

# Quantum Chemistry in Near-term Quantum Computers

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IBM Quantum, IBM Research Europe, Zurich

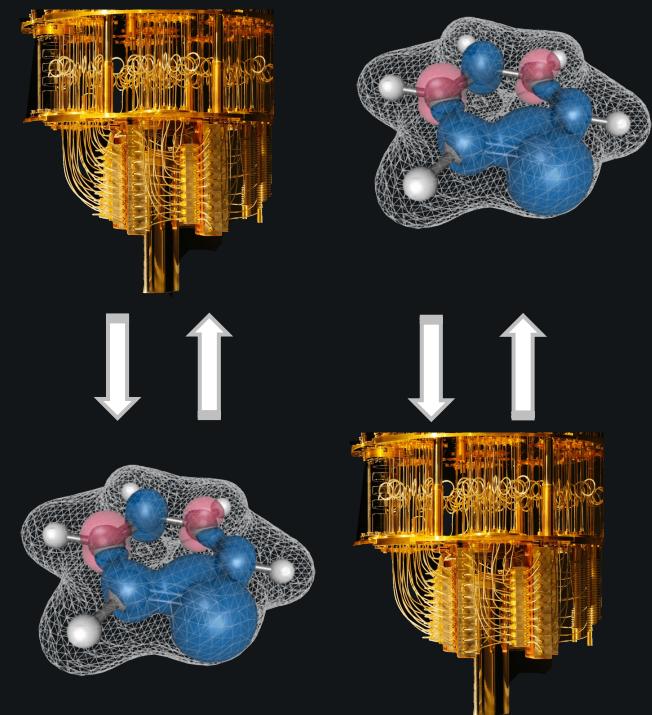
# IBM Quantum, IBM Research Europe

## IBM Quantum



# Outline

- Quantum Chemistry: why is quantum chemistry important?
- How do we approach quantum chemistry in near term quantum computers?
- Is the solution exact and how can we acquire better solutions?
- What software can we use?
- Are there applications beyond the electronic structure problem?



# Introduction

“I'm not happy with all the analyses that go with just the classical theory, *because nature isn't classical*, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical ...”

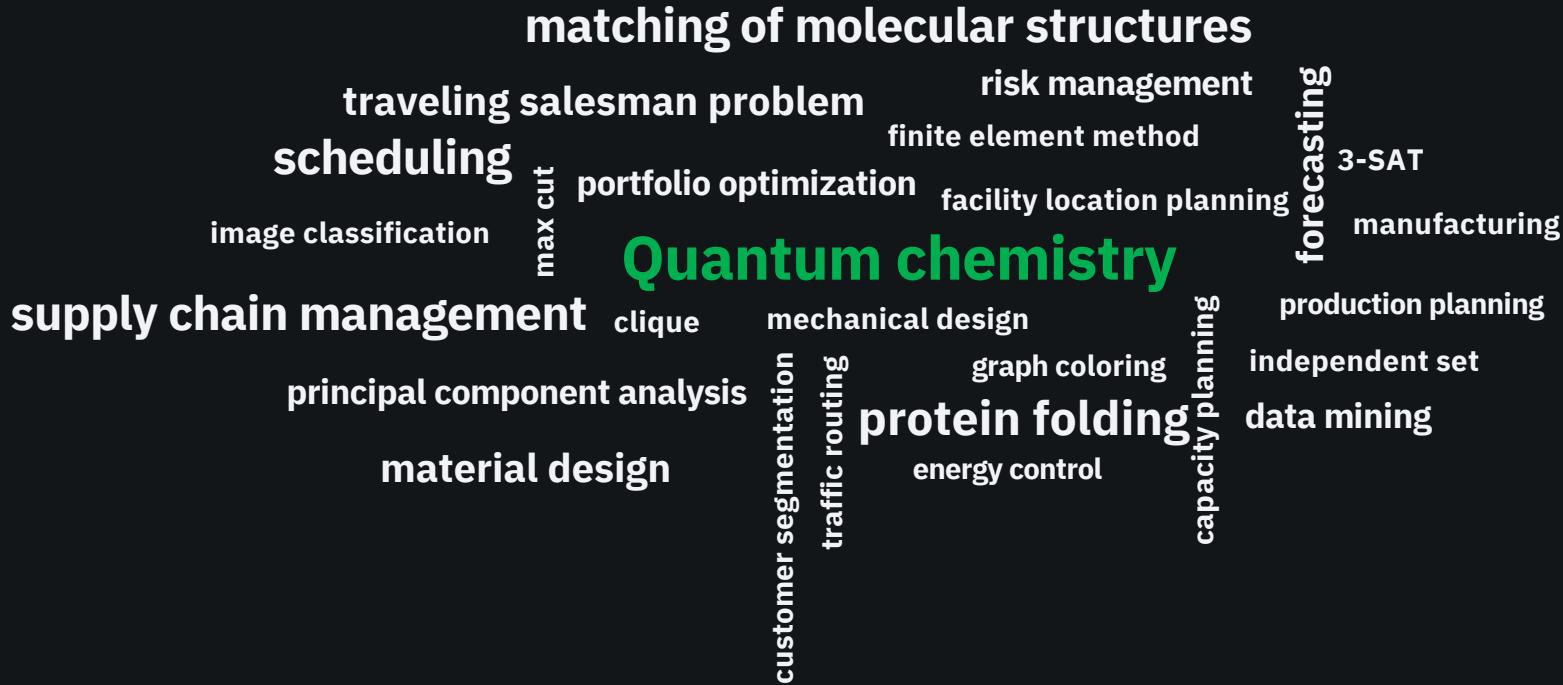
*International Journal of Theoretical Physics*, Vol 21, Nos. 6/7, 1982

Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology,  
Pasadena, California 91107





# What is quantum chemistry ?

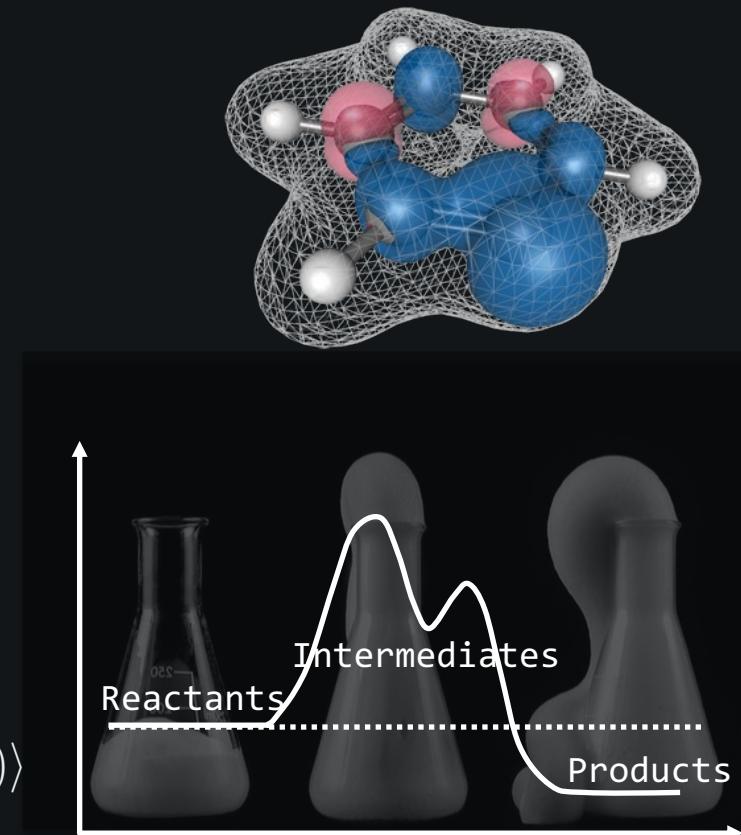
Use computer simulations to assist in solving chemical problems:

- Molecular structure
- Reaction rates
- Reaction pathways

$$H_{\text{el}} = -\frac{1}{2} \sum_{i=1}^N \nabla_i^2 - \sum_{i=1}^{N_{\text{el}}} \sum_{A=1}^{N_{\text{nu}}} \frac{Z_A}{r_{iA}} + \sum_{i=1, j>i}^{N_{\text{el}}, N_{\text{el}}} \frac{1}{r_{ij}}$$

$$H_{\text{el}} \Psi(r_1, r_2, \dots, r_N) = E_0 \Psi(r_1, r_2, \dots, r_N)$$

$$\Psi(r_1, r_2, \dots, r_N) = \sum_I C_I |\phi_{I_1}(r_1) \phi_{I_2}(r_2) \dots \phi_{I_N}(r_N)\rangle$$



# Why quantum chemistry is a challenge?

Solving interacting fermionic problems is at the core of most challenges in computational physics and high-performance computing: the exact electronic wavefunction for a system with  $N$  electrons expanded in  $M$  orbitals (basis functions) scales “**exponentially**”

$$\Psi(r_1, r_2, \dots, r_N) = \sum_I C_I |\phi_{1I}(r_1)\phi_{2I}(r_2) \dots \phi_{NI}(r_N)\rangle$$

