Quantum Simulations of Fermionic Hamiltonians with Efficient Encoding and Ansatz Schemes

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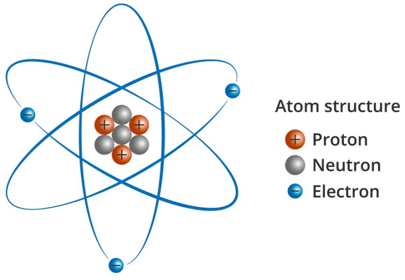
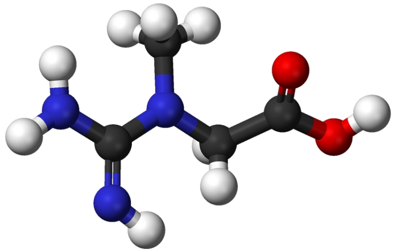
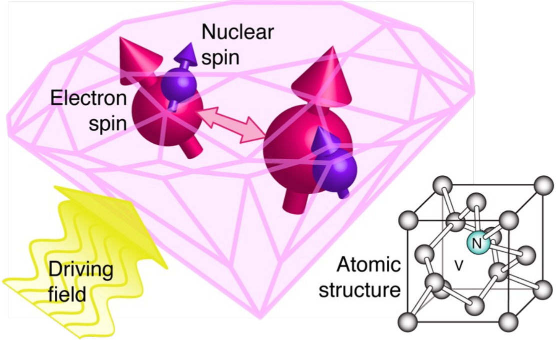
Motivation

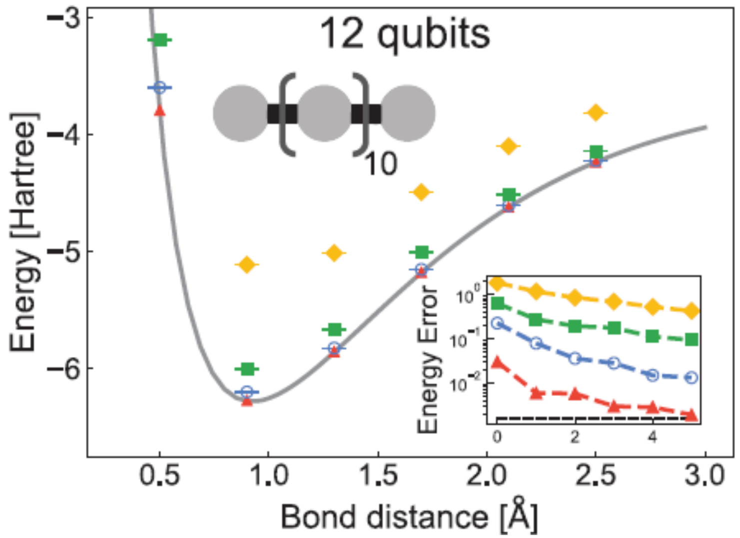
- Solving for eigenstates of Hamiltonians describing physical systems

$$H = \sum_{ij} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k$$









Arute, Frank, et al. Science 369.6507 (2020): 1084-1089.

Kandala, Abhinav, et al. Nature 567.7749 (2019): 491-495.

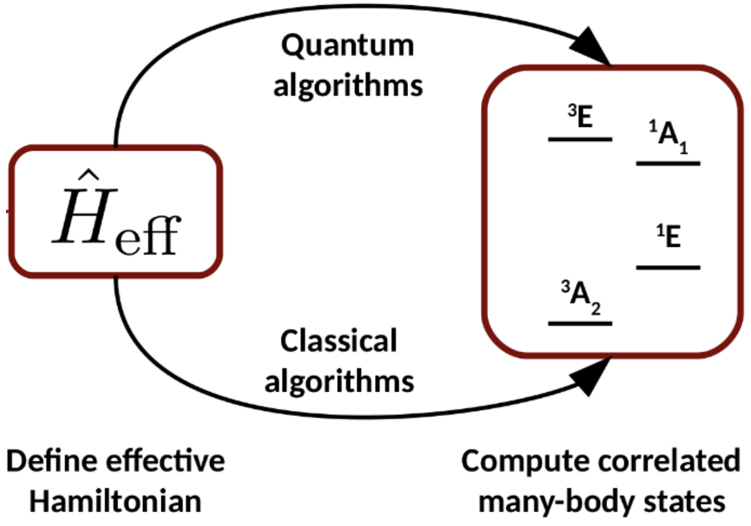
Outline

- Open challenges in solving the electronic structure problem of spin defects and possible solutions
- Results of quantum simulations
- Conclusions and outlook

Benchen Huang, Marco Govoni, and Giulia Galli. *PRX Quantum* 3.1 (2022): 010339.
Benchen Huang, Nan Sheng, Marco Govoni, and Giulia Galli, *JCTC* 2023 (accepted) *arXiv:2212.01912* (2022).
Christian Vorwerk*, Nan Sheng*, Marco Govoni, **Benchen Huang**, and Giulia Galli, Nat. Comput. Sci. 2, 424 (2022).

Simulating Spin Defects in Solids

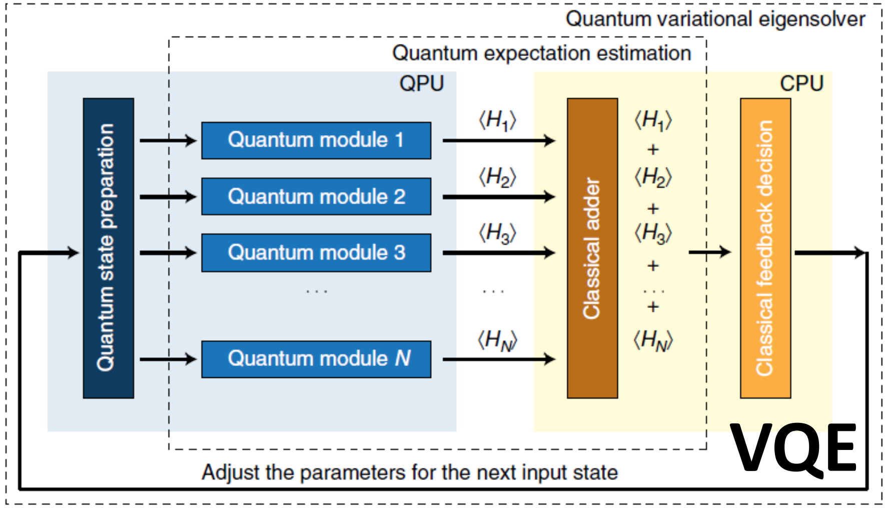
$$H = \sum_{ij} h_{ij}\, a_i^\dagger a_j + \frac{1}{2}\sum_{ijkl} V_{ijkl}\, a_i^\dagger a_j^\dagger a_l a_k$$



- We adopt a recently developed quantum defect embedding theory (QDET) to simulate many-body correlated states of defects
- Low level of theory (environ.): G_0W_0; high Level of theory (H_{eff}): Full Configuration Interaction

He Ma, Marco Govoni, and Giulia Galli. *npj Computational Materials* 6.1 (2020): 85.
He Ma, Nan Sheng, Marco Govoni, and Giulia Galli. *JCTC* 17.4 (2021): 2116-2125.
Nan Sheng, Christian Vorwerk, Marco Govoni, and Giulia Galli. *JCTC* 18.6 (2022): 3512-3522.
Christian Vorwerk, Nan Sheng, Marco Govoni, Benchen Huang, and Giulia Galli. Nature Computational Science 2.7 (2022): 424-432.

