurs because electrons with opposite spins in the same orbital experience stronger Coulomb repulsion. The same principle can be extended to artificial atoms composed of a few coupled donor dots, where the competition between exchange interactions and Coulomb interactions determines the spin-filling sequence.

A similar principle applies in the dopant array. Here, the exchange interactions occur between electrons on neighboring sites, rather than between orbitals within a single confinement potential. As a result, the spin configuration of the array is determined by the interplay between on-site repulsion, long-range Coulomb interaction, and exchange coupling. This makes the analogy to Hund's rule more appropriate for a system like the 3×3 dopant array, which behaves as a collective artificial atom whose spin filling follows an extended version of atomic Hund's principle with tunable interactions.

To probe the spin-filling sequence of the 3×3 dopant array, we employ a similar method by tracking the slopes of the charge addition lines as a function of magnetic field. Among the three fabricated arrays, we focus on the strongly coupled array with a lattice constant of $a = 4.1$ nm for two main reasons. First, the closely packed donor sites produce a delocalized electron distribution, making this configuration more analogous to a large artificial atom compared with the sparser arrays, where the electron states remain

mostly localized. The interplay between exchange interactions and Coulomb interactions are also more likely to trigger non-trivial spin configurations.

Secondly, the Coulomb diamond diagram of the strongly coupled array exhibits closed and regularly spaced diamonds. This enables measurable tunneling currents even at small source–drain biases, allowing us to track charge addition and spin transitions without applying a large bias voltage that could otherwise alter the atomic-scale energy landscape and give bias dependent “atom” structures.

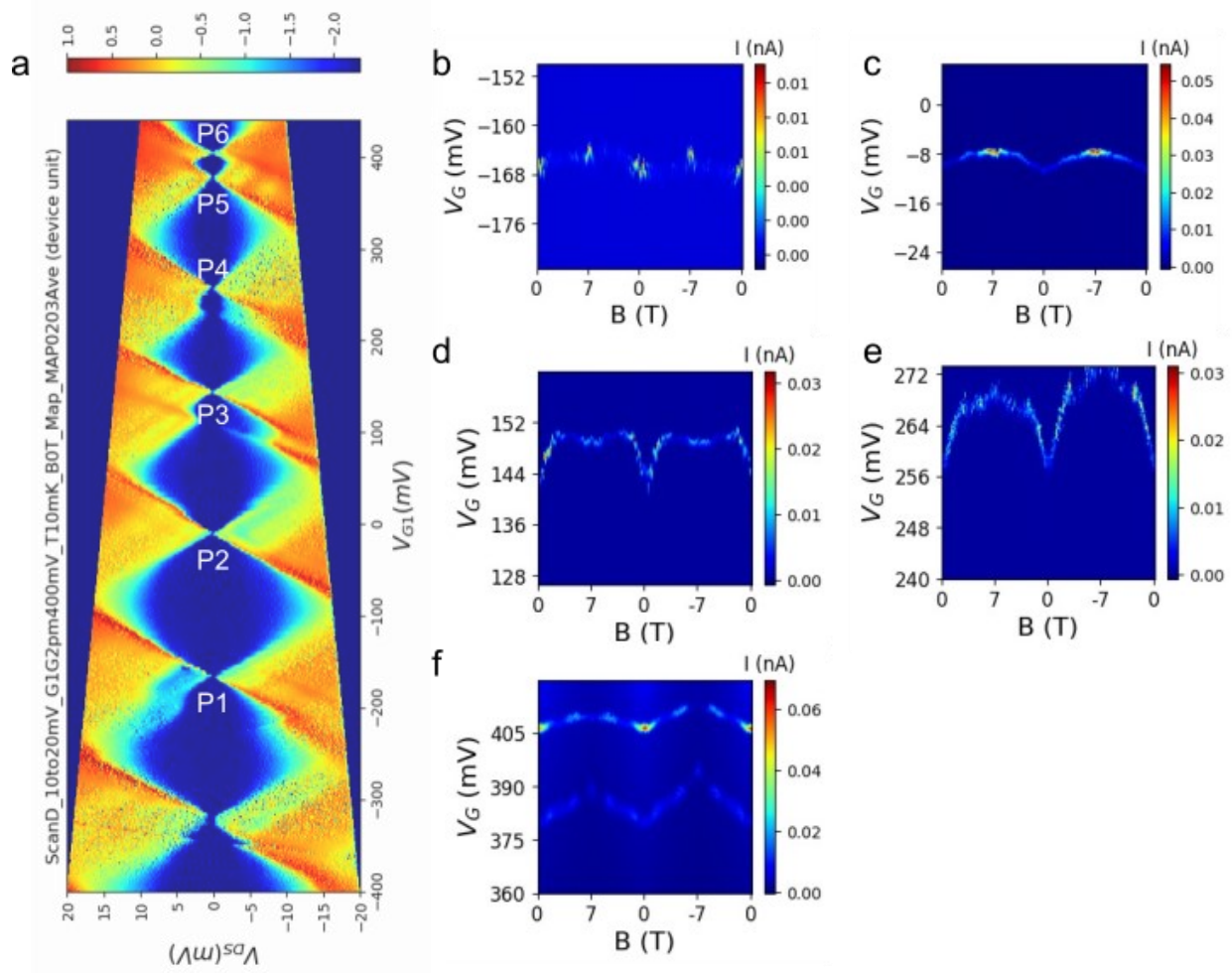


Figure 6.10 Magnetotransport measurement of the strongly coupled 3×3 dopant array ($a = 4.1$ nm) at an estimated electron temperature of $T_e = 300$ mK. (a) Log-scale Coulomb stability diagram showing regularly spaced, closed diamonds corresponding to uniform charging energies. The five peaks labeled P1–P6 are tracked as a function of magnetic field. (b–f) Magnetospectroscopy of electron additions from P1 to P6, measured at a small source–drain bias of $V_{ds} = 0.1$ mV over a magnetic-field range of -7 T $\leq B \leq +7$ T.

The spectra exhibit largely symmetric behavior with respect to field polarity. Multiple kinks are visible, arising from ground-state transitions as the magnetic field increases.

Figure 6.10 summarizes the magnetotransport measurements performed on the strongly coupled 3×3 array. The device plane is oriented such that it is parallel to the direction of the external magnetic field to exclude effects from the Peierls term ²⁰⁵. The regularly spaced Coulomb diamonds shown in Fig. 6.10(a) indicate well-defined and uniform charging energies. Five representative charge addition peaks labelled P1–P6 were selected for magnetospectroscopy. In Fig. 6.10(b–f), the regions near the conductance peaks were swept as a function of magnetic field from -7 T to $+7$ T at a small source–drain bias of $V_{ds} = 0.1$ mV. The resulting traces display clear kinks and distinct values of slopes, corresponding to ground state transitions as Zeeman splitting shifts the relative energies between different spin configurations.

The approximately symmetric behavior at positive and negative magnetic fields further confirms the spin nature of these transitions.

To quantize the peak shifts in the voltage space, the position of each conductance peak was determined by locating the magnetic-field-dependent maximum in the tunneling current. These peak positions were then converted into chemical potentials of the added electrons using the lever arms extracted from the shapes of the Coulomb diamonds. Alternatively, we also look at the addition energy E_{add} between two consecutive electrons $E_{add} = \mu(N + 1) - \mu(N)$ and its dependence on the magnetic field:

$$\frac{\partial E_{add}}{\partial B} = \frac{\partial \mu_{N+1}}{\partial B} - \frac{\partial \mu_N}{\partial B} = -g\mu_B(S_{tot}(N + 1) - S_{tot}(N - 1)) \quad (6.13)$$

where $S_{tot}(N + 1)$ and $S_{tot}(N - 1)$ are the total spin of the $N+1$ state and $N-1$ state. This equation illustrates the difference between systems with and without interaction. Without many-body interactions, the spin of newly added electron has no correlation with the spin of the already filled electrons, therefore $\Delta S_{tot}(N)$ can only take the value of $\pm 1/2$ and $\frac{\partial E_{add}}{\partial B}$ can only take the value of $\{0, -g\mu_B, +g\mu_B\}$ corresponding to the two consecutive electrons have spin $\{(\downarrow, \downarrow \text{ or } \uparrow, \uparrow), (\uparrow, \downarrow), (\downarrow, \uparrow)\}$. In the presence of

many-body interactions, the total spin of the system ground state can change by more than $\pm 1/2$ due to correlation, resulting in more interesting behavior such as transition lines with a much higher slope such as $\pm 3/2 g\mu_B$ or even $\pm 5/2 g\mu_B$. In other words, charge-transition slopes exceeding $\pm 1/2 g\mu_B$ signify strong electron–electron correlations, which underpin the Hund’s-rule-like spin ordering observed in this artificial atom.

Figure 6.11 shows the extracted peak positions converted to chemical potential, together with the corresponding addition-energy spectrum, obtained by taking the difference between consecutive peaks. The curves are vertically offset for clarity, allowing all transitions to be displayed in a single plot. Each segment between kinks is fitted to the nearest integer multiple of $1/2 g\mu_B$, revealing the characteristic Zeeman slopes associated with different spin configurations.

Examining the range between $B=0$ T and $B=7$ T, the first two peaks exhibit slopes of approximately $+\frac{1}{2} g\mu_B$, consistent with the addition of spin-up electrons. The third and fourth peaks show unusually large positive slopes at low fields (0–2.5 T), best matched to $+\frac{5}{2} g\mu_B$. This behavior suggests that, in addition to the added electron being spin-up, two spin-down electrons within the array flip to spin-up, driven by strong electron correlation. Above 2.5 T, the third peak reverses to a negative slope of $-\frac{1}{2} g\mu_B$, indicating that the added electron is now spin-down, while the fourth peak transitions to a slope of $+3/2 g\mu_B$, corresponding to the addition of a spin-up electron accompanied by an internal spin flip within the array. The behavior of the fifth and sixth peaks can be similarly interpreted with a positive slope of $+\frac{3}{2} g\mu_B$ and $+\frac{1}{2} g\mu_B$ respectively.

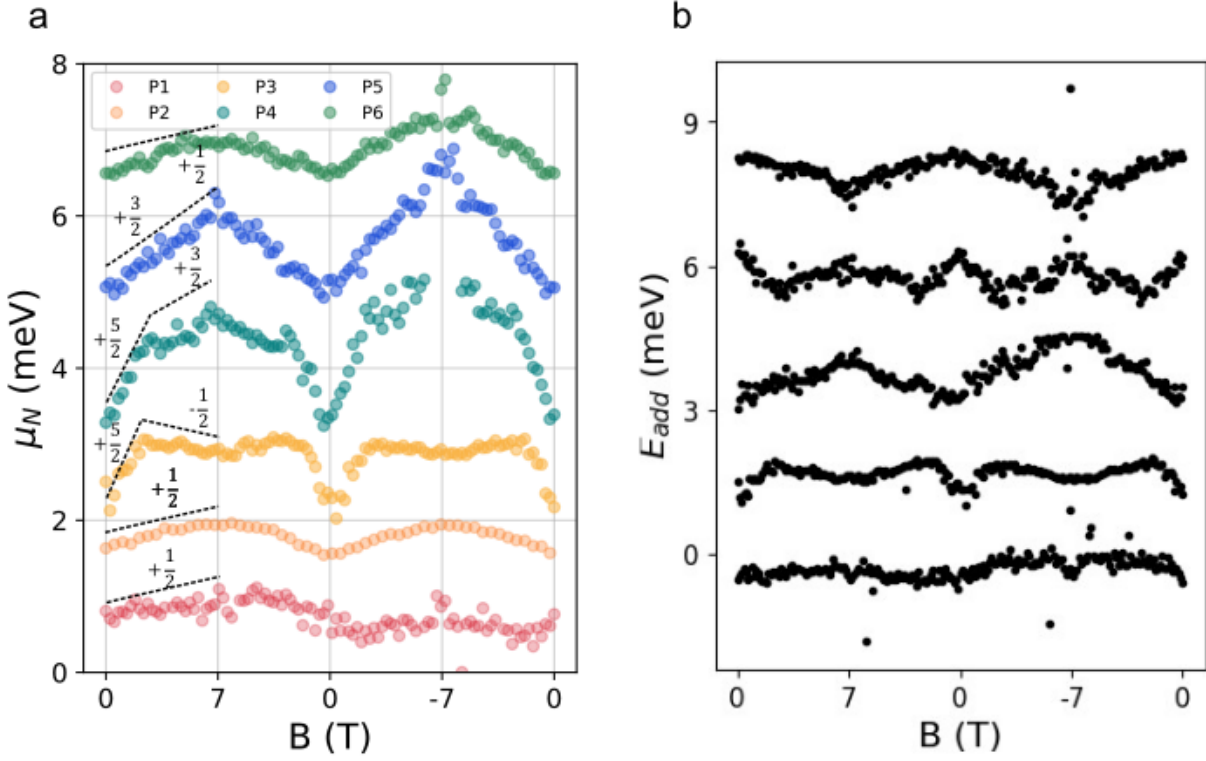


Figure 6.11 (a) Electrochemical potential of the N th electron added to the array, extracted from the position of Coulomb peaks in the magnetospectroscopy data, slopes are annotated in units of $g\mu_B$. (b) Electron addition energy, obtained as the difference in electrochemical potential between consecutive electrons in (a) $E_{add} = \mu_{N+1} - \mu_N$. The data are vertically offset for clarity.

From another cooldown of the same device, we performed RF-reflectometry measurements to probe electron addition. Figure 6.12 presents the Coulomb-diamond maps obtained through DC current, RF magnitude, and RF phase, using an input RF power of approximately -95 dBm. Although slight variations (position and shape of the Coulomb peaks) appear due to changes in the surrounding charge environment, the overall transport characteristics of the device remain consistent across cooldowns.

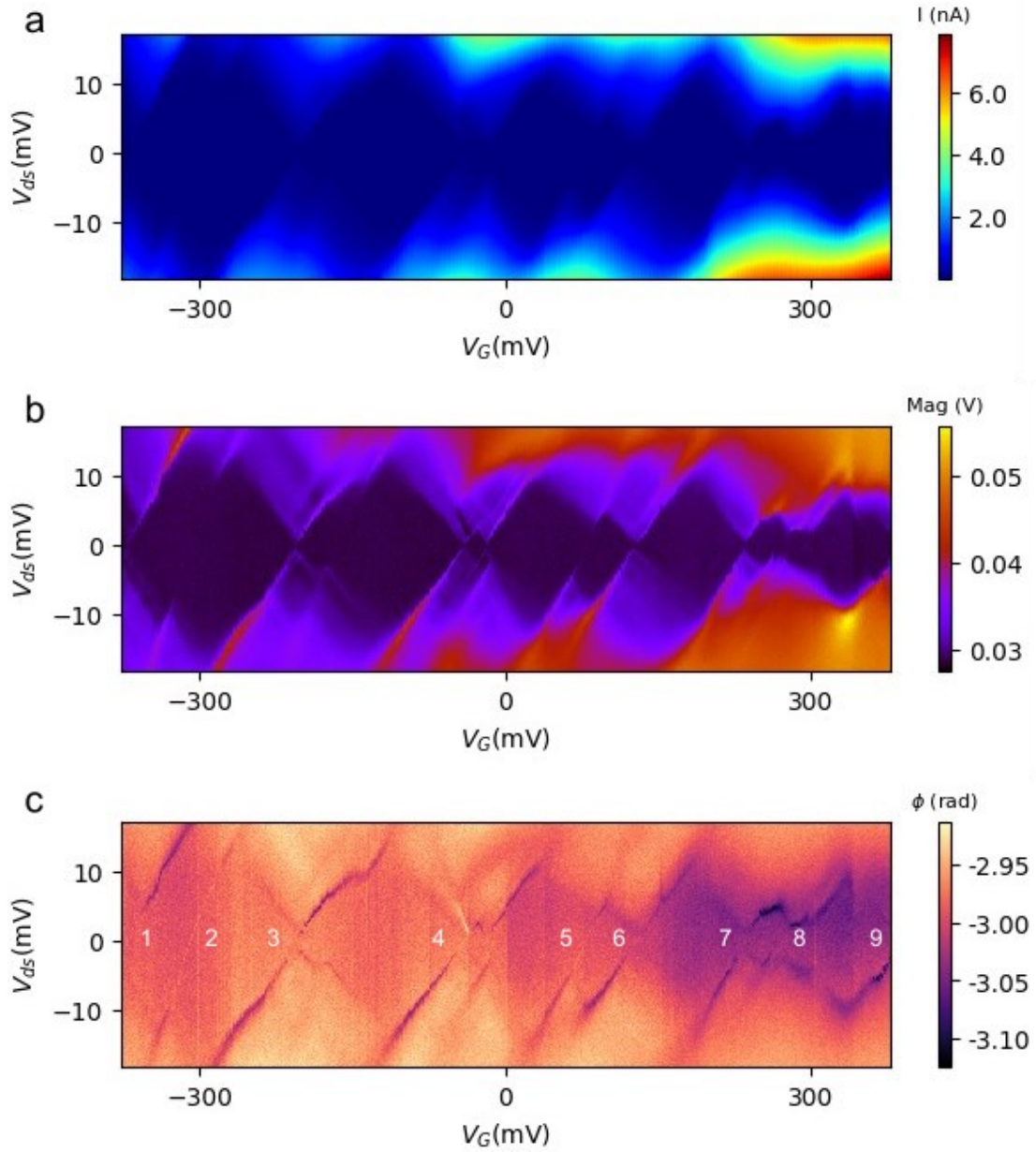


Figure 6.12 RF reflectometry measurement of the same device in a separate cooldown, with an input power of $P_{in} = -95$ dBm. (a) DC current, (b) RF magnitude, and (c) RF phase of the Coulomb diamond diagram. The reflectometry signal is sensitive to the capacitive response of the array, enabling the detection of charge transitions even at zero source–drain bias, where no DC current flows. Nine notable transitions are labeled in (c).

The details of RF reflectometry measurements will be discussed in the next chapter. The major advantage of the technique here is that it is sensitive to both conductance and capacitance within the array, enabling charge transition to be detected even at zero source drain bias. In the previous magnetotransport measurement, many Coulomb diamonds are not closed at zero bias which can be result from finite density of state in the lead or localization of electronic state within the array. The Coulomb peaks were tracked at a small but finite bias (0.1 mV). At zero bias, these peaks reduce to charge transition lines in the RF signal reflecting electrons hopping back and forth between the array and a lead but not tunneling through. The widths of these lines are proportional to the electron temperature in the leads which are smaller than the finite bias used to measure current and therefore provide a more precise position of the transition. Figure 6.13 shows the details of the nine peaks in Figure 6.12(c) and the corresponding magnetic field induced shifts extracted from the RF magnitude and phase channels.

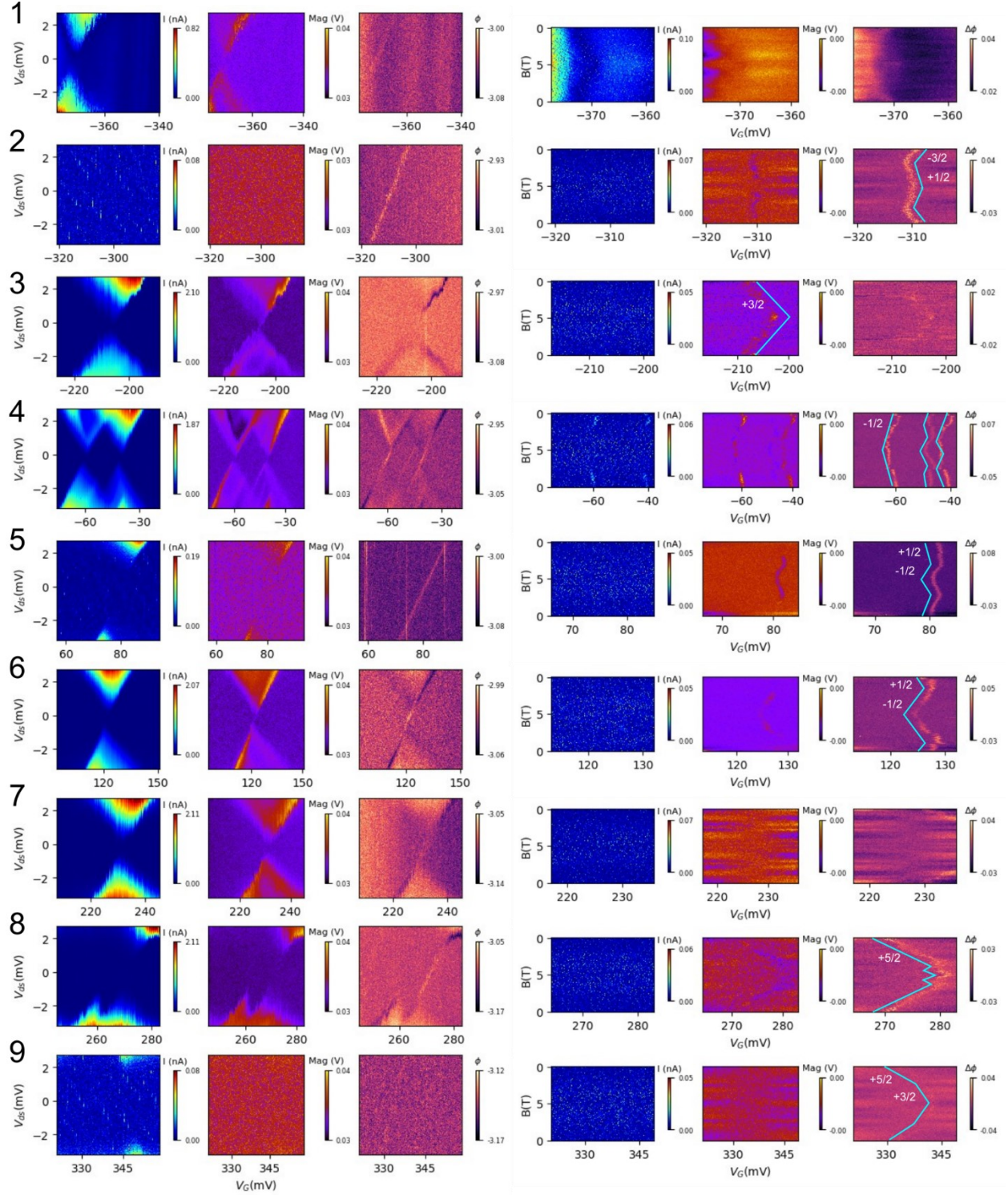


Figure 6.13 Details of the magneto-RF reflectometry measurements at the nine identified charge transitions. The left panels show zoomed-in Coulomb-diamond diagrams corresponding to each transition. Most peaks remain open at zero bias, some exhibit significantly larger openings for example peak 5. The right panels track the positions of the charge-transition lines as a function of magnetic field at

zero source–drain bias, with the slopes annotated by the solid cyan lines. Peaks 1 and 7 produce very weak signals across all channels and do not yield sufficiently clear features for reliable tracking.

Out of all peaks, alternating slopes with kinks, deviation from even-odd filling and larger magnetic field dependences ($\frac{3}{2}g\mu_B, \frac{5}{2}g\mu_B$) are observed in the RF signals consistent with the previous magnetotransport results. Peaks 1 and 7 show very weak responses across all channels, which can be attributed to reduced tunnel coupling between the corresponding electronic states and the leads. The separation between the upper and lower diamonds provides a qualitative measure of the degree of localization. For example, Peak 2 behaves as a highly localized state that does not support transport, while the other peaks exhibit varying degrees of diamond opening. This observation reflects the fact that, despite strong inter-site coupling, the 3×3 array differs from a fully metallic island and residual localization still affects the shape of charge-transition features.

