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1. REPORT DATE (DD-MM-YYYY) 18-08-2023	2. REPORT TYPE Final Report	3. DATES COVERED (From - To) 15-May-2017 - 30-Nov-2022
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4. TITLE AND SUBTITLE Final Report: Theoretical Study of Silicon-Based Quantum Information Processing	5a. CONTRACT NUMBER W911NF-17-1-0257
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER

6. AUTHORS	5d. PROJECT NUMBER
	5e. TASK NUMBER
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES State University of New York (SUNY) at B The UB Commons 520 Lee Entrance, Suite 211 Amherst, NY 14228 -2567	8. PERFORMING ORGANIZATION REPORT NUMBER
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9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES) U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211	10. SPONSOR/MONITOR'S ACRONYM(S) ARO
	11. SPONSOR/MONITOR'S REPORT NUMBER(S) 70707-PE-OC.8

12. DISTRIBUTION AVAILABILITY STATEMENT Approved for public release; distribution is unlimited.
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13. SUPPLEMENTARY NOTES The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.
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14. ABSTRACT
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15. SUBJECT TERMS
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16. SECURITY CLASSIFICATION OF:	17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT UU	b. ABSTRACT UU	c. THIS PAGE UU	Xuedong Hu
			19b. TELEPHONE NUMBER 716-645-5444

# RPPR Final Report

## as of 29-Aug-2023

Agency Code: 21XD

Proposal Number: 70707PEQC

Agreement Number: W911NF-17-1-0257

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EIN: 141368361

**Report Date:** 28-Feb-2023

Date Received: 18-Aug-2023

**Final Report** for Period Beginning 15-May-2017 and Ending 30-Nov-2022

**Title:** Theoretical Study of Silicon-Based Quantum Information Processing

**Begin Performance Period:** 15-May-2017

**End Performance Period:** 30-Nov-2022

**Report Term:** 0-Other

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**Distribution Statement:** 1-Approved for public release; distribution is unlimited.

**STEM Degrees:** 1

**STEM Participants:** 6

**Major Goals:** The objective of our research program is to help facilitate the realization of spin-based quantum computing in Si nanostructures. Our proposed research program consists of two main directions: coherent manipulation of a single spin qubit, and exchange coupling between spin qubits. Both are crucial in our long term goal of building a high-fidelity large-scale Silicon- and spin-based quantum computer. On the front of single-spin explorations, our major goals are to study spin coherence and control fidelity in the presence of static magnetic field gradient, and search for optimal conditions for spin control and coherence. On the front of multiple spin qubits, our major goal is to study the interplay between exchange coupling and valley mixing, and explore whether multi-electron states in a dot/donor(s) can be used to encode a more robust spin qubit. On the front of noise and decoherence, we would like to study how interface defects could produce charge and magnetic noise. The goals set forth in this research program are all focused on helping identify optimal designs for high-fidelity single-qubit and two-qubit gates in a Silicon-spin-based quantum computer.

**Accomplishments:** In this theoretical research program we have studied several important current issues in Silicon-based semiconductor quantum computing architectures, including the effects of an on-chip micromagnet, the effects of valley-orbit coupling in Si, and decoherence and control issues in spin qubit transport.

Micromagnets have become an important element for spin qubit control in Si quantum dots, enabling fast and high fidelity single-qubit gates. We have studied the effects of a micromagnet, specifically the magnetic field gradient it produces, on spin coherence. We find that, in contrast to intrinsic spin-orbit coupling (iSOC), such field gradient allows spin pure dephasing due to charge noise (which has since been shown to be the dominant decoherence channel for spin qubits in some situations). It also leads to a different dependence by spin relaxation rate on the external field. On the other hand, the field gradient also opens new avenue for spin control, such as via a longitudinal driving field. Lastly, we have developed a new Master Equation for describing non-Markovian effects of charge noise on a spin qubit in a double dot with a micromagnet.

We have performed single- and two-qubit decoherence studies of the flip-flop qubit made from a donor and an interface quantum dot in Si. This system turns out to be mathematical similar to the problem of a double dot in a magnetic field gradient. We showed that charge noise could significantly impact the two-qubit operations, and proposed an alternative operating regime to minimize leakage and decoherence effects.