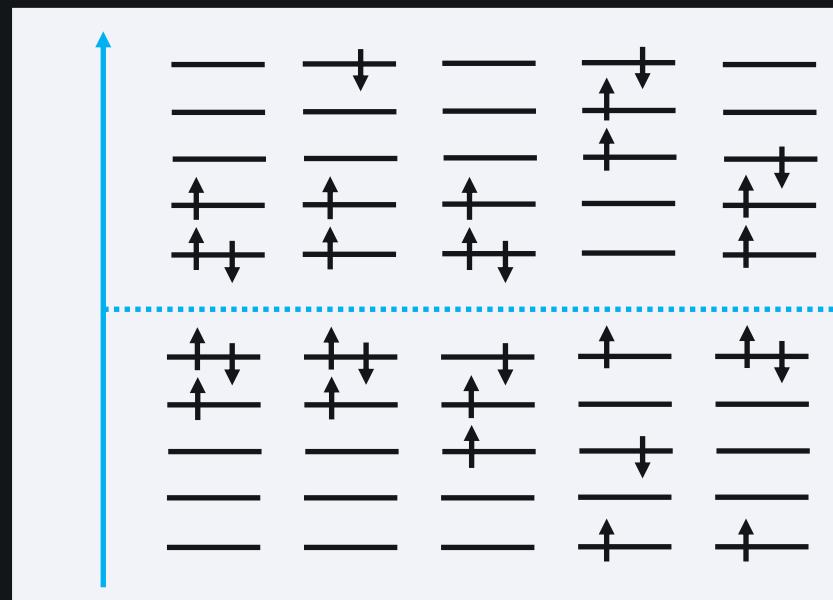
The meaning of exponential scaling

$M$ : # basis functions

$$\frac{M!}{(M - N)! N!}$$

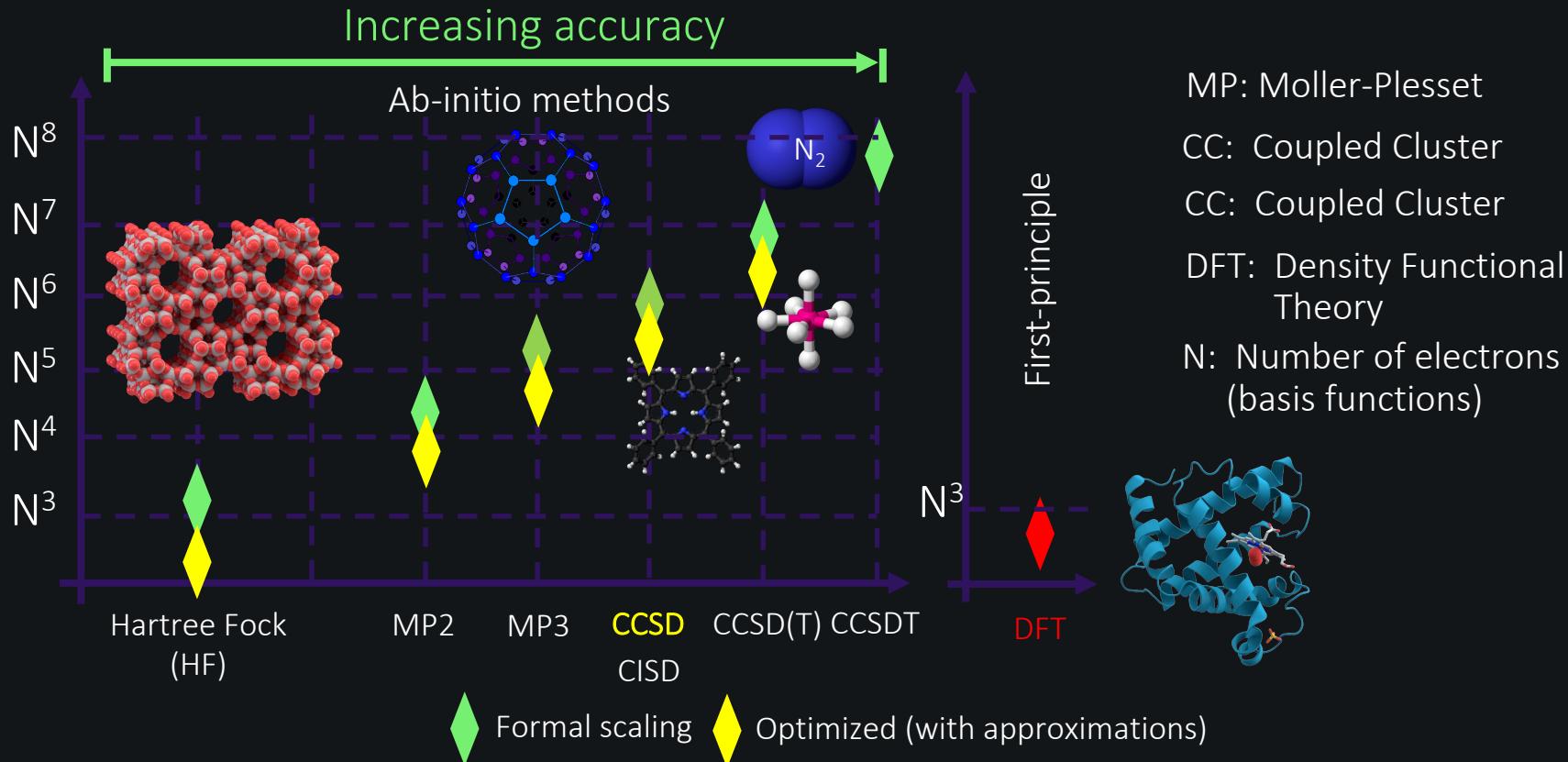
$N$ : # electrons

“There are  $\approx 10^{12}$  different possibilities to distribute 21 electrons in 43 spin orbitals.”  
[Markus Reiher]



# Why quantum chemistry is a challenge?

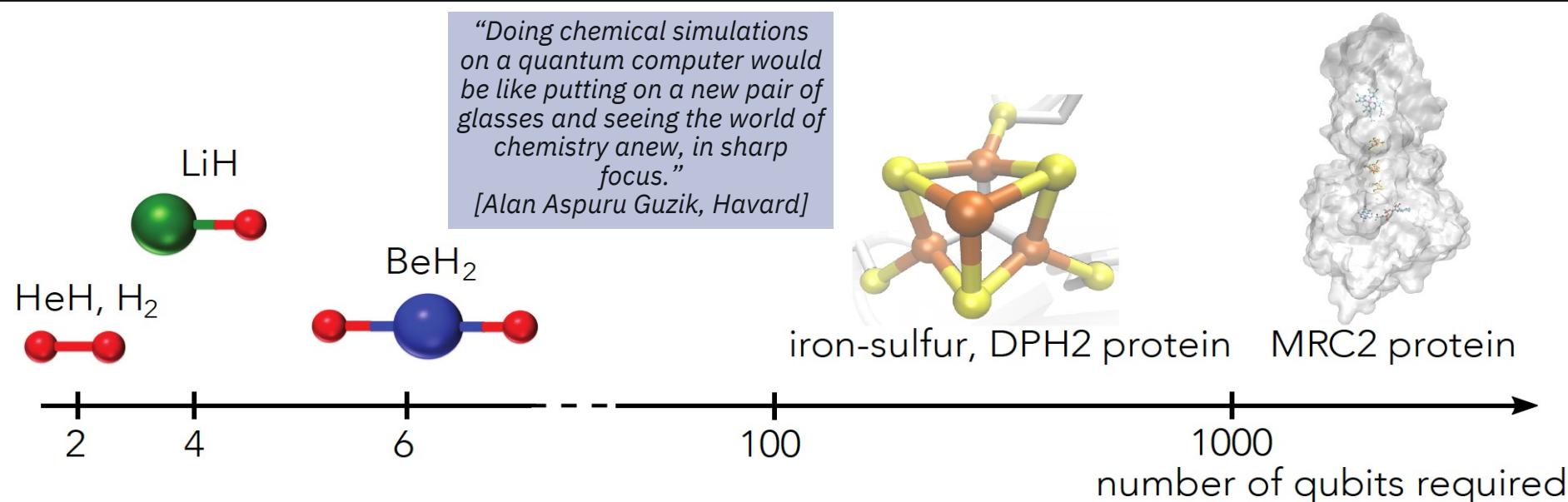
Classically, **several approximations** have been derived to break the exponential scaling



# Why quantum chemistry is important?

Problems that require a more accurate description of the electronic structure (better than DFT):

- **Industrial processes:** catalysis; design; CO<sub>2</sub> sequestration; photochemistry
- **Chemistry/Biology/Medicine:** electronic structure combined with ML for drug discovery



# What kind of problems are we interested in?

Some examples of interesting and important problems that we are using a quantum computer for are:

- Electronic Structure Problem
  - Ground State and Excited States
  - Properties of Molecular Systems
- Chemical Reaction Understanding
- Quantum and Classical Dynamics
- Optimization problems in Natural Sciences
  - Material Design
  - Protein Folding

# What is the input of the problem and how do we map it in a quantum computer?

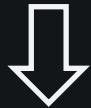
Fermionic Hamiltonian

$$\hat{H}_{elec} = \sum_{pq} h_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

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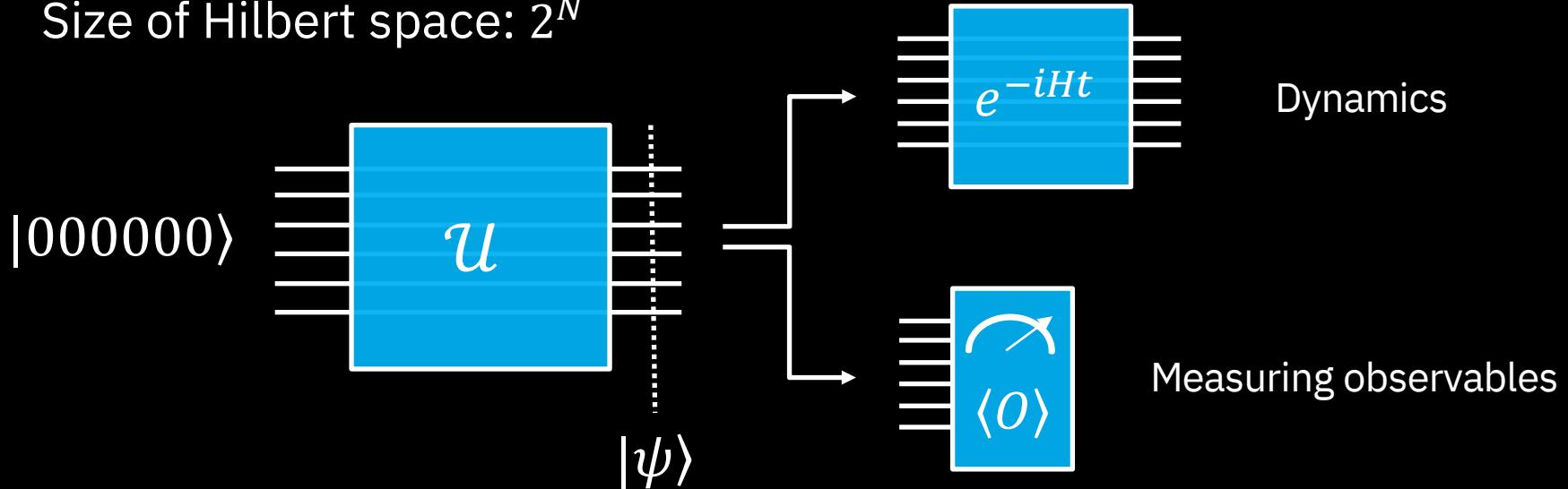


Qubit Hamiltonian

$$\hat{H}_{elec} = \sum_i c_i \hat{P}_i$$

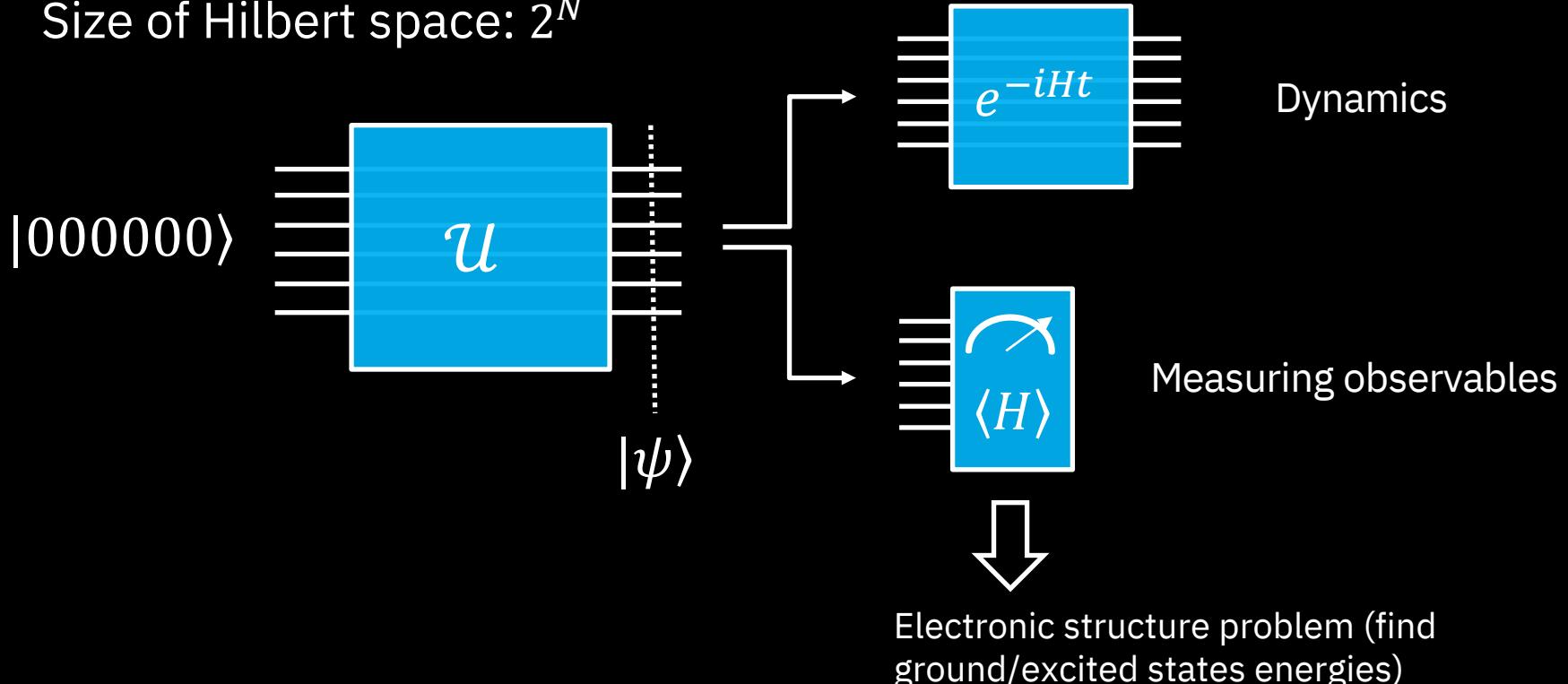
# Quantum chemistry on a quantum computer: the circuit model