As discussed earlier, the observed slope transitions and spin-flip features highlight the influence of both exchange and Coulomb interactions in determining the spin configuration of the 3×3 array, which is highly sensitive to the precise atomic arrangement of the donor sites. Due to the limited gate-voltage range, we are unable to probe the spin configurations associated with the first few electrons or with higher electron fillings beyond the accessible window. Consequently, rather than attempting a quantitative reconstruction of the complete electron addition spectrum which would otherwise require exploring millions of possible configurations, we focus on demonstrating that distinct spin-filling patterns can emerge through controlled tuning of exchange and Coulomb interaction strengths. To build an intuitive understanding of these mechanisms before discussing the full array, we first illustrate an example of spin filling in a triple quantum dot with simplified interaction parameters.

Consider the system of the three quantum dots (D1, D2, and D3) in the weak-coupling limit ($t/U \ll 1$). To lift the degeneracy between sites, the central dot D2 is assigned a slightly lower chemical potential, $\mu_2 =$

$-\delta$, while the electron–ion core interactions are taken as constant and neglected. The long-range Coulomb interactions between electrons are defined as $U_{12} = U_{23} = a$ and $U_{13} = b$, where a , b , U , and δ are the only adjustable parameters in this simplified toy model with a constant external magnetic field. Figure 6.14 shows the resulting ground-state spin configurations of the system at different total electron occupation numbers. Since t is set to zero, the energy of each occupation configuration is just the algebraic sum of the Coulomb interactions and chemical potentials.

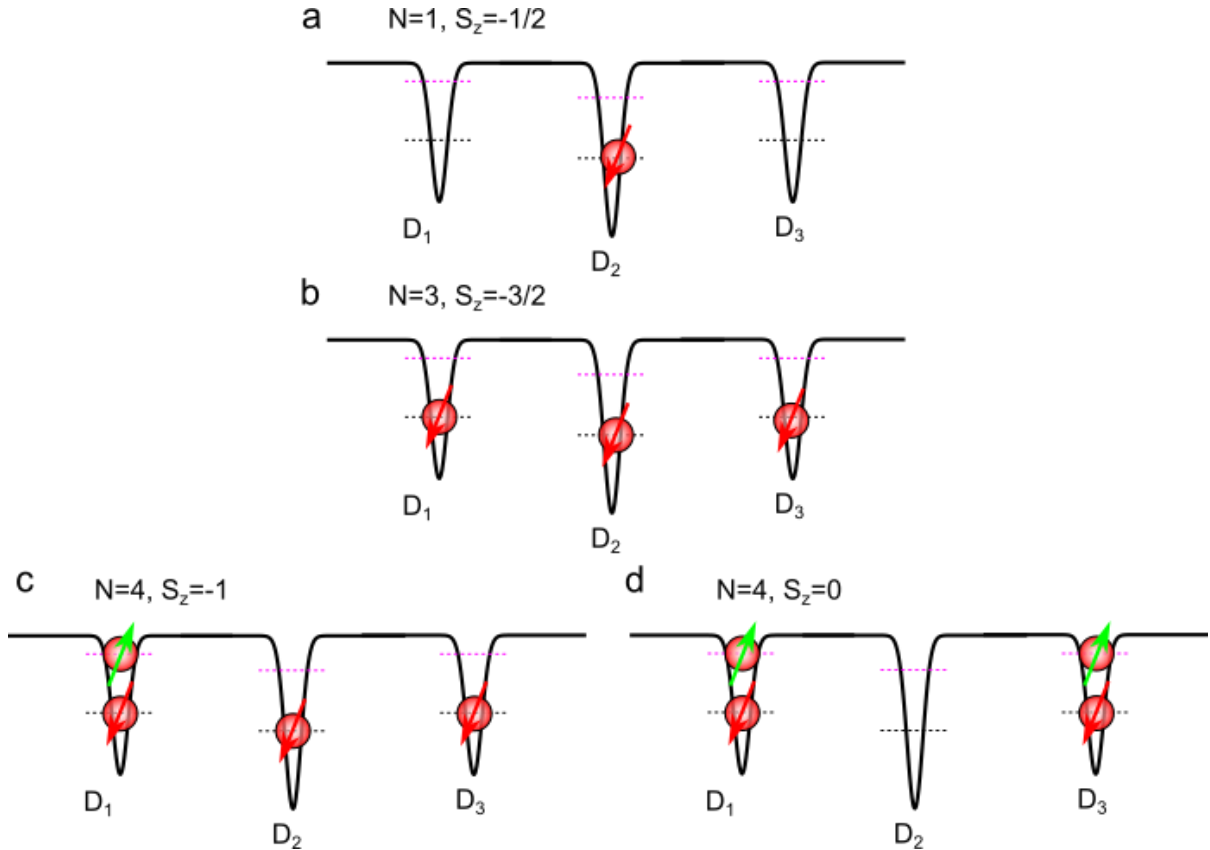


Figure 6.14 Spin-filling sequence of a linear triple-dot system in the small- t limit under a constant magnetic field. Each dot has an identical on-site Coulomb energy U . The nearest-neighbor and next-nearest-neighbor Coulomb repulsions are a and b , respectively. The middle dot is given a slightly lower chemical potential $\mu_2 = -\delta$ to lift degeneracy. (a) The first electron occupies D2 with spin down. (b) The second and third electrons fill D1 and D3 with spin down, yielding a total spin $S_z = 3/2$. (c–d) Addition of the fourth electron leads to two possible configurations: (c) $S_z = -1$ or (d) $S_z = 0$, depending on which has the lower total energy. If configuration (d) is realized, the transition from $N = 3$ to $N = 4$ results in

$\Delta S_{\text{tot}} = +3/2$, producing a large charge-transition slope similar to that observed in the 3×3 magnetotransport measurements.

For $N = 1$, the first electron occupies the central dot D2 with spin down (Fig 6.14(a)). The second and third electrons successively fill D1 and D3, also with spin down. When a finite tunneling amplitude t is introduced, the exchange interaction favors spin-up occupation for the second and third electrons at low magnetic fields, leading to partial spin polarization that transitions to an all-spin-down configuration at higher fields as Zeeman energy dominates. At $N = 3$, the total spin is $S_z = -3/2$ and the total energy is $E = -\delta + 2a + b$ (Fig 6.14(b)). The addition of a fourth electron gives rise to multiple possible spin configurations, depending on the relative strength between the Coulomb interaction and exchange interaction. In Fig. 6.14(c), the fourth electron occupies D1, resulting in a total energy of:

$$E_{4,-1} = -\delta + U + 3a + 2b \quad (6.14)$$

and a total spin $S_z = -1$. In contrast, in Fig. 6.14(d), the four electrons rearrange to form double occupancies on D1 and D3, leaving D2 unoccupied. This configuration has a total energy of

$$E_{4,0} = 2U + 4b \quad (6.15)$$

and a total spin $S_z = 0$. The energy difference between the two configurations is therefore

$$\Delta E = E_{4,0} - E_{4,-1} = U + 2b - 3a + \delta \quad (6.16)$$

If $3a - 2b > U + \delta > 2a - b$, which can occur when the three dots are positioned close enough, the system adopts the $S_z = 0$ spin configuration of Fig 6.14(d) as the ground state of $N=4$, producing $\Delta S_{\text{tot}} = +3/2$ at the charge transition from $N=3$ to $N=4$. This simple example illustrates how spin rearrangements could occur in a minimal system due to strong electron-electron correlation, resulting in enhanced transition slopes observed experimentally in the 3×3 array.

A similar analysis can be extended to the 3×3 dopant arrays to examine their spin-filling behavior. In the presence of intrinsic disorder in the site chemical potentials, finite exchange interactions, and possible valley–orbital states, the spin-filling spectrum can exhibit distinct patterns for each array, including kinks at specific magnetic field strengths that mark spin-configuration crossovers in the underlying ground states. For instance, Figure 6.15 shows a numerical simulation performed by Garnett Bryant based on the Hubbard model without disorder and long-range Coulomb interactions, which varies the tunnel coupling t to determine the ground-state spin configuration at half-filling ($N = 9$). The results revealed a fully spin-polarized ground state for small t/U and an anti-polarized state for large t/U , with a crossover occurring near $t/U \approx 0.13$.

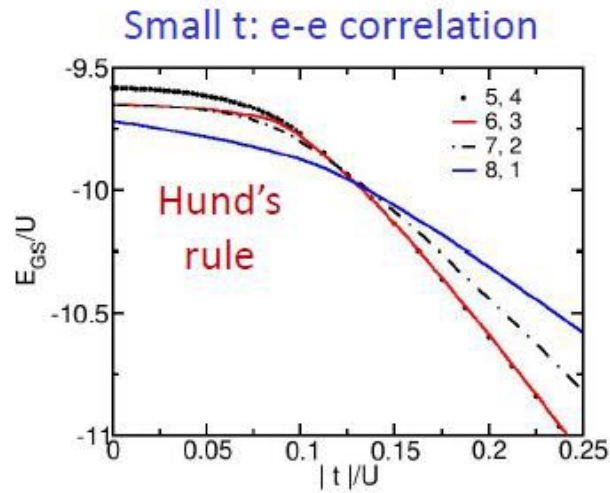


Figure 6.15 Ground-state energy at half-filling for a disorder-free 3×3 dopant array as a function of t/U , calculated by Garnett Bryant. The notations (n, m) in the legend denote the lowest energy configuration with n spin-down and m spin-up electrons. For $0 < t/U < 0.13$, the ground state is $(8,1)$, corresponding to a maximally polarized state. This interval manifests as the analogue of Hund's rule for the array. For $t/U > 0.13$, the ground state transitions to an anti-polarized configuration, where exchange interactions dominate over on-site repulsion.

We present extended Fermi-Hubbard model simulations of the charge and spin configurations for the strongly coupled array, accounting for the effects of realistic disorder. We use the same Hamiltonian introduced in Equation 6.2, with the addition of a Zeeman term:

$$E_Z = \frac{1}{2} \sum_{i,\sigma} (-1)^\sigma g \mu_B n_{i\sigma}$$

Since this term is diagonal in the occupation basis, it does not modify the many-body eigenstates but instead shifts their energies linearly with magnetic field. Among the Hubbard parameters, the on-site interaction energies U_i and corresponding binding energies E_{bi} carry the greatest uncertainty, as shown in Fig. 6.5(a). To account for this, we perform simulations using reduced, expected and increased values of $U_i = 26$ meV, 46 meV, and 86 meV, while keeping all other parameters fixed. Figure 6.16 shows the simulated electron configurations for the case of uniform $U_i = 46$ meV and $t = 8$ meV, as the filling increases from $N=3$ to $N=12$ at $B=1.0$ T, obtained by sweeping the gate voltages along the diagonal axis ($V_{G1} = V_{G2}$).

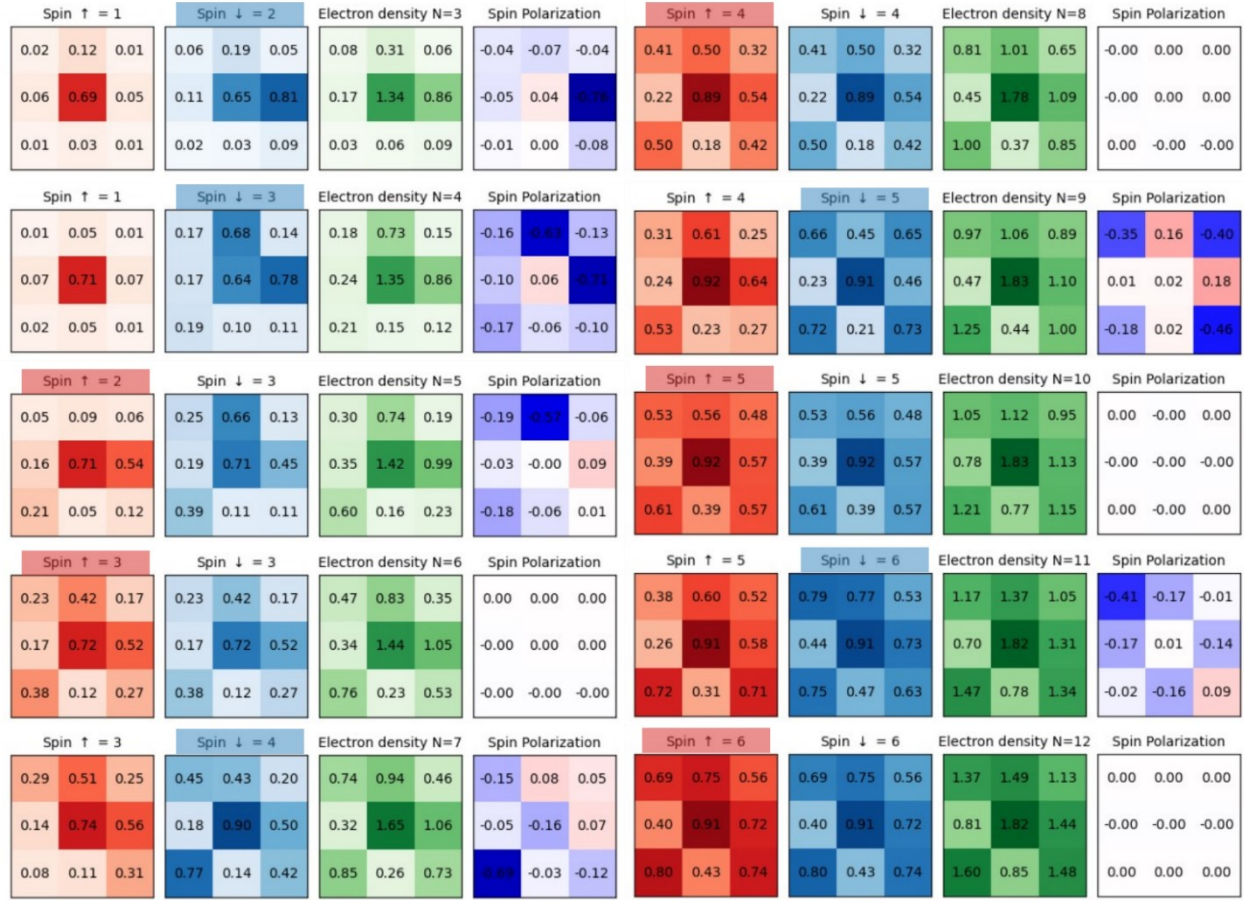


Figure 6.16 Simulated spin and charge configuration of array #3. Simulation parameters: $U_i=46\text{meV}$, $t=8\text{meV}$, $B=1.0\text{T}$. The electron filling number is increased from $N=3$ to $N=12$ by increasing the voltages on both gates. The spin of each added electron is indicated by a colored box. The resulting filling sequence is $\{\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\}$.

The simulated result yields a spin filling sequence of $\{\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\}$. Deviation from simple even-odd filling appears between $N=3$ and $N=6$, although no transitions with $\Delta S_{tot} > 1/2$ are observed. For $U_i = 26 \text{ meV}$, where the effective ratio t/U_i is larger, the simulation produces an exact even-odd spin-filling sequence of $\{\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\}$ from $N=4$ to $N=13$. In contrast, for $U_i = 86 \text{ meV}$, the resulting sequence $\{\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\}$ from $N=3$ to $N=12$ shows stronger deviations from even-odd filling as Coulomb interactions dominate.

This section examined how the spin-filling sequence observed in the 3×3 array arises from the interplay among Zeeman splitting, Coulomb repulsion, exchange coupling, and the specific donor arrangement. Future device designs should aim to minimize disorder and thereby reduce uncertainty in these interaction terms, enabling precise control over electron correlations. With such improvements in atomic precision and uniformity, it may become possible to realize many hallmark phenomena of condensed-matter physics, such as Nagaoka ferromagnetism^{176,206}, further strengthening the potential of dopant-based analog quantum simulators.

6.4 Fermi-Hubbard simulation beyond the 3×3 arrays

The fabrication of the 3×3 arrays serve as a prototype for more advanced designs targeting specific Hamiltonians or quantum systems. The most prominent challenge against scaling to larger arrays lies in addressing disorder, particularly variations in the exact donor number within each site and the spatial configuration of dopants within individual clusters. As discussed in the previous section, achieving atomic precision in lithographic patterning using the STM methods developed in Chapter 4 does not, by itself, eliminate disorder. The phosphorus incorporation process remains stochastic, and even successfully incorporated dopants may undergo diffusion during the overgrowth phase at elevated temperatures^{126,207}. This randomness introduces nonuniform binding and addition energies across the array, deviating the device from the idealized Hubbard model, which assumes uniform site potentials. Scaling to larger systems effectively expands the landscape of disordered chemical potentials rather than mitigating it.

Until truly deterministic control over both the dopant number and spatial configuration at each site is achieved, it is valuable to consider what forms of analog quantum simulation can be pursued within the constraints of the current fabrication process. Given that a certain degree of disorder is, at present, unavoidable, one natural direction is to embrace it and investigate its impact on quantum transport in two dimensions. Disorder and quantum interference play a central role in defining the transport behavior of low-

dimensional systems. A paradigmatic example is Anderson localization^{103,208}, where destructive interference among scattered wavefunctions leads to an exponential suppression of conductance. Although the theoretical foundations of localization in two dimensions are well established that all single-particle states become localized in terms of a localization length. Direct experimental realization and characterization in engineered solid-state platforms remain rare. Therefore, bridging the gap between microscopic disorder models and measurable transport signatures in controllable quantum systems represents an important step toward this goal.

6.4.1 Fabrication of a 32x32 square lattice quantum dot array

To this end, we fabricated a 32×32 dopant-based quantum dot array in a square lattice using automated STM lithography and characterized its transport behavior under an applied source–drain bias.

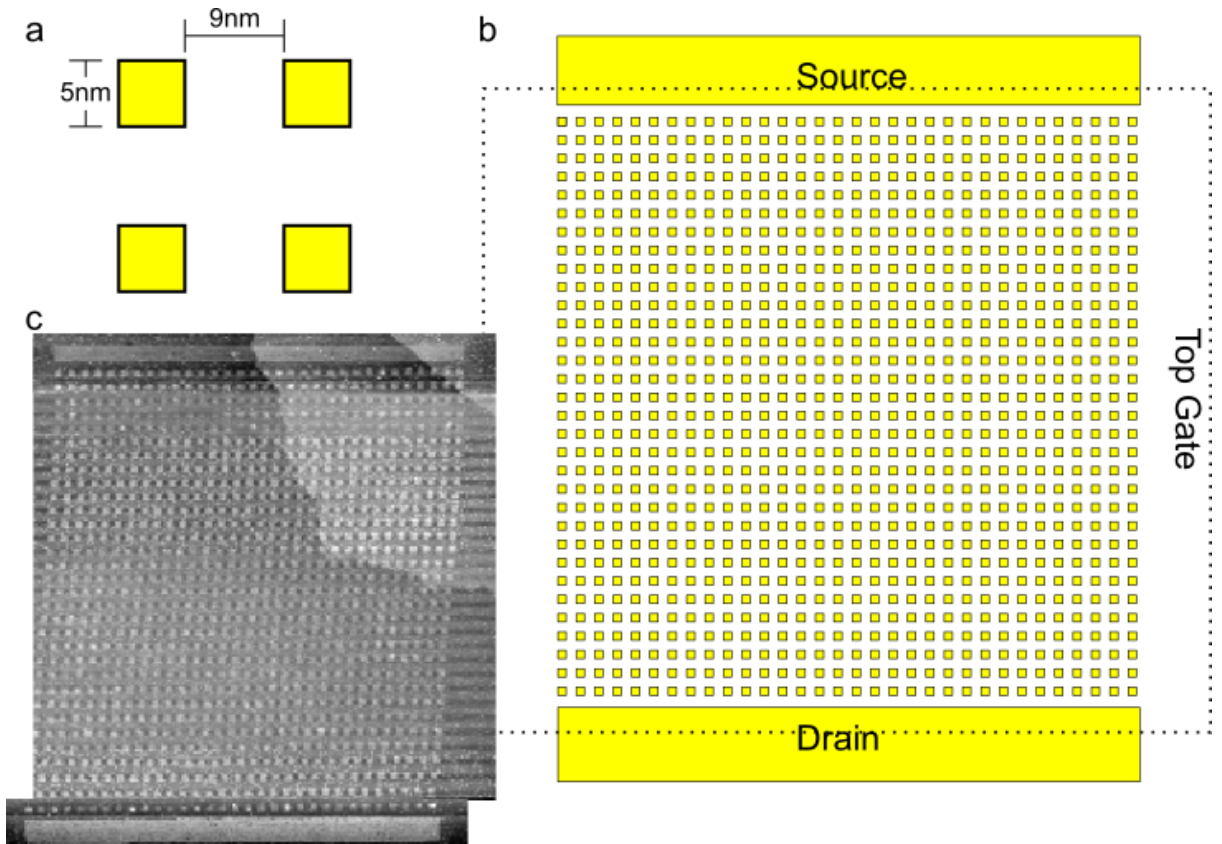


Figure 6.17 Schematic and STM image of the 32×32 dopant array. (a) Each quantum dot is defined as a $5 \text{ nm} \times 5 \text{ nm}$ square island rather than a few-donor cluster. The estimated number of phosphorus donors

per island is $N_D \sim 50$. Neighboring sites are separated by $d \approx 9$ nm, corresponding to an estimated tunnel coupling of $t \sim 2$ meV. (b) Schematic of the array connected to a pair of source and drain leads for transport measurements. An additional global top gate, deposited above a ~ 20 nm thick hafnium oxide dielectric layer over the silicon surface, is used to tune the overall chemical potential (filling factor) of the array. (c) STM image of the fabricated 32×32 array. The apparent skew is due to residual sample drift accumulated during the extended patterning process.

Figure 6.17 illustrates the overall layout of the 32×32 array consisting of $5 \text{ nm} \times 5 \text{ nm}$ square islands coupled to source and drain leads, similar in geometry to the 3×3 arrays discussed earlier. The key difference lies in the gate configuration: rather than employing a symmetric pair of in-plane plunger gates, we utilize a global top gate to control the chemical potential across the entire array. The influence of in-plane gates decays rapidly with distance, resulting in negligible capacitive coupling to sites on the opposite side of the array. In contrast, the global top gate provides dominant capacitive coupling to the entire array, with only a slight reduction in coupling strength for sites located near the source and drain leads. By varying the top-gate voltage, the overall electron filling of the array can be continuously tuned, while adjusting the source–drain bias allows probing of the transport dynamics within the lattice.

To quantify the top-gate coupling, we perform finite-element electrostatic simulations and extract a lever arm $\alpha \approx 0.45$ between the top gate and the quantum dot sites. The average charging energy of the $5 \text{ nm} \times 5 \text{ nm}$ islands is $E_c = 25$ meV for the sites, with an uncertainty of approximately $\Delta E_c \sim \pm 3$ meV due to local variations in donor number and patch size. The quantum confinement energy is negligible compared to the charging energy due to the relatively large island size (or large donor numbers) leading to mostly uniform addition energies. These results are consistent with the previous quantum simulators realized in the Si:P platform¹⁹¹.