One of the distinctive properties of Si quantum dots is the presence of low-lying valley excited states, with valley splitting typically in the order of 0.1 meV while orbital excitation energy typically about 1 meV. During this program we have studied several aspects of the valley physics in Si. Specifically, we find that a single interface step on an

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otherwise smooth interface could lead to significant suppression of valley splitting and dramatic change in valley mixing phase. We find that exchange coupling in a Si double dot can be significantly suppressed if valley mixing phase is different across the double dot by  $\pi$ , even when the magnitude of valley splitting in both dots are large. On the other hand, if valley splitting is very small in one of the dots, exchange may not work at all since different pairs of singlet-triplet states usually have different exchange splittings. Lastly, in the context of measuring tunnel coupling in a Si double dot, we find that the prevalent approach used by most experimentalists now, which is based on a GaAs double dot, has to be modified to include valley effects. Otherwise the estimated tunnel coupling could be off by a significant fraction, sometimes completely wrong. In short, while in a single Si quantum dot valley splitting is the main effect of valley physics, in a double quantum dot both magnitude and phase of valley-orbit coupling are important parameters to consider.

We have performed systematic studies of spin qubit transport by focusing on the problem of spin transfer in a double quantum dot, both in GaAs and in Si. We have identified some of the most important factors that would affect spin transfer fidelity, from avoiding spin relaxation hot spot, to the correction to g-factor by the double dot potential, and possible difference in g-factor in the two dots. We have identified parameter regimes (in terms of tunnel coupling, valley splitting, and applied magnetic field) where spin transfer fidelity would most likely suffer from spin relaxation and dephasing. The observations from this study also prompted us to search for better control of spin transport, and arrived at the idea of adiabatic resonance, where the electron would periodically return to its instantaneous eigenstates as the system Hamiltonian evolves with time. We believe this concept can have important potential impact on how we control spin transport in the future.

In the context of spin transport, we have also studied how surface acoustic waves (SAW) could carry electrons controllably in a semiconductor nanostructure, specifically in GaAs. We have performed a careful examination of the eigenmodes of SAW, and identified additional modes that have not been considered so far in the context of quantum information processing. While these modes may not affect electron transport, they could play a role in spin decoherence, and could possibly interact with transmon qubits in the context of superconducting quantum computing.

We have been involved in a wide range of collaborations with both experimental and theoretical colleagues during the current research program, which have led to some useful results in the study of spin qubits. For example, in a collaboration with John Nichol group at University of Rochester, we have studied how a short spin chain can act as a bus and mediate coupling and entanglement for spin qubits, and how certain states of a spin bus cannot help with quantum state transfer; In a collaboration with Dimi Culcer group at University of New South Wales, we identified certain acceptor hole spin states as a good candidate for a controllable and coherent qubit; In a collaboration with Seigo Tarucha group from Riken we studied transport of entangled spin states in a triple dot system and found that pure dephasing could actually facilitate entanglement transfer; In a collaboration with Keiji Ono group at Riken we have demonstrated two-hole electric dipole spin resonance in a commercial p-channel SiMOS Field Effect Transistor; In a collaboration with Guoping Guo group from USTC we identified the phenomenon of Pauli spin blockade (PSB) in a three-electron double dot (normally PSB is observed in a two-electron double dot); We have also demonstrated very fast hole-spin Rabi oscillation in a Germanium nanowire double quantum dot; In collaboration with Susan Coppersmith group at University of Wisconsin and Hong-Wen Jiang group from UCLA, we identify unintended quantum dots in Si/SiO<sub>2</sub> heterostructures as a possible reason for breaking spin blockade.

**Training Opportunities:** During the 5 years period of this program, six graduate students have worked on related problems, with one obtaining his PhD degree and another his MS degree. Two postdoctoral scholars have contributed a significant portion to the research results. Most have attended conferences or program reviews to report their results.

The PI has helped organized two domestic workshops on decoherence and quantum computing at Stevens Institute of Technology to disseminate research results and develop potential collaborations.

**Results Dissemination:** We have published 25 refereed papers during this program, given 10 invited and 28 contributed presentations at international conferences, and 11 seminars and colloquiums in universities and national labs both domestically and internationally.