Size of Hilbert space:  $2^N$

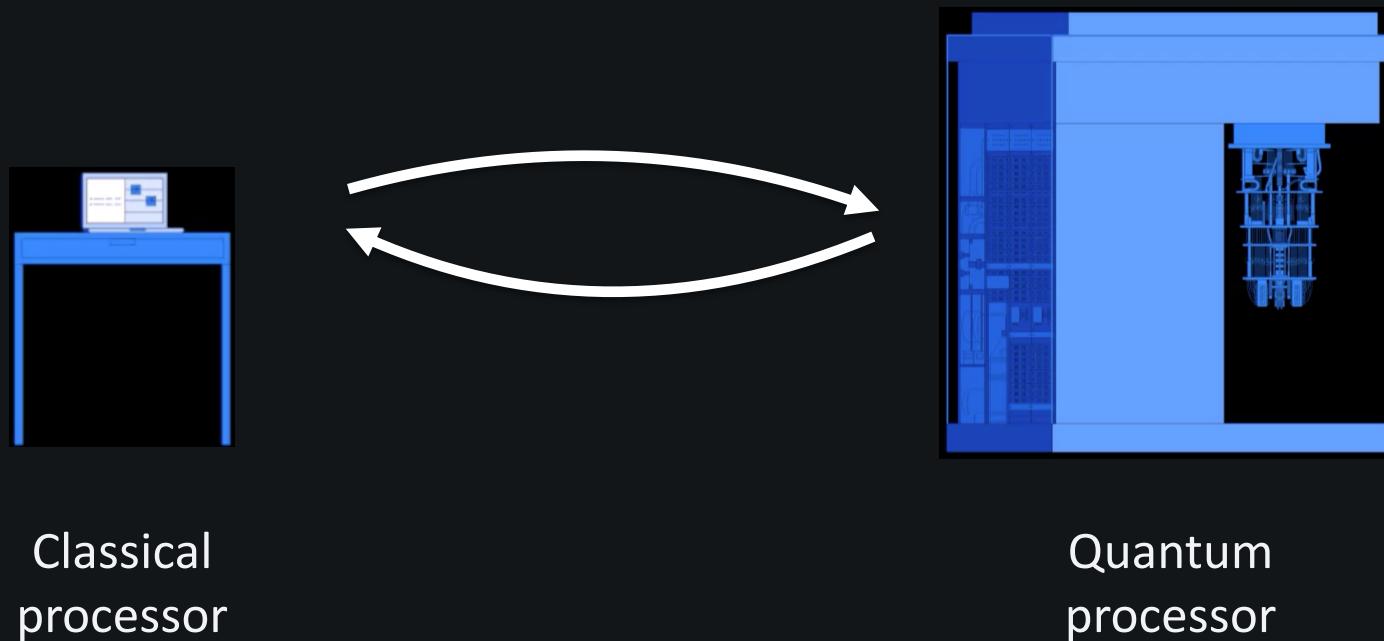


# Quantum chemistry on a quantum computer: the circuit model

Size of Hilbert space:  $2^N$



Near-term quantum chemistry relies on hybrid quantum-classical algorithms.

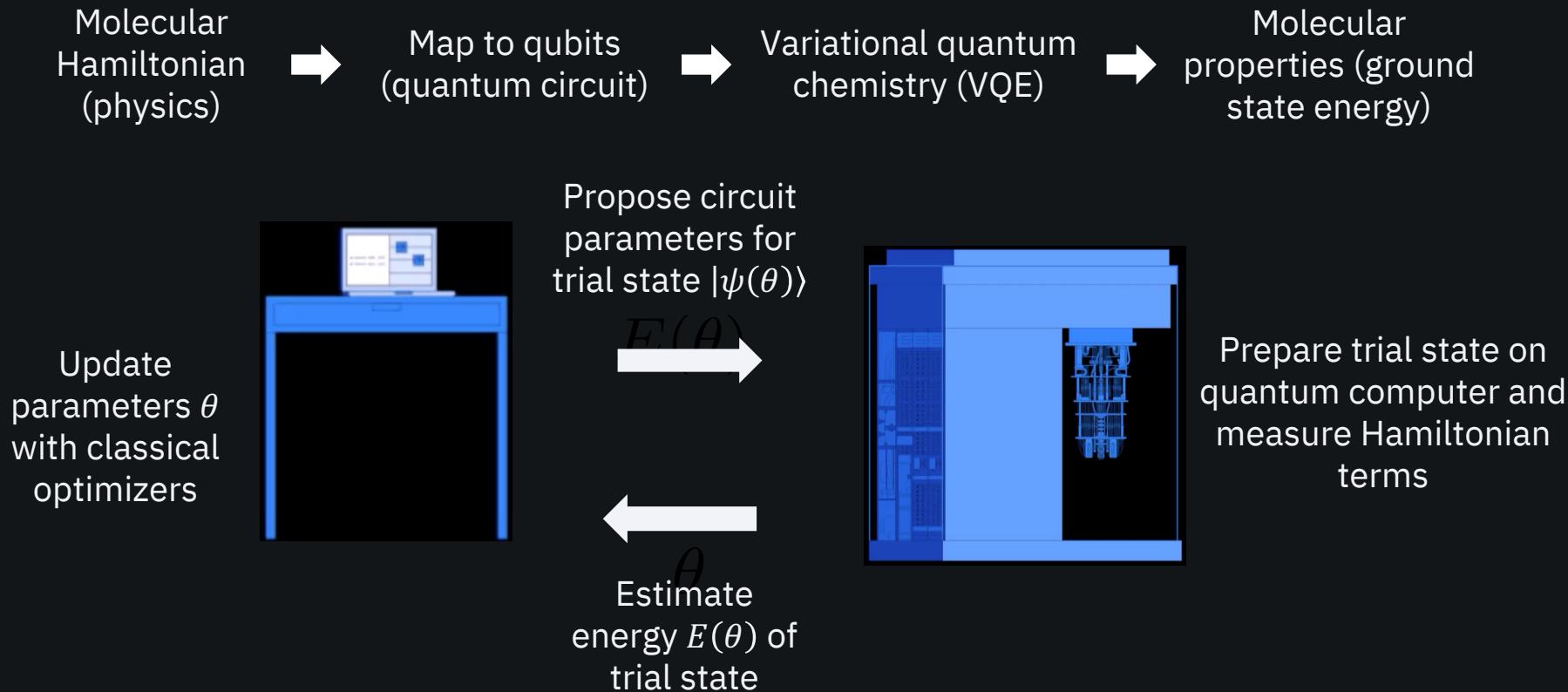


Near-term quantum chemistry relies on hybrid quantum-classical algorithms.

### Advantages:

- Use **short-depth quantum circuits** that fit into our coherence time of the qubits
- Can potentially **improve on best classical estimates** by using non-classical trial states
- Store a quantum state with **exponentially fewer resources** than required classically

# Near-term quantum chemistry relies on hybrid quantum-classical algorithms.



# Variational Quantum Eigensolver

Fermionic Hamiltonian

$$\hat{H}_{elec} = \sum_{pq} h_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

mapping



Qubit Hamiltonian

$$\hat{H}_{elec} = \sum_i c_i \hat{P}_i$$



classical

Calculate energy

$$E = \sum_i c_i \langle \Psi(\theta) | P_i | \Psi(\theta) \rangle \geq E_{\text{exact}}$$

Adjust parameters

$$\{\theta_i\}$$



Prepare trial state

$$|\Psi(\theta)\rangle$$

Measure expectation values

$$\langle \Psi(\theta) | P_i | \Psi(\theta) \rangle$$

quantum

Solution  $\{\theta_{opt}\}$

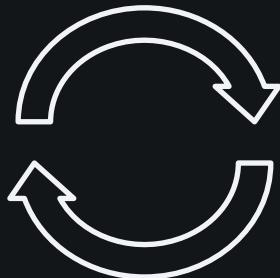
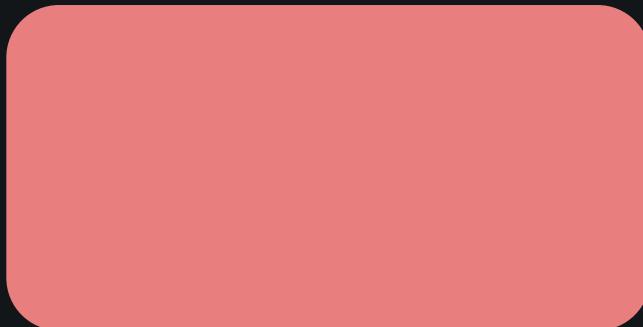
There are still many things to be optimized...

# Variational Quantum Eigensolver

Fermionic Hamiltonian

*Can we transfer more complexity to the problem definition? (e.g. transcorellated, MC schemes ...)*

classical



quantum



# Variational Quantum Eigensolver

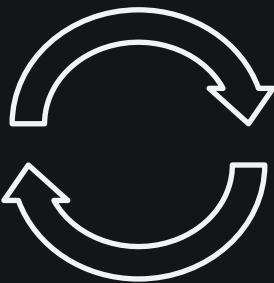
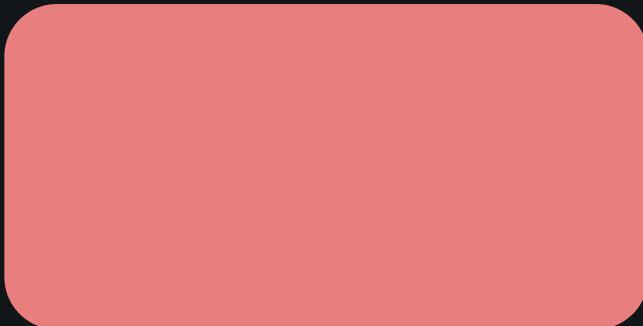
Fermionic Hamiltonian