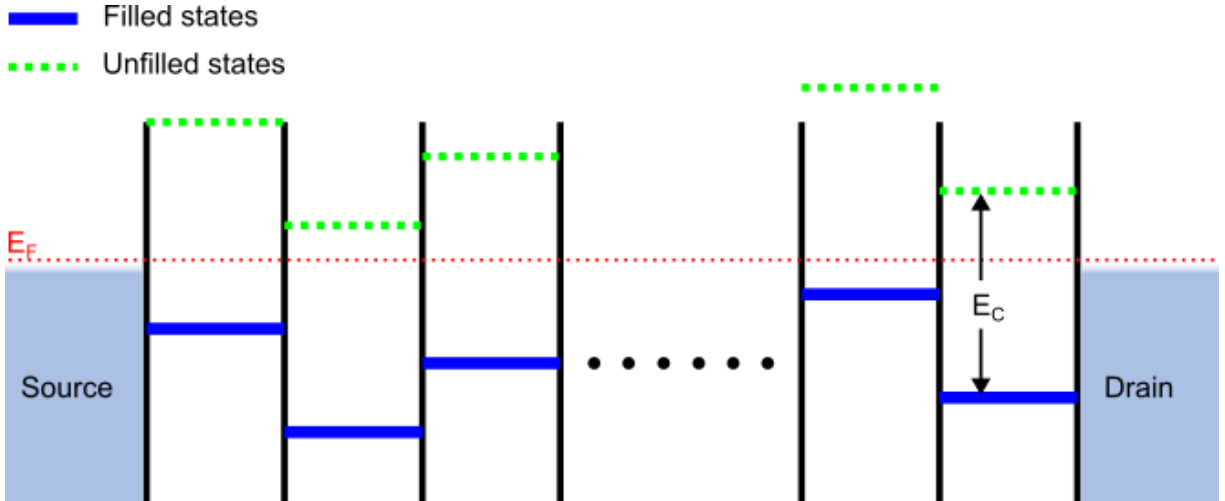


Figure 6.18 Illustration of the maximally disordered chemical potential landscape. Each site is characterized by an electron addition spectrum consisting of a uniform ladder of energy levels separated by the charging energy E_C , with a small quantum confinement energy. Filled levels are shown as blue solid lines, while unoccupied levels are shown as green dashed lines. Electrons occupy these levels up to the Fermi level E_F (red dashed line) defined by the source and drain leads. Due to variations in local donor configurations and electrostatic environments, each site experiences a random chemical potential offset on the order of E_C , resulting in a maximally disordered chemical potential landscape across the array.

Although the lithographic pattern of each island appears uniform, the underlying chemical potential landscape across the array is effectively maximally disordered, as illustrated in Figure 6.18. In this regime, the on-site addition energies, long-range Coulomb interactions, and inter-site tunnel couplings remain largely uniform owing to the regular island size and consistent inter-dot spacing. The disorder arises from random offsets in the local chemical potential of individual sites which originate from the stochastic freeze-out of electrons in silicon during device cooldown. Each site retains a residual offset charge until charge neutrality is approached at the Fermi level. The exact offset depends sensitively on the local dopant configuration and the electrostatic environment of each island, leading to a random distribution that ranges from zero up to approximately the charging energy, thereby generating a maximally disordered chemical potential landscape.

6.4.2 Transport measurement result

Figure 6.19(a) shows the measured current–voltage (I–V) characteristics of the 32x32 dopant-based quantum dot array at temperature $T=4\text{K}$. At small source–drain bias, the current is strongly suppressed, producing a well-defined transport gap around zero bias. This gap is not a conventional band gap arising from a single-particle dispersion, but rather an effective gap that reflects the absence of extended conduction channels near the Fermi level²⁰⁹. Transport is initially suppressed because disorder-induced localized states fail to form percolating paths across the array. As the applied bias increases, the current rises sharply, producing a nonlinear, nearly exponential response. The turn-on above the threshold bias reflects the emergence of groups of localized states whose overlapping wavefunctions create percolating channels that enable finite transmission. This diode-like I–V behavior distinguishes the disordered quantum dot lattice from conventional semiconductor diodes, where current rectification instead arises from built-in junction asymmetry^{210,211}.

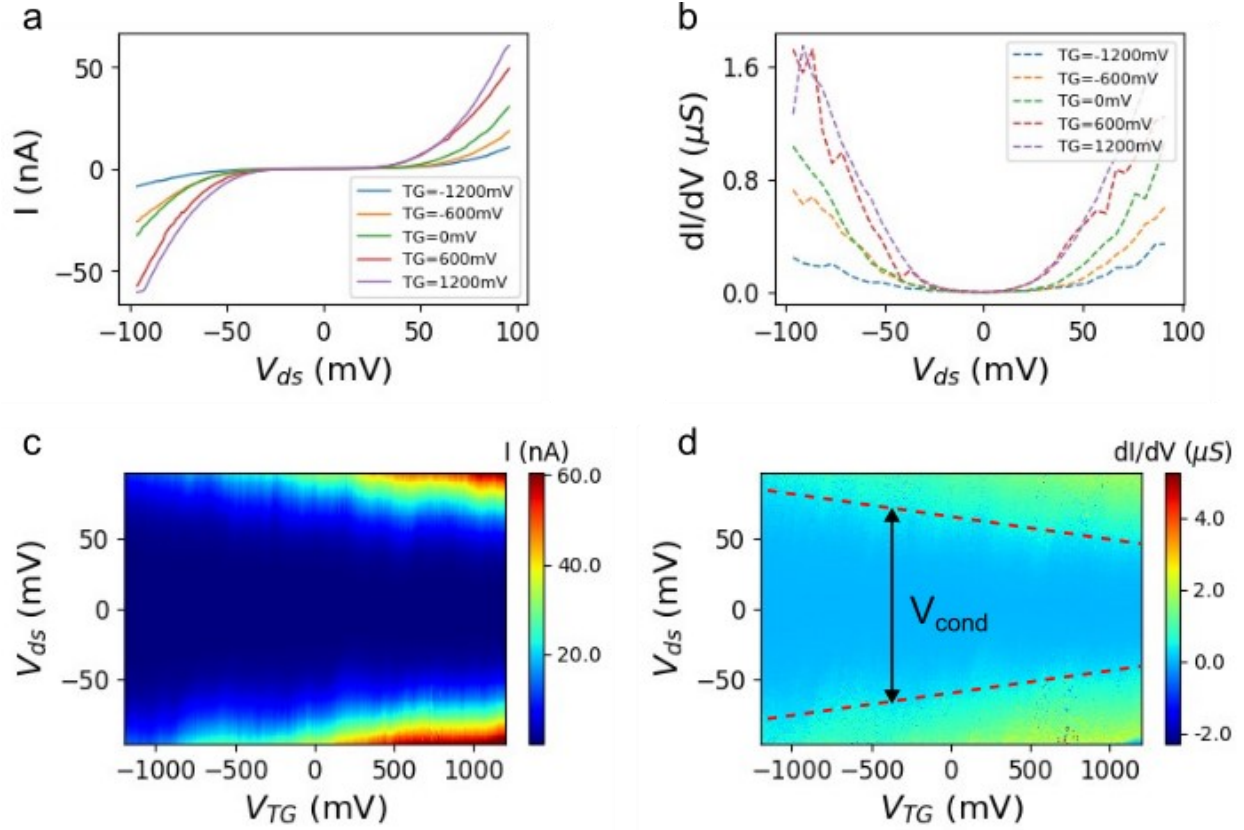


Figure 6.19 IV characteristics of the 32×32 quantum dot array with a global top gate. (a) Measured tunneling current and (b) differential conductance (dI/dV) spectra at various top-gate voltages within a source–drain bias window of ± 100 mV. The array remains largely non-conducting below a threshold of approximately 20 mV, above which the current rises almost exponentially. The turn-on effect is notably stronger for positive top-gate voltages compared to negative ones. (c, d) Conductance and dI/dV maps as a function of top-gate voltage (V_{TG}) in the range of -1.2 V to $+1.2$ V, showing a continuous modulation of the array’s transport characteristics. A visible conductance “gap,” corresponding to $\frac{dI}{dV} \approx 1.0 \mu S$ is labeled V_{cond} which progressively narrows as V_{TG} increases.

We further investigated the role of the global top gate by sweeping its voltage from -1.2 V to $+1.2$ V. As shown in Fig. 6.19(c, d), the width of the transport gap decreases continuously as the gate voltage is increased. This behavior can be understood in terms of the filling factor of the array. As the top gate voltage increases, more electrons are occupied in the array sites. Electrons added at higher filling levels have wavefunctions that are spatially more extended than those of the lower filling levels. This enhances the

tunnel coupling between neighboring sites and effectively strengthens the connectivity of the disordered lattice. The improved overlap between localized states reduces the bias threshold required for resonant conduction, producing the observed narrowing of the transport gap. This feature illustrates the potential of using a global top gate to tune the tunnel coupling strength in Si:P devices.

To probe the fine structure of transport resonances, we performed high-resolution measurements of current as a function of both source–drain bias and top gate voltage over a smaller range. As shown in Fig. 6.20(b), the conductance maps exhibit a dense pattern of diamond-shaped features reminiscent of the Coulomb diamonds in single-electron transistors. These structures arise from discrete charging and level alignment within the array, where each localized state behaves as an effective quantum dot with its own addition energy and blockade region. The collective charging effects of many such localized sites produce the dense, fragmented diamond pattern observed experimentally. This indicates that despite the regular lattice design, intrinsic disorder and site-to-site potential variations break transport into multiple percolation channels²¹², each characterized by its own charging spectrum.

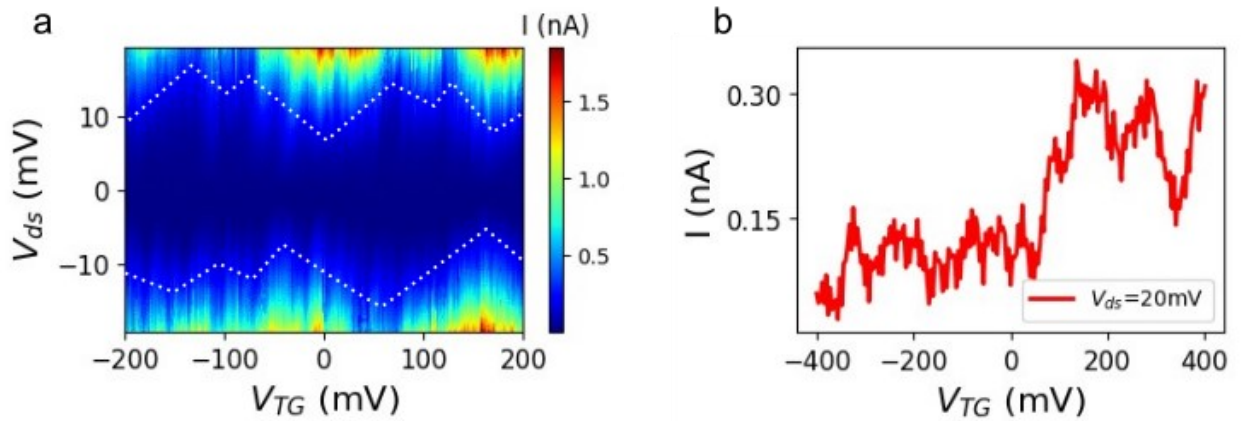


Figure 6.20 Small range top-gate voltage sweeps revealing detailed features in conductance. (a) Conductance map showing a zoomed-in view of densely packed, irregular Coulomb diamond fragments. The outlines of individual diamonds are indicated by white dashed lines. (b) Line trace of conductance versus top-gate voltage (V_{TG}) from -400 mV to $+400$ mV at a source–drain bias of $V_{DS} = +20$ mV, displaying clear Coulomb oscillations. These oscillations indicate that transport through the array occurs via multiple localized conduction channels, representing the continuous-limit extension of the weakly coupled 3×3 array discussed in the previous section.

6.4.3 Simulation of transport through localized states

To rationalize the experimental observations, we modeled the device as a two-dimensional disordered tight-binding lattice with parameters chosen to reflect the 32 x 32 dopant-based array. Each site was described by a single orbital with nearest-neighbor hopping t , subject to on-site disorder ϵ_i drawn uniformly from the range $(-W/2, W/2)$ where $W = E_c$ consistent with the max variability of site chemical potentials as the average charging energy of the array. Open boundary conditions were used in both directions to represent the finite array geometry and direct source–drain coupling.

Energy Spectrum and Localization

We first computed the single-particle spectrum of the Hamiltonian in the absence of interactions ($U_{ij} = 0$).

The Hamiltonian of the system is:

$$H = \sum_{\langle i \rangle} \epsilon_i c_i^\dagger c_i + \sum_{\langle i, j \rangle} (-t c_i^\dagger c_j + h.c.) \quad (6.17)$$

This approximation serves as a simplified description of the array and can be justified as the estimated long range Coulomb interaction between the nearest neighbors is small compared to the disorder in chemical potential ($U_{i,i+1} \ll W$). When this condition cannot be met, the interaction terms could also bring in the Many-Body Localization (MBL) effect which is out of scope of this analysis. For a clean system ($W = 0$), the spectrum reproduces the characteristic tight-binding band spanning $(-4t, 4t)$. When disorder is included, the eigenstates exhibit Anderson localization depending on the strength of the disorder, as confirmed by participation ratio (PR) analysis. The participation ratio^{103,213} quantifies how spatially extended an eigenstate is across the lattice and is defined as

$$PR = \frac{1}{\sum_i |\psi_i|^4} \quad (6.18)$$

where ψ_i is the normalized wavefunction amplitude at site i . For an extended state, $|\psi_i|^2 \sim 1/N$ (N is the total number of sites), therefore $PR \sim N$. For localized states, only finite number of sites have non-zero amplitude which results in $PR \sim 1$.

We simulate the clean system versus the maximally disordered system with $t = 2.0$ meV and $W = E_c = 20$ meV. Figure 6.21 shows the density of states, histogram of participation ratios and the wavefunction of a typical eigenstate in the two systems. Across the entire band, PR/N values remain close to unity for the disorder free system while being substantially below unity for the maximally disordered system, indicating that no truly extended states exist in the system.

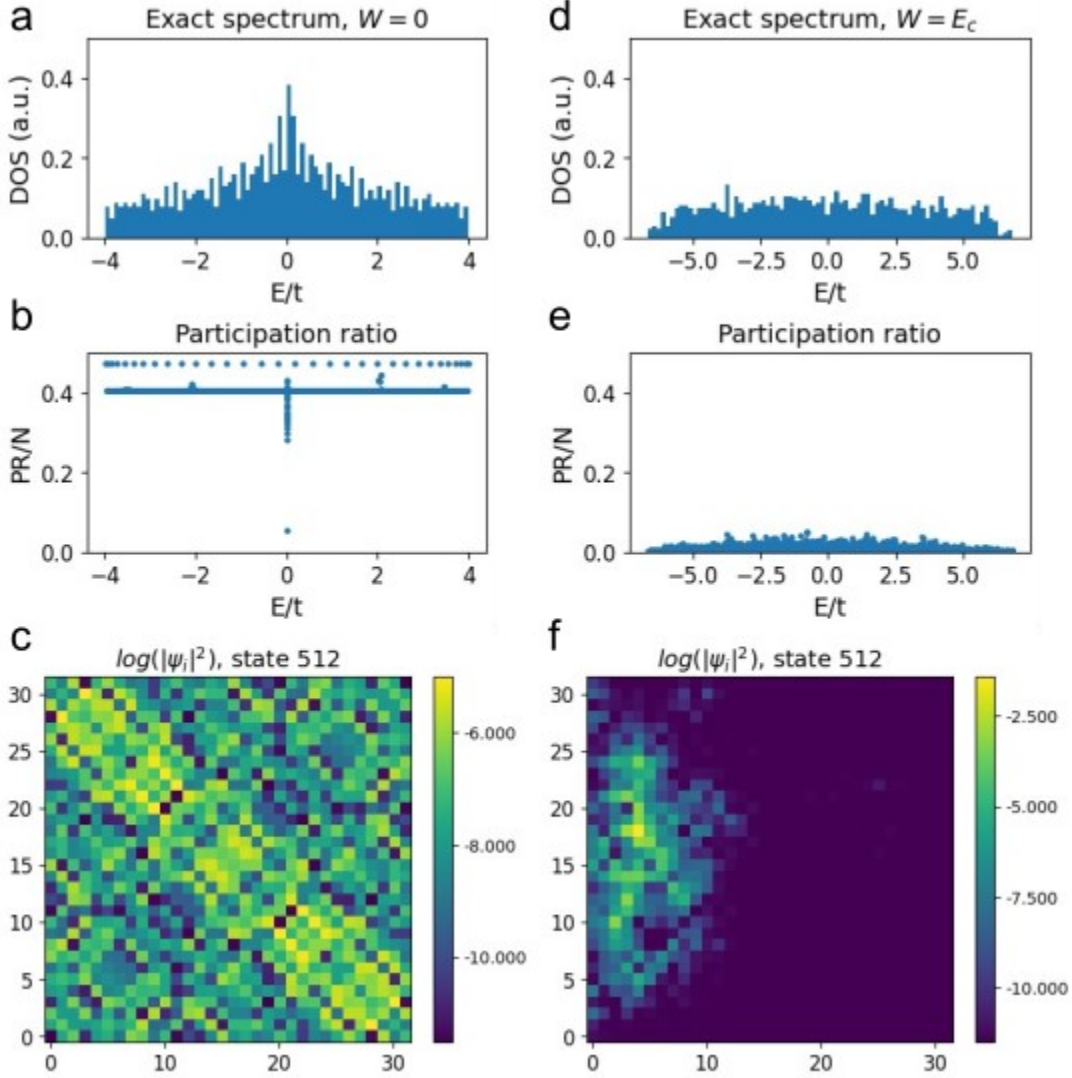


Figure 6.21 Simulated energy spectrum and localization characteristics of the disorder-free and maximally disordered systems. Simulations were performed with $t = 2$ meV and $W = 10t$, where on-site energies are uniformly distributed as $\varepsilon_i \in (-W/2, W/2)$ in the disordered case. Panels (a–c) show the density of states, participation ratio, and logarithmic amplitude of a representative single-particle wavefunction for the disorder-free lattice. Panels (d–f) present the corresponding quantities for the maximally disordered lattice. The disordered system exhibits a more uniform density of states and reduced participation ratios across nearly all eigenstates, indicating strong localization induced by disorder. This localization is also evident in the spatial amplitude distribution of an eigenstate near zero energy.

As pointed out earlier in the discussion of the 3×3 arrays, a direct conductance path requires electronic states whose density is nonzero at both the source and drain edge, that is, spatially extended states. The absence of measurable current at zero source–drain bias thus supports the interpretation that extended states are absent as in Figure 6.21(e), and that transport likely occurs through a set of resonant states with varying localization lengths. In the present device, the localized states, specifically their spatial positions and localization lengths, cannot be directly probed, but only inferred through transport measurements. Future device designs could incorporate multiple charge sensors positioned at different locations within the array and coupled via radio-frequency (RF) reflectometry to probe localization charge states.

6.4.4 Summary & Discussion

The diode-like I–V characteristics observed in our dopant-based quantum dot lattice arise from the interplay between disorder-induced localization and bias-driven transport. In the linear-response regime, the conductance is strongly suppressed because of the lack of extended conduction channels near the Fermi level. As the applied bias increases, percolation paths that extend across the array connecting multiple overlapping localized states start to appear and allow electrons to transport, resulting in a sharp onset of current. This threshold-like behavior emerges not from band bending or built-in junctions, as in conventional diodes, but from the statistical properties of localized states in a disordered lattice.

Our modeling using the single particle tight-binding framework visualizes the spatial profile of the localized states giving the tunnel couplings and disorder level. The calculated transmission spectrum consists of sharp resonances associated with localized clusters. Integration over the bias window indicates that the number of percolation paths also rise nonlinearly. Participation ratio analysis confirms that most states remain localized, supporting that conduction is not due to delocalization by the higher bias.

In conclusion, the 32×32 tunnel coupled quantum dot array provides direct experimental evidence of bias-driven conduction thresholds arising from Anderson localization in a finite-size solid-state system. These

results establish dopant-based quantum dot arrays as a solid-state playground for exploring mesoscopic transport phenomena at the atomic scale and open avenues toward devices with engineered disorder.

6.5 Quantum Field and Lattice Gauge Simulations Using Electron–Nuclear Spin Coupled Systems

6.5.1 Motivation

Beyond electron-based Hubbard-type simulators, dopant-based architecture in silicon offers an additional and uniquely powerful degree of freedom: the nuclear spin, which served as the original qubit in Kane’s proposal. The hyperfine interaction between a bound electron and its host nucleus naturally couples these two degrees of freedom, extending the simulator’s reach from condensed-matter–style Hamiltonians to quantum field theory (QFT) models where different fields such as matter and gauge fields can interact with each other. In a recent work ²¹⁴, the author proposed an analog quantum simulator consisting of donor arrays in which electrons bound to phosphorus donors form a fermion field, while the associated nuclear spins act as dynamical rotors providing an effective background field. The hyperfine energy mediates interactions analogous to those between matter fields and bosonic gauge or scalar fields in a continuum QFT. As the donor sites are separate and discrete, the array can be seen as a physical realization of a lattice gauge field theory.

This new architecture therefore offers a potential route toward studying fundamental mechanisms in high energy physics such as dynamical mass generation, chiral symmetry breaking, and confinement with a high level of control and scalability.

6.5.2 Hamiltonian mapping

Following Rad et al ²¹⁴, the starting point is the physical Hamiltonian of a 1D single donor array where each donor bounds exactly one electron that includes electronic hopping, Coulomb interactions, Zeeman terms, and hyperfine coupling:

$$H = H_k + H_\mu + H_{ff} + H_{sf} + H_s \quad (6.19)$$

where H_k is the electron kinetic energy from inter-donor tunneling, H_μ is the chemical potential landscape, H_{ff} the electron–electron interaction. The first three terms are identical to the extended-Fermi Hubbard model. H_{sf} represents the hyperfine coupling between electron and nuclear spins, and is the critical term which makes this simulator possible:

$$H_{sf} = g \sum_i s_i^z I_i^z \quad (6.20)$$

where s_i^z is the electron spin and I_i^z is the nuclear spin at site i . H_s is the Zeeman term at the presence of external magnetic fields:

$$H_s = - \sum_i h_n \cdot I_i + \sum_i h_e \cdot s_i \quad (6.21)$$

where $h_n = \gamma_n B$, $h_e = \gamma_e B$ are the gyromagnetic coupling of the nuclear and the electron.

This physical Hamiltonian can be shown to map, in the low-energy limit, onto the lattice discretized Hamiltonian of the rotor Jackiw–Rebbi (RJR) model²¹⁵ which is a minimal field theory describing a Dirac fermion coupled to a dynamical mass (rotor) field:

$$H_{\text{RJR}} = \int dx \left[-ic \Psi^\dagger \gamma^i \partial_i \Psi - g \Psi^\dagger (\gamma^0 \boldsymbol{\ell} + \boldsymbol{\phi}) \Psi - \mathbf{h} \cdot \boldsymbol{\ell} \right] \quad (6.22)$$

Here, $\Psi = (\psi_+, \psi_-)^T$ denotes the Dirac or fermionic field represented by pairs of adjacent donor-bound electrons, while $\boldsymbol{\phi}$ and $\boldsymbol{\ell}$ represents the collective orientation and fluctuations of the nuclear spins respectively, acting as the dynamical rotor field. The coupling constant g is proportional to the hyperfine interaction strength, and $\mathbf{h}$ maps to the external magnet field. In this mapping, the nuclear-spin field modulates the local electronic potential via the hyperfine coupling, playing the role of a scalar or gauge field for the fermion. The simulator starts with all electrons polarized and fixed in the spin down state $|\downarrow\rangle$.

6.5.3 Experimental feasibility

The relevant parameters of the silicon donor system place it well within an experimentally accessible regime for observing the predicted field-theory behavior. For phosphorus donors in silicon, the electron–nuclear hyperfine constant is $A = 117 \text{ MHz}$ ($\approx 0.48 \text{ } \mu\text{eV}$), while achievable tunnel couplings between neighboring donors range from $t \approx 0.5$ to 8 meV for inter-donor separations of $4\text{--}10 \text{ nm}$. Magnetic fields of $1\text{--}3 \text{ T}$ are sufficient to polarize the electronic spins while leaving the nuclear spins effectively free to form collective states. These values yield coupling ratios g/t spanning $10^{-7}\text{--}10^{-5}$, which are quite small.

Initialization of the nuclear-spin field can be achieved using dynamic nuclear polarization through optical or electrical pumping. Once polarized, the nuclear spins can retain coherence for seconds to minutes^{129,136} at cryogenic temperatures in an isotopically purified ^{28}Si environment. This allows adiabatic manipulation of the electron subsystem while treating the nuclear spins as quasi-static during measurement.

Transport spectroscopy similar to that described in Sections 6.3–6.4 can reveal the onset of mass gaps and confined phases. A reduction in zero-bias conductance or the appearance of oscillatory sidebands in differential conductance spectra would signal electron localization induced by the nuclear-spin field.