**Honors and Awards:** The PI received the Exceptional Scholar Award for Sustained Achievement from University at Buffalo in 2021.

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**Protocol Activity Status:**

**Technology Transfer:** Nothing to Report

**PARTICIPANTS:**

**Participant Type:** PD/PI

**Participant:** Xuedong Hu

**Person Months Worked:** 2.00

Project Contribution:

National Academy Member: N

**Funding Support:**

**Participant Type:** Postdoctoral (scholar, fellow or other postdoctoral position)

**Participant:** Xinyu Zhao

**Person Months Worked:** 12.00

Project Contribution:

National Academy Member: N

**Funding Support:**

**Participant Type:** Postdoctoral (scholar, fellow or other postdoctoral position)

**Participant:** Chon Fai Kam

**Person Months Worked:** 2.00

Project Contribution:

National Academy Member: N

**Funding Support:**

**Participant Type:** Graduate Student (research assistant)

**Participant:** Luke Pendo

**Person Months Worked:** 4.00

Project Contribution:

National Academy Member: N

**Funding Support:**

**Participant Type:** Graduate Student (research assistant)

**Participant:** John Truong

**Person Months Worked:** 2.00

Project Contribution:

National Academy Member: N

**Funding Support:**

**Participant Type:** Graduate Student (research assistant)

**Participant:** Bilal Tariq

**Person Months Worked:** 4.00

Project Contribution:

National Academy Member: N

**Funding Support:**

**Participant Type:** Graduate Student (research assistant)

**Participant:** Courtney Fitzgerald

**Person Months Worked:** 2.00

Project Contribution:

**Funding Support:**

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National Academy Member: N

**Participant Type:** Graduate Student (research assistant)

**Participant:** Zongye Wang

**Person Months Worked:** 2.00

**Funding Support:**

Project Contribution:

National Academy Member: N

**Participant Type:** Graduate Student (research assistant)

**Participant:** Akash Patel

**Person Months Worked:** 1.00

**Funding Support:**

Project Contribution:

National Academy Member: N

## International Travel:

AUS	70 days
FRA	60 days
JPN	40 days
CHN	30 days

## International Collaboration:

CHN  
AUS  
BRA  
ESP  
JPN

## ARTICLES:

**Publication Type:** Journal Article

Peer Reviewed: Y      **Publication Status:** 1-Published

**Journal:** Physical Review Applied

Publication Identifier Type: DOI

Publication Identifier: 10.1103/PhysRevApplied.8.064035

Volume: 8

Issue: 6

First Page #:

Date Submitted: 8/29/18 12:00AM

Date Published: 12/1/17 5:00AM

Publication Location:

**Article Title:** Tunable Hybrid Qubit in a Triple Quantum Dot

**Authors:** Bao-Chuan Wang, Gang Cao, Hai-Ou Li, Ming Xiao, Guang-Can Guo, Xuedong Hu, Hong-Wen Jiang, C

**Keywords:** multielectron, hybrid qubit, frequency control

**Abstract:** We experimentally demonstrate quantum-coherent dynamics of a triple-dot-based multielectron hybrid qubit. Pulsed experiments show that this system can be conveniently initialized, controlled, measured electrically, and has a good ratio  $Q \approx 29$  between the coherence time and gate time. Furthermore, the current multielectron hybrid qubit has an operation frequency that is tunable in a wide range, from 2 to about 15 GHz. We also provide a qualitative understanding of the experimental observations by mapping them onto a three-electron system. The demonstration of the high tunability in a triple dot system could be potentially useful for future quantum control.