mapping

Qubit Hamiltonian

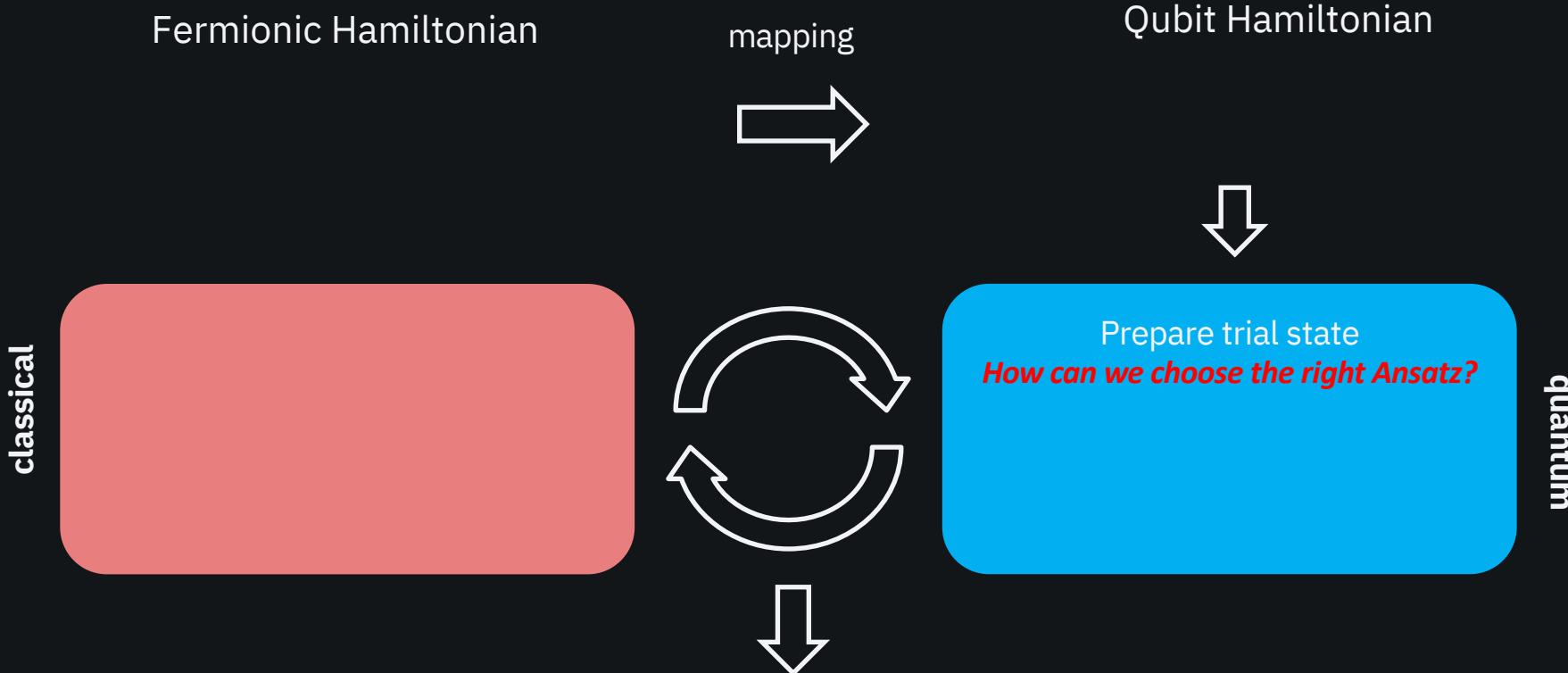
*Can we find more efficient mapping for the qubit Hamiltonian?*

classical



quantum

# Variational Quantum Eigensolver



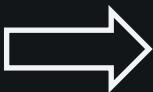
# Variational Quantum Eigensolver

classical

Fermionic Hamiltonian

mapping

Qubit Hamiltonian

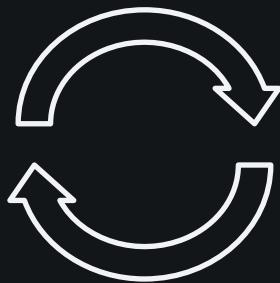


Prepare trial state

Measure expectation values

*Can we use different aggregation  
functions for non quantum-mechanical  
quantities?*

quantum



# Variational Quantum Eigensolver

classical

Fermionic Hamiltonian

mapping

Qubit Hamiltonian

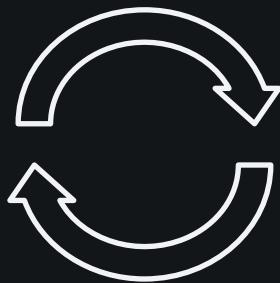
Calculate energy  
Can we mitigate for the different errors happening?

Adjust parameters



Prepare trial stat

Measure expectation values



quantum

# Variational Quantum Eigensolver

Fermionic Hamiltonian

mapping

Qubit Hamiltonian



*What is the best optimizer?*

classical

Calculate energy

Adjust parameters



Prepare trial stat

Measure expectation values

quantum



# Variational Quantum Eigensolver

classical

Fermionic Hamiltonian

mapping

Qubit Hamiltonian



Calculate energy

Adjust parameters



Prepare trial stat

Measure expectation values

quantum

Solution  $\{\theta_{opt}\}$ *What do we do with the solution?*

# Input of the Problem

**1. Solve Hartree Fock calculation for the orbitals**

$$F(\{\phi_i(r)\})\phi_i(r) = \epsilon_i\phi_i(r)$$

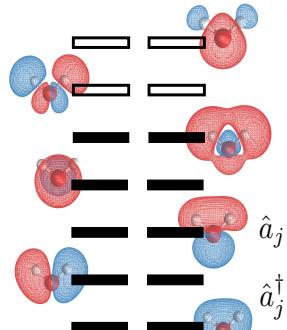
**2. Compute all necessary 1- and 2-body integrals**

$$h_{pq} = \int dr \phi_p^*(r) \left( -\frac{1}{2} \nabla^2 - \sum_I \frac{Z_I}{|R_I - r|} \right) \phi_q(r)$$

$$h_{pqrs} = \int dr_1 dr_2 \frac{\phi_p^*(r_1) \phi_q^*(r_2) \phi_r(r_2) \phi_s(r_1)}{|r_1 - r_2|}$$

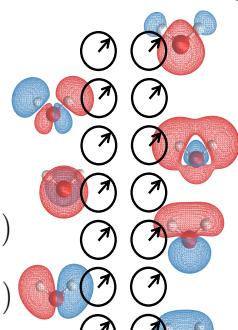
Fermions

$$\{a_i, a_i\} = 0, \{a_i^\dagger, a_i^\dagger\} = 0, \{a_i, a_j^\dagger\} = \delta_{i,j}$$



Spins

$$[\sigma_i, \sigma_i] = 0, [\sigma_i^\dagger, \sigma_i^\dagger] = 0, [\sigma_i, \sigma_j^\dagger] = \delta_{i,j}$$



mapping

Jordan-Wigner

$$\hat{a}_j = \bigotimes_{i=1}^{j-1} \hat{\sigma}_i^z \otimes (\hat{\sigma}_j^x + i\hat{\sigma}_j^y)$$

$$\hat{a}_j^\dagger = \bigotimes_{i=1}^{j-1} \hat{\sigma}_i^z \otimes (\hat{\sigma}_j^x - i\hat{\sigma}_j^y)$$

$$\hat{H}_{elec} = \sum_{pq} h_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

Classical pre-processing

Mappings

Jordan-Wigner

Bravyi-Kitaev

Parity

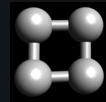
BK Superfast Encoding

...

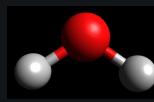
Number of Pauli Tensor Strings in the second quantized Hamiltonian:  $\mathcal{O}(N^4)$

# Reducing resource requirements

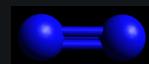
Extending VQE to larger/strongly correlated molecular systems...



$\text{H}_4$  (4 e<sup>-</sup>/8 MOs)

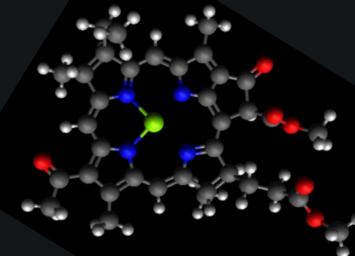


$\text{H}_2\text{O}$  (10 e<sup>-</sup>/14 MOs)



$\text{N}_2$  (14 e<sup>-</sup>/20 MOs)

.....



## Noisy Intermediate-Scale Quantum (NISQ) computers

(50-100 qubits + noise)

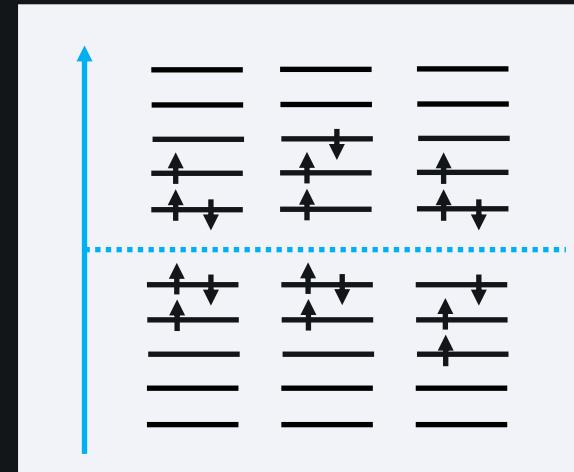
- Coherence time of qubits ~50μs. Single-qubit gate ~10ns and 2-qubit gate ~100ns → 500 CNOTs

e.g., LiH (10 qubits)

- UCCSD Ansatz: 2592 CNOTs
- Number of Pauli terms: 276

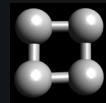


- **Reduction of active space**
- UCC Ansatz truncation
- Rotation of Hamiltonian to more efficient basis

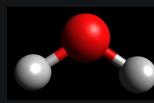


# Reducing resource requirements

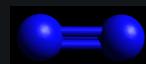
Extending VQE to larger/strongly correlated molecular systems...



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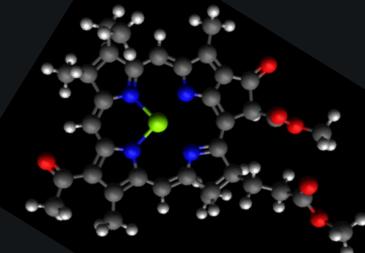


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## Noisy Intermediate-Scale Quantum (NISQ) computers

(50-100 qubits + noise)

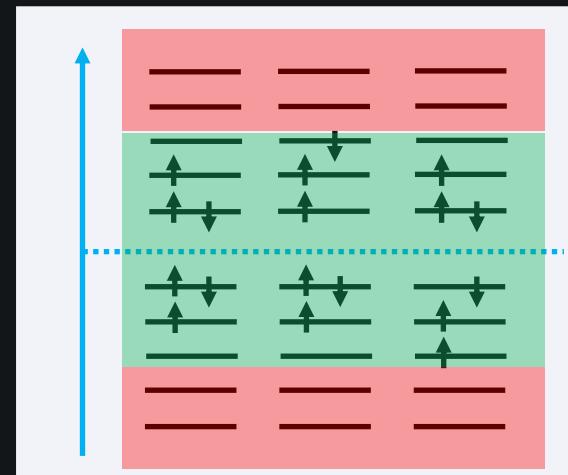
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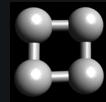


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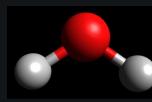


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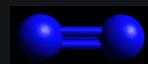
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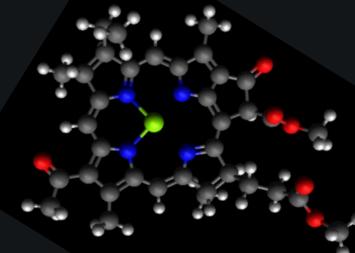