On the fabrication side, similar challenges arise, as the proposed nuclear-spin array architecture demands atomic-scale precision. This requires not only the creation of atomically precise lithographic patterns (as described in Chapter 4) but also the preservation of exact phosphorus lattice positions during encapsulation. For single donors, the tunnel coupling and exchange interaction between neighboring sites are highly sensitive to both separation and crystallographic orientation where even a one-lattice-constant displacement can cause significant variations in coupling strength. Understanding these atomic-scale displacements and exploring the use of multi-donor clusters to reduce such sensitivity remain important directions for future work.

6.6 Summary

In this chapter, we explored a progression of dopant-based analog quantum simulators in silicon, ranging from small-scale electronic Hubbard arrays to hybrid electron–nuclear spin architectures capable of emulating lattice gauge models. The atomically engineered 3×3 dopant array represents the first two-dimensional realization of an extended Fermi–Hubbard model in silicon. By systematically varying the lattice constant, we tuned the hopping amplitude and the interaction-to-kinetic-energy ratio U/t , observing a continuous transition from a metallic regime to a Mott-like insulating state and finally to the atomic limit. The measured charge stability diagrams and transport characteristics were well captured by extended Hubbard simulations, confirming that dopant-based arrays can faithfully reproduce many-body phenomena in a solid-state platform with nanometer-scale control.

Scaling to a 32×32 dopant array extends this framework toward mesoscopic dimensions, where the array behaves as a weakly coupled network of quantum dots with transport dominated by multiple localized conduction channels. The emergence of dense, irregular Coulomb diamond fragments and clear Coulomb oscillations under top-gate modulation manifest a percolative conduction regime. These experiments mark an important step toward realizing large, tunable artificial lattices, where global gate control can modulate collective behavior across hundreds of sites. However, achieving truly uniform coupling across such a large array remains a significant fabrication challenge, one that can only be addressed by assuring absolute atomic precision in both the lithography and dopant incorporation process.

Looking forward, coupling the electronic lattice to the nuclear spin degree of freedom introduces a new frontier for analog quantum simulation. The hyperfine-coupled electron–nuclear spin system forms a natural platform for simulating gauge field theory models such as the rotor Jackiw–Rebbi Hamiltonian, enabling studies of dynamical mass generation, confinement, and emergent gauge fields within a solid-state environment. Yet, the success of such simulators again depends critically on our ability to position donors with sub-lattice precision and to maintain that precision through encapsulation as small atomic displacements can drastically alter tunnel couplings and hyperfine interactions. Continued advances in

STM-based hydrogen lithography, deterministic dopant incorporation, and atom-resolved metrology are therefore essential to move from proof-of-concept devices to quantitatively controlled quantum simulators. Finally, future generations of dopant-based simulators will require local charge and spin readout capabilities beyond conventional transport measurements. Integrating multiple charge sensors into large arrays will make it possible to directly probe site-resolved charge configurations and correlations. Techniques such as radio-frequency (RF) reflectometry and dispersive readout will play a central role in achieving this capability, enabling high-bandwidth, non-invasive measurements of local electronic states. These advances will allow dynamic probing of quantum correlations and collective excitations in real time, paving the way for scalable, site-resolved analog quantum simulation in silicon. The development and implementation of these charge-sensing and RF reflectometry techniques will be the focus of the next chapter.

Chapter 7: Optimizing RF-reflectometry measurements for large impedance silicon quantum devices

7.1 Introduction

Dopant-based spin qubits in silicon are a promising platform for scalable quantum computing^{16,41}. Recently, high-fidelity single- and two-qubit gate operations have been demonstrated^{36,216–218}, with electron spin coherence times reaching beyond 1s. Qubit state readout is typically performed via energy-selective spin-to-charge conversion, where the spin states are mapped onto distinguishable charge states of a nearby charge sensor, for example, the on and off state of a single-electron transistor (SET)^{54,128}. In this case, the tunneling currents can be measured using a transimpedance amplifier. However, the long coaxial cables connecting the device at the millikelvin stage to the room-temperature amplifier introduce significant parasitic capacitance, which forms a low-impedance path for low-frequency (kHz) noise and limits the measurement bandwidth²¹⁹. In dry dilution refrigerators, pulse-tube vibrations couple triboelectric noises²²⁰ into the lines which further degrades the signal-to-noise ratio (SNR), making fast and high-fidelity detection challenging.

Radiofrequency (RF) reflectometry has become a standard technique for high-bandwidth, non-invasive readout in semiconductor quantum devices^{221–223}. In this approach, an RF resonant circuit, implemented on a printed circuit board (PCB) or integrated directly on the device chip, couples to the quantum impedance from the device. State-dependent variations in the device impedance are transduced into changes in both the amplitude and phase of the reflected RF signal, enabling sensitive detection of charge or spin states²²⁴. A key advantage of RF reflectometry is that it requires only a single electrical lead to deliver the probe signal, in contrast to conventional DC current readout that typically requires separate source and drain connections. This reduction in wiring not only minimizes device footprint and circuit complexity but also alleviates the scaling challenges associated with routing multiple leads in large multi-qubit architectures, where wiring density and thermal load become critical limitations^{225,226}. Moreover, in a heterodyne

detection scheme, the RF method is intrinsically immune to the low-frequency noise introduced by cable capacitance, providing a significant improvement in signal quality over DC approaches.

The sensitivity of the RF resonant circuit is critical, especially when discerning weak signals from minor impedance changes. A wide range of resonator architectures have been developed for different qubit platforms, from simple surface-mount lumped-element designs²²⁷ to hybrid implementations incorporating superconducting spiral inductors^{228,229}. Regardless of the specific design, the central objective in the case of semiconductor spin qubits is to maximize charge sensitivity or signal contrast to enable fast, high-fidelity readout with minimal integration time, while keeping the probe power low to minimize electron temperature^{230–232}.

The design and impedance matching strategy must also be tailored to the electrical characteristics of the device under test. For example, gate-defined CMOS or III-V heterostructure quantum devices typically have resistances from tens to several hundred kilo-ohms²³³, offering substantial impedance contrast between states. This large contrast provides a high SNR to enable rapid, high-fidelity readout. In contrast, scanning tunneling microscope (STM) patterned devices often exhibit on-state resistances in the mega-ohm range¹¹⁹. Fabrication variations such as slightly increased tunnel barrier widths could lead to even higher resistances¹⁴¹. For these high-impedance devices, the RF measurement chain requires meticulous characterization to ensure that the small impedance-dependent signal variations remain distinguishable above the noise floor within a reasonable data acquisition time.

In this work, we study the advantages and limitations of an RF resonant circuit based on a single wire-wound inductor, for charge sensing in dopant-based quantum devices. Our measurements capture the intrinsic sensitivity of the resonator to impedance changes of both conductive and capacitive types, independent of other components in the full measurement chain. We develop a lumped-element model that captures the essential behavior of the circuit and allows simulation of RF responses due to device state changes. A tunable varactor-based matching network^{234,235} is used to identify the optimal impedance-matching condition, after which fixed-value capacitors are selected for low temperature device

measurements in a dilution refrigerator. Charge sensitivity of the RF setup is benchmarked using a single-electron transistor (SET), quantified by the minimum integration time required to distinguish between its on and off state. Under optimal conditions, we achieve a minimum measurement time of 600 ns at input RF power level of -86 dBm.

7.2 Results

7.2.1 Circuit Implementation and Parameter Extraction

We implemented a minimal RF matching network consisting of a single wire-wound surface-mount (SMD) inductor positioned close to the device bonding pad [Fig 7.1(a)]. Together with the parasitic capacitance C_p of the PCB trace, the inductor L forms the resonant tank circuit required for RF reflectometry. This network transforms the device impedance Z_{dev} toward the $50\ \Omega$ transmission line impedance, minimizing reflected power. For STM-patterned single-electron transistors (SETs), where the on-state resistance can reach the $M\Omega$ range, proper impedance transformation is essential for achieving measurable contrast.

To accurately describe the RF response, we map the circuit behavior onto a lumped-element model [Fig 7.1(b)]. The inductor used (Coilcraft 0603HL821) has a nominal inductance of 820 nH, a manufacturer-specified quality factor $Q \sim 10$ at 200 MHz, and a DC series resistance of $\sim 1.5\ \Omega$. The PCB substrate is made with 10 mil CLTE-AT with a dielectric loss tangent of 0.0013. Although the operating RF frequency (~ 200 MHz) is well below the inductor's self-resonance frequency ($f_{sr} = 290$ MHz), these non-idealities significantly influence the circuit's effective quality factor and matching condition. We therefore consider two alternative lumped-element representations for the inductor.

Model 1 (simplified) represents the inductor as an ideal inductor L in series with a DC resistance R_L , while the parasitic capacitance C_p is modeled in parallel with a dielectric loss resistor R_p . The input impedance of the open-ended (without a device) circuit is:

$$Z_{tot} = R_L + j\omega L + \frac{R_p}{1 + j\omega C_p R_p} \quad (7.1)$$

From this model, the resonance frequency is approximately at $\omega_0 \sim 1/\sqrt{LC_p}$, and the impedance at resonance is determined by the balance between R_L and R_p , $R_{eff} = R_L + \frac{L}{C_p R_p}$. By fitting the measured reflection coefficient S_{11} to this model, effective values of C_p and R_p can be extracted. To reproduce the measured resonance frequency of $f_0 = 192.0$ MHz, we set $C_p = 0.84$ pF. However, as shown in Fig 7.1(d, e), while Model 1 reproduces the magnitude of S_{11} ($|\Gamma|$), it incorrectly predicts an over-coupled resonance profile, inconsistent with the measured under-coupled trajectory in the Smith chart. This discrepancy indicates that Model 1 underestimates the true energy loss within the inductor.

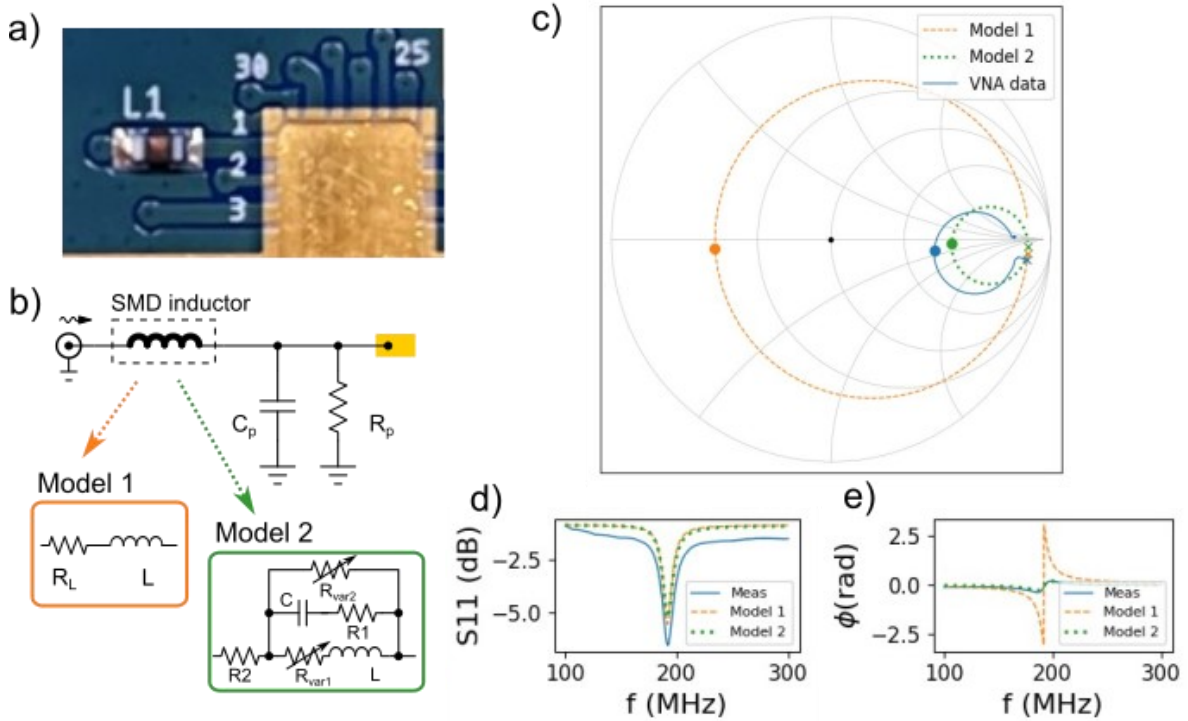


Figure 7.1 Parameter extraction for an RF resonator circuit. (a) Photograph of the PCB showing the surface-mount wire-wound inductor (Coilcraft 0603HL821, labeled L1) and nearby bonding pads. (b) Lumped-element circuit model of the matching network. The inductor is described either by a simple series R_L , L representation (orange box, Model 1) or by a more realistic SPICE-based network including self-resonance and core loss (green box, Model 2). C_p denotes the parasitic trace capacitance and R_p the

dielectric loss of the substrate. (c) Measured reflection coefficient $|\Gamma|$ (blue, VNA data) plotted on a Smith chart, compared with simulations from Model 1 (orange) and Model 2 (green). (d) Corresponding frequency dependence of $|S_{11}|$ in dB and phase ϕ . While both models reproduce the resonance dip, Model 1 predicts an over-coupled response that deviates significantly from experiment, whereas Model 2 captures both amplitude and phase, correctly describing the under-coupled behavior.

Model 2 (realistic) incorporates additional loss mechanisms within the inductor, following the manufacturer's SPICE model. In this description, the inductor is represented by a series resistance R_L , two frequency-dependent parallel resistance R_{var1} and R_{var2} accounting for ceramic core losses, and a parasitic capacitance C associated with self-resonance. The resulting input impedance is:

$$Z_{tot} = R_2 + (j\omega L + R_{var1}) \parallel \left(\frac{1}{j\omega C} + R_1 \right) \parallel R_2 + \frac{R_p}{1 + j\omega C_p R_p} \quad (7.2)$$

We used manufacturer-recommended parameters for C and $R_1, R_2, R_{var1}, R_{var2}$, while adjusting C_p to ~ 0.45 pF to reproduce the measured resonance frequency. The dielectric loss resistance R_p was estimated from the known loss tangent²³⁶ using:

$$R_p = \frac{1}{\omega C_p \tan \delta} \quad (7.3)$$

As shown in Fig. 7.1(c), Model 2 accurately reproduces both the magnitude and phase of the measured reflection coefficient and correctly captures the under-coupled regime. accounting for inductor self-resonance and core loss is essential for realistic modeling. Accordingly, we adopt Model 2 for all subsequent simulations and parameter extraction.

7.2.2 Simulated Response to Device State Changes

With the realistic inductor model established, we next simulate how the resonator responds to state changes in a quantum device. In the lumped-element picture [Fig. 7.2(a)], the device is modeled as additional admittance elements coupled to the resonant network through wire bonds. Depending on the operating

point, a single-electron transistor (SET) can contribute both resistive (R_S) and capacitive (C_S) components to the matching network. These quantum admittances²³², expressed as $Y(\omega) = G(\omega) + i\omega C(\omega)$, modified the reflected coefficient Γ , generating a measurable signal contrast $\Delta\Gamma$ from which the device state can be inferred. The normalized contrast $\frac{\Delta\Gamma}{\Delta Y} = (\Gamma_{on} - \Gamma_{off})/\Delta Y$ serves as the figure of merit to be optimized and defines the intrinsic sensitivity of the resonator in distinguishing device state changes.

We also examine how the resonator quality factor influences sensitivity by comparing two inductors: the Coilcraft 0603HL821 ($Q \sim 10$) and the Coilcraft 0805HP821 ($Q \sim 60$). Figure 7.2(b) shows the open-ended S_{11} traces (no device connected) measured with a VNA. In both cases, the resonance frequency lies near 200 MHz, but the higher Q 0805HP821 produces a sharper resonance dip and shifts the resonator into the over-coupled regime due to its reduced internal loss. Circuit parameters for both inductors were extracted using Model 2 and then applied to simulate the resonator's response to changes in device admittance.

Figures 7.2(c) and 7.2(d) show simulated responses to a resistive perturbation ($\Delta G = 1 \mu S$) and a capacitive perturbation ($\Delta C_q = 1$ fF) on the device, respectively. For both inductors, the resonator is offset from its perfect matching condition, so the added quantum admittance induces only a small variation in Γ near the resonance frequency. A resistive change manifests as a peak in the magnitude response $|\Gamma|$ near resonance, with the sign of the peak determined by whether the resonator is operating in the over- or under-coupled regime. By contrast, a capacitive change primarily shifts the phase response ϕ , producing a dispersive line shape centered at resonance. These results indicate that the phase channel is particularly sensitive to quantum capacitance, whereas the magnitude channel provides a more robust probe of conductance changes.

The chosen values for ΔG and ΔC_q reflect the typical impedance scale of STM-patterned Si:P devices, set by the tunneling barriers required for electron confinement. These impedances are significantly larger than those encountered in other semiconductor qubit platforms. For example, gate defined CMOS quantum dot SETs typically exhibit on-state resistances of 10 – 100 k Ω while GaAs quantum dot SETs often fall in the few k Ω range yielding a much larger on/off contrast in the reflected RF signal. The small signal contrast

inherent to STM-patterned devices places stricter requirements on the resonator sensitivity and directly limits the achievable readout speed.

We denoted the relation between the signal contrast and the quantum admittance at $f = f_0$ by $\Delta|\Gamma| = \sigma_G G_s$ and $\Delta\phi = \sigma_C C_s$ where σ_G and σ_C represent conductance and capacitance sensitivity. In the small-signal regime, these sensitivities can be approximated using the lumped-element circuit model²³⁷:

$$\Delta|\Gamma| = \frac{2R_{eff}Z_0}{(R_{eff} + Z_0)^2} R_p G_s \quad (7.4)$$

$$\Delta\phi = \frac{-2Q_L}{C_p} C_s \quad (7.5)$$

Where $Q_L = (Q_{int}^{-1} + Q_{ext}^{-1})^{-1}$ is the total quality factor. The equations indicate two primary strategies for enhancing resonator sensitivity: (1) tuning the circuit closer to its matching condition to enhance conductance sensitivity. (2) increasing the circuit's quality factor to enhance capacitance sensitivity. However, the two are not independent as changes in the circuit parameters (R_L and C_p) affect both the quality factor and the matching condition simultaneously. From the lumped element model perspective, we extract σ_G and σ_C directly from the numerically simulated signal contrast to include non-idealities such as inductor losses. The results are used to explore the trade-off between the two sensitivities, serving as a guide for selecting component values best suited to a given type of measurement.

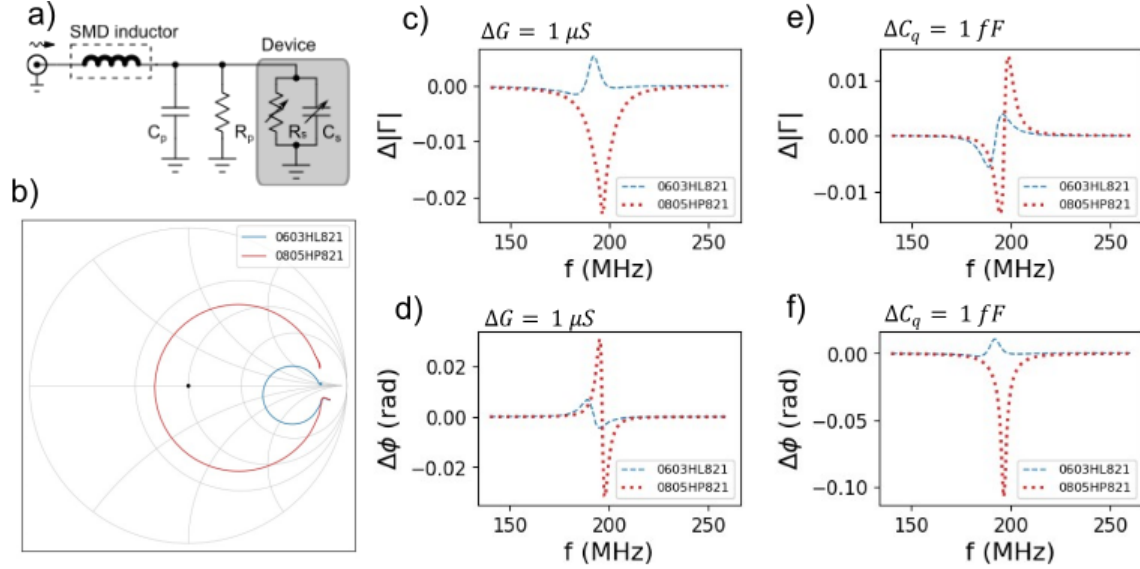


Figure 7.2 Simulated resonator response to device impedance changes. (a) Schematic of the resonator circuit, with the device modeled as lumped conductive and capacitive elements inside the gray box. (b) Smith chart of the resonator response for a higher Q (0805HP821) and lower Q (0603HL821) inductor with the same inductance value $L = 820$ nH, over the frequency range 100-300 MHz. (c), (d) Simulated $\Delta|\Gamma|$ and $\Delta\phi$ for a quantum conductance change of $\Delta G = 1 \mu S$. (e), (f) Simulated $\Delta|\Gamma|$ and $\Delta\phi$ for a quantum capacitance change of $C_s = 1$ fF. The magnitude channel is more effective for detecting small conductance variations, whereas the phase channel provides higher sensitivity to small capacitance changes.

7.3.3 Impedance Matching with Varactor Tuning

To modify the impedance matching condition, we incorporated two sets of varactors (MA46h204-1056) into the circuit with the higher Q inductor. Fig. 7.3(a) and 7.3(b) shows the photo and schematic of the matching network with added varactors C_m and C_t whose capacitance are controlled by the reverse bias V_m and V_t , respectively. C_m is primarily used for impedance matching while C_t mainly tunes the resonant frequency. The selected varactor provides a tunable capacitance range from 20 pF ($V_{RB} = 2V$) down to 2 pF ($V_{RB} = 20$ V). Since C_t has a minimum value of 2 pF, the effective resonator capacitance $C_{p'} = C_p + C_t$

increases from ~ 0.5 pF to ~ 3 pF, shifting the resonance frequency below 100 MHz. Introducing this voltage-controlled element provides a direct way to characterize resonator sensitivity, since a change in C_t can emulate the impedance variation of a real device. By tuning both C_m and C_t , different matching conditions can be realized.