**Distribution Statement:** 3-Distribution authorized to U.S. Government Agencies and their contractors

Acknowledged Federal Support: Y

# RPPR Final Report

as of 29-Aug-2023

**Publication Type:** Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

**Journal:** Physical Review Letters

Publication Identifier Type: DOI

Publication Identifier: 10.1103/PhysRevLett.119.156802

Volume: 119 Issue: 15

First Page #:

Date Submitted: 8/29/18 12:00AM

Date Published: 10/1/17 12:00AM

Publication Location:

**Article Title:** Hole Spin Resonance and Spin-Orbit Coupling in a Silicon Metal-Oxide-Semiconductor Field-Effect Transistor

**Authors:** K. Ono, G. Giavaras, T. Tanamoto, T. Ohguro, X. Hu, F. Nori

**Keywords:** two-hole spin resonance, p-SiMOSFET, spin blockade, spin-orbit coupling

**Abstract:** We study hole spin resonance in a p-channel silicon metal-oxide-semiconductor field-effect transistor. In the subthreshold region, the measured source-drain current reveals a double dot in the channel. The observed spin resonance spectra agree with a model of strongly coupled two-spin states in the presence of a spin-orbit-induced anticrossing. Detailed spectroscopy at the anticrossing shows a suppressed spin resonance signal due to spin-orbit-induced quantum state mixing. This suppression is also observed for multiphoton spin resonances. Our experimental observations agree with theoretical calculations.

**Distribution Statement:** 3-Distribution authorized to U.S. Government Agencies and their contractors

Acknowledged Federal Support: Y

**Publication Type:** Journal Article Peer Reviewed: Y **Publication Status:** 1-Published

**Journal:** Scientific Reports

Publication Identifier Type: DOI

Publication Identifier: 10.1038/s41598-018-20706-5

Volume: 8 Issue: 1

First Page #:

Date Submitted: 8/29/18 12:00AM

Date Published: 2/1/18 5:00AM

Publication Location:

**Article Title:** Spin-orbit coupling and electric-dipole spin resonance in a nanowire double quantum dot

**Authors:** Zhi-Hai Liu, Rui Li, Xuedong Hu, J. Q. You

**Keywords:** electric dipole spin resonance, nanowire, double quantum dot, spin-orbit coupling

**Abstract:** We study the electric-dipole transitions for a single electron in a double quantum dot located in a semiconductor nanowire. Enabled by spin-orbit coupling (SOC), electric-dipole spin resonance (EDSR) for such an electron can be generated via two mechanisms: the SOC-induced intradot states mixing and the interdot spin-flipped tunneling. The EDSR frequency and strength are determined by these mechanisms together. For both mechanisms the EDSR transition rates are strongly dependent on the external magnetic field. Their competition can be revealed by increasing the magnetic field and/or the interdot distance for the double dot. To clarify whether the strong SOC significantly impact the electron state coherence, we also calculate relaxations from excited levels via phonon emission. We show that spin-flip relaxations can be effectively suppressed by the phonon bottleneck effect even at relatively low magnetic fields because of the very large g-factor of strong SOC materials like InSb.

**Distribution Statement:** 3-Distribution authorized to U.S. Government Agencies and their contractors

Acknowledged Federal Support: Y





**RPPR Final Report**  
as of 29-Aug-2023

**Partners**

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I certify that the information in the report is complete and accurate:

Signature: Xuedong Hu

Signature Date: 8/18/23 3:02PM

The overall objective of our research program is to help facilitate the realization of spin-based quantum computing in Si nanostructures. Our proposed research program consists of two main directions: coherent manipulation of a single spin qubit, and exchange coupling between spin qubits. Both are crucial in our long term goal of building a high-fidelity large-scale Silicon- and spin-based quantum computer. On the front of single-spin explorations, our major goals are to study spin coherence and control fidelity in the presence of static magnetic field gradient, and search for optimal conditions for spin control and coherence. On the front of multiple spin qubits, our major goal is to study the interplay between exchange coupling and valley mixing, and explore whether multi-electron states in a dot/donor(s) can be used to encode a more robust spin qubit. On the front of noise and decoherence, we would like to study how interface defects could produce charge and magnetic noise. The goals set forth in this research program are all focused on helping identify optimal designs for high-fidelity single-qubit and two-qubit gates in a Silicon-spin-based quantum computer.

Through this theoretical research program we have studied several important current issues in Silicon-based semiconductor quantum computing architectures, including the effects of an on-chip micromagnet, the effects of valley-orbit coupling in Si, and decoherence and control issues in spin qubit transport. Below is a list of our results and the corresponding publications.