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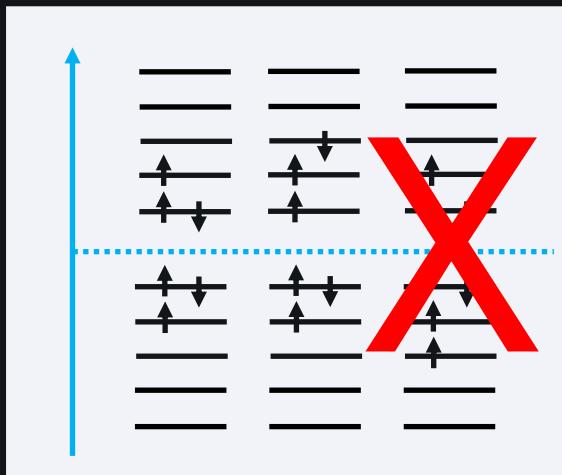
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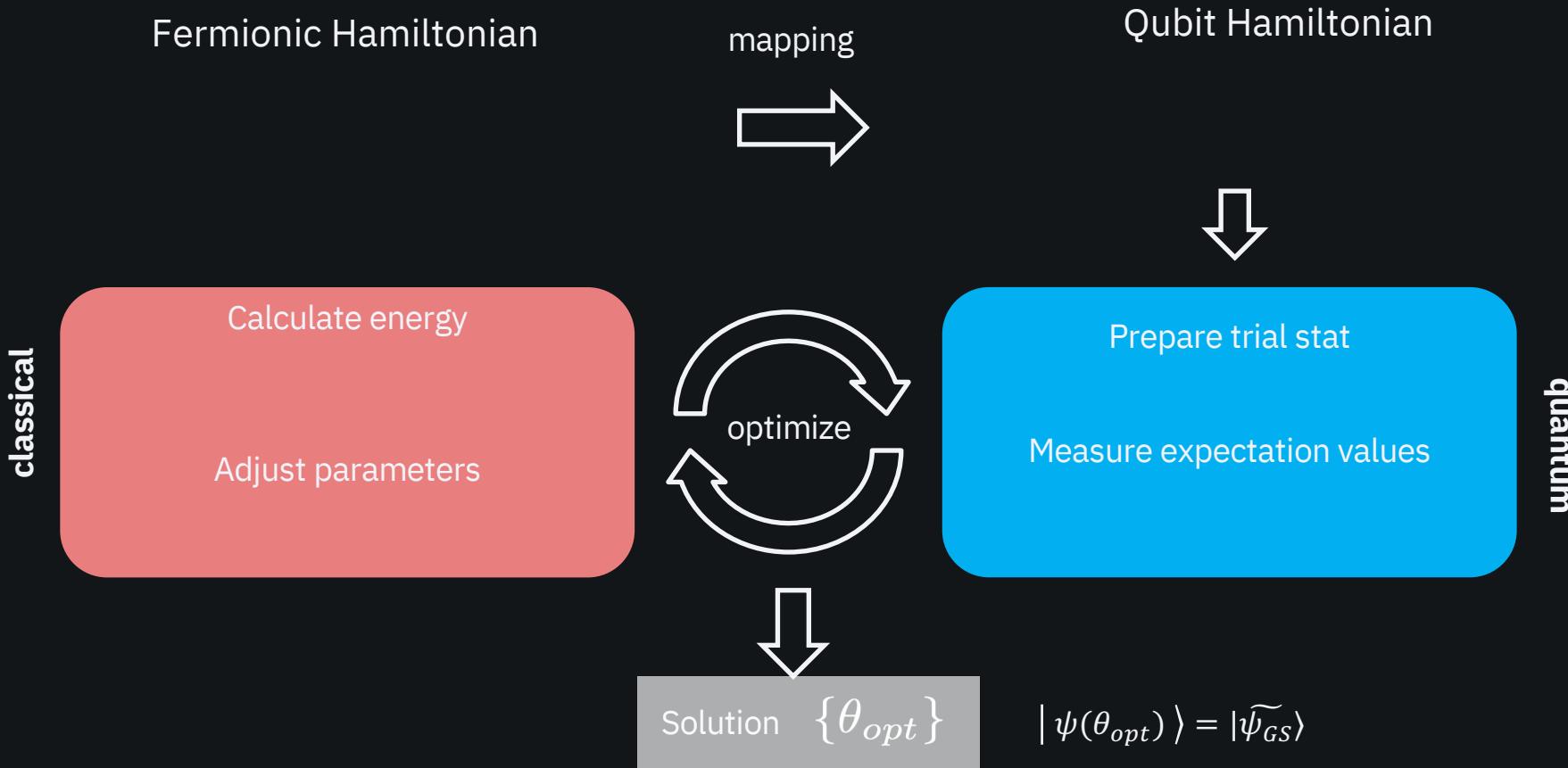
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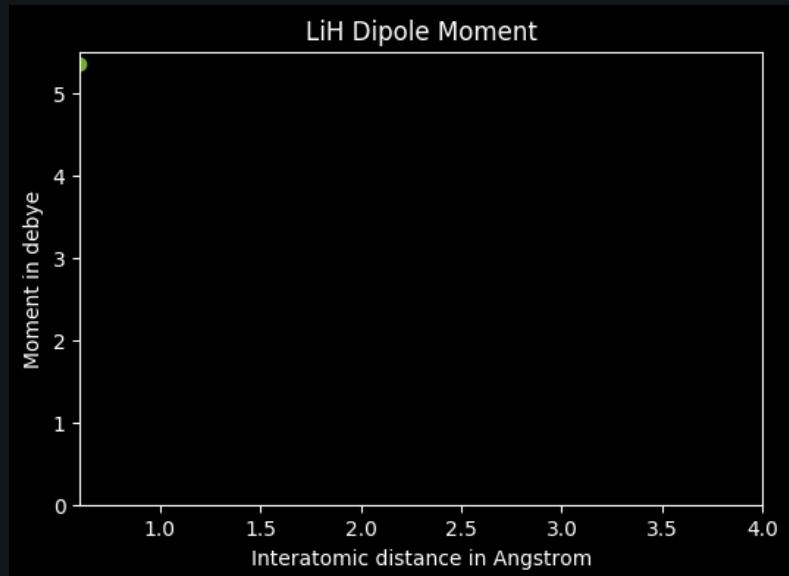
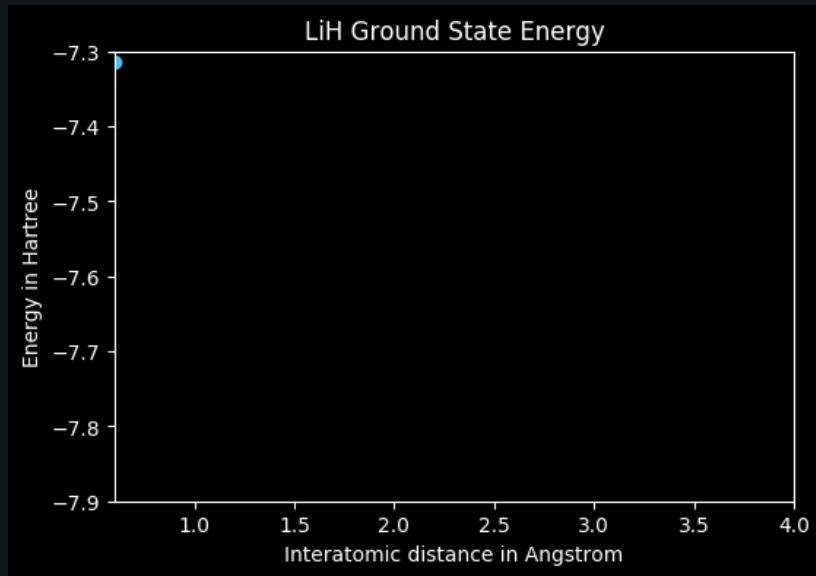
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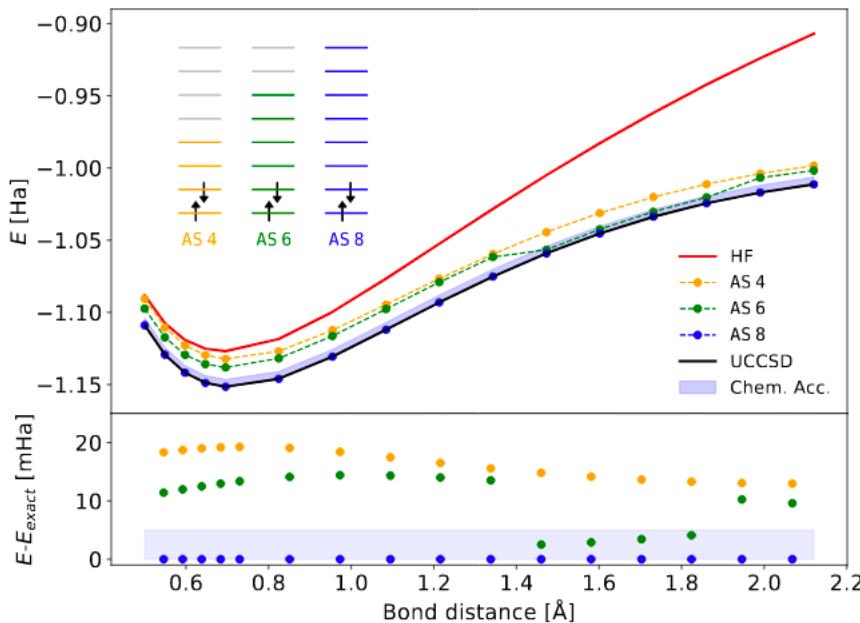
# Solution of the Problem