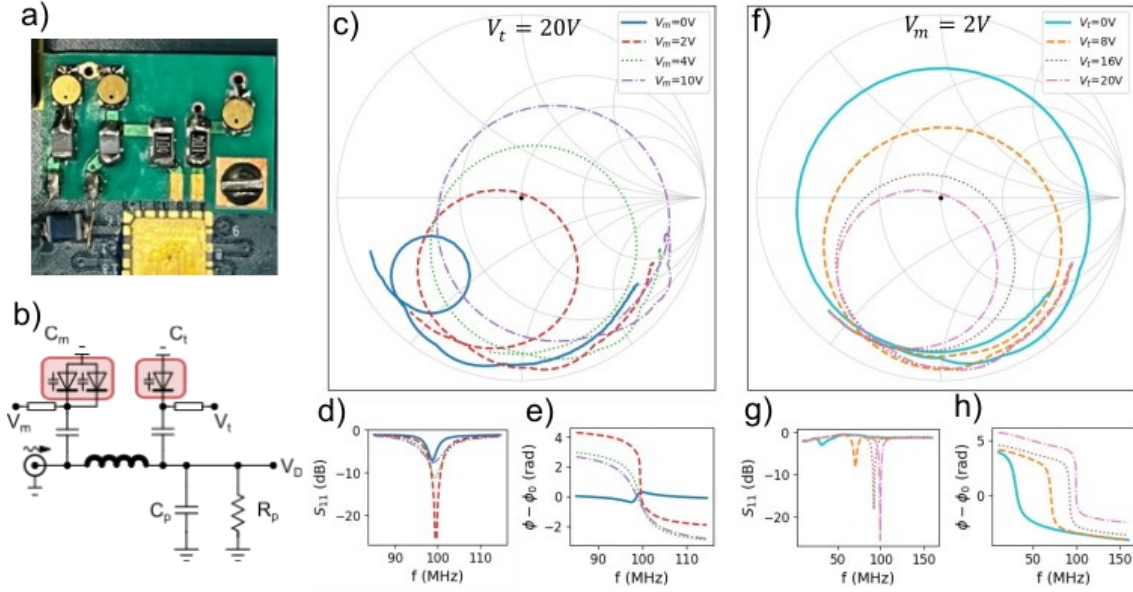


Figure 7.3 Impedance matching using varactor diodes. (a) Photograph of the tuning circuit with varactors C_m and C_t . (b) Circuit diagram of the modified matching network. The higher Q inductor has ignorable core loss and thus no parallel loss resistor. The two bias tees, each consisting of a 100 k Ω resistor and a 1.5 nF capacitor, provide reverse bias to the varactors. Each varactor (MA204) has a tuning range of 2 – 20 pF. (c-e) Measured Smith chart, S_{11} and phase of the resonator response at fixed $V_t = 20$ V varying V_m . (f-h) Measured Smith chart, S_{11} and phase of the resonator response at fixed $V_m = 2$ V varying V_t . Changes on C_m primarily adjusts the impedance matching, while C_t mainly tunes the resonance frequency. The perfect matching condition is achieved at $V_m = 1.9$ V with $V_t = 20$ V.

Figures 7.3(c) and 7.3(f) show the Smith chart of the resonator response in the open-ended configuration for different values of V_m and V_t , with the corresponding S_{11} and phase ϕ plotted in Fig 7.3(d, g) and 7.3(e, h). Within the tuning range, the circuit can be brought to perfect matching. In Fig 7.3(c), V_t is fixed at 20

V while V_m is varied. As C_m decreases, the resonator transitions from over-coupled to under-coupled, reaching perfect matching at $V_m = 1.9$ V. In Fig 7.3(f), V_m is fixed at 2 V and V_t is varied. Increasing C_t lowers the resonance frequency significantly while also modifying the matching condition.

To reproduce these behaviors, we extended the lumped-element model to include the additional tuning components and extra parasitic capacitance from the new metal traces. For this multi-parameter simulation, we define a criterion for a reasonable fit as one where the discrepancy on Γ between the simulation and measured data is below a threshold (resonant frequency $< 1\%$, $|\Gamma|$ at resonance < 2 dB, Q factor $< 5\%$) across the relevant frequency range. After several iterations, we identified a set of parameters that faithfully reproduces the measured frequency response across the full tuning range of C_m and C_t .

We next tune the value of C_t by modulating V_t to emulate the response of a quantum capacitance. For a small ΔV_t , the resulting capacitance change is roughly equal to the perturbation expected from STM-patterned quantum devices. For a thermal broadened dot reservoir charge transition ($\hbar\gamma \ll kT_e$), the tunneling capacitance $C_p = \frac{\alpha^2 q^2}{4kT_e}$ which is typically on the order of 1 fF at $T_e = 300$ mK in a dilution

refrigerator. The varactor capacitance follows roughly $C_t = 23/V_t^{\frac{3}{4}} pF \cdot V^{3/4}$ across its tuning range. At $V_t = 20$ V, a modulation of $\Delta V_t = 5$ mV corresponds to $\Delta C_t \sim 0.5$ fF, comparable to a tunneling capacitance. Fig 7.4(a, b) presents the measured amplitude and phase contrasts $\Delta|\Gamma|, \Delta\Phi$ of $\Delta V_t = 50$ mV at $V_t = 20$ V as a function of V_m and frequency. The phase contrast $\Delta\Phi$ changes sign when crossing the perfect matching condition (via V_m) while the magnitude contrast $\Delta|\Gamma|$ changes sign when crossing the resonant frequency and decreases in intensity as the system moves away from matching. The optimal phase contrast (i.e., capacitance sensitivity) is obtained close to, but not exactly at, the perfect matching point, where the phase is unstable due to critical coupling. We also note while $\Delta|\Gamma|$ is limited and proportional to the effective “quantum capacitance” ΔC_t , the phase shift $\Delta\phi$ can approach unity near matching, where the Smith chart trajectory crosses the origin.

Figure 7.4(c, d) shows simulated contrasts for $\Delta V_t = 5$ mV using the lumped-element model, demonstrating quantitative agreement with experiment. A switchable resistance in the $M\Omega$ range was not implemented to directly probe conductance sensitivity. Instead, we infer it by representing the device with a shunt resistor in the simulation as a reasonable estimate for the real circuit response. The corresponding simulated amplitude and phase responses are shown in Fig 7.4(e, f). The optimal amplitude contrast (i.e., conductance sensitivity) occurs at the resonant frequency, with only a weak dependence on the matching condition.

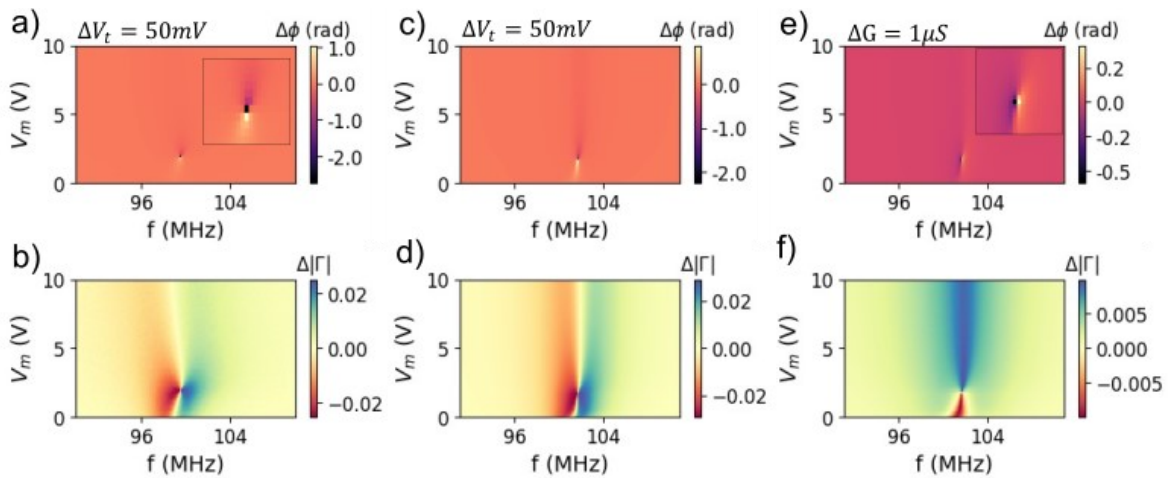


Figure 7.4 Measured and simulated signal contrast under device impedance changes. Measurements were taken by varying V_m at a fixed $V_t = 20$ V. (a, b) Measured phase and amplitude contrast for a perturbation of $\Delta V_t = 50$ mV, emulating a device capacitance change. The inset highlights the region close to resonance and matching condition. (c, d) Simulated phase and amplitude response for $\Delta V_t = 50$ mV using the lumped-element model. (e, f) Simulated phase and amplitude response for a conductance change of $\Delta G = 1 \mu S$ ($R_s = 1 M\Omega$).

7.3.4 Low-Temperature SET Measurements

Building on the room-temperature characterization and modeling, we selected the higher Q inductor (0805HP821) and replaced the varactors with fixed-value SMD capacitors to tune the matching network close to its impedance-matching point. Charge stability diagrams of an STM-patterned SET device were then measured in a dilution refrigerator at a base temperature of 10 mK using RF reflectometry. The

measurement setup is shown in Fig. 7.5(a). The RF lead is connected to the SET drain, while the tunneling current through the source is captured by a transimpedance amplifier at room temperature, enabling simultaneous acquisition of RF and transport data. A Cosmic Microwave CITLF3 amplifier, mounted at the 4 K stage with a noise temperature of ~ 4 K, served as the first amplification stage, followed by additional room-temperature amplification and finally demodulation with a Polyphase AD0105 to extract the I/Q signals.

Fig. 7.5(b-d) presents the tunneling current, RF magnitude and RF phase in the Coulomb blockade regime. The numerically obtained differential conductance $G = dI/dV$ is correlated to $\Delta|\Gamma|$ through the conductance sensitivity coefficient $\Delta|\Gamma|$. At $V_{ds} = 3$ mV, the on-state has a differential conductance $G < 1 \mu\text{S}$, placing the device in the high impedance small signal regime discussed in this paper. The phase channel shows a weaker response, consistent with operation at the resonance frequency where the SET admittance is predominantly conductive, at which the RF magnitude provides a clearer signature of the conductance change.

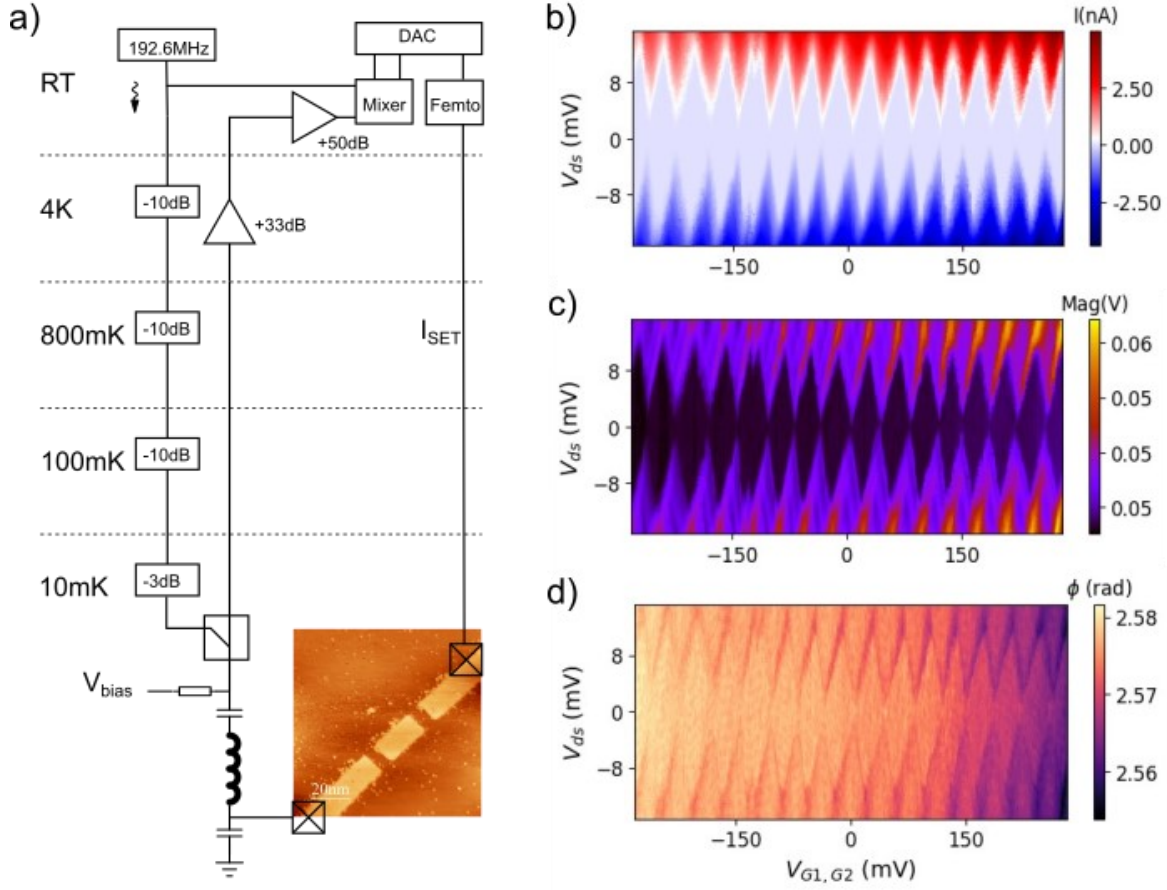


Figure 7.5 Low-temperature RF reflectometry measurements on an STM-patterned SET device. (a) Experimental setup for RF measurements in a dilution refrigerator. (b–d) Tunneling current, RF magnitude, and RF phase in the Coulomb blockade regime. (e) Correlation between $\Delta|I|$ and the differential conductance dI/dV , yielding a conductance sensitivity of $\sigma_G = 6.25 \times 10^4 \Omega$ for this setup.

7.3.5 Charge sensing SNR Analysis

We next examine the overall charge sensitivity of the measurement setup by including noise contributions from the signal chain and characterizing the effective bandwidth of the SET when used as a charge sensor for a nearby donor dot. The input RF power at the matching network was fixed at $P_{\text{in}} = -86$ dBm. Owing to resonance, the actual RF voltage amplitude that appear at the device lead is estimated to be $V_{\text{rf}} = 100 \mu\text{V}$. While this power level may increase the local electron temperature of the SET through dissipation

and reduce spin readout fidelity²³⁸, for charge sensing they enhance signal contrast at the expense of only a moderate temperature rise. To evaluate charge sensitivity, we set the gate voltages to the on- and off-states of a Coulomb peak at $V_{ds} = 3$ mV and record the reflected signals in the I/Q plane. Each quadrature measurement contributes a count to a two-dimensional I/Q histogram, yielding two distinct clusters corresponding to the on and off states, broadened by noise. The signal-to-noise ratio (SNR) is defined as the ratio between the separation of the cluster means and the standard deviation of the individual clusters.

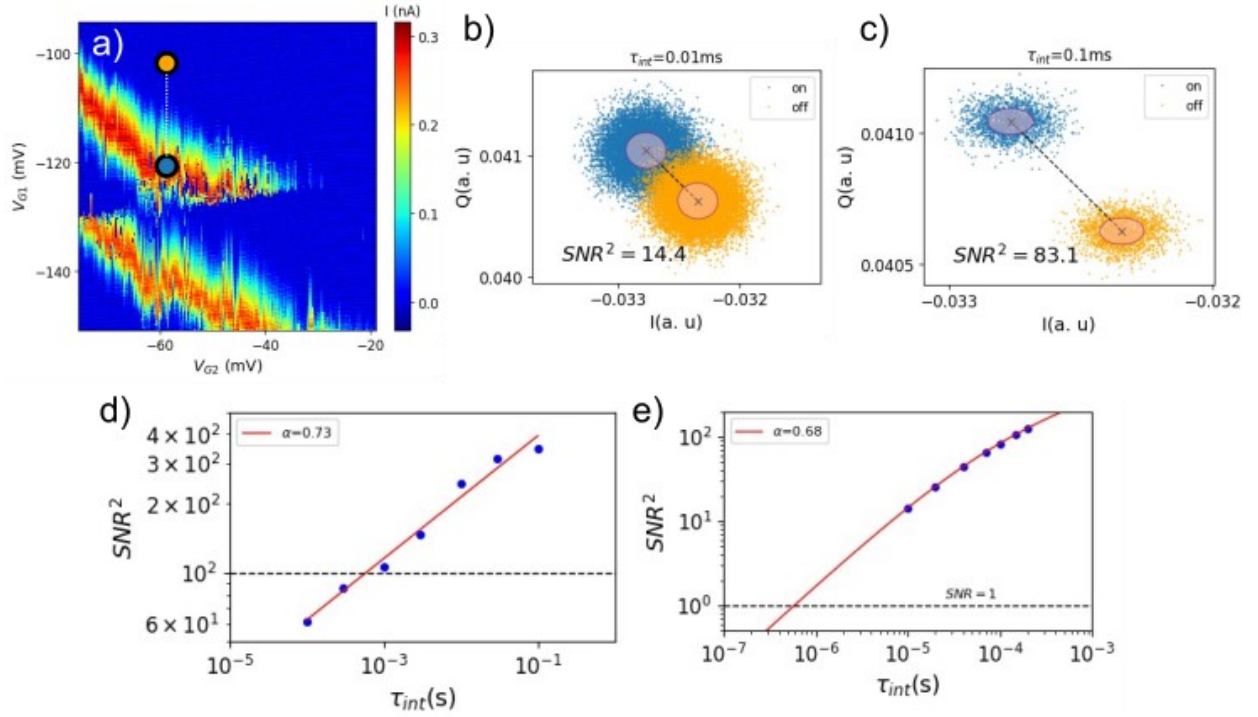


Figure 7.6 Signal-to-noise ratio (SNR) as a function of integration time. (a) Charge stability diagram near a donor-dot transition. The RF response is repeatedly measured at the SET on-state (blue circle) and off-state (orange circle) for different integration times. (b, c) Two-dimensional histograms of single-shot I/Q measurements with integration times of 10 μ s and 100 μ s. Blue and orange clusters correspond to the on and off states, respectively. (d, e) SNR as a function of integration time τ . At longer τ , the behavior is dominated by low-frequency charge noise, while at shorter τ charge noise is effectively frozen and $SNR^2 \propto \tau$. Extrapolation of the fit to $SNR=1$ yields a minimum integration time of $\tau_{min} = 600$ ns.

Figure 7.6 shows the SNR of the on/off states as a function of integration time τ . The I/Q data were acquired at 500 kSa/s after a low-pass filter with cutoff frequency of 250 kHz. In the presence of thermal white noise and low-frequency environment flicker/charge noise, the SNR exhibits a characteristic dependence on the integration time²³⁹, $SNR^2 = S_0\tau/(1 + A_f\tau^\alpha)$ where S_0 represents the white-noise power and A_f parameterizes the contribution of low-frequency noise.. For longer integration times ($\tau > 100 \mu\text{s}$), the charge noise dominates by shifting the I/Q cluster means of the on and off state within each acquisition interval, yielding $SNR^2 \sim \tau^{1-\alpha}$ with α measured to be 0.73 at the operating position. At shorter integration times, slower charge noise becomes effectively static, and the linear scaling $SNR^2 \propto \tau$ is recovered, dominated by thermal white noise. In this regime, the measurement charge sensitivity is determined solely by the intrinsic conductance sensitivity of the impedance matching network and limited by the noise of the amplifier chain, which is dominated by the 4 K noise temperature of the first-stage cryogenic amplifier. Extrapolating the curve to $SNR = 1$, we obtain a minimum integration time of $\tau_{min} = 600 \text{ ns}$. Further improvements on the minimum integration time can be achieved by increasing the SET on-state conductance or reducing the noise temperature of the first-stage amplifier^{240,241}.

7.3 Conclusion

In this work, we investigated the performance of a simple RF reflectometry circuit based on a single wire-wound surface-mount inductor for charge sensing in high-impedance silicon quantum devices. Using a detailed lumped-element model, we captured the effects of inductor core loss, self-resonance, and PCB dielectric loss, and demonstrated that realistic modeling is essential to accurately reproduce measured reflection coefficients. Comparison of low- and high-Q inductors confirmed that improving the internal quality factor enhances charge sensitivity.

By integrating a tunable varactor-based matching network, we characterized the reflected signal contrast under different impedance-matching conditions. Both measurement and simulation showed that sensitivity

to small admittance changes vanishes at exact matching and reaches an optimum slightly off match. Phase contrast is more suitable for detecting quantum capacitance, while magnitude response is more suitable for conductance variations.

Finally, we benchmarked the resonator in a dilution refrigerator using a STM patterned single-electron transistor device with $M\Omega$ -scale on-state impedance. Despite the small conductance, we achieved charge readout with a minimum integration time of ~ 600 ns or a charge sensitivity of $S_C = 1.0 \mu\text{e}/\sqrt{\text{Hz}}$, consistent with the intrinsic conductance sensitivity of the matching network and the noise temperature of the first-stage cryogenic amplifier.

These results establish the fundamental limits and optimization strategies for wire-wound inductor-based RF resonators in large-impedance silicon quantum devices. Our approach demonstrates a practical pathway to enhance charge sensitivity through careful selection of inductor quality factors and impedance-matching conditions. Moreover, the methods developed here are broadly applicable and can be extended to advanced resonator architectures, including superconducting spiral inductors, to enable faster and higher-fidelity spin readout in future silicon quantum technologies.

Chapter 8: RF reflectometry measurements of charge configuration in a Si:P quantum dot array

8.1 Introduction

The Fermi-Hubbard model has been an indispensable tool for the exploration of condensed matter physics in a variety of material systems. When accounting for the interactions, the model can capture essential electron correlation effects and complex many-body phenomenon such as high- T_c superconductivity²⁴², spin liquids²⁴³ and other exotic phenomena. Despite the simple formulation of the Hamiltonian, solutions to the Fermi-Hubbard model can quickly become non-trivial as the Hilbert space grows exponentially with the system size and numerical methods^{160,244,245} fail.

In parallel, techniques to simulate the Fermi-Hubbard model on a physical analog quantum simulator have emerged in different platforms such as optical lattices^{174,246,247} and solid-state quantum dots^{171,176,191}. A carefully designed physical lattice is assembled to emulate the behavior of a Hubbard Hamiltonian where a discrete site in the Hamiltonian naturally corresponds to a physical site such as an atom or a quantum dot. The parameters of the Hubbard Hamiltonian, such as the tunnel coupling constants and on-site/long-range interactions, may be controlled during the fabrication process or during the measurement and operation, depending on the specific platform. For dopant-based quantum dot systems, Hubbard parameters are typically controlled by tuning the lattice constants and donor numbers on each site, realizing different lattice geometries, etc. STM-based Hydrogen lithography technique^{53,54,70} enables sub-nm precision in the lithography and placement of the dopants. Recently, enhanced atomic precision techniques^{48,123} have been demonstrated that enable tip facilitated⁴⁹ dopant incorporation which results in exact donor number per site with high yield, avoiding the randomness resulting from stochastic thermal incorporation. Combining precision lithography with deterministic incorporation enables engineering of nearly defect-free dopant lattices in silicon. Recent advances in machine learning and automated patterning are expected to further

improve robustness and streamline STM device fabrication, strengthening the prospects for analog quantum simulation.

A key challenge in studying Hubbard physics in dopant arrays is probing charge and spin configurations at the level of individual sites, which is also critical for identifying fabrication-induced disorder. Typically, low temperature transport measurements are performed by coupling the array to a pair of source drain lead to map out the charge stability spectrum in the Coulomb blockade regime. In a previous study ¹⁷², we demonstrated the fabrication of a series of 3x3 quantum dot arrays with different lattice constants and characterized their electron addition energy spectrum and dependencies on the tunneling coupling constants. Although qualitative and limited quantitative agreement with an extended Hubbard simulation has been established, transport measurement alone only provides limited insight: non-equilibrium dynamics, Coulomb or spin blockade, and electron localization obscure site-specific charge redistribution. This is especially the case for the weakly coupled array as electrons are mostly localized on individual sites resulting in weak tunneling currents. A more direct probe of ground-state configurations is therefore needed. RF reflectometry ²³⁷ is becoming a powerful charge sensing technique with a variety of implementations such as RF-SET (single electron transistor) ^{46,239}, RF-QPC (quantum point contact) ²¹⁹, and SLQD (single lead quantum dot) ²⁴⁸, etc. with distinct advantages over transport measurements. The RF signal can be applied to existing control gates, reducing device footprint and wiring complexity, while charge transitions manifest as quantum capacitance or conductance without cable-capacitance bandwidth limits. This enables fast and sensitive detection of charge dynamics in multi-dot systems.

In this paper, we use RF reflectometry to probe charge configurations within a weakly coupled STM patterned few-dopant quantum dot array. Since the RF response induced at charge degeneracy points is broadened by tunnel coupling or thermal energy, we obtain more precise mutual charging energies and electron addition energy spectra beyond what transport can provide. Distinct capacitive couplings to the leads allow us to identify the exact sites of electron addition and charge rearrangements. By tracking individual transitions, we can, in principle, reconstruct the full charge configuration of the array as a function of applied gate voltages. We also study the impact of RF input power on effective electron

temperature by analyzing the line shape of charge transition phase signals and confirm that line broadening arises primarily from heat dissipation at the RF lead, with a temperature gradient observed across the array. Finally, we observe asymmetric suppression of the interdot charge transition (ICT) signal between an edge and a central dot as a signature of Pauli spin-blockade and measure a singlet-triplet relaxation time of 7.5 μs . These results demonstrate the capability to probe electron correlations and transient dynamics in 2D dopant arrays using RF reflectometry and suggest that optimized RF gate placement could further enhance sensitivity and enable high-fidelity spin readout.