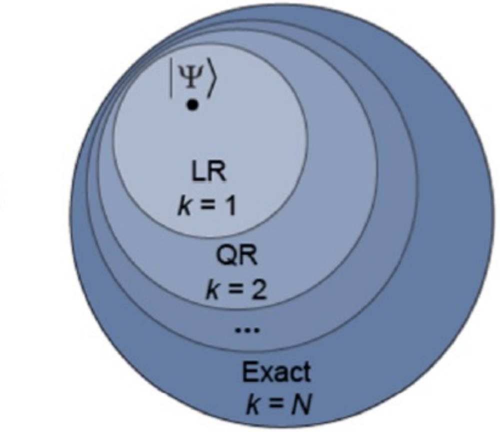
Computational Protocol



Ground State: Variational Quantum Eigensolver (**VQE**)

- Encode chemical information onto qubits
- Define a parameterized quantum circuit
- Use a classical optimizer to optimize the params

Alberto Peruzzo, et al. Nature communications 5.1 (2014): 1-7.



Span $\left\{\sigma_1^{\alpha_1}\sigma_2^{\alpha_2}\ldots\sigma_k^{\alpha_k}|\Psi\rangle \middle| \alpha \in [I,\sigma_x,\sigma_y,\sigma_z]\right\}$

$$\begin{cases} H_{ij}^{QSE} = \langle\Psi|\hat{O}_i^\dagger \hat{H}\hat{O}_j|\Psi\rangle \\ S_{ij}^{QSE} = \langle\Psi|\hat{O}_i^\dagger \hat{O}_j|\Psi\rangle \end{cases}$$

($\hat{O}_i$ is the qubit encoded excitation operators)

Solve $H^{QSE}C = S^{QSE}C\varepsilon$

QSE

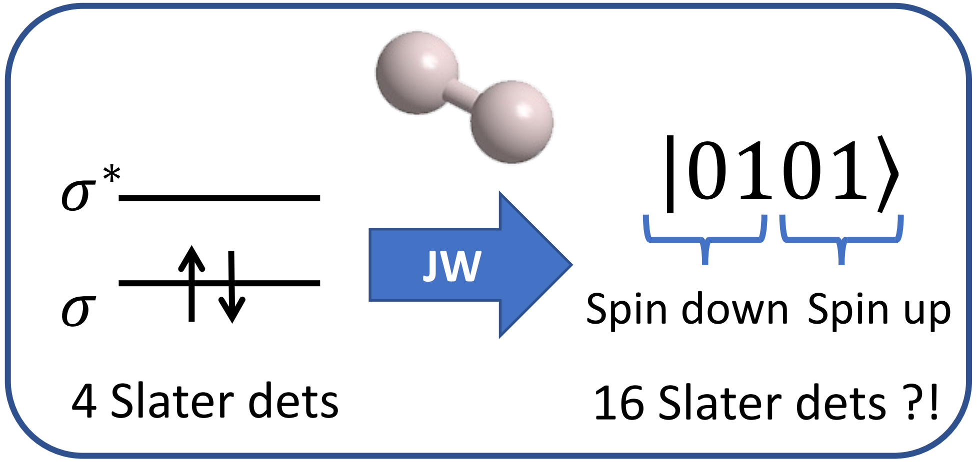
Excited States: Quantum Subspace Expansion (**QSE**)

- Compute matrix elements through quantum measurements
- Diagonalize the generalized eigenvalue problem on a classical computer

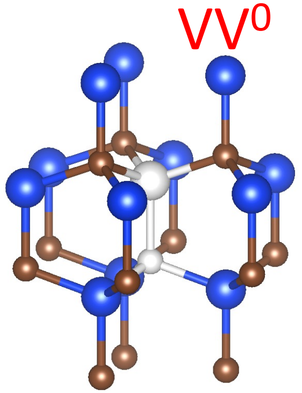
McClean, Jarrod R., et al. Physical Review A 95.4 (2017): 042308.

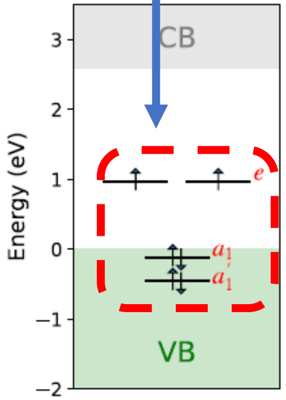
Challenges for Conventional Approaches

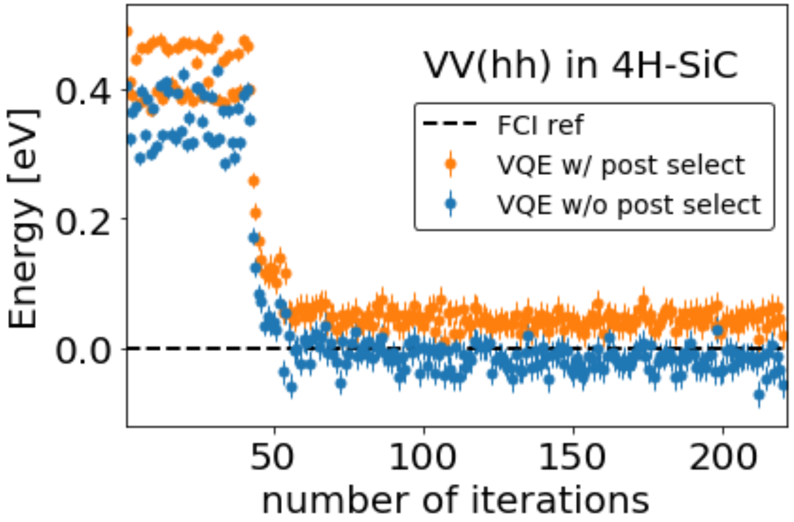
Challenge I: **unphysical state problem** from conventional encoding



Minimum model





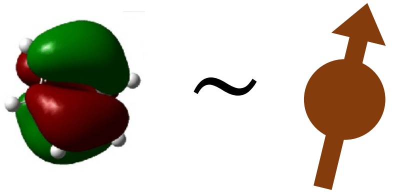


- $\boldsymbol{H}_{\mathbf{eff}} \subseteq \boldsymbol{H}_{\mathbf{q}}$
- Violation of the variational principle
- Problem partially mitigated by post-processing the measure outcomes

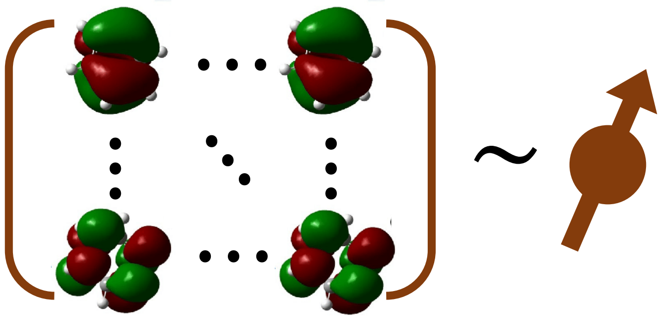
Benchen Huang, Marco Govoni, and Giulia Galli. *PRX Quantum* 3.1 (2022): 010339.