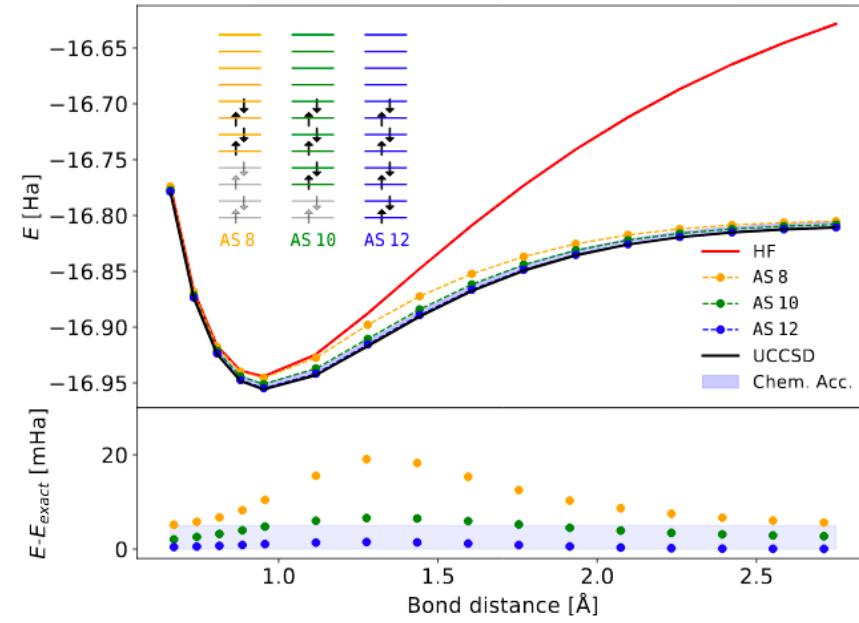
# Output of the Problem



# VQE Results for molecular systems

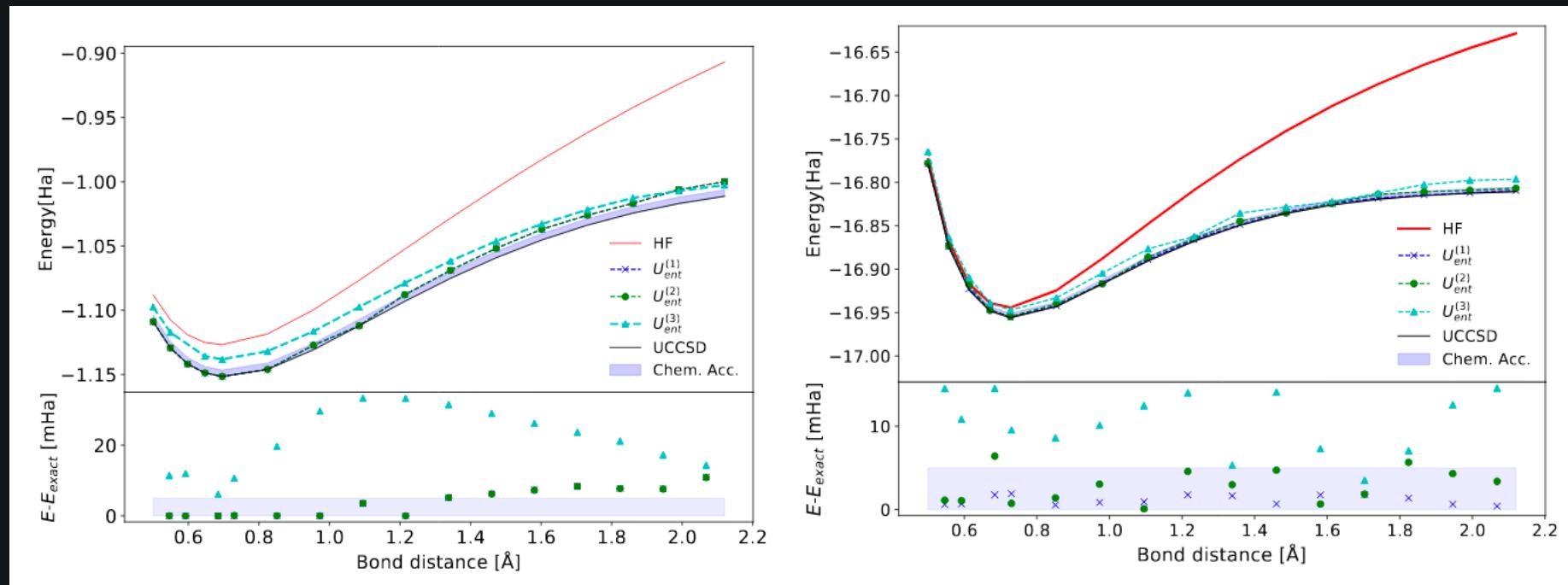


$\text{H}_2$ , 631G Basis Set



$\text{H}_2\text{O}$ , STO3G Basis Set

# VQE Results for molecular systems



$\text{H}_2$ , 631G Basis Set

$\text{H}_2\text{O}$ , STO3G Basis Set

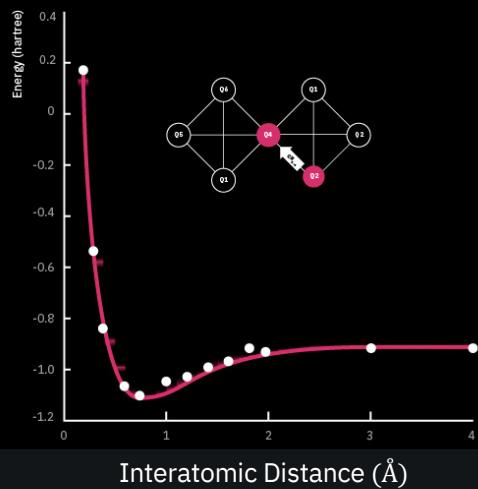
Presence of noise can have impact...

# Computing the ground state energy for small molecules

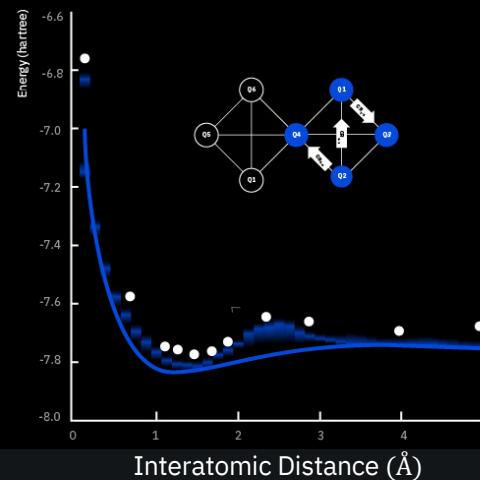
A. Kandala, A. Mezzacapo, K. Temme, M. Takita, M. Brink, J. M. Chow, J. M. Gambetta. Nature **549**, 242 (2017)



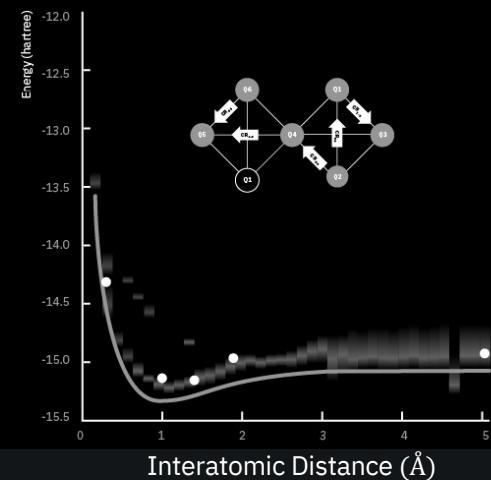
Hydrogen ( $H_2$ ): 2 Qubits



Lithium Hydride (LiH): 4 Qubits



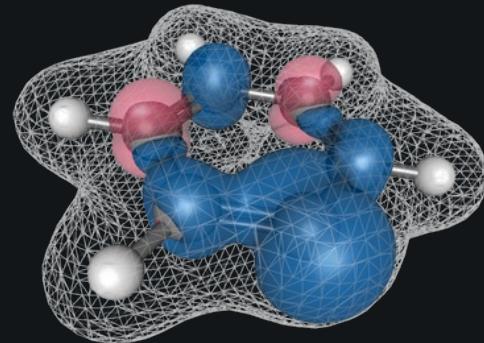
Beryllium hydride ( $BeH_2$ ): 8 Qubits



But even with an approximate / noisy result we can measure multiple properties (observables) of the system...

# Other quantities that we want to measure

- Energy
- Dipole moment
- Angular momentum
- Particle number
- Magnetization
- Forces



# Is the solution exact?

- There is no guarantee that the chosen ansatz will take you to the ground state of the system
- The ground state may not be described by the family of the variational ansatzes being used

Solution 1: Try constraining the Hamiltonian to keep in the right sector

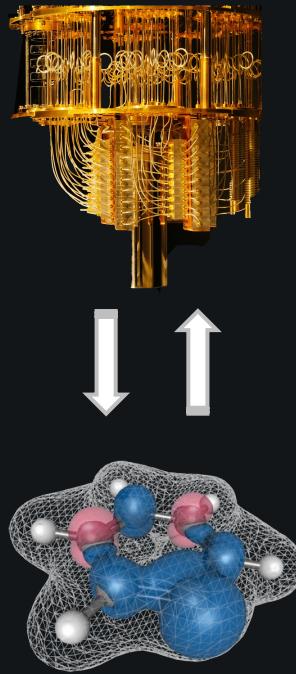
Solution 2 : Make the ansatze richer by increasing the depth

Finding the ground state of a k-local Hamiltonian is a QMA complete problem

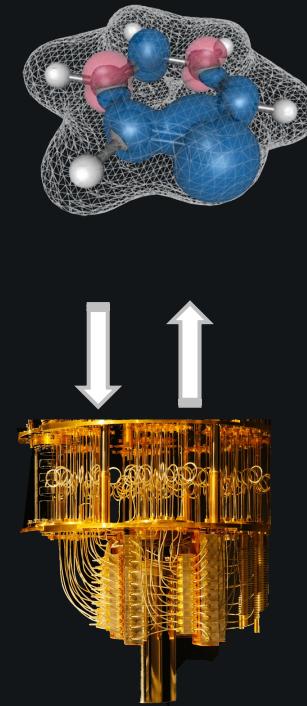
*More Information about this to come in one of the next lectures...*



Can we make the solution better?



# Break



# Mid-term Summary

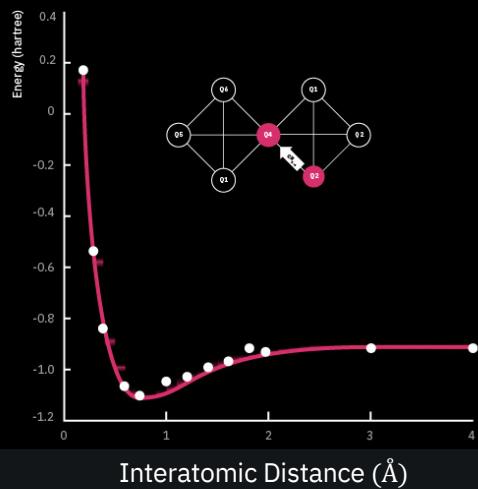
- Quantum Chemistry is important
- Quantum Chemistry in the near term quantum computers relies on Hybrid Quantum Classical algorithms
- Certain Approximation can be applied to make the simulations better fitted for near term quantum computers
- Can we make the solutions better?

# Computing the ground state energy for small molecules

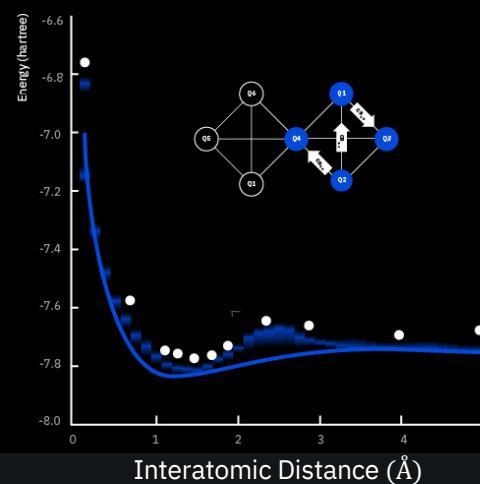
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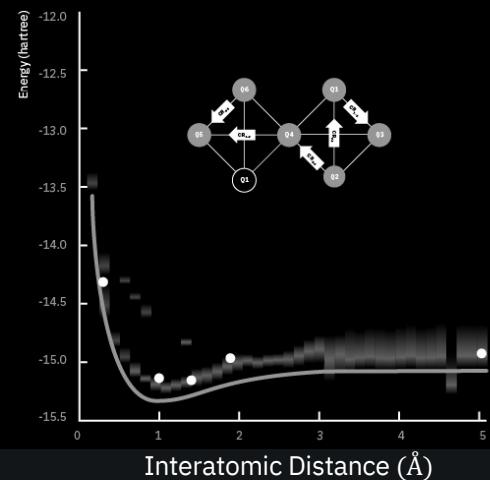
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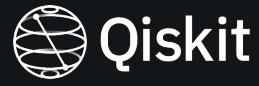
Beryllium hydride ( $BeH_2$ ): 8 Qubits



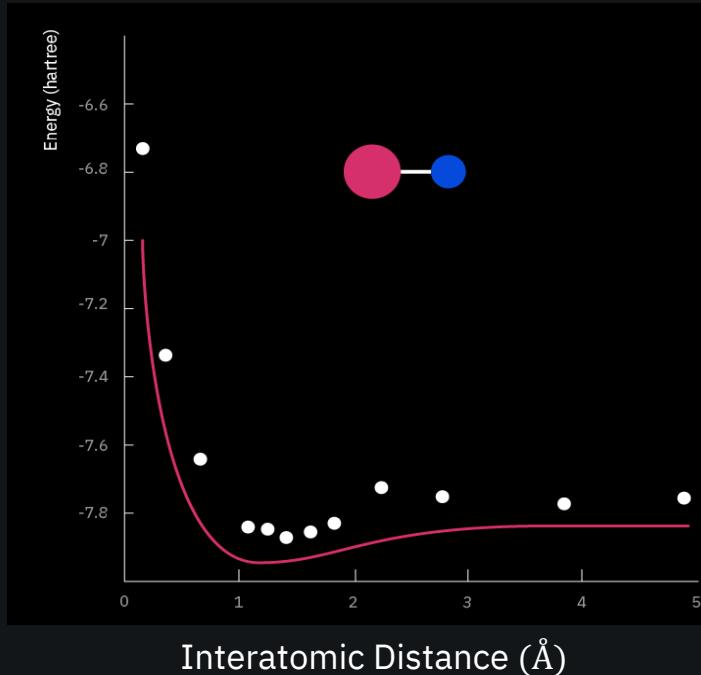


Can we make the solution better?