8.2 Results

The device measured in this paper is a weakly coupled 3x3 array with an average lattice constant $a = 10.7$ nm. Figure 8.1(a) shows an STM image of the central region of the device. The lithography masks for the 3x3 quantum dot array are patterned individually and form incorporation sites that are estimated to hold 2 to 3 Phosphorus atoms. The rows are defined as along the source-drain direction and the columns are defined as along the transverse direction. The nine sites are named by their corresponding position defined in Figure 8.1(b) from $D11$ to $D33$ where the row is specified by the first index and the column by the second. The dots on the first column are tunnel coupled to the source and the dots on the third column are tunnel coupled to the drain for transport measurements. Two in-plane gates ($G1, G2$) are placed symmetrically about the array in order to tune the electrochemical potential landscape across the array. The input RF signal is combined with DC bias voltage via a bias tee and applied to the drain lead. A tank circuit consisting of an 820 nH inductor and on-board parasitic capacitance is used to match the device impedance to the 50 Ω coax line impedance with a resonant frequency of 191.6 MHz and a quality factor of $Q \sim 20$, shown in Figure 8.1(a). The reflected RF signal is read from a homodyne setup following an amplification chain. The transport current is measured using a room temperature transimpedance amplifier connected to the source.

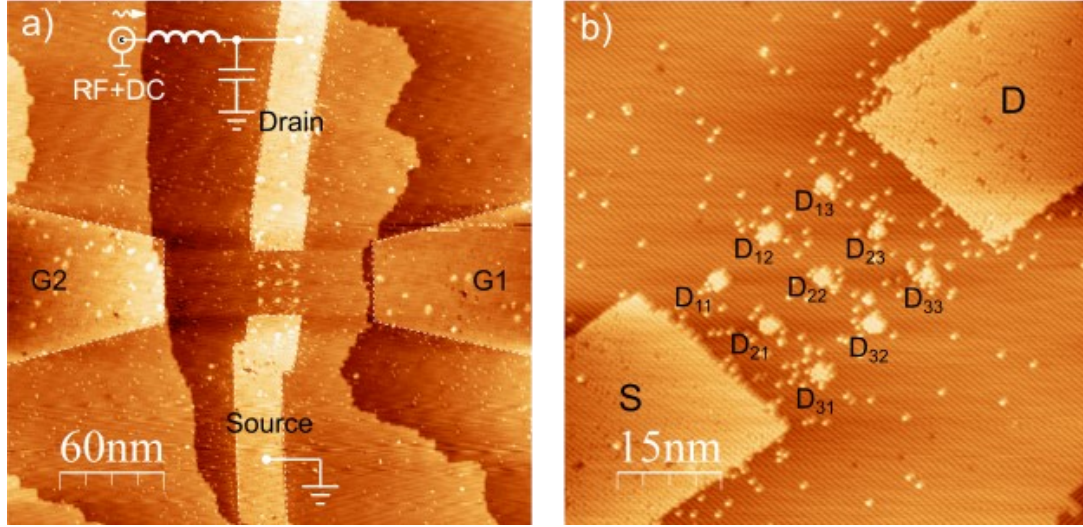


Figure 8.1 a) STM image of the weakly coupled 3x3 array device. b) Zoomed in image at the central dot region. The dots are named by row and column from D11 to D33 with an average lattice constant of 10.7 nm. The edge dots are directly tunnel coupled to the source and drain lead with similar tunneling gaps.

Figure 8.2 shows the charge stability diagram measured at $V_{ds} = 4$ mV. The RF signal has an estimated amplitude of $V_{rf} = 20$ μ V at input power $P_{in} = -86$ dBm. Line segments in the RF phase response Figure 8.2(a) arise from additional quantum capacitance generated at charge transitions. Two types of transitions can be distinguished: dot-lead and interdot. The edge dots are directly tunnel coupled to the source or drain, and when their chemical potential aligns with the lead Fermi level, electrons tunnel non-adiabatically between the lead and the dot producing a detectable tunneling capacitance provided the tunnel rate γ exceeds the RF drive frequency ω_0 , $\gamma \gg \omega_0$. In contrast, interdot charge transitions (ICTs) occur when the chemical potentials of two dots (or multi-dot eigenstates) coincide. If the two dots are directly tunnel coupled, the RF excitation adiabatically modulates their ground state energy, yielding a detectable quantum capacitance. Figure 8.2(b) shows the transport current on a logarithmic scale. The currents flow in narrow strips with charge transition lines as support. Each of these channels represents a conducting path for an

electron to load from one edge and then unload from the other edge. As we increase the source-drain bias, these current strips become wider and new strips appear due to more available conducting paths. The overall low conductance except at isolated hot spots reflects the relatively large lattice constant, which weakens tunnel coupling and localizes electrons on individual sites. Since resonant tunneling requires the near perfect alignment between two overlapping many-body eigenstates which only occur occasionally, the current is mostly suppressed at lower source-drain biases.

With the RF phase signal tracking the ground state electron configuration and the transport capturing the non-equilibrium dynamics^{196,199}, the two channels provide complementary information on the underlying Hubbard physics. When the operating RF frequency is slightly off the resonant frequency, finite tunneling current may also induce a small phase shift by conductance. However, this contribution is minor compared to the quantum capacitance signal, and the RF phase signal still faithfully captures any charge rearrangement events. To interpret the observed charge configuration and transition patterns, we simulated the device behavior using an extended Fermi–Hubbard model by varying the tunnel coupling t between the nearest neighbor sites. The fact that most of the line features are straight and the transitions between different slopes are sharp is a manifestation of the array being in the weak tunneling coupling regime (atomic limit) where $t \ll U$ and the electrons are mostly localized on each individual site except at the close affinity of a charge degeneracy point.

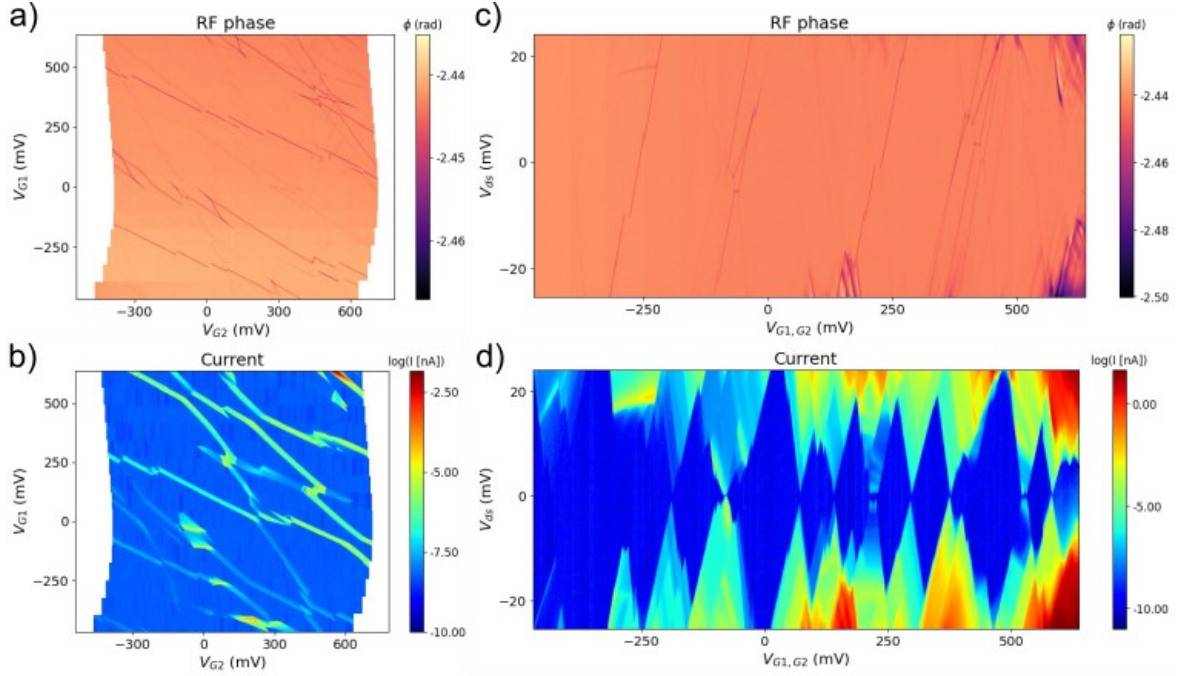


Figure 8.2 Charge stability diagram and finite bias spectroscopy $P_{in} = -86$ dBm. (a) Reflected RF signal phase, (b) DC transport current measured across the entire gate range. Data acquisition is done in a block-by-block sequence to avoid large jumps in the gate voltage which can cause hysteresis. Each block is then stitched together to produce the full map. (c), (d) Finite bias spectroscopy measured along the axis $V_{G1} = V_{G2}$.

8.2.1 Identifying the charge configuration

Previously we quantified the spectrum of array charging energies as a function of tunnel coupling based on transport measurements alone. Here, by combining transport with RF reflectometry, we resolve electron additions at individual sites and obtain a more precise electron addition energy spectrum of the array. We first perform capacitance modeling of the device using the post lithography STM image as input geometry. From the simulated capacitance matrix, we determine the lever arms of all four leads and the mutual charging energies between sites and use these values as reference to identify measured charge transition lines. Since the lever arms depend primarily on the physical separation d , decreasing approximately as a polynomial function the dots within the same row share similar capacitive coupling to both $G1$ and $G2$

while the dots within the same column share similar capacitive coupling to the source and drain. In the RF phase signal Figure 8.2(a), the most prominent features are multiple extended line segments with a negative slope $s = \Delta V_{G1} / \Delta V_{G2}$ which are attributed to the charge transitions between the source drain lead and the edge dots. The measured slopes group into distinct sets of values, corresponding to the first ($s \sim -1.45$), second ($s \sim -0.81$) and third ($s \sim -0.45$) row. These values agree with the capacitance simulation results $s = -\alpha_2 / \alpha_1$ where $\alpha_{1,2}$ is the calculated lever arm of $G_{1,2}$ to each site. The remaining line features come from interdot charge transitions (ICTs) between two adjacent sites (nearest or next nearest neighbor) with a non-zero tunnel coupling.

Figure 8.3 shows the charge stability map near a double interdot degeneracy region. Two sets of charge transition lines with a negative slope are clearly visible, each corresponding to an electron addition onto row 1 (red) and row 2 (blue). A third addition line (green) is absent from the RF phase response but is inferred from a distinct change in the transport pattern in Figure 8.3(b), where its slope is consistent with row 1. Altogether, three electrons are added into the array, increasing the total electron number from N to $N+3$. The degeneracy between the blue and the green legs shows a faint signal indicating that the two corresponding sites are adjacent and tunnel coupled. However, the tunnel coupling is much smaller than the mutual charging energy, $t \ll U_{ij}$, as the triple-point region is negligible compared to the degeneracy region. By contrast, the degeneracy between the red and blue legs shows no RF response suggesting the two dots are very weakly tunnel coupled. This can also be seen from the smaller mutual charging energy obtained from the line separation across the degeneracy.

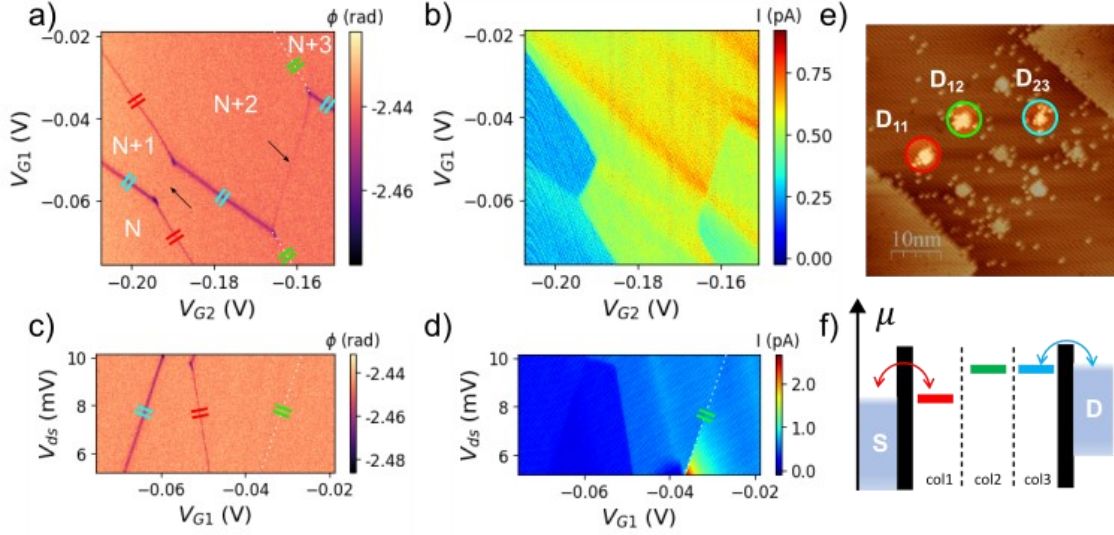


Figure 8.3 Identifying electron addition sites near a double ICT region. (a) and (b) RF phase response and transport current measured at $V_{ds} = 10$ mV. Three electron addition lines and two ICTs (labelled by black arrows) are observed. Transport current shows distinct patterns at each charge configuration. (c) and (d) varying bias spectroscopy measured along the diagonal axis of (a) with $\Delta V_{G1} = \Delta V_{G2}$. (e) Identified electron addition sites D11, D12 and D23 are highlighted in red, green and blue as explained in the main text. The corresponding electron addition lines are labeled with the same colors in (a) and (c). The D12 (green) addition is invisible in the phase signal as it is not directly tunnel coupled to the source nor the drain. (f) Schematic illustration of charge addition: column 1 dots align with the source, column 3 dots align with the drain, and column 2 dots may align with either.

To identify also the precise column of these electron additions, we track how the charge transition lines shift under varying source–drain bias. In Figure 8.3(c) and 8.3(d), RF phase and transport current are measured along the diagonal line in Figure 8.3(a) where $\Delta V_{G1} = \Delta V_{G2}$. To keep the left edge dots to align with the source (ground), the combined leveraging from the gates must compensate for the leveraging from the drain voltage, yielding a negative sloped charge transition line in the finite bias spectroscopy map with $s_L = -(\alpha_1 + \alpha_2)/\alpha_D$. Conversely, to keep the right edge dots in resonant with the drain, the combined leveraging from the gates must push the dot chemical potential to follow the drain, producing a positive sloped charge transition line with $s_R = (\alpha_1 + \alpha_2)/(1 - \alpha_D)$. This is analogous to a single electron transistor where the left (right) edges of the Coulomb diamonds represent the alignment of the island with its source (drain) ¹⁴¹.

In Figure 8.3(d), we extract the line slopes and confirm the column indices for each addition electron. The green leg charge transition has a positive slope according to Figure 8.3(d) which suggests it is aligned to the drain. Combining both row and column information, the three electron addition sites are $D11$ (red), $D12$ (green) and $D23$ (blue) and highlighted in Figure 8.3(e). Mutual charging energies between the two pairs of dots are calculated using the simulated lever arms: $U_{11,23} = 2.4$ meV, $U_{12,23} = 5.2$ meV, consistent with the separation distance of the pairs. The same measurement techniques and site-identification methods can be extended to more complex many-body eigenstates in larger or more strongly coupled arrays. In such systems, electron delocalization leads to hybridized charge configurations and richer transition patterns as the many body wavefunction evolves with gate voltages, yet RF reflectometry remains a powerful approach for resolving the expectation value of the electron's spatial position. The transition from the atomic limit to a more delocalized state can be readily identified from changes in the patterns of charge transitions.

8.2.2 Characterization of electron temperature as a function of input RF power

In this section, we investigate the effect of input RF power on the effective electron temperature within the array by measuring the line width of each dot-lead charge transition lines at different input RF powers. For a quantum dot tunnel coupled to an electron reservoir with a tunnel rate γ driven by an external RF excitation V_{rf} of frequency ω_0 , the quantum capacitance, C_q , and conductance, g_q caused by charge movement in the temperature broadened regime ($k_B T_e \gg \hbar\gamma$) are given by ^{227,232,249}:

$$C_q = \frac{\alpha^2 q_e^2}{4k_B T_e} \left(1 + \frac{\omega_0^2}{\gamma^2}\right)^{-1} \cosh^{-2}\left(\frac{\Delta\mu}{2k_B T_e}\right) \quad (8.1)$$

$$g_q = \frac{\alpha^2 q_e^2}{4k_B T_e} \left(1 + \frac{\gamma^2}{\omega_0^2}\right)^{-1} \cosh^{-2}\left(\frac{\Delta\mu}{2k_B T_e}\right) \quad (8.2)$$

where q_e is the electron charge, $\Delta\mu$ is the chemical potential of the dot relative to the lead and α' is the ratio of induced chemical potential difference $\Delta\mu_{rf}$ from the RF excitation, $\Delta\mu_{rf} = e\alpha'V_{rf}$. The peak value of

C_q and g_q give a direct estimate of the electron temperature and tunnel rate. Additionally, the width of the peak is only proportional to the electron temperature, as indicated by the argument of the cosh function. The above equations are valid for small RF excitation amplitudes such that $\Delta\mu_{rf} \ll k_B T_e$ and the broadening due to $\Delta\mu_{rf}$ can be ignored. Since the measurement of sensitive impedance changes usually requires averaging over many data points to ensure an acceptable signal-to-noise ratio, sometimes larger RF excitation (larger $\Delta\mu_{rf}$) is needed to reduce the total integration time for charge sensing. For spin sensitive measurements, however, the effects of finite RF excitation require careful examination as the typical Zeeman energies used for silicon electron spin qubits are on the order of $\sim 100 \mu\text{eV}$ which can be easily overwhelmed by a significant increase in the electron temperature. (On the other hand, if the RF excitation only broadens the transition line without increasing the electron temperature, better SNR can be achieved.) To account for the effect of finite RF excitation ($\Delta\mu_{rf} \geq k_B T_e$) for larger RF input power measurements, we adopt a master equation²⁵⁰ which describes the tunneling process between a quantum dot and a lead:

$$\dot{P}_1(t) + \gamma P_1(t) = \frac{\gamma}{1 + \exp\left(\frac{\Delta\mu(t)}{k_B T_e}\right)} \quad (8.3)$$

where $P_1(t)$ is the probability of the electron on the dot and $\Delta\mu(t) = \Delta\mu_0 + e\alpha' V_{rf} \sin(\omega_0 t)$ is the time dependent chemical potential between the dot and the lead. The tunneling capacitance can be calculated from the derivative of $P_1(t)$ with respect to the excitation voltage: $C_q = e\alpha \frac{dP_1(t)}{dV_{rf}(t)}$. Note the $k_B T_e$ in the master equation represents the actual electron temperature of the dot-lead system when the RF excitation is on, which could be higher than the base electron temperature $k_B T_0$ when the RF excitation is off. The solution of equation (8.3) simplifies into equation (8.1) when $\Delta\mu_{rf}$ is small, but not for general excitation amplitudes. In which case the charge addition line is broadened by both the finite $\Delta\mu_{rf}$ and the thermal energy. Therefore, the apparent line width sets the upper bound for the electron temperature of the system.

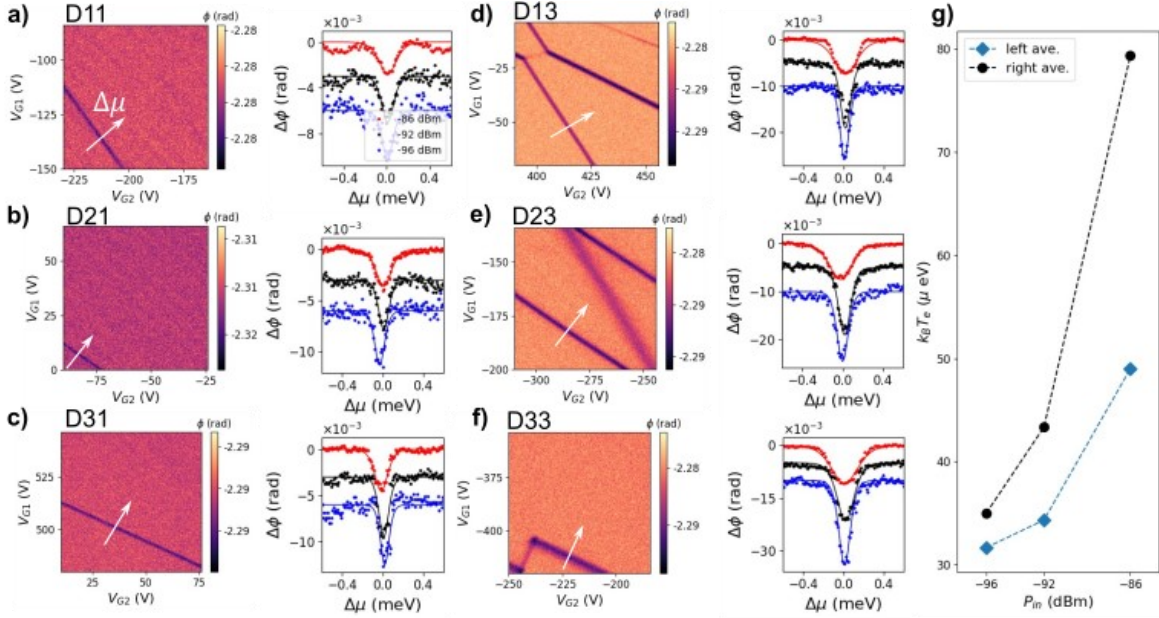


Figure 8.4 Effective electron temperature of individual edge sites at different input RF powers. (a) to (c) and (d) to (f) Charge addition lines of the left edge dots (D11, D21, D31) and right edge dots (D31, D32, D33). The shape of the lines is measured at $P_{in} = -86$ dBm (red), -92 dBm (black) and -96 dBm (blue) in the right panel along the white arrows in the left panel which are orthogonal to the charge addition lines. The lines are fitted using equation (1) to get the electron temperature, $FWHM = 3.526k_B T_e$. (g) the average electron temperature of the left side and right side plotted as a function of input RF power. The right edge dots show a clear higher electron temperature as those are directly tunnel coupled to the RF lead.