Possible Solution: Qubit-Efficient Encoding

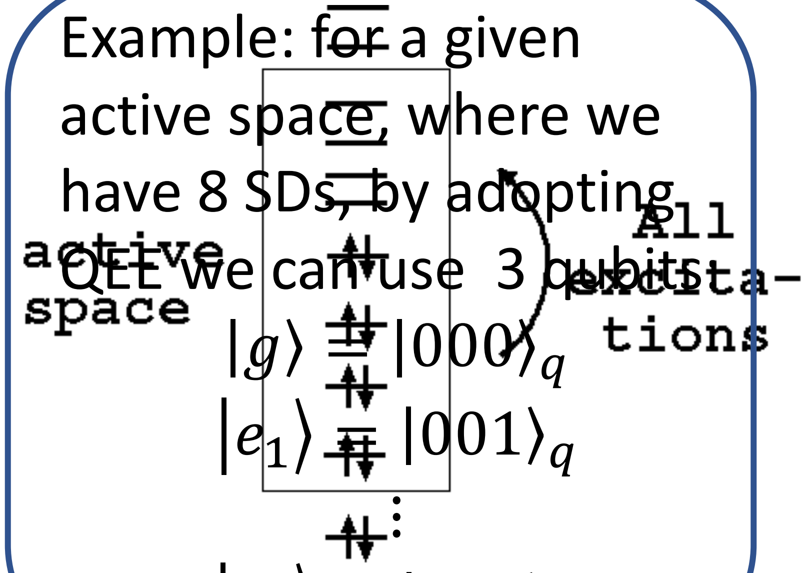
- Conventional scheme encodes spin orbitals into qubits:



- **Solution**: We encode Slater determinants (SD)into qubits, qubit-efficient encoding (QEE):



Example: for a given active space, where we have 8 SDs, by adopting QEE we can use 3 qubits



$|g\rangle$ $|000\rangle_q$

$|e_1\rangle$ $|001\rangle_q$

⋮

$|e_7\rangle$ $|111\rangle_q$

1. QEE by construction spans a space that is identical to the physical Hilbert space → eliminates the unphysical state problem
2. QEE requires $N_q = \lceil \log_2 Q \rceil$ qubits, where Q is the number of Slater determinants.

Yu Shee, Pei-Kai Tsai, Cheng-Lin Hong, Hao-Chung Cheng, and Hsi-Sheng Goan. Physical Review Research 4.2 (2022): 023154.

Challenges in the Construction of Ansatz

Challenge II: Choosing a good ansatz for NISQ (noisy) devices

- **Unitary Coupled-Cluster (UCC) ansatz**

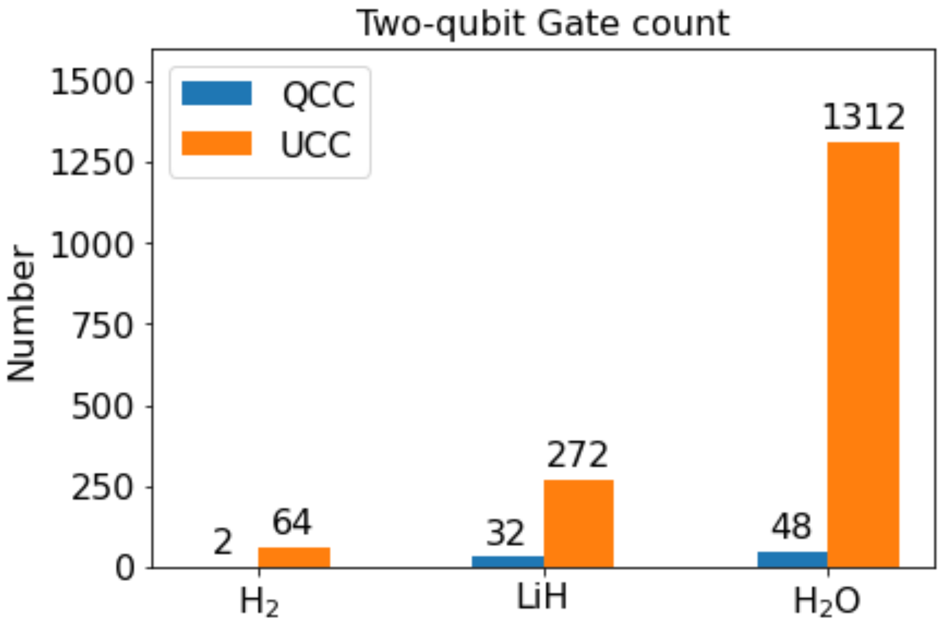
$$|\Psi\rangle = e^{T-T^\dagger}|\Psi_{\mathrm{HF}}\rangle,$$

$$e^{T-T^\dagger} \approx \prod_k e^{-\frac{i\theta_k \hat{P}_k}{2}} = e^{\frac{i}{2}\theta_0 Y_2 Z_1 X_0} \times \cdots, \hat{P}_k = \{I, X, Y, Z\}^{\otimes N}$$

The CNOT gate complexity[1] is: $\sim \boldsymbol{O}\left(\boldsymbol{N}^{3\sim5}\right)$

Kühn, Michael, et al. *JCTC* 15.9 (2019): 476 4-4780.

Is there an optimal way to determine which $\hat{P}_k$s contribute the most to the ground state energy?