Micromagnets have become an important element for spin qubit control in Si quantum dots, enabling fast and high fidelity single-qubit gates. We have studied the effects of a micromagnet, specifically the magnetic field gradient it produces, on spin coherence. We find that, in contrast to intrinsic spin-orbit coupling (iSOC), such field gradient allows spin pure dephasing due to charge noise (which has since been shown to be the dominant decoherence channel for spin qubits in some situations). It also leads to a different dependence by spin relaxation rate on the external field. On the other hand, the field gradient also opens new avenue for spin control, such as via a longitudinal driving field. We have published one paper and one preprint on these results. Lastly, we have developed a new Master Equation for describing non-Markovian effects of charge noise on a spin qubit in a double dot with a micromagnet. This part of the study is not yet written up as we continue to seek physical explanations of some of the mathematical steps and expressions.

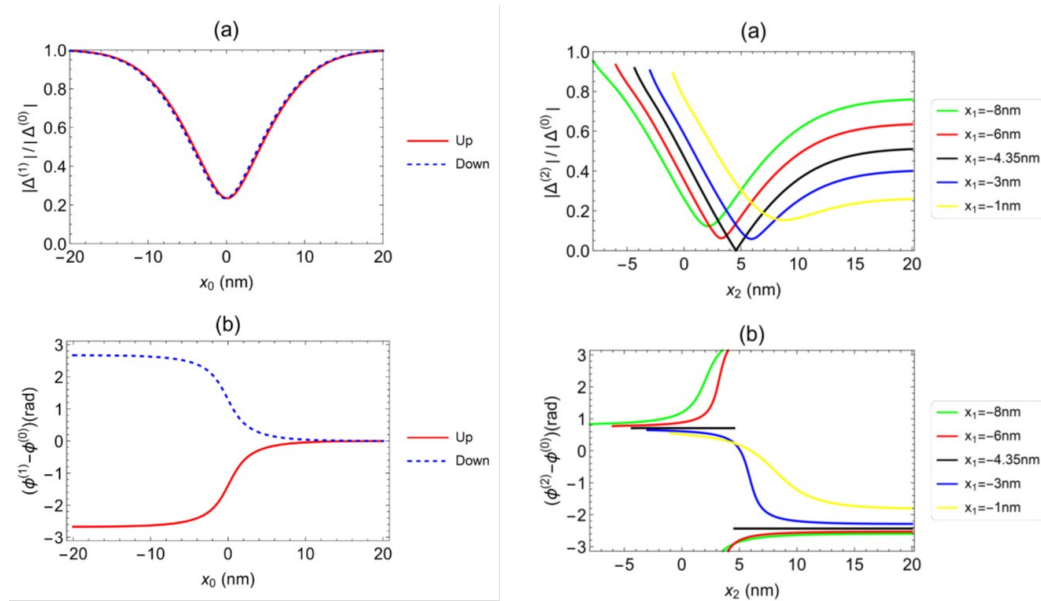
- Fast spin-valley-based quantum gates in Si with micromagnets, P. Huang and X. Hu, arxiv:2010.14844. *NPJ Quantum Information* **7**, 162 (2021).
- Impact of Time-Reversal Symmetry on spin decoherence and control in a synthetic spin-orbit field, P. Huang and X. Hu, arxiv:2008.04671. *New J. of Phys.* **24**, 013002 (2022).
- Non-Markovian dynamics of an electron spin qubit in a magnetic field gradient, X. Zhao and X. Hu, preprint in preparation.

We have performed single- and two-qubit decoherence studies of the flip-flop qubit made from a donor and an interface quantum dot in Si. This system turns out to be mathematical similar to the problem of a double dot in a magnetic field gradient. We showed that charge noise could significantly impact the two-qubit operations, and proposed an alternative operating regime to minimize leakage and decoherence effects.