Figure 8.4(a-c) and 8.4(d-f) show the RF phase response measured at the charge transition lines for the left edge dots (D11, D21, D31) and the right edge dots (D13, D23, D33). The line sweeps are measured at $P_{in} = -96$ dBm, -92 dBm and -86 dBm in order to investigate contributions to the line width from electron temperature and finite excitation amplitude. The detuning axes are scaled to the relative chemical potential $\Delta\mu$ using the corresponding lever arms and the degeneracy is shifted to $\Delta\mu = 0$ meV. RF amplitude response was measured but showed almost no signal (see Supplementary note), suggesting that the tunnel rates γ are much greater than the RF frequency used (191.6 MHz) for all six edge dots and the induced

quantum admittances are almost purely capacitive. At $P_{in} = -96$ dBm, the amplitude of RF excitation is small compared to the electron temperature for all six dots and the small signal approximation is valid. From Eq. (1), we extract an electron temperature of $k_B T_e \sim 32$ μ eV from the full width at half maximum (FWHM) of the transition lines across all six dots and use this as the baseline condition where input RF power has a negligible effect on electron temperature. At higher P_{in} , we observe both more broadening and lower peak values in the charge transition lines. Figure 8.4(g) plots the average apparent electron temperature from the FWHM of the left edge dots (black circle) versus the right edge dots (blue diamond) as a function of the input RF power. A clear trend of larger broadening or higher electron temperature is seen on the right edge dots. This difference can be explained by two attributes. First, the left edge dots are tunnel coupled to the source so the RF lever arm $\alpha' = (\alpha_D - 0) = 0.21$ while the right edge dots are tunnel coupled to the drain resulting in $\alpha' = (1 - \alpha_D) = 0.45$. This geometric factor alone yields $(0.45/0.21)^2 \sim 4.6$ times larger peak response and ~ 2.2 times larger finite amplitude broadening on the right edge dots than the left edge dots. Secondly, the dissipation of RF power at the drain caused the local electron temperature to rise while the source is still thermalized to almost base temperature as no direct dissipation occurs. This creates an effective temperature gradient across the array where the middle column dots are at intermediate temperature but cannot be directly measured. To estimate the actual electron temperature at $P_{in} = -92$ dBm and -96 dBm, we perform the numerical integration of the master equation. This provides a criterion for when the actual electron temperature is increasing. The measured phase response for D13 and D23 at $P_{in} = -92$ dBm and $P_{in} = -96$ dBm show similar peak values but a ~ 10 μ eV difference in line width which suggests the actual electron temperature does not increase by much (close to 30 μ eV), and the extra broadening is mainly due to the finite voltage amplitude from which we estimate $\Delta\mu_{rf} \sim 10$ μ V at $P_{in} = -92$ dBm and correspondingly $\Delta\mu_{rf} \sim 20$ μ V at $P_{in} = -86$ dBm. The peak phase shift on D33 already decreases going from -96 dBm to -92 dBm. This is likely because the actual dopant incorporation position is slightly closer to the drain than D13 and D23, leading to a higher electron temperature. The line broadening of the right edge dots at $P_{in} = -86$ dBm is 80 μ eV much greater than the estimated RF

excitation amplitude, confirming the actual electron temperature is close to the apparent line width. From measurement perspective, $P_{in} = -92$ dBm is the optimal RF input power for this experiment as it maximizes the SNR without significantly increasing the electron temperature.

8.2.3 Spin-blockade and singlet-triplet relaxation

We investigate spin configurations in the array by probing interdot charge transitions at finite magnetic fields. One distinct phenomenon of electron tunneling between two quantum dots is spin-blockade. For small few dopant (2~3 Phosphorus atoms) quantum dots in silicon, tight binding calculations⁹⁰ predict an even-odd spin filling for the first few electrons for most dopant configurations. Experimentally, valley-orbital excited states^{82,251} in silicon quantum dots on the order of hundreds of microelectron volts to millielectron volts have been observed. By comparing the charge stability diagrams at 0 T and 2 T, we identify a few degeneracy points where an ICT phase signal disappears, likely due to Pauli spin-blockade. Figures 8.5(a) and 8.5(b) show one such region measured at $V_{ds} = 0$ mV. Using the procedure described in section 2.1, we identify the two dots relevant to this interdot charge transition to be $D13$ and $D22$. The charge addition lines of $D22$ have no RF phase signal due to weak tunnel coupling to the source and drain leads. Since the exact electron number on each dot is unknown due to limited gate range, we refer to the relative electron number on the two dots as (N_{13}, N_{22}) over any paired electrons that already exist on each dot. At zero magnetic field, a symmetric RF phase signal is observed across the charge degeneracy axis suggesting the two sides share the same spin configuration. The disappearance of the signal at 2 T is attributed to Pauli spin-blockade, where the ground states across the degeneracy have different spin configurations preventing electron tunneling. In the simplest scenario, the energy diagram including a singlet and triplet states are plotted as a function of detuning ϵ in Figure 8.5(d). At zero magnetic field, the ground state is the spin singlet across the detuning (ϵ) axis and its curvature at the anti-crossing ($\epsilon = 0$ meV) generates a measurable quantum capacitance. As the magnetic field increases, the triplet state energy is split by the Zeeman energy $E_z = g\mu_B B$ where μ_B is the Bohr magneton and g is the electron g-factor. The

$T_-(1,1)$ state eventually becomes the ground state at the (1,1) configuration while the ground state at the (0,2) configuration remains a singlet, resulting Pauli spin-blockade at the degeneracy. Between 0 T and 2 T, we observe an asymmetric disappearance of the ICT phase response towards the (0,2) charge configuration in Figure 8.5(b), which defines the $+\epsilon$ direction of the detuning axis as the singlet-triplet exchange energy $\Delta_{ST} = E_{T_0} - E_S$ increases with ϵ .

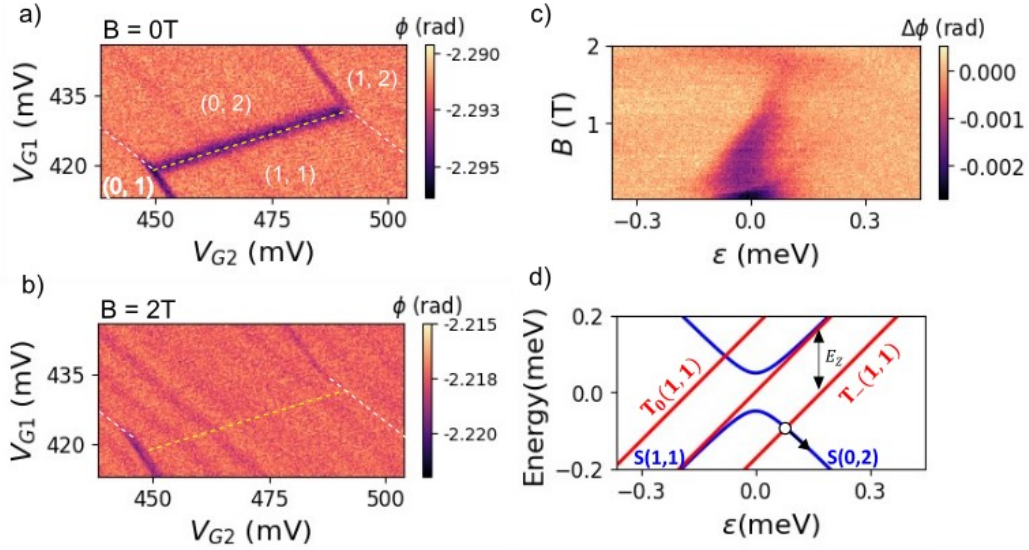


Figure 8.5 Spin-blockade between a pair of dots within the array. (a, b) charge stability diagram across the ICT taken at 0 T and 2 T. The pair of dots in degeneracy correspond to D13 and D22 following the method in 2.1. (c) Asymmetric disappearance of the ICT phase signal as a function of the magnetic field B. (d) Energy spectrum across the (0,2) - (1,1) interdot charge transition with the singlet and triplet states. The crossover from the singlet ground state to the $T_-(1,1)$ ground state occurs at the white circle and shifts along the arrow with increasing magnetic field, causing spin-blockade.

The quantum capacitance of an electron shared between two tunnel coupled quantum dots is described by^{28,34}.

$$C_q = - \sum_i q_e \alpha'' \frac{d^2 E_i}{dV_{rf}^2} P_i \quad (8.4)$$

where α'' is the ratio between the detuning ε and the RF excitation voltage applied on the drain $\varepsilon = e\alpha''V_{rf}$. The summation is over all many body states with energy $E_i(\varepsilon)$ which have a non-zero probability P_i to be occupied. In the case of no thermal excitation onto the higher energy states occurs, equation (8.4) simplifies into $C_q = \frac{\alpha'^2 q \varepsilon^2 t_c^2}{4} ((\frac{\varepsilon}{2})^2 + t_c^2)^{-3/2}$ where t_c is the tunnel coupling. By fitting the width of the ICT signal, we extract an effective tunnel coupling of $t_c = 35 \pm 5 \mu\text{eV}$ corresponding to the two few-donor dots separated by 14 nm. This value is much larger than the tunnel coupling between two single P donors, due to the larger spread of electron wavefunction over the donor clusters^{96,252}. The ICT phase signal disappears when the singlet energy $E_S = -\sqrt{(\varepsilon/2)^2 + t_c^2}$ is equal to the triplet energy $E_{T-} = \delta_{TS} - g\mu_B B + \frac{\varepsilon}{2}$ where δ_{TS} is the energy offset between $T(1,1)$ and $S(1,1)$ (e.g. $\delta_{TS} = E_{T0(1,1)} - E_{S(1,1)}$). Knowing the value of t_c , the transition shape shown in Figure 8.6(g) is consistent with a g = factor of 2 (where $g=2$ was used to generate the dashed green line).

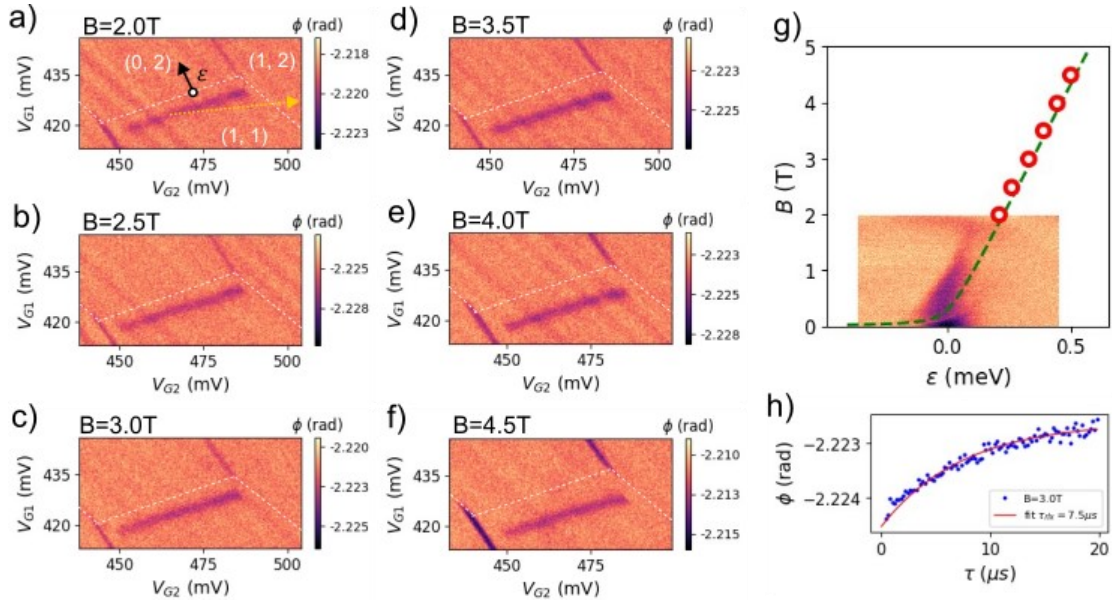


Figure 8.6 Recovering singlet ICT signal above $B=2$ T through dynamic repopulation, $V_{ds} = 0$ mV. a) to f) shows the transient RF response after applying a gate voltage pulse (vector along the dotted yellow arrow in a)) at each point from $B = 2.0$ T to $B = 4.5$ T. Data are acquired and averaged over a time window of $8 \mu s$ after the pulse ends. The blockaded ICT signal reappears as the system probabilistically resets into the spin-singlet state upon unloading an electron from the $(1, 2)$ configuration. The distance between the ground state transition (white dashed line with circle) and the transient ICT line along the detuning axis increases visibly at higher fields. g) Single-triplet ground state transition (green dashed line) with $g=2$ and $t = 35 \mu eV$ overlayed on the asymmetric disappearance of the ICT signal as a function of B . Red circles mark the offsets of the transient ICT lines extracted from a) through f). h) Spin relaxation time of $7.5 \mu s$ at $B=3$ T, extracted from an exponential fit.

Beyond 2 T, no additional ICT phase signal associated with a $T(1,1) - T(0,2)$ transition is observed likely because the $T(0,2)$ state is much higher in the energy spectrum. To probe the dynamics, we repopulate the double-dot system with a singlet state and measure its transient RF phase response before the singlet relaxes to the triplet ground state $T_-(1,1)$. This is achieved by applying a short voltage pulse into the $(1,2)$ configuration to load an electron, after which the system probabilistically resets into a singlet or triplet. The yellow dotted arrow in Figure 8.6(a) indicates the gate pulse vector, and the RF phase data at each point is obtained by averaging over an $8 \mu s$ time window immediately after the pulse, repeated over many cycles. When a singlet is loaded, its quantum capacitance at the anti-crossing produces a transient RF signal that is detectable before relaxation. Figure 8.6(a-f) shows the transient RF phase response at different magnetic fields. The increasing singlet-triplet exchange energy Δ_{ST} is reflected in the growing offset ε_D between the transient signal line and the ground state transition. These discrete offsets align with the extrapolated singlet-triplet crossover curve in Figure 8.6(g), tracking the linear Zeeman shift with $g = 2$. Figure 8.6(h) shows the transient ICT phase signal in the time domain at $B = 3.0$ T, from which an exponential fit yields a relaxation time of $\tau_{rlx} = 7.5 \mu s$.

8.3 Summary

In summary, we have demonstrated RF reflectometry as a powerful probe of charge and spin configurations in a 3×3 dopant-based quantum dot array. Reflected RF phase signals resolve both discrete electron addition lines and interdot charge transitions, yielding a more detailed charge map and a more precise electron addition spectrum than transport alone. Supported by electrostatic capacitance modeling, we identify the exact sites of electron addition from the leads. From interdot transition widths, we extract next-nearest-neighbor tunnel couplings of $35 \mu\text{eV}$ between two few-dopant dots, which serve as reference values for theoretical predictions and the engineering of controlled couplings. We examine the effect of input RF power on the line shape of induced quantum capacitances and observe a temperature gradient radiating from the RF lead. At finite magnetic field, we observed Pauli spin-blockade between two dots and measured a singlet to triplet spin relaxation time on the order of few microseconds. These results demonstrate the capability to sense specific charge/spin configurations in multiple quantum dot arrays using a single RF lead and provide insights for integrating RF readout leads into larger size analog quantum simulators in the future.

8.4 Methods

Device Fabrication and Measurement setup

The 3×3 few-dopant quantum dot arrays are fabricated in an ultrahigh vacuum (UHV) environment with a base pressure below 3×10^{-11} Torr using an STM tip to create atomic-scale lithographic patterns of the device by removing individual hydrogen atoms on a hydrogen-terminated, Si (100) 2×1 reconstructed surface. The substrate is then saturation-dosed with PH₃ gas at room temperature, where PH₃ molecules selectively adsorb only onto the lithographic regions where chemically reactive Si dangling bonds are exposed. A subsequent rapid thermal anneal process at 350°C for 1 min incorporates the adsorbed phosphorus atoms into the Si surface lattice sites while preserving the hydrogen resist to confine dopants

within the patterned regions. We embed the incorporated dopant atoms into a single crystalline silicon environment using low temperature Si epitaxial overgrowth with an optimized locking layer ⁷³ to suppress dopant movement at the atomic scale during epitaxial overgrowth. Finally, ohmic contacts to the buried device are formed using a low thermal budget contacting technique ⁴⁷.

All measurements are done in a dilution refrigerator with a base temperature of 10 mK. Electron temperature of 300 mK has been characterized using an STM-fabricated SET (single electron transistor) device under similar setup conditions. The RF input signal is attenuated within the fridge, goes through a directional coupler before combining with the DC bias via a bias tee. An LC tank circuit consists of a chip inductor (820 nH, $Q \sim 20$) and PCB parasitic capacitance matches the device impedance to the 50 Ω line impedance. The RF input power entering the tank circuit is chosen between -86 dBm and -96 dBm to balance between better signal contrast and electron temperature increase. The reflected RF signal is amplified by 1 x CITLF-3 mounted at the 4K stage and 3 x Mini-circuit PN103LN+ chained together at room temperature before being demodulated by a Polyphase 0105. The I/Q signal is digitized by a NI6363 or a Keysight M3102A module. DC voltage supply and slower pulses are generated by SIM928s and NI6363. Fast pulses are generated by an AWG5000 or a Keysight M3202A triggered by the NI6363 and attenuated by ~ -15 dB inside the fridge before entering a bias tee.

8.5 Supplementary

8.5 1 Estimation of capacitance matrix and mutual charging energies

Experimentally measured charge stability diagrams yield reliable slopes of charge transition lines. However, absolute values of charging energies and lever arms cannot be extracted as directly as in the case of a single electron transistor (SET), where the charging energy is determined from the Coulomb diamond size. To obtain these parameters for the fabricated devices, the electrostatics module of COMSOL Multiphysics was employed to simulate the potential landscape.

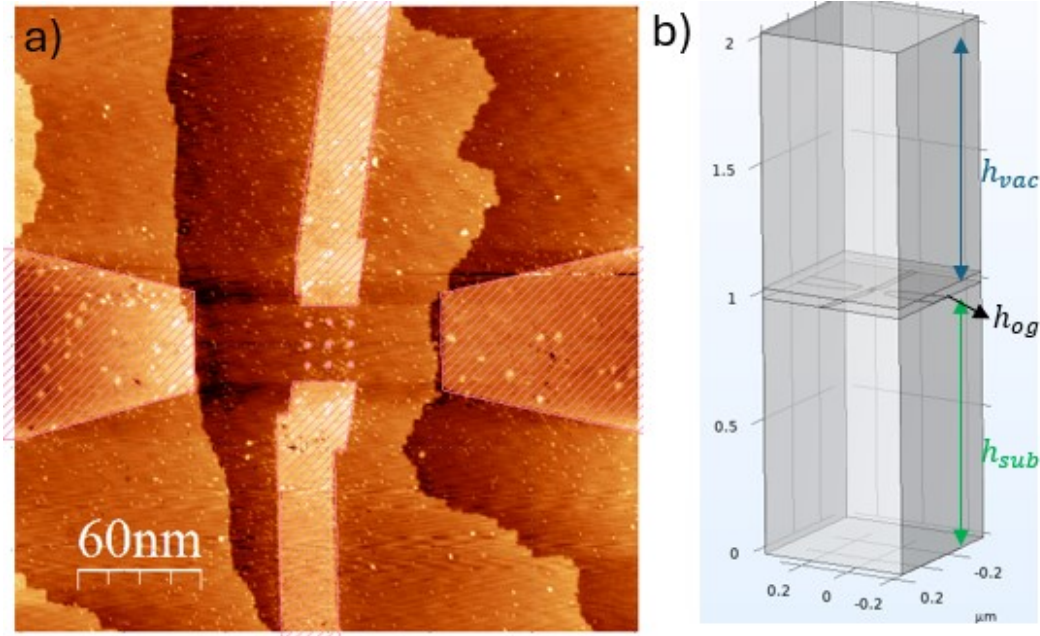


Figure 8.7 Electrostatic capacitance simulation using COMSOL Multiphysics. (a) The exact 2D geometry of the patterned device is reconstructed from STM images. The dots are modelled as bounding boxes centered on each site with lateral size of 2-3 nm. (b) 3D geometry and domain used for the electrostatic FEM simulation. Only the center 600 nm $\times$ 600 nm region is included. The device is buried under a 40 nm silicon overgrowth layer. The thickness of the vacuum layer (h_{vac}) and the silicon substrate layer (h_{sub}) are increased until their effects converge. Each gate and dot are treated as separate floating terminals for calculating the mutual capacitance matrix.

Post-lithography STM images were used to reconstruct the device geometry for finite element simulation. The simulation domain was defined as a 600 nm $\times$ 600 nm box centered on the array. The extended fanout of the four leads was truncated, and the device plane was positioned at the mid-plane of the z-direction which consists of 1000 nm of silicon substrate, a 40 nm silicon overgrowth layer, and 1000 nm of vacuum. Leads were modeled with a 2 nm thickness and a 1.5 nm seam to account for the finite spread of the donor wavefunctions. The quantum dots were represented as bounding boxes that match their lithographic masks in the device plane. Boundary conditions were set with the bottom plane grounded and all other planes open. Each dot and gate were treated as an independent terminal for calculation of the Maxwell capacitance matrix, from which lever arms and mutual charging energies were obtained (Table 8.1 and 8.2).

Table 8.1 Lever arms of each gate to all sites in the 3x3 array.

	$D11$	$D12$	$D13$	$D21$	$D22$	$D23$	$D31$	$D32$	$D33$
α_{G1}	0.085	0.105	0.087	0.112	0.136	0.111	0.165	0.191	0.162
α_{G2}	0.123	0.152	0.132	0.089	0.111	0.092	0.074	0.088	0.073
α_D	0.203	0.348	0.538	0.207	0.360	0.564	0.208	0.347	0.535
α_S	0.566	0.367	0.220	0.571	0.367	0.212	0.530	0.346	0.207

Table 8.2 Charging energies (meV) derived from the capacitance matrix. All dots are set to 3nm×3nm in lateral size. Diagonal elements correspond to the on-site Coulomb interactions U_{ii} and off-diagonal elements correspond to long-range Coulomb interactions U_{ij} .

	$D11$	$D12$	$D13$	$D21$	$D22$	$D23$	$D31$	$D32$	$D33$
$D11$	61.4	8.79	3.12	7.57	5.29	2.44	2.52	2.56	1.59
$D12$		63.1	8.94	5.28	9.28	5.29	2.59	3.53	2.59
$D13$			61.5	2.48	5.37	7.62	1.62	2.60	2.55
$D21$				60.9	8.60	2.96	7.65	5.33	2.49
$D22$					62.9	8.62	5.36	9.30	5.36
$D23$						61.1	2.49	5.31	7.65
$D31$							61.2	8.96	3.18
$D32$								63.4	8.92
$D33$									61.6

To minimize the boundary effects due to finite-domain the simulation box height is increased in 200 nm steps until the results change compared to the previous step is below 5%. The dot size d was also varied to evaluate its impact on lever arms and charging energies. The results show that the on-site interaction U_{ii} is strongly dependent on dot size, increasing from 61 meV at 3 nm to 79 meV at 2 nm, consistent with the diverging self-energy of a point charge ($U \propto 1/r$). In contrast, the mutual charging energies U_{ij} are largely insensitive to dot size, as the dot size d is much smaller than the lattice constant a ($d \ll a$). To correct for unphysical U_{ii} , we replaced its values with on-site charging energies expected for few-dopant clusters from prior atomistic tight-binding calculations, while retaining the calculated U_{ij} values.

Uncertainties in the lever arms were estimated by calculating the potential landscape within the device plane, sequentially setting each gate to 1.0 V while grounding the others and excluding the quantum dots.

The lever arm of each dot was taken as the potential at the center of its bounding box, while the upper and lower bounds were determined from the maximum and minimum potential values across the box, corresponding to the points closest to and farthest from the gate.

As described in the main text, the slopes of charge addition lines are determined by the ratios of the dots lever arms. Different rows exhibit distinct lever arms with respect to gates G1 and G2, while different columns show distinct lever arms relative to the source and drain. The calculated lever-arm ratios for each dot are plotted in Fig. S2 and serve as a reference for identifying measured charge transitions. Although the absolute lever-arm values obtained from electrostatic simulations may differ from experiment by an overall scale factor of ~ 1 , the ratios are expected to be more reliable since the common scale factor cancels out.