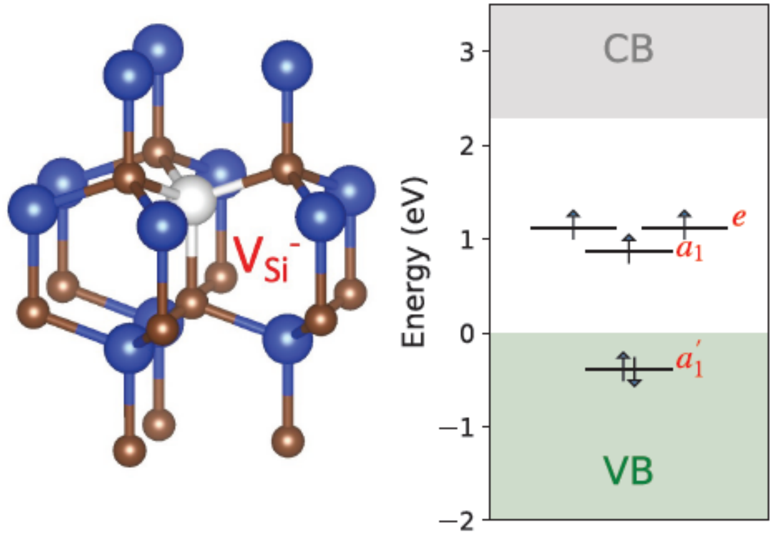


Solution: **Qubit Coupled-Cluster (QCC) ansatz**

- Pre-screening process proposed in Ref 1 to select $\hat{P}_k$s
- All Pauli operators $\hat{P}_k$s are **ranked** to construct ansatz circuit $\hat{U}$
- The ranking procedure dramatically reduces the two-qubit gate count

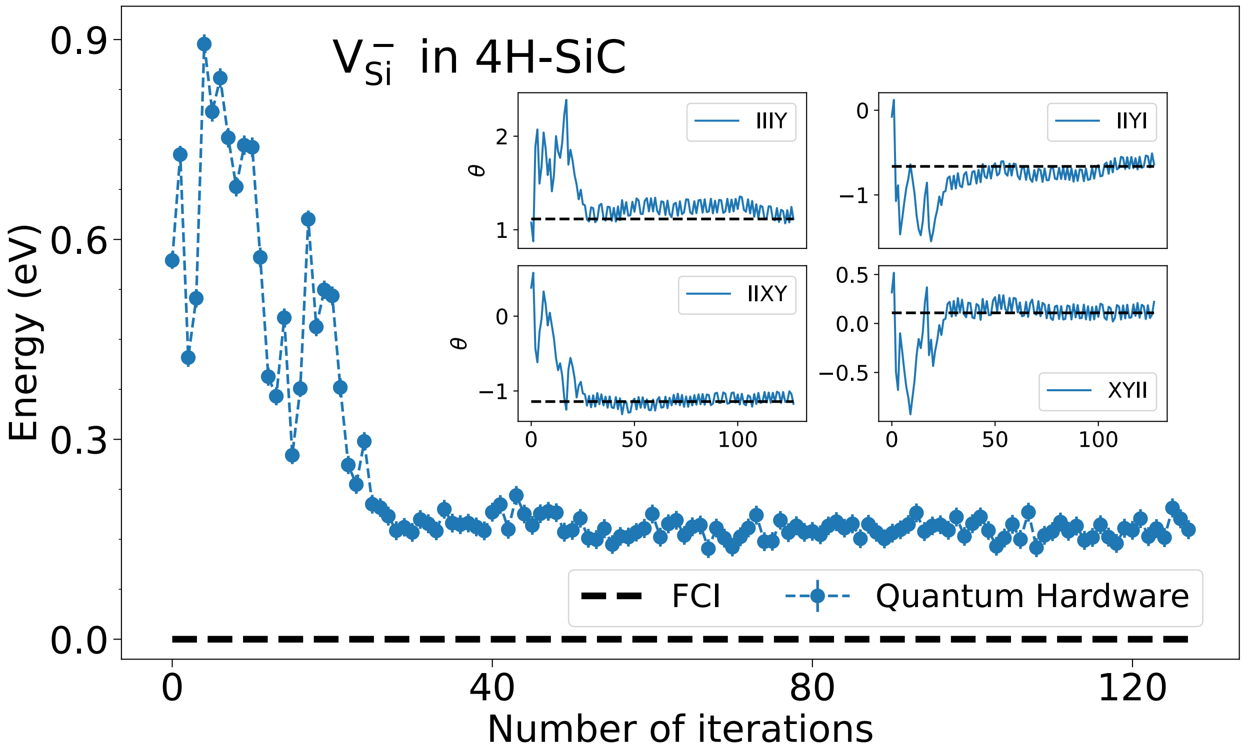
[1]Ilya G. Ryabinkin, Tzu-Ching Yen, Scott N. Genin, and Artur F. Izmaylov. *JCTC* 14.12 (2018): 6317-6326.

Results: V_{Si}^{-} in 4H-SiC



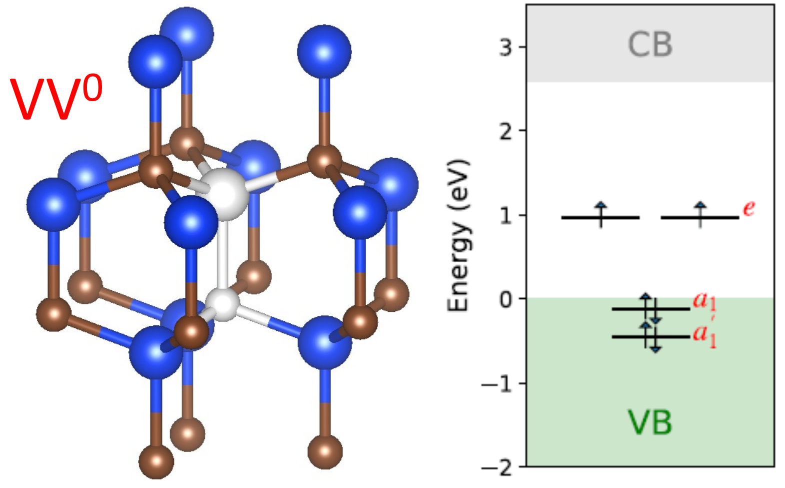
Active space: (5e, 4o)

Hamiltonian H_{eff} is derived from quantum defect embedding theory[1].