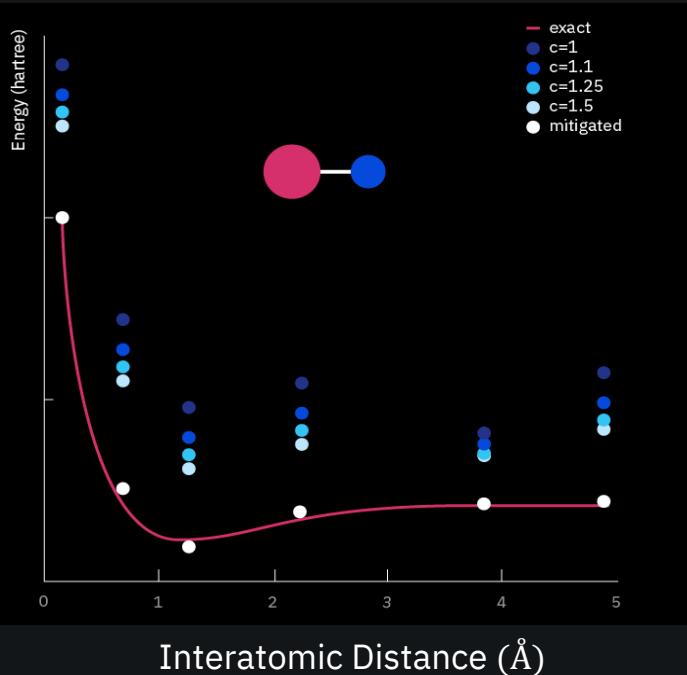
# Can we make the solution better?



2017



2019



# Can we make the solution better?

## From the hardware side:

- roadmap to fault-tolerance

Detecting arbitrary quantum errors via stabilizer measurements on a sublattice of the surface code

Demonstration of weight-four parity measurements in the surface code architecture

Hardware-efficient Quantum Optimizer for Small Molecules and Quantum Magnets

Experimental demonstration of fault-tolerant state preparation with superconducting qubits

Maika Takita, Andrew W. Cross, A. D. Córcoles, Jerry M. Chow, and Jay M. Gambetta  
IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA

Robust quantum computation requires encoding delicate quantum information into degrees of freedom that are hard for the environment to change. Quantum encodings have been demonstrated in many physical systems by observing and correcting storage errors, but applications require not just storing information; we must accurately compute even with faulty operations. The theory of fault-tolerant quantum computing illuminates a way forward by providing a foundation and collection of techniques for limiting the spread of errors. Here we implement one of the smallest quantum codes in a five-qubit superconducting transmon device and demonstrate fault-tolerant state preparation. We characterize the resulting codewords through quantum process tomography and study the free evolution of the logical observables. Our results are consistent with fault-tolerant state preparation in a protected qubit subspace.

## Solving problems with Quantum Computers

## From the algorithmic side:

- reduce overheads
- error mitigation
- new algorithms

Trading classical and quantum computational resources

Error mitigation for short depth quantum circuits

Tapering off qubits to simulate fermionic Hamiltonians

Sergey Bravyi,<sup>1</sup> Jay M. Gambetta,<sup>1</sup> Antonio Mezzacapo,<sup>1</sup> and Kristan Temme<sup>1</sup>

<sup>1</sup>IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA

(Dated: January 31, 2017)

We discuss encodings of fermionic many-body systems by qubits in the presence of symmetries. Such encodings eliminate redundant degrees of freedom in a way that preserves a simple structure of the system Hamiltonian enabling quantum simulations with fewer qubits. First we consider  $U(1)$  symmetry describing the particle number conservation. Using a previously known encoding based on the first quantization method a system of  $M$  fermi modes with  $N$  particles can be simulated on a quantum computer with  $Q = N \log_2(M)$  qubits. We propose a new version of this encoding tailored to variational quantum algorithms. Also we show how to improve sparsity of the simulator Hamiltonian using orthogonal arrays. Next we consider encodings based on the second quantization method. It is shown that encodings with a given filling fraction  $\nu = N/M$  and a qubit-per-mode ratio  $\eta = Q/M < 1$  can be constructed from efficiently decodable classical LDPC codes with the relative distance  $2\nu$  and the encoding rate  $1 - \eta$ . A family of codes based on high-girth bipartite

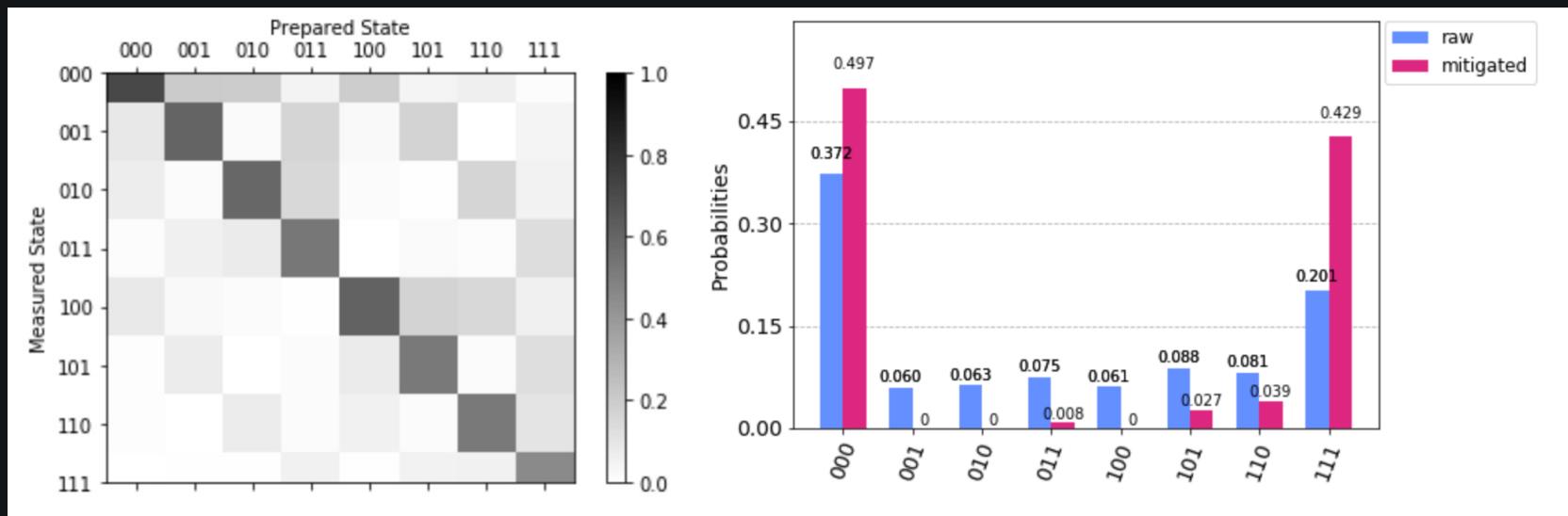
## From the software side:

- Quantum software

# Can we make the solution better?

Error Mitigation Techniques can be used to get a better result from a noisy hardware

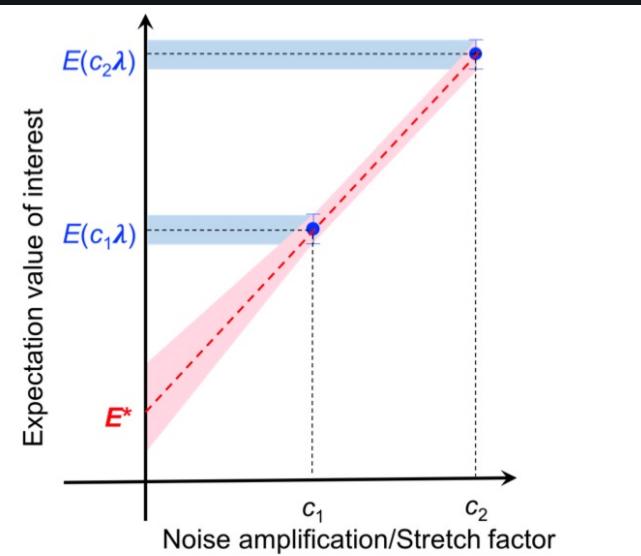
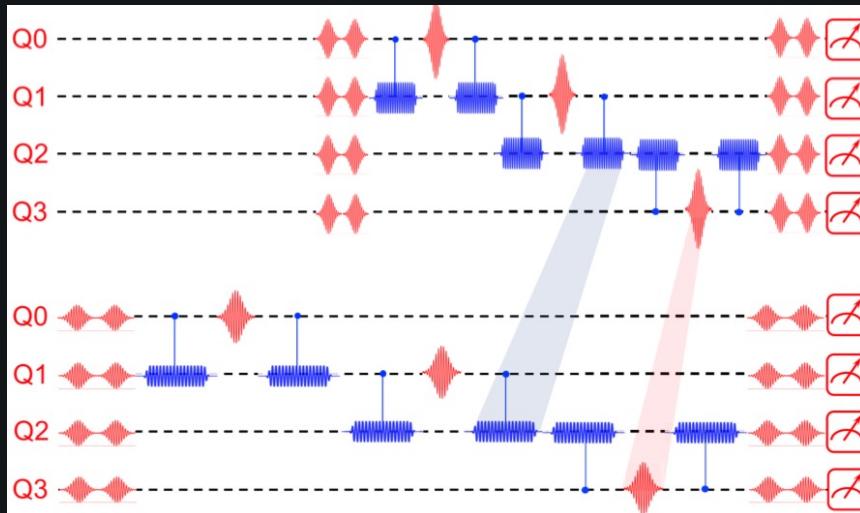
- Readout Error Mitigation technique



# Can we make the solution better?

Error Mitigation Techniques can be used to get a better result from a noisy hardware

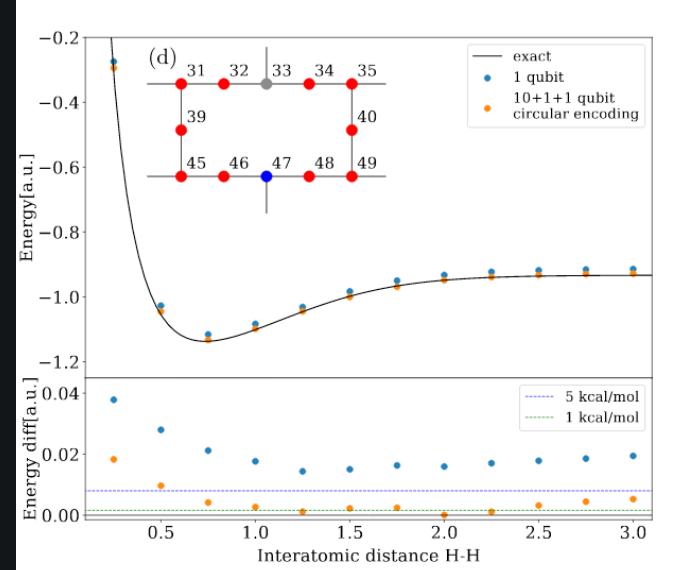
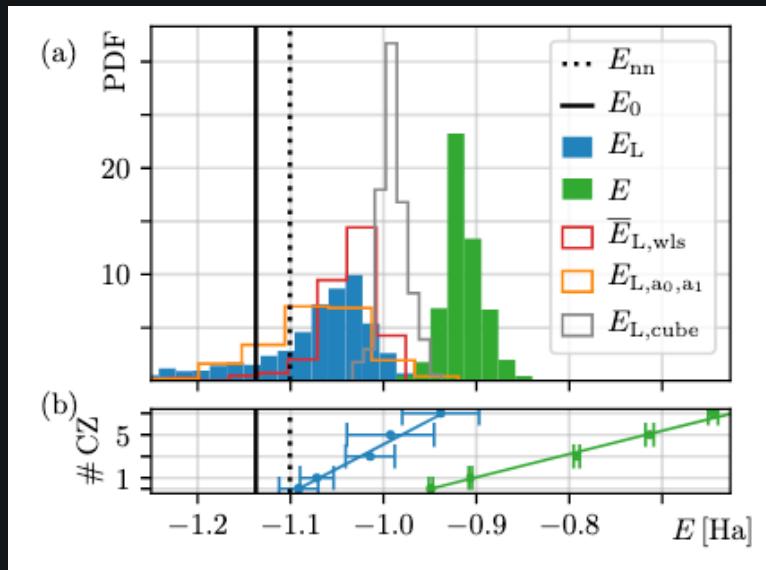
- Zero Noise Extrapolation