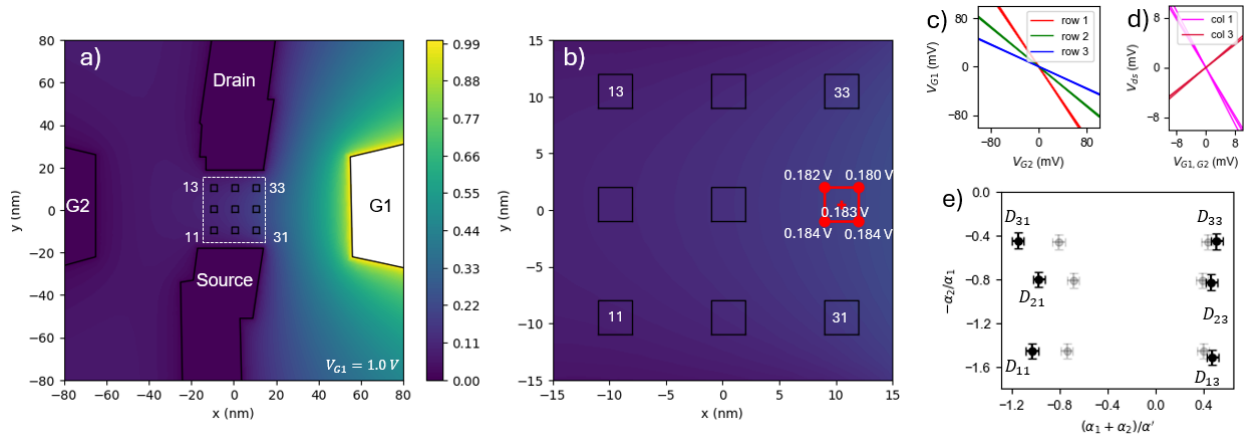


Figure 8.8 Calculation of the gate lever arm and uncertainty estimation. (a) The potential landscape within the device plane with V_{G1} set to 1.0 V and other gates set to ground. The lever arm of G1 to each dot can be read from the voltage potential at the position of the dot. (b) Zoom of the center region in (a). The lever arm of G1 to D32 (α_{32}^{G1}) is equal to the potential at the center of the dot. The maximum and minimum potential values at the boundary (corner) of the dot are acquired as the upper and lower bound of the lever arm. (c) Charge transition slopes within the same row have similar values. (d) Source-drain bias moves the charge transitions of column 1 dots and column 3 dots in the opposite way. (e) Dot-lead charge transition slopes of all dots, used as a reference when identifying measured charge transition lines

8.5.2 Fermi-Hubbard simulation in the classic limit

To analyze the charge transition boundary patterns, we simulated the 3x3 array using an extended Fermi–Hubbard model with parameters obtained from last section. Each site is treated as a single spin orbital capable of accommodating up to two electrons. While an exact diagonalization of the Hamiltonian is required to obtain the full energy spectrum, the measured charge stability diagram of the 3x3 array, characterized by distinct slopes and minimal curvature at charge triple points from the RF phase signal, indicates that the average tunnel coupling t is much smaller than the on-site and long-range Coulomb interactions ($t/U \ll 1$). To approximate the positions and patterns of the charge transition boundaries, we therefore set $t = 0$, reducing the full Hilbert space to the occupation configuration basis where only diagonal terms are non-zero and each site can host 0, 1, or 2 electrons. The resulting simulated charge occupations and transitions for each dot are shown in Figure 8.9.

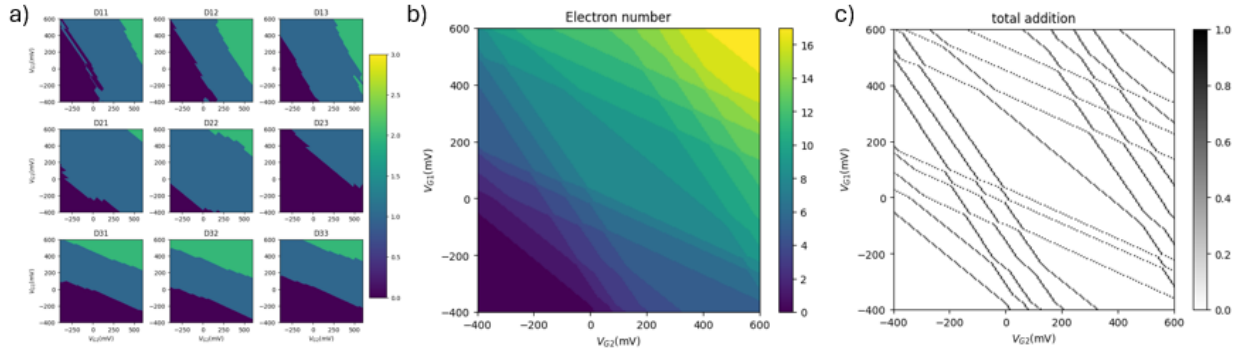


Figure 8.9 Simulated charge stability diagram simulation with $t=0$ meV in the extended Fermi-Hubbard model. (a) Charge occupation of individual sites. (b) Total electron number and (c) charge transition boundaries of $\Delta N_e = +1$.

Classifying each transition as either dot–dot or dot–lead, we applied equation (8.1) or (8.4) from the main text to obtain the quantum capacitance at the degeneracy points. Net additions onto the center-column dots were treated as second-order processes and assumed to yield no RF response. While we do not attempt a quantitative match between simulation and experiment, many of the simulated line structures closely

resemble features observed in the measured RF phase data. An example is shown in Figure 8.10, with the electron occupation on each site explicitly depicted.

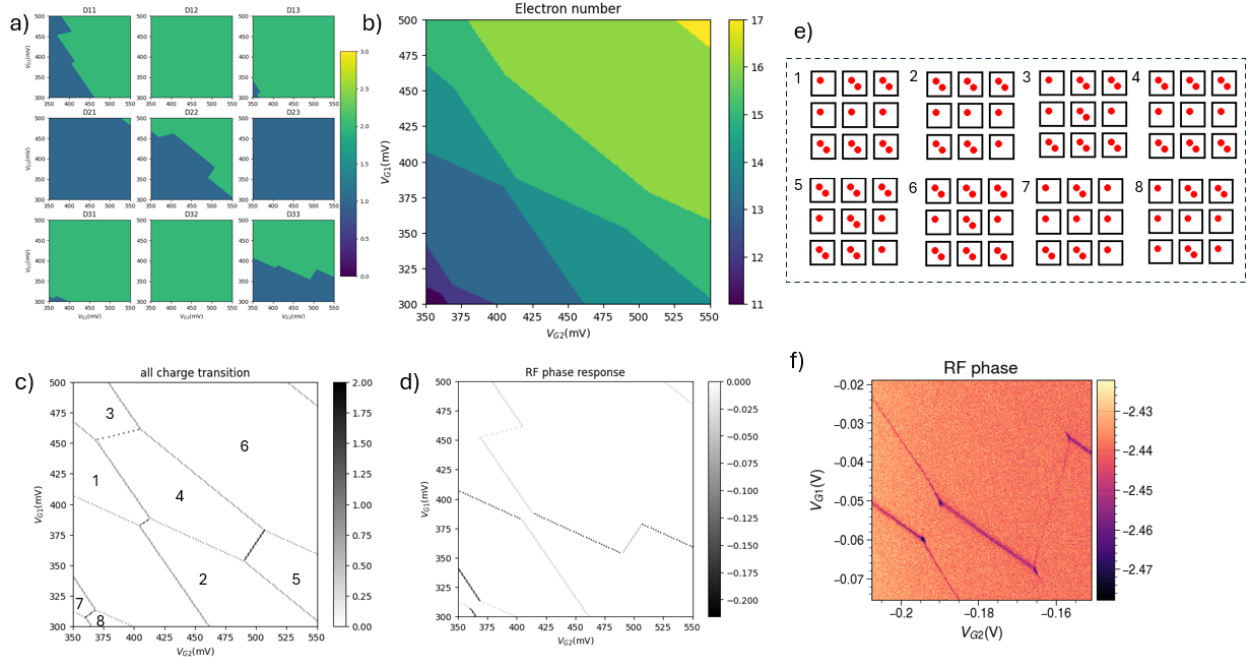


Figure 8.10 Zoomed-in view of a simulated charge-occupation map showing multiple interdot charge transitions. (a) Individual dot occupation numbers. (b) Total electron occupation across the array. (c) All charge-transition boundaries, including net electron additions from the leads and interdot charge transitions (ICTs). (d) Charge transitions converted to quantum capacitance, with nearest- and next-nearest-neighbor hopping terms (t and t') set to nonzero values. (e) Electron occupation on each site for the charge configurations shown in (c). (f) Measured charge-stability diagram discussed in the main text, exhibiting patterns similar to those in (d).

8.5.3 Magneto-spectroscopy measurement

In Fig. 8.11 we present the full magneto-spectroscopy measurement at the charge stability diagram discussed in the main text, tracking the evolution of charge transition lines as a function of the magnet field B . The magnetic field is from $B = 0$ T to $B = 5$ T in steps of 0.1 T.

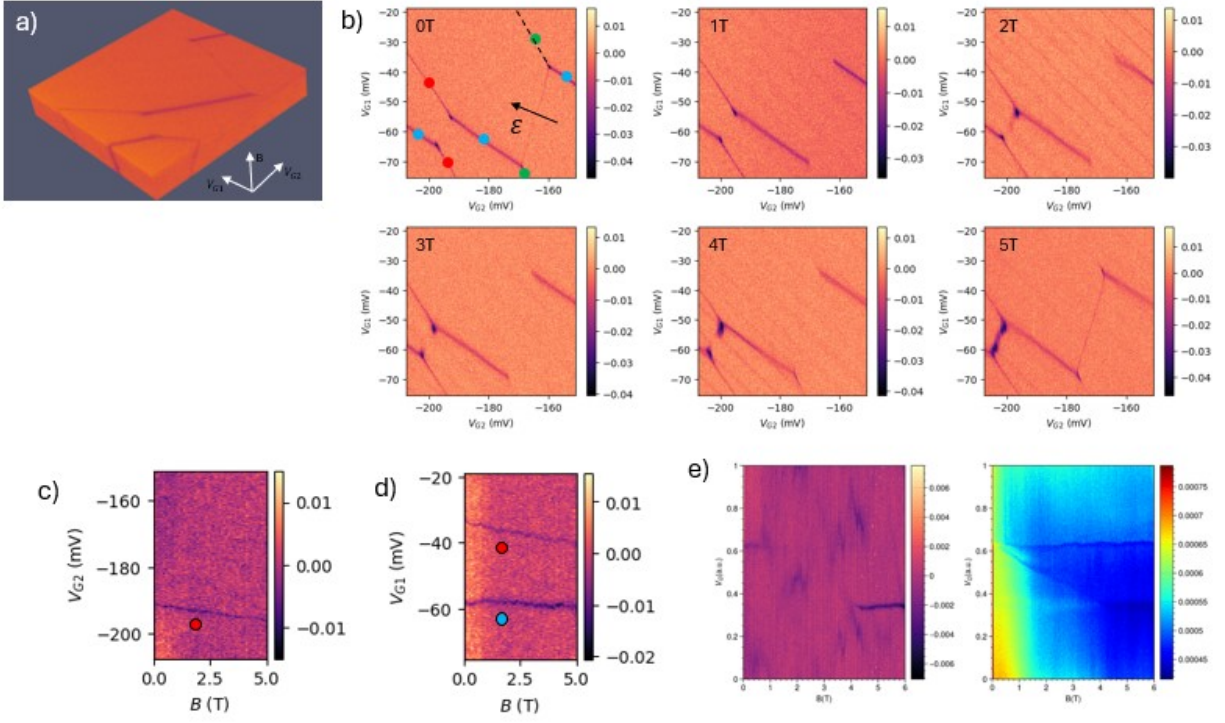


Figure 8.11 Magneto-spectroscopy at the charge configuration discussed in section 8.2.2. a) 3D representation of the charge stability data (RF phase) with B from 0 T to 5 T on the z axis. b) Slice of data at $B=0\text{ T}$, 1 T, 2 T, 3 T, 4 T, 5 T. c) and d) Slice of data taken at the front and left face of 3D charge stability map. The electron adding to D11 (red dot) always has spin down from its negative slope. The electron addition line of D23 (blue) has a kink at $B \sim 0.6\text{ T}$ where its slope switches from positive to negative, suggesting a transition in the ground state spin configuration. e) Slice of data taken across the detuning axis in b). The ICT signal initially disappears at $B=0.6\text{ T}$ and reappears above $B=4.2\text{ T}$. This indicates a spin-blockade event at 0.6 T consistent with the kink in d) and a lift of the blockade at 4.2 T where the ground state spin configuration across the degeneracy becomes the same again.

Chapter 9: Summary and Future Works

9.1 Summary of the Dissertation

This dissertation presents a comprehensive study on the development of atomically precise silicon devices for the complementary goals of quantum information processing and analog quantum simulation, spanning fabrication, measurement, and theoretical modeling.

Chapters 2–4 lay the technical foundation for the dissertation.

In Chapter 2, we presented the full atomically precise fabrication workflow that has been continuously refined in our laboratory. Particular emphasis was placed on explicitly defining the parameters used at each critical step of the process including wafer selection, preparation of atomically flat Si (100) surfaces, RTA dopant incorporation, and low-temperature encapsulation overgrowth. Achieving reliable quantum devices hinges on the quality of the starting silicon wafer, the precision of the STM lithography mask, and the crystal purity of the overgrown silicon layer. Beyond the established Si:P fabrication process, significant effort has been devoted to exploring alternative approaches aimed at improving device quality with respect to charge noise, gate range, and gate linearity. Preliminary data from for example, substituting lightly boron-doped substrates with nominally intrinsic silicon, show promising improvements in gate range. Such enhancements may enable complete depletion of few-donor quantum dots and more reliable access to the single-electron regime.

Chapter 3 reviews the theoretical framework governing the behavior of dopant atoms in silicon. Starting from the basic electronic band structure and the single-donor effective-mass wavefunction, we examine the quantum properties and transport mechanisms of dopant-defined nanostructures, including continuous two-dimensional patches and few-donor cluster structures that form the fundamental building blocks of Si:P quantum devices. These concepts then serve as the basis for understanding how circuit level components, such as tunnel junctions and single-electron transistors, can be constructed and operated as highly sensitive charge sensors.

Chapter 4 focuses on automating STM lithography, a crucial step for achieving reproducible and scalable atomically precise device fabrication. In essence, STM lithography involves steering the tip along predefined paths derived from rasterized two-dimensional patterns while applying the appropriate bias voltage and tunneling current to selectively remove hydrogen atoms. However, fluctuations in tip condition, along with drift and creep effects, make the process highly non-trivial. To address these challenges, we developed a step-by-step workflow with clearly defined objectives for patterning both atomically precise structures and large fan-out leads, significantly reducing the need for manual intervention.

Chapters 5–8 present the major experimental results achieved throughout this dissertation.

Chapter 5 focuses on efforts to achieve high-fidelity single-shot spin readout using a donor-dot SET architecture intended for single-qubit operation. We demonstrate time-resolved charge sensing, characterize spin-dependent tunneling dynamics, and measure the spin relaxation time as a function of magnetic field. The primary obstacle to achieving high-fidelity readout is identified as excess charge noise in the device environment, which induce random tunnel events and shortens the T_1 time.

Chapter 6 expands from single-donor devices to engineered dopant arrays designed to emulate Hubbard-type physics. Section 6.3 summarizes key results from prior work demonstrating a 2D extended Fermi–Hubbard model using a series of 3×3 dopant dot arrays with theoretical interpretation and transport measurements. The section also presents measurements of the spin-filling sequence in a strongly coupled 3×3 donor array, supported by numerical simulations that capture the interplay between tunnel coupling, on-site energy variation, and exchange interactions. Section 6.4 introduces ongoing work on quantum transport through a large-scale 32×32 dopant array, highlighting signatures of disorder-induced localization and the challenges of scaling atomic-precision devices to mesoscopic dimensions.

Chapter 7 focuses on metrology, introducing an optimized RF-reflectometry architecture tailored for high-impedance silicon quantum devices. By systematically evaluating the effects of impedance-matching conditions, circuit quality factors, and sample-loading contributions, we identify operating regimes that maximize sensitivity while maintaining sufficient bandwidth. These improvements enable fast charge

readout of a SET device with an on-state conductance of $0.2\ \mu\text{S}$, achieving a minimal integration time of 600 ns which significantly outperforms direct tunneling current measurements.

Chapter 8 applies RF reflectometry to probe the charge configuration of few-donor quantum dot arrays. Using dispersive sensing techniques, we map out charge transitions, interdot tunnel coupling, and capacitive interactions with high temporal resolution. These measurements demonstrate how RF-based techniques can reveal microscopic charge configurations and dynamical processes that are difficult to access with conventional DC transport, establishing an essential diagnostic tool for next-generation dopant-based quantum simulators.

9.2 Challenges and Future works

This section delineates several avenues for future research and identifies the technical challenges associated with them. While some of these proposals are achievable in the near term, others necessitate further maturation in fabrication techniques, measurement capabilities, and theoretical understanding.

9.2.1 Coherent Electron and Nuclear Spin Manipulation

In Chapter 5, we demonstrated single-shot spin readout via energy-selective tunneling for an electron bound to a donor cluster. The next stage of development is to advance this architecture toward a fully functional single qubit by enabling coherent spin manipulation. Single-qubit rotations can be achieved by applying an oscillating magnetic field B_x orthogonal to the static external field. When the drive frequency matches the Larmor frequency associated with the Zeeman splitting $E_Z = g\mu_B B_0$, coherent control becomes possible. For donor-based electron-spin qubits, a static field of approximately $B_0=1.5\ \text{T}$ is typically required to ensure $E_Z \gg k_B T_e$ and to provide a sufficiently long T_1 . This corresponds to a Zeeman energy of $E_Z = 173\ \mu\text{eV}$ and a Larmor frequency of $f_0 = 41.8\ \text{GHz}$.

To achieve this experimentally, our group is currently integrating an on-chip antenna—serving as the ESR excitation line—directly onto functional devices. The Rabi frequency scales with the amplitude of the

oscillating magnetic field according to $f_{Rabi} = \gamma_e B_x / h$ where $\gamma_e = g\mu_B \approx 28$ GHz/T is the electron gyromagnetic ratio. The immediate next step is to verify that the addition of the ESR line preserves the electrostatic characteristics of the device. Once this is confirmed, the microwave drive power and frequency can be tuned to observe the expected modulation in the probability of detecting the spin-up state.

The same on-chip antenna can also be used to drive NMR transitions of the donor nuclear spins. For an electron bound to a phosphorus donor, the coupled electron–nuclear spin system is described by the Hamiltonian ¹²⁹:

$$H = \gamma_e S_Z B_0 - \gamma_n I_Z B_0 + A \mathbf{S} \cdot \mathbf{I} \quad (9.1)$$

where $\gamma_n \approx 17.26$ MHz is the nuclear gyromagnetic ratio, $\mathbf{S}, \mathbf{I}$ are the electron and nuclear spin operator and A is the hyperfine interaction, typically on the order of 100 MHz and tunable via the Stark shift. At a magnetic field of $B_0 = 1.5$ T, we have $\gamma_e B_0 \gg A \gg \gamma_n B_0$, the electron and nuclear spin resonance frequency split into $f_{e1,2} = \gamma_e B_0 \mp A/2$ and $f_{n1,2} = A/2 \pm \gamma_n B_0$ respectively. Driving the system near these frequencies enables conditional rotations of both electron and nuclear spins as each transition is addressable depending on the state of the other spin. Similarly, readout of the nuclear spin can be performed indirectly by using the electron spin as an ancilla.

For systems containing multiple electrons within a donor cluster, the same Hamiltonian applies with a hyperfine term for each electron–nuclear pair. This produces a more complex pattern of resonance splitting, but also enables controlled gates between individual nuclear spins, allowing the realization of a multi-qubit quantum register within a single donor cluster ²⁵³.

An additional application arises from comparing experimentally measured Rabi spectra with numerical simulations. The donor configuration within a cluster can potentially be reconstructed from the spectral signatures ²⁵⁴. This technique can be used to calibrate how much the incorporated donors shift during the encapsulation process.

9.2.2 Realizing the Strongly Correlated Regime in Large 2D Simulators

In Chapter 6, we demonstrated the realization of 2D extended Fermi-Hubbard model using a minimal system of 3×3 arrays. A natural next step for this platform is the development of a large-scale 2D dopant-based analog Hubbard simulator capable of reaching the strongly correlated regime and probing emergent phases such as superconductivity. Theoretical and numerical studies^{255,256} consistently identify the doped, repulsive- U Hubbard model on a uniform 2D square lattice as the minimal model exhibiting robust d-wave pairing tendencies. To target this physics, future devices should aim for lattice sizes of at least 10×10 sites, where finite-size effects no longer dominate short-range pairing correlations, and for a hopping amplitude in the few meV range with an on-site Coulomb repulsion $U/t \sim 6-10$ ²⁵⁷⁻²⁵⁹. The ability of controlled hole doping to the level of 10–20% away from half filling is also essential, as this regime corresponds to the maximum enhancement of singlet pairing correlations in the Hubbard model. Through careful selection of lattice spacing and island size, these parameter targets are accessible within the existing STM-lithography framework. An example of such mesoscopic simulators is the 32×32 array presented in section 6.4.

However, a central challenge in realizing superconductivity-relevant arrays is the need to maintain a uniform chemical potential across all lattice sites, which is a fundamental assumption in most Hubbard model simulations. Dopant-defined quantum dots inherently exhibit site-to-site variations in local chemical potential on the order of several meV which is comparable to or even larger than the target hopping parameter t . Even small variations in the on-site potential $\Delta\epsilon$ can distort the intended Hubbard landscape, effectively introducing disorder that competes with pairing and suppresses coherent many-body correlations. One potential route to achieving global chemical-potential uniformity in a 2D (island-size) quantum dot array is to employ a dense gate architecture capable of compensating residual offsets through site-level tuning. As an intermediate step, future work could focus on smaller arrays, for instance 5×5 , to demonstrate multi-gate control strategies that maintain $\Delta\epsilon \ll t$, ideally below $\sim 10\%$ of the hopping energy across the entire array. For larger arrays, one should also examine that the electron coherent length is larger than the correlation length.

Another viable approach is to target a single donor per site, thereby eliminating the binding-energy variability inherent to multi-donor configurations and ensuring a more uniform chemical potential. This strategy, however, demands atomic precision lithography mask and deterministic single-dopant placement. While this uniformity reduces uncertainties in $\Delta\epsilon$, it introduces greater sensitivity in the hopping amplitude t , which depends exponentially on donor separation. The fabrication methods developed in Chapter 4 provide a foundation for this single-donor approach, yet new encapsulation techniques must be developed to ensure that donors remain stationary once incorporated.

9.2.3 Realizing a Lattice Gauge Field Theory Simulator

In Section 6.5, we briefly introduce the concept of using a coupled electron–nuclear spin system to emulate a discrete realization of the rotor Jackiw–Rebbi model, following the proposal by Rad et al.²¹⁴ In this framework, the nuclear spins act as a dynamical gauge field that couples to the matter field (electrons) through the hyperfine interaction. Different spatial configurations of the nuclear spins correspond to distinct gauge-field backgrounds, which in turn modify the ground-state properties of the electronic system. As a result, the matter field may exhibit different phases, including phenomena such as dynamical mass generation characterized by Néel-type ordering.

Realizing this proposal experimentally requires atomically precise placement of phosphorus donors at designated lattice sites within the silicon crystal, presenting a formidable challenge for current atomically precise fabrication techniques, even with the assistance of STM automation. Nevertheless, smaller yet perfectly defined systems, such as a 2×2 array of single donors, may already be sufficient to capture key signatures of the model and serve as a proof-of-principle demonstration. Observing distinct phases through transport or RF-based measurements further requires substantially lower electron temperatures, as the relevant energy scale set by the hyperfine interaction is relatively small.

Encouraging progress has been made toward this goal. Our group member Jonathan Wyrick has demonstrated tip-induced donor incorporation for a 2×2 single-donor array with placement accuracy

approaching ± 1 lattice site. A critical next step is ensuring that the incorporated donors remain fixed during the subsequent silicon overgrowth process. This achievement represents a significant milestone toward the realization of atomically precise devices with true lattice perfection. Preparation and control of the nuclear spin states can, in principle, be achieved via NMR using a carefully designed on-chip antenna and proper design of the gate geometry.

Beyond minimal systems such as the 2×2 array, the fabrication of larger two-dimensional lattices or extended one-dimensional chains with perfect donor placement lies well beyond the capabilities of manual STM lithography alone. A viable path forward will likely require the integration of fully automated STM patterning workflows with the insights gained from tip-facilitated donor incorporation, enabling scalable fabrication of defect-free donor arrays for quantum simulation of gauge-field dynamics.

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