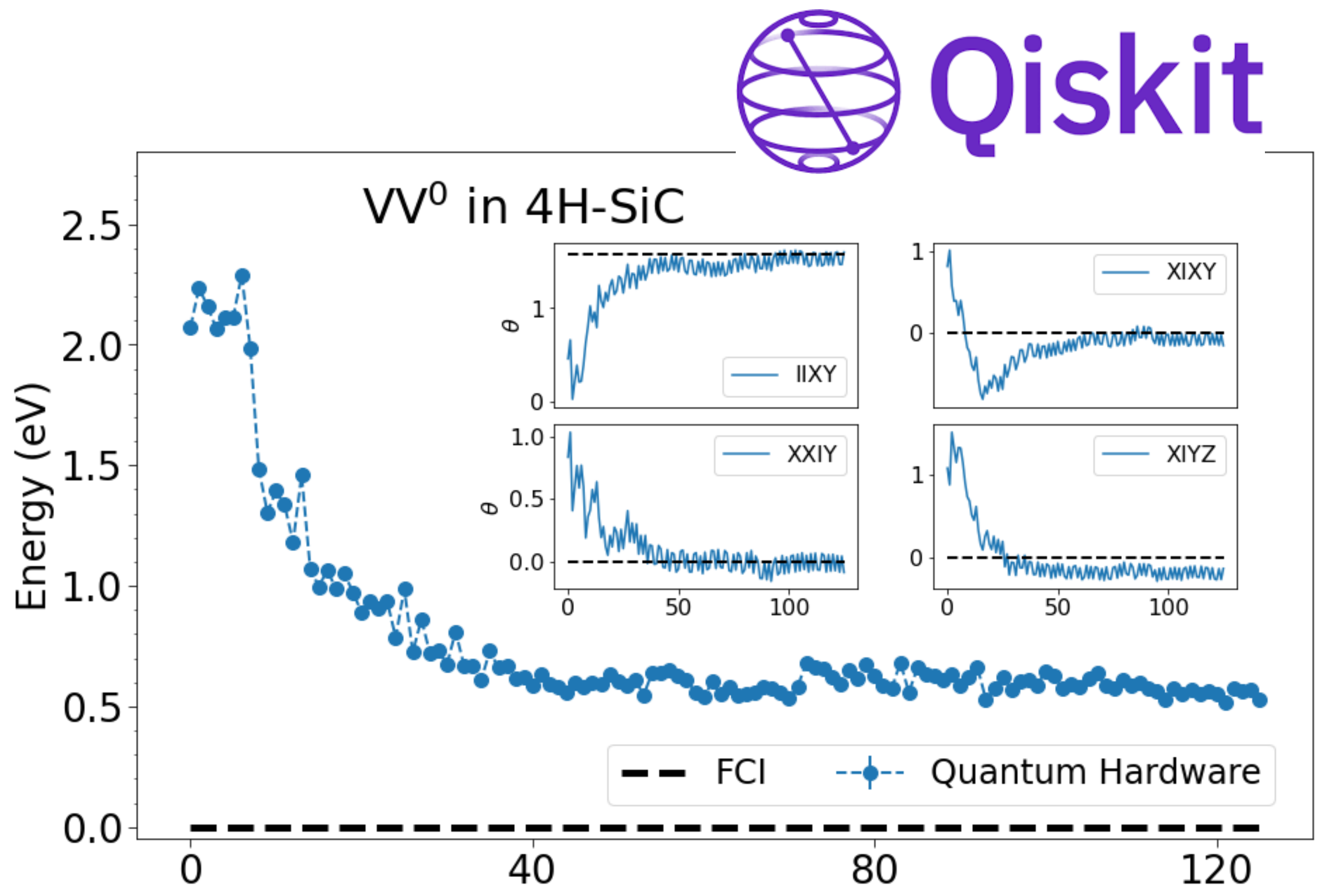


[1]Nan Sheng, Christian Vorwerk, Marco Govoni, and Giulia Galli. *JCTC* 18.6 (2022): 3512-3522.
Benchen Huang, Nan Sheng, Marco Govoni, and Giulia Galli. *JCTC* 2023 (accepted) *arXiv:2212.01912* (2022).

Results: VV^0 in 4H-SiC



Active space: (14e, 8o)
(beyond the minimum model)



How can we mitigate the error?

Benchen Huang, Nan Sheng, Marco Govoni, and Giulia Galli. *JCTC* 2023 (accepted) *arXiv:2212.01912* (2022).

Zero Noise Extrapolation

1. Write the measured expectation value as:

$$\langle H\rangle(\lambda) = \langle H\rangle(0) + \sum_k^n c_k \lambda^k + O(\lambda^{n+1})$$

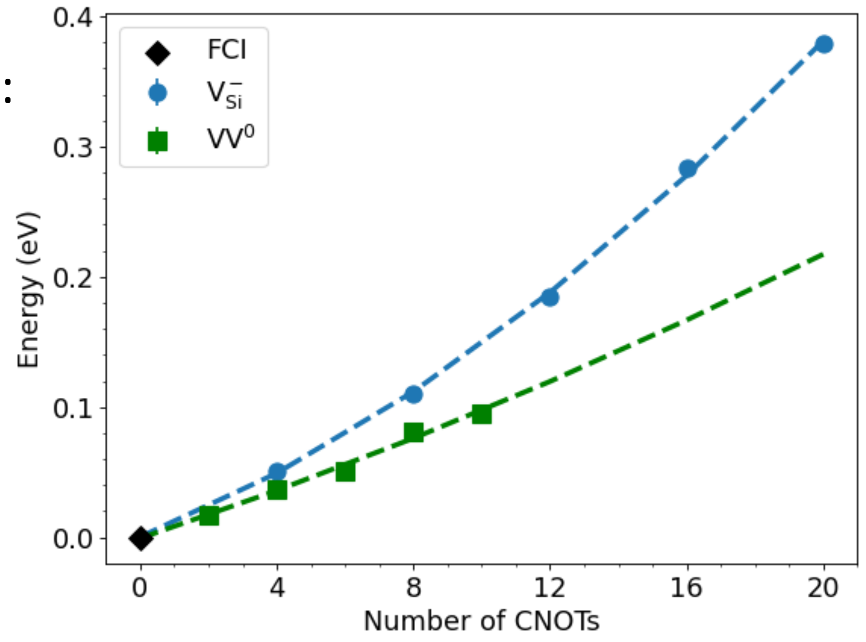
2. Boost the noise in a controllable fashion and then extrapolate to get the zero-noise limit.

- Exponential Block replication* for **all Coupled Cluster type ansatz**:

QCC (UCC): $\hat{U}(\vec{\theta}) = \prod_k e^{-\frac{i\theta_k \hat{P}_k}{2}}, \qquad \hat{P}_k \in \{I, X, Y, Z\}^{\otimes N}$

$$\hat{U}(\vec{\theta}) = \prod_k \left(\prod_n e^{-\frac{i\theta_k \hat{P}_k}{2n}} \right)$$