# Can we make the solution better?

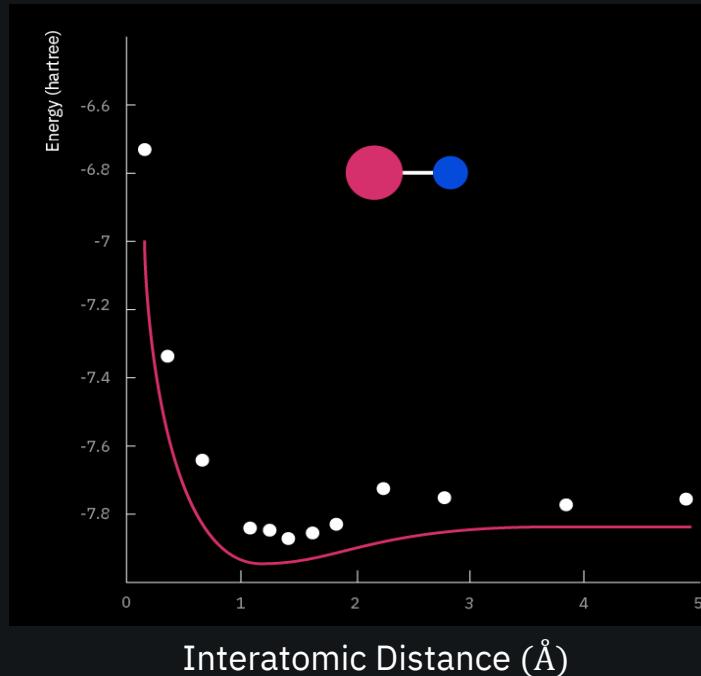
Error Mitigation Techniques can be used to get a better result from a noisy hardware

- Algorithmic Error Mitigation Techniques

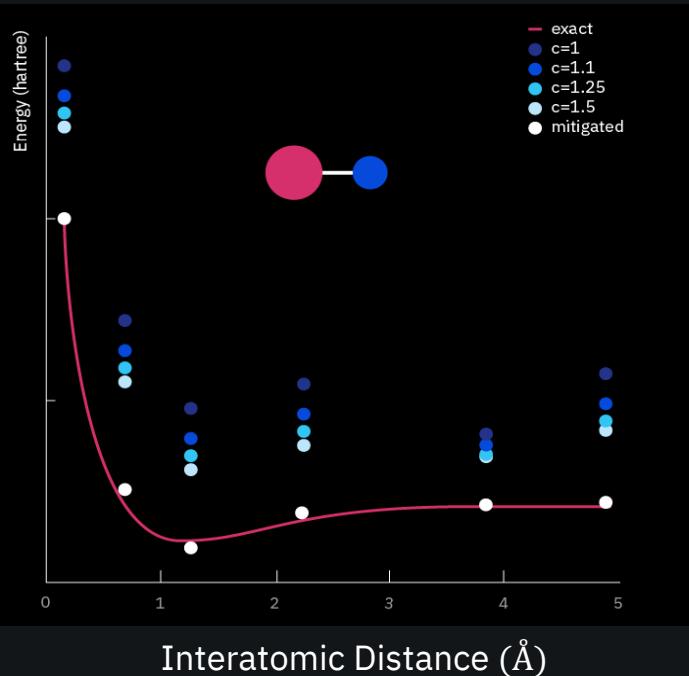


# Error Mitigation Techniques

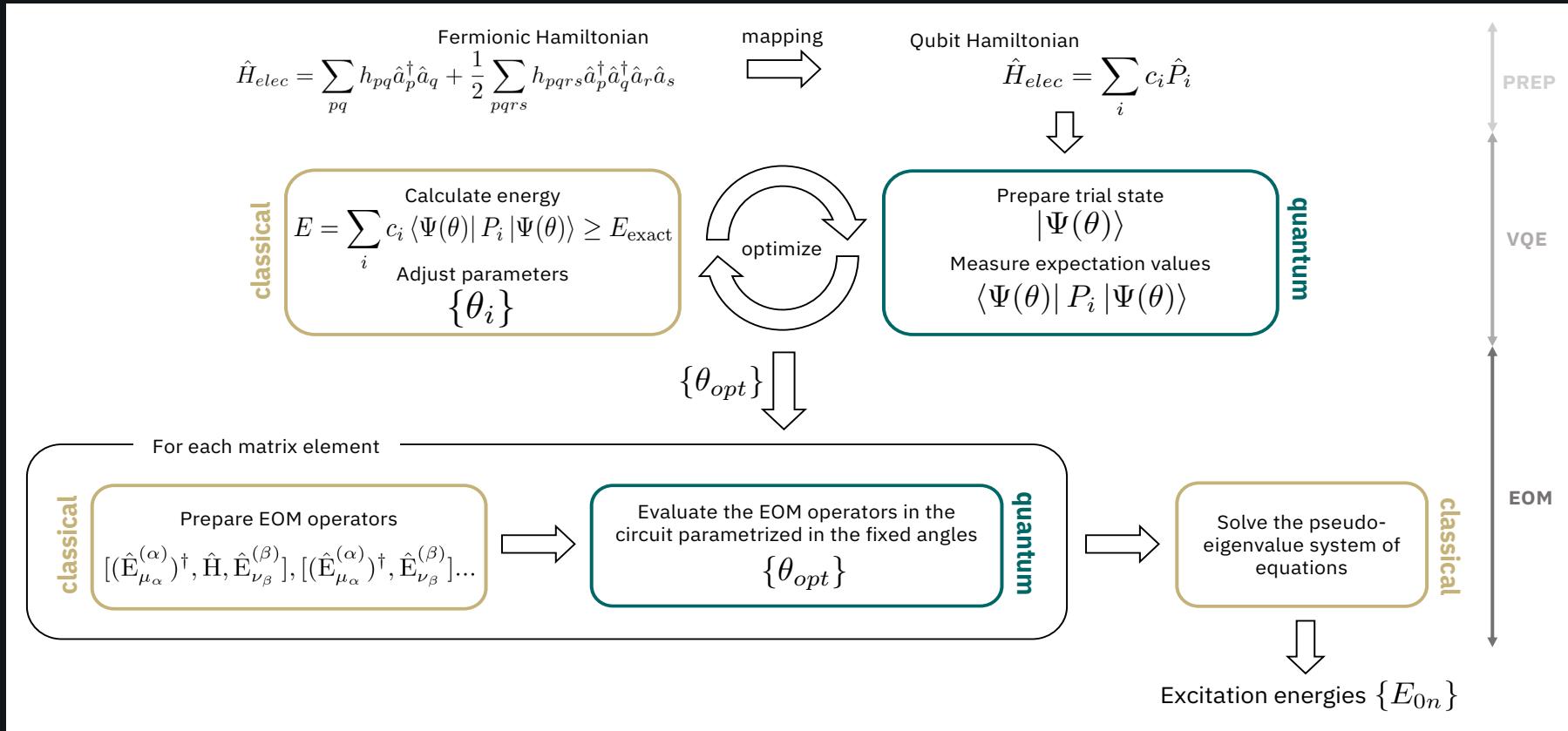
2017



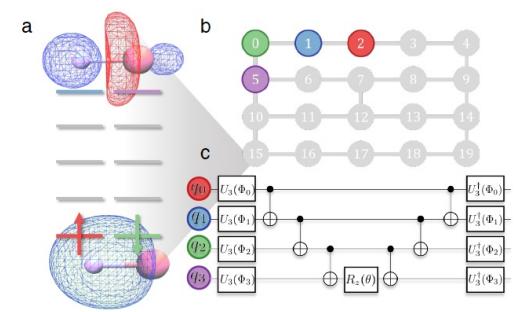
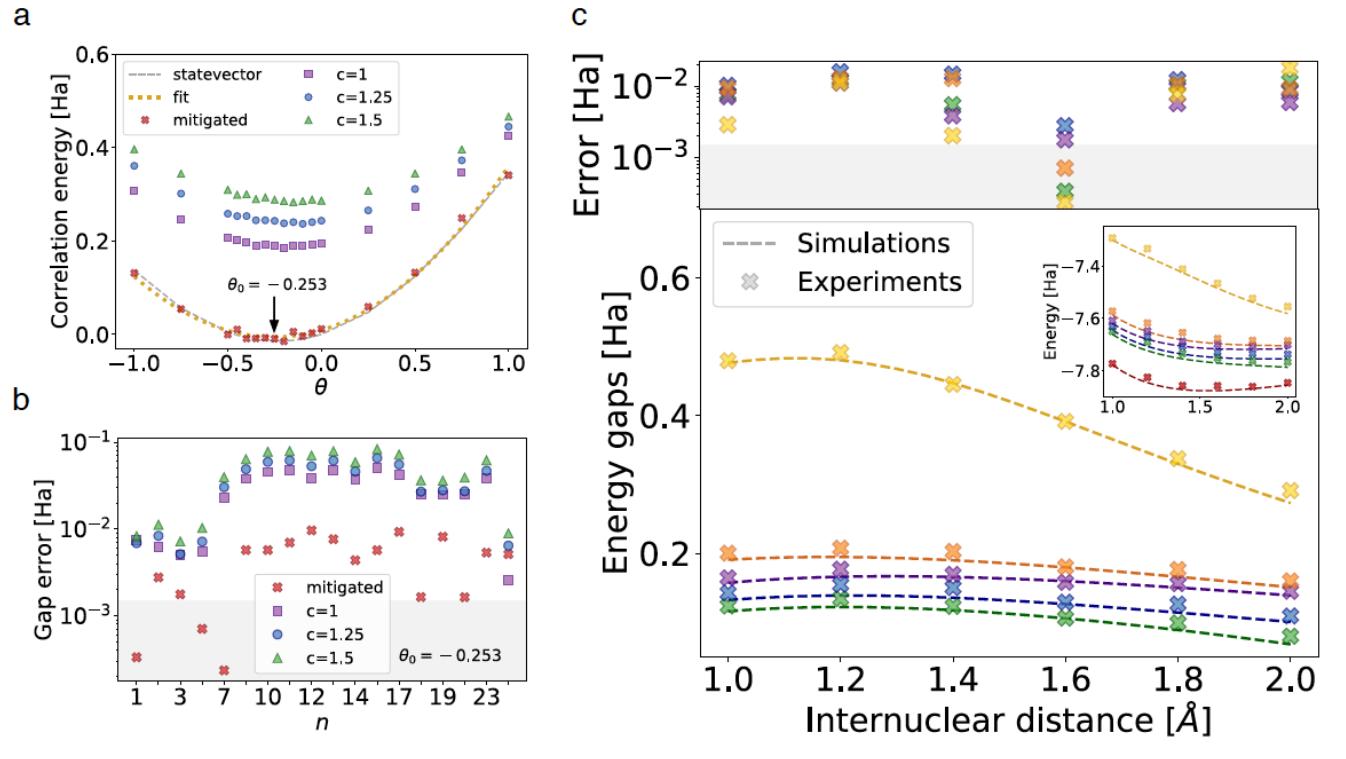
2019



# Extend the solution to Excited States