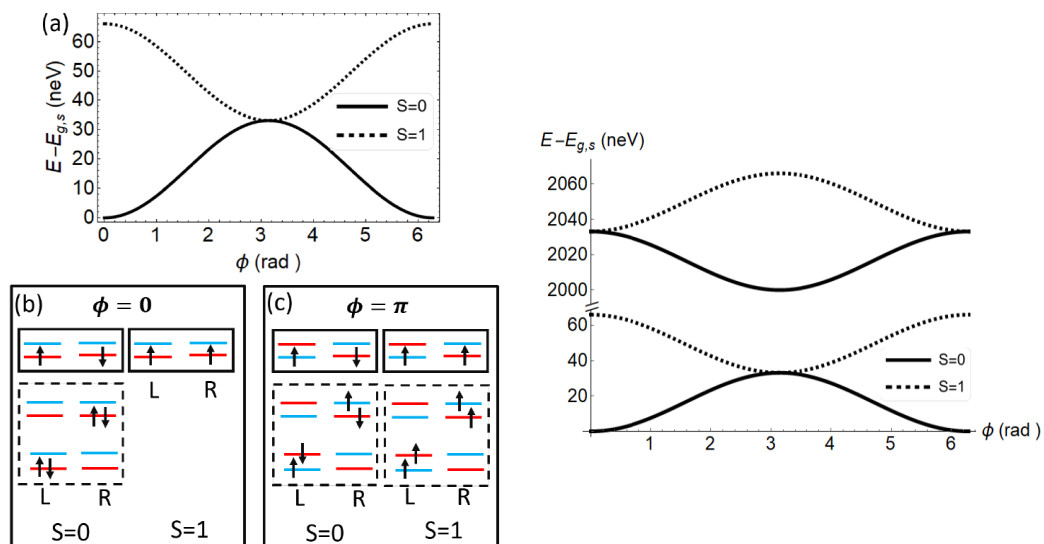
- Decoherence of Coupled Flip-Flop Qubits Due to Charge Noise, J. Truong and X. Hu, arXiv:2104.07485.

One of the distinctive properties of Si quantum dots is the presence of low-lying valley excited states, with valley splitting typically in the order of 0.1 meV while orbital excitation energy typically about 1 meV. During this program we have studied several aspects of the valley physics in Si. Specifically, we find that a single interface step on an otherwise smooth interface could lead to significant suppression of valley splitting and dramatic change in valley mixing phase. We find that exchange coupling in a Si double dot can be significantly suppressed if valley mixing phase is different across the double dot by  $\pi$ , even when the magnitude of valley splitting in both dots are large. On the other hand, if valley splitting is very small in one of the dots, exchange may not work at all since different pairs of singlet-triplet states usually have different exchange splittings. Lastly, in the context of measuring tunnel coupling in a Si double dot, we find that the prevalent approach used by most experimentalists now, which is based on a GaAs double dot, has to be modified to include valley effects. Otherwise the estimated tunnel coupling could be off by a significant fraction, sometimes completely wrong. In short, while in a single Si quantum dot valley splitting is the main effect of valley physics, in a double quantum dot both magnitude and phase of valley-orbit coupling are important parameters to consider.

- B. Tariq and X. Hu, “Effects of Interface Steps on the Valley Orbit coupling in a Si/SiGe quantum dot”, arXiv:1904.11944. *Physical Review B* **100**, 125309 (2019).
- Impact of the valley orbit coupling on exchange gate for spin qubits in silicon quantum dots, B. Tariq and X. Hu, arXiv:2107.00732. *NPJ Quantum Information* **8**, 53 (2022).
- Measurement of tunnel coupling in a Si double quantum dot based on charge sensing, X. Zhao and X. Hu, arXiv:2103.06409. *Phys. Rev. Applied* **17**, 064043 (2022).