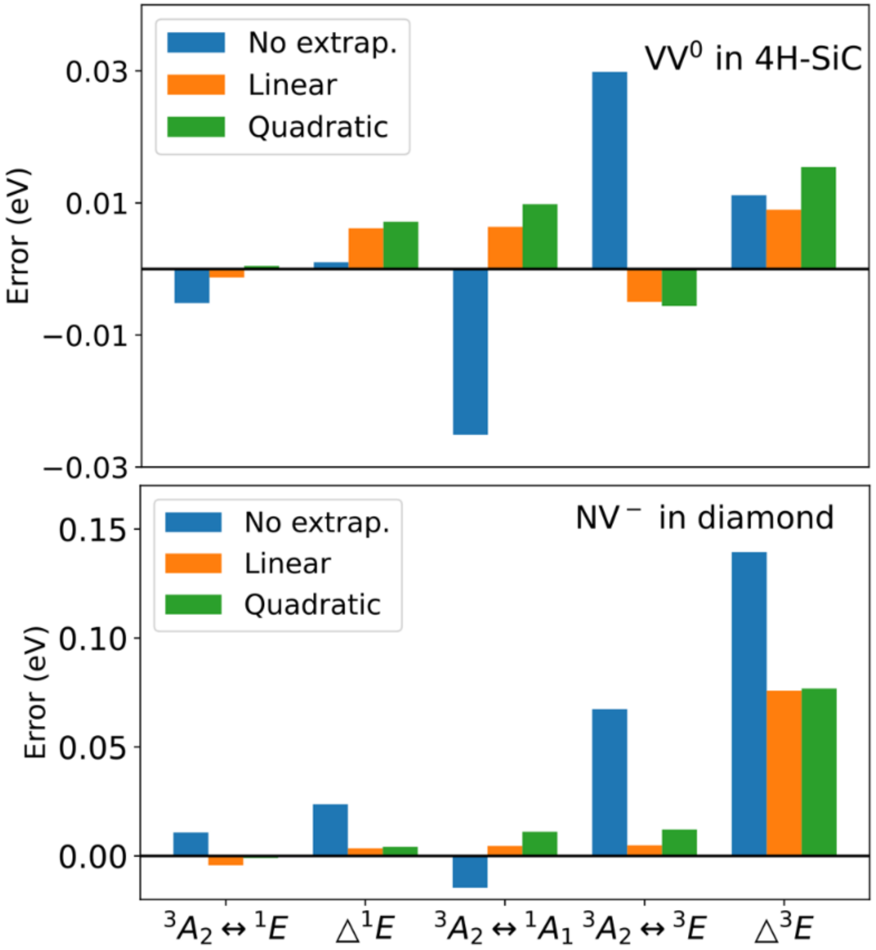
*Splitting the exponential does **not affect** the Trotter error.



Suguru Endo, Simon C. Benjamin, and Ying Li. *Physical Review X* 8.3 (2018): 031027.
Benchen Huang, Nan Sheng, Marco Govoni, and Giulia Galli. *JCTC* 2023 (accepted) *arXiv:2212.01912* (2022).

Computed Electronic Excitations of Spin Defects

- In addition to ground state optimized energy with VQE, we computed electronic excitations of spin defects using the Quantum Subspace Expansion algorithm.
- Use of noise extrapolation greatly improves the accuracy of calculated transitions on quantum hardware in most cases.
- All the results were obtained using *4* qubits on the *IBM Guadalupe* quantum computer.

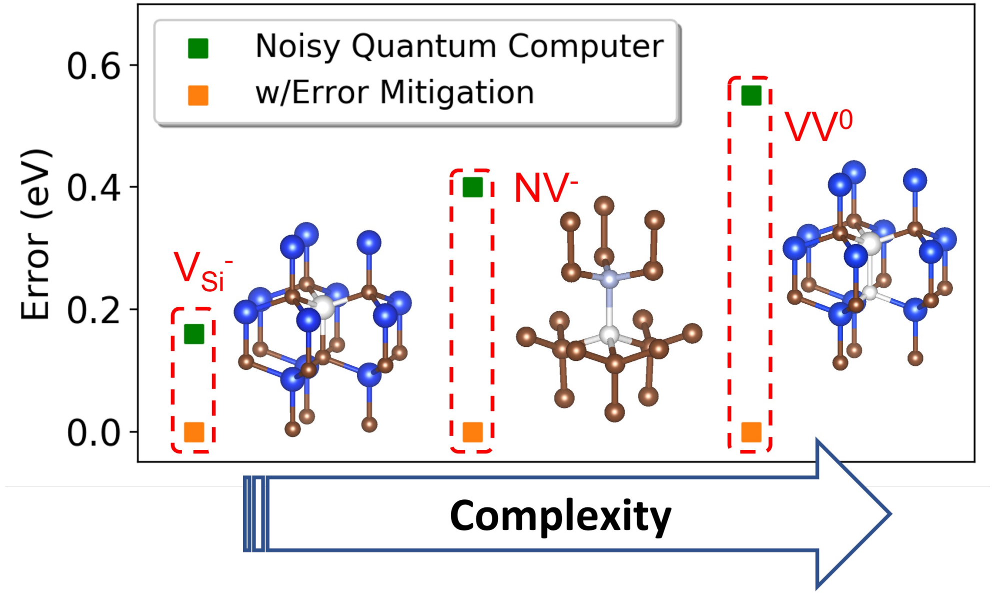


Benchen Huang, Nan Sheng, Marco Govoni, and Giulia Galli. *JCTC* 2023 (accepted) *arXiv:2212.01912* (2022).

Conclusions and Outlook

- We combined a qubit-efficient encoding and a qubit coupled-cluster ansatz to go beyond the minimum model in simulations of the electronic properties of spin defects in solids.

- Our strategy led to a substantial improvement in the scaling of circuit gate counts and in the number of required qubits, and to a decrease in the number of required variational parameters, thus increasing the resilience to noise.



- Use of noise extrapolation greatly improves the accuracy of ground state energy and calculated transitions on quantum hardware.

Acknowledgements

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Backup I: Qubit-Efficient Encoding

	JW, BK, parity	QEE
# qubits	$N_q = N$	$N_q = \lceil \log Q \rceil \le N$
# size of H_q	$O\left(N_q^4\right) \sim O(N^4)$	$O\left(2^{2N_q}\right) \sim O(Q^2) \sim O(N^{2c})$

N is the number of spin orbitals;
m is the number of electrons;
c is the number of holes;
N_q is the number of qubits;
Q is the total number of Slater determinants.

$$Q = \frac{N!}{m!\,(N-m)!}$$

Benchen Huang, et al. *arXiv:2212.01912* (2022).

Possible solutions: Qubit Coupled-Cluster Ansatz

Trotterized UCC: $\hat{U}(\vec{\theta}) = e^{T-T^\dagger} \approx \prod_k e^{-\frac{i\theta_k \hat{P}_k}{2}}, \qquad \hat{P}_k \in \{I, X, Y, Z\}^{\otimes N}$

Can we work directly on the Pauli strings $\hat{P}_k$ that make up the exponentials, instead of finding those by transforming the creation and annihilation operators?

- Find those $\hat{P}_k$s that contribute most to the energy minimization: $E = \langle \Psi_0 | \hat{U}^\dagger H \hat{U} | \Psi_0 \rangle$.
- For operators satisfying $\hat{P}_k^2 = 1$,

$$e^{i\theta \hat{P}_k/2} H e^{-i\theta \hat{P}_k/2} = H - i\frac{\sin\theta}{2}\left[H, \hat{P}_k\right] + \frac{1-\cos\theta}{2}\hat{P}_k\left[H, \hat{P}_k\right]$$

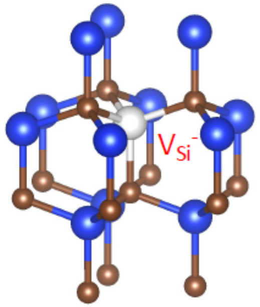
- A pre-screening process is proposed[1], where the derivative of $\hat{P}_k$ w.r.t. $E\left[\theta; \hat{P}_k\right] = \langle \Psi_0 | e^{i\theta \hat{P}_k/2} H e^{-i\theta \hat{P}_k/2} | \Psi_0 \rangle$ is:

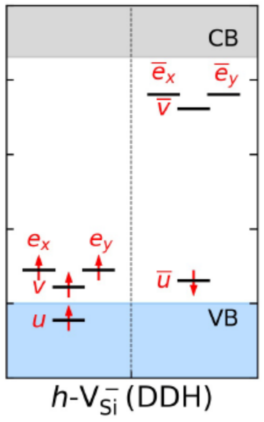
$$\left.\frac{dE\left[\theta; \hat{P}_k\right]}{d\theta}\right|_{\theta=0} = \left\langle \Psi_0 \middle| -\frac{i}{2}\left[\hat{H}, \hat{P}_k\right] \middle| \Psi_0 \right\rangle$$

- Pre-screening process: all $\hat{P}_k$s are ranked according to the computed derivatives to construct $\hat{U}$.

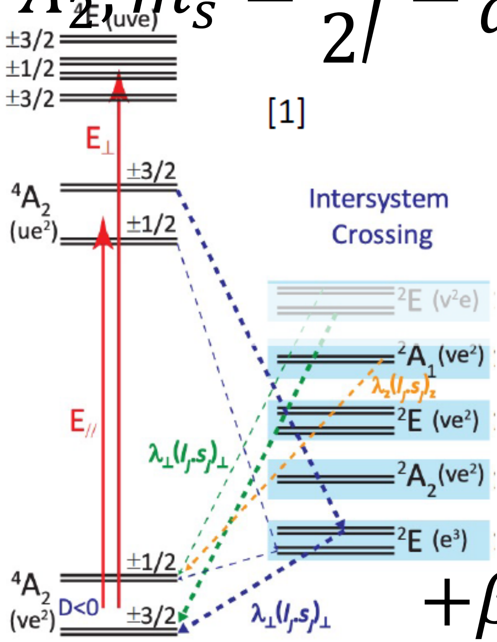
[1]Ryabinkin, Ilya G., et al. JCTC 14.12 (2018): 6317-6326.

Results: V_{Si}^- from FCI



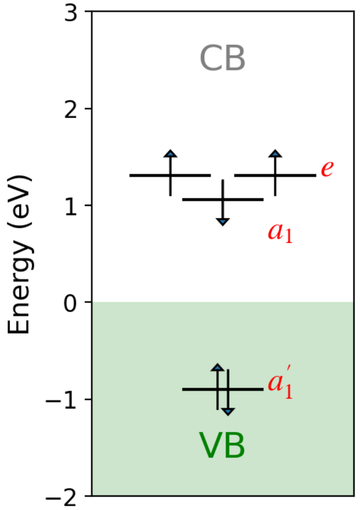


h-V_{Si}^- (DDH)



[1]

$$\left|{}^4A_2, m_s = \frac{1}{2}\right\rangle = \alpha\Big($$



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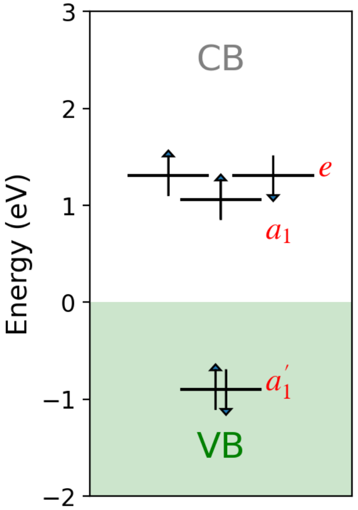

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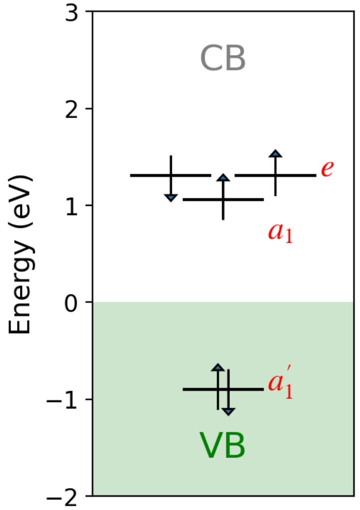

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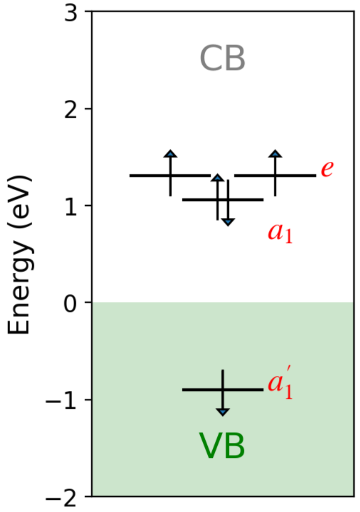

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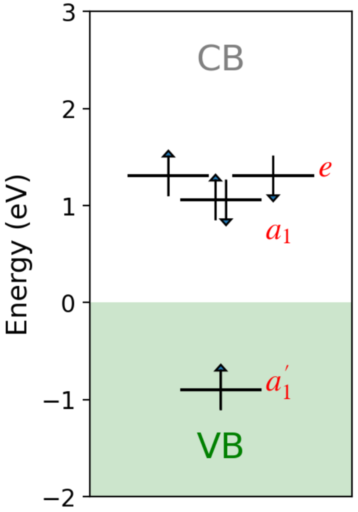

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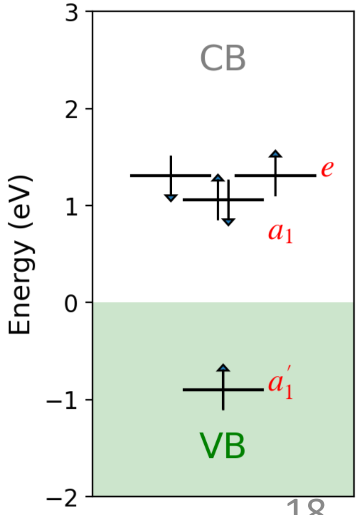