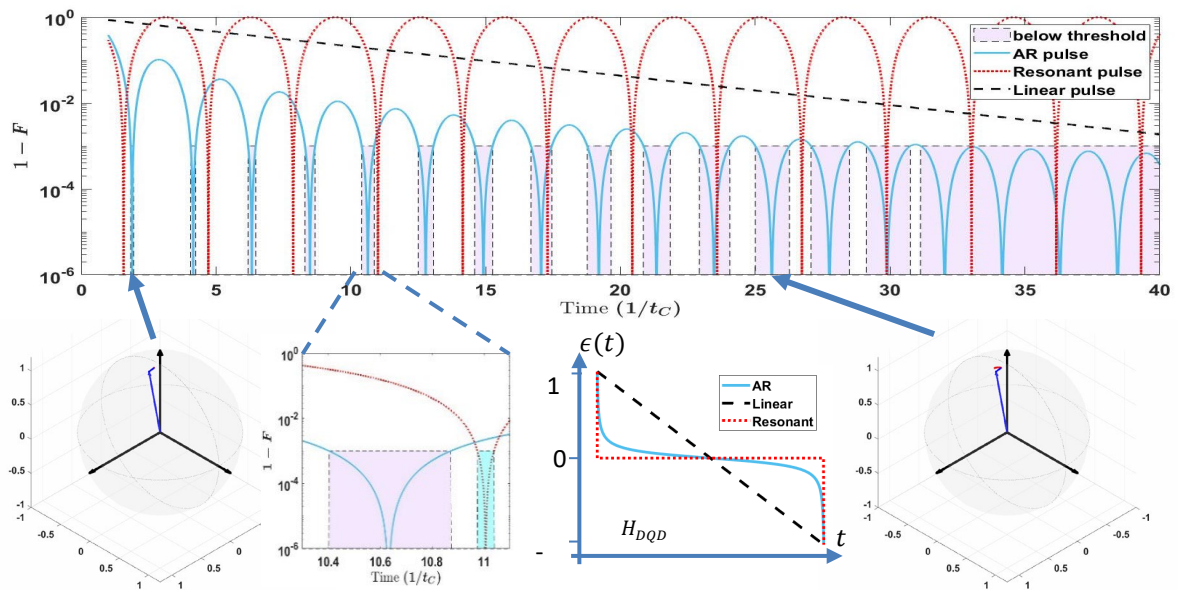
**Figure 1.** Magnitude and phase of valley-orbit coupling in a quantum dot with one [panels (a) and (b)] or two [panels (c) and (d)] interface steps, as functions of the location(s) of the step(s). Panel (a) shows that  $|\Delta_{VO}|$  can be reduced by 75% if a step is present at the center of the dot, while panel (b) shows that its phase can vary by almost  $\pi$ . “Up” and “Down” here refer to the direction of the step. Panel (c) shows that  $|\Delta_{VO}|$  can be significantly suppressed if the two steps fall in certain regions, while Panel (d) shows that its phase can vary in a wide range, too. B. Tariq and X. Hu, Phys. Rev. B **100**, 125309 (2019).



**Figure 2.** Panels (a) shows the energies of the lowest singlet and triplet states (S-orbitals only) as functions of the interdot valley phase difference. Panels (b) and (c) give a pictorial representation on how the state compositions are different at the phase difference of 0 and  $\pi$ . Panel (d) gives the energy spectrum for the lowest four states in a Si double dot. The solid lines are singlet state and dashed lines are triplet, respectively. Notice that in general the singlet-triplet splitting is different among the ground and excited pairs, so that during time evolution the phase accumulation will be different. B. Tariq and X. Hu, npj Quantum Information **8**, 53 (2022).

We have performed systematic studies of spin qubit transport by focusing on the problem of spin transfer in a double quantum dot, both in GaAs and in Si. We have identified some of the most important factors that would affect spin transfer fidelity, from avoiding spin relaxation hot spot, to the correction to  $g$ -factor by the double dot potential, and possible difference in  $g$ -factor in the two dots. We have identified parameter regimes (in terms of tunnel coupling, valley splitting, and applied magnetic field) where spin transfer fidelity would most likely suffer from spin relaxation and dephasing. The observations from this study also prompted us to search for better control of spin transport, and arrived at the idea of adiabatic resonance, where the electron would periodically return to its instantaneous eigenstates as the system Hamiltonian evolves with time. We believe this concept can have important potential impact on how we control spin transport in the future.

- X. Zhao and X. Hu, “Toward high-fidelity coherent electron spin transport in a GaAs double quantum dot”, arXiv:1707.05217. *Scientific Reports* **8**, 13968 (2018).
- X. Zhao and X. Hu, “Coherent electron transport in silicon quantum dots”, arXiv:1803.00749. This paper was submitted and then split into parts, leading to a *Phys. Rev. Applied* article on measurement of tunnel coupling and a preprint on adiabatic resonance.
- X. Zhao, K. Xia, and X. Hu, “Fast Quantum Control through Adiabatic Resonance”, preprint in preparation.