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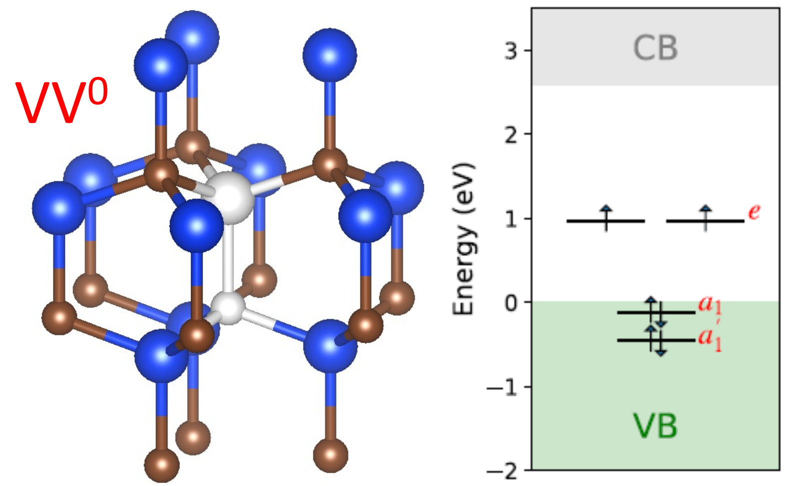
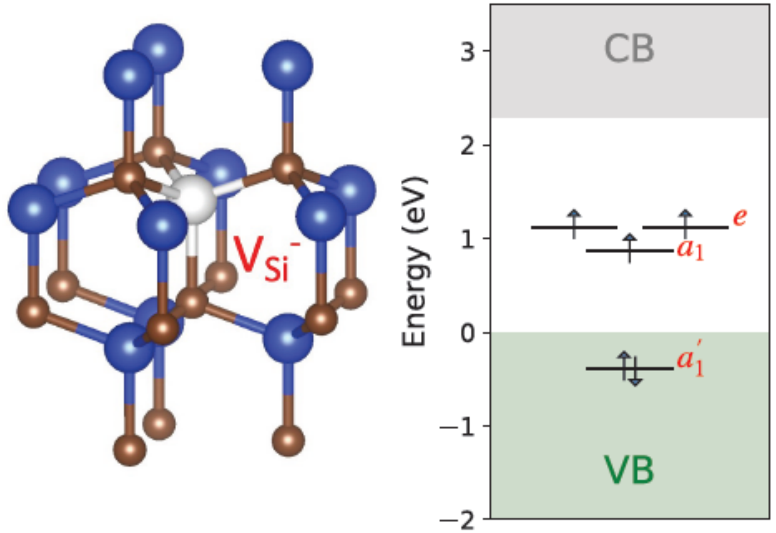
Results: VV^0 and V_{Si}^- pre-screening



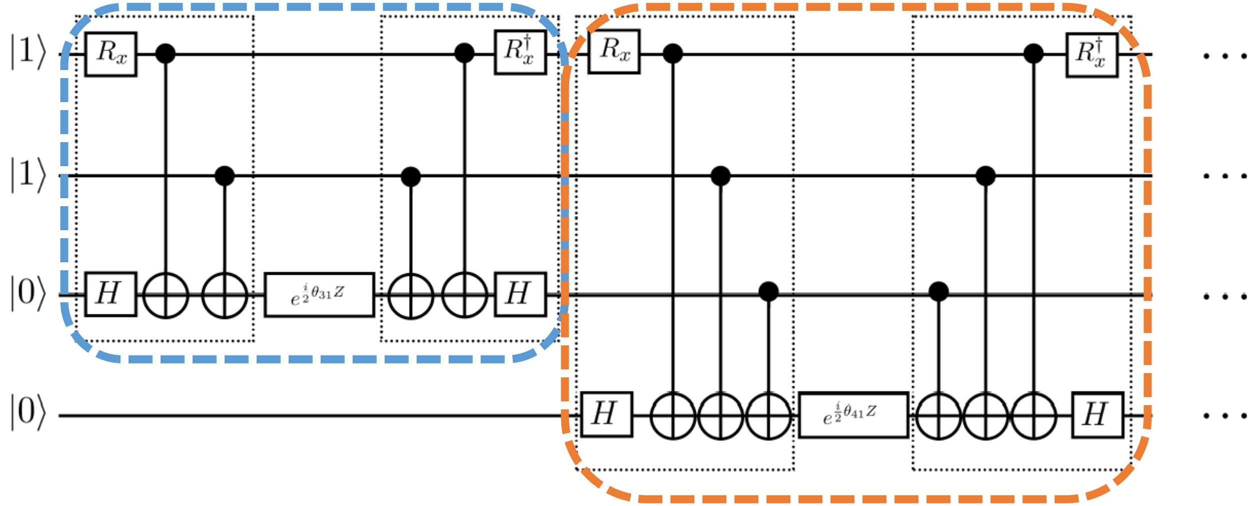


Rank	VV^0		
	entangler	Noiseless (10^{-3})	Noisy (10^{-3})
1	IIXY	9.243	9.170
2	XIYZ	8.177	8.100
3	XXIY	8.165	8.065
4	XIXY	6.587	6.529

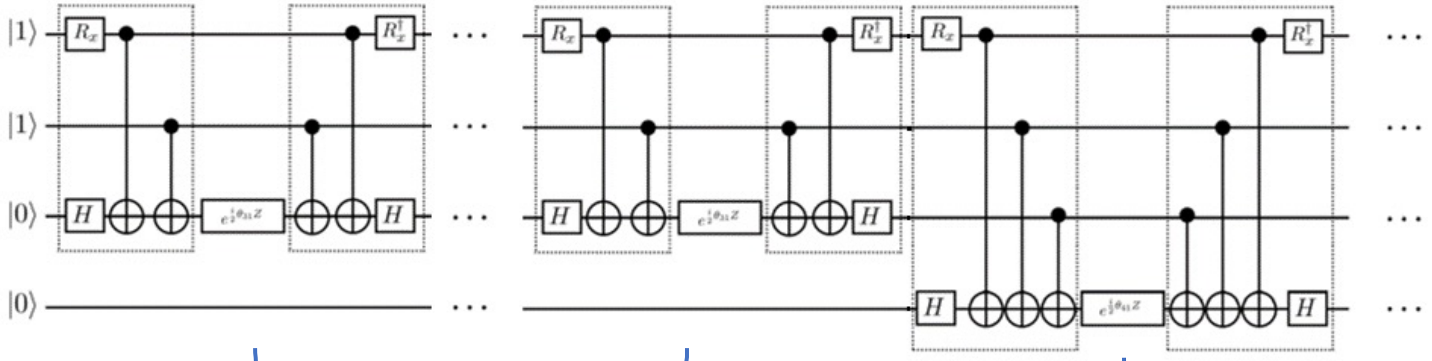
Rank	V_{Si}^-		
	entangler	Noiseless (10^{-3})	noisy (10^{-3})
1	XYII	6.969	6.754
2	IIYI	6.693	6.601
3	IYII	4.352	4.357
4	IIXY	4.350	4.350

Zero Noise Extrapolation

$$\boxed{e^{\frac{i}{2}\theta_{31}Y_1Z_2X_3}} \times \boxed{e^{\frac{i}{2}\theta_{41}Y_1Z_2Z_3X_4}} \times \ldots$$



$$\underbrace{e^{\frac{i}{2}\frac{\theta_{31}}{n}Y_1Z_2X_3} \times \ldots \times e^{\frac{i}{2}\frac{\theta_{31}}{n}Y_1Z_2X_3}}_{\text{n terms}} \ldots$$



n blocks

n blocks