**Figure 3.** Adiabatic resonance (AR) in a two-level system (such as a double dot charge qubit). The top panel shows the infidelity for the system to return to the adiabatic path via different protocols. The fidelity threshold is set at  $10^{-3}$ . The horizontal axis is the total evolution time, in the unit of tunneling time for the double dot. The Resonant protocol (red dotted line) brings the DQD to zero detuning instantaneously and parks the system there until tunneling brings the electron from one dot to the other; the Linear protocol (black dashed line) changes the detuning linearly with time and is used as the adiabatic benchmark. Lastly, the blue solid line gives the AR protocol, which has fast speed and high tolerance of timing errors.

In the context of spin transport, we have also studied how surface acoustic waves (SAW) could carry electrons controllably in a semiconductor nanostructure, specifically in GaAs. We have performed a careful examination of the eigenmodes of SAW, and identified additional modes that have not been considered so far in the context of quantum information processing. While these modes may not affect electron transport, they could play a role in spin decoherence, and could possibly interact with transmon qubits in the context of superconducting quantum computing. There is no publication for this work yet. The student has only started to prepare a preprint on mode calculations.

We have been involved in a wide range of collaborations with both experimental and theoretical colleagues during the current research program, which have led to some useful results in the study of spin qubits. For example, in a collaboration with John Nichol group at University of Rochester, we have studied how a short spin chain can act as a bus and mediate coupling and entanglement for spin qubits, and how certain states of a spin bus cannot help with quantum state transfer; In a collaboration with Dimi Culcer group at University of New South Wales, we identified certain acceptor hole spin states as a good candidate for a controllable and coherent qubit; In a collaboration with Seigo Tarucha group from Riken we studied transport of entangled spin states in a triple dot system and found that pure dephasing could actually facilitate entanglement transfer; In a collaboration with Keiji Ono group at Riken we have demonstrated two-hole electric dipole spin resonance in a commercial p-channel SiMOS Field Effect Transistor; In a collaboration with Guoping Guo group from USTC we characterized giant anisotropy in spin relaxation due to spin-orbit coupling; We have also demonstrated very fast hole-spin Rabi oscillation in a Germanium nanowire double quantum dot; In collaboration with Susan Coppersmith group at University of Wisconsin and Hong-Wen Jiang group from UCLA, we identify unintended quantum dots in Si/SiO<sub>2</sub> heterostructures as a possible reason for breaking spin blockade.

- Long-distance superexchange between semiconductor quantum-dot electron spins, H. Qiao et al., arxiv:2009.06071. *Physical Review Letters* **126**, 017701 (2021).
- J.C. Abadillo-Uriel, J. Salfi, X. Hu, S. Rogge, M.J. Calderon, and D. Culcer, “Entanglement control and magic angles for acceptor qubits in Si”, arXiv:1706.08858. *Applied Physics Letters* **113**, 012102 (2018).
- T. Nakajima, M.R. Delbecq, T. Otsuka, S. Amaha, J. Yoneda, A. Noiri, K. Takeda, G. Allison, A. Ludwig, A.D. Wieck, X. Hu, F. Nori, and S. Tarucha. *Nature Communications* **9**, 2133 (2018).
- K. Ono, G. Giavaras, T. Tanamoto, T. Ohguro, X. Hu, and F. Nori, “Hole spin resonance and spin-orbit coupling in a silicon metal-oxide-semiconductor field-effect transistor”, arXiv:1707.03106. *Physical Review Letters* **119**, 156802 (2017).
- X. Zhang et al., “Giant Anisotropy of Spin Relaxation and Spin-Valley Mixing in a Si Quantum Dot”, arxiv:1912.08365. *Physical Review Letters* **124**, 257701 (2020).
- Ultrafast Operations of a Hole Spin Qubit in Ge Quantum Dot, K. Wang et al., arxiv:2006.12340. *Nature Communications* **13**, 206 (2022).
- C. King et al., “Lifting of Spin Blockade by Charged Impurities in Si-MOS Double Quantum Dot Devices”, arXiv:1807.11064. *Physical Review B* **101**, 155411 (2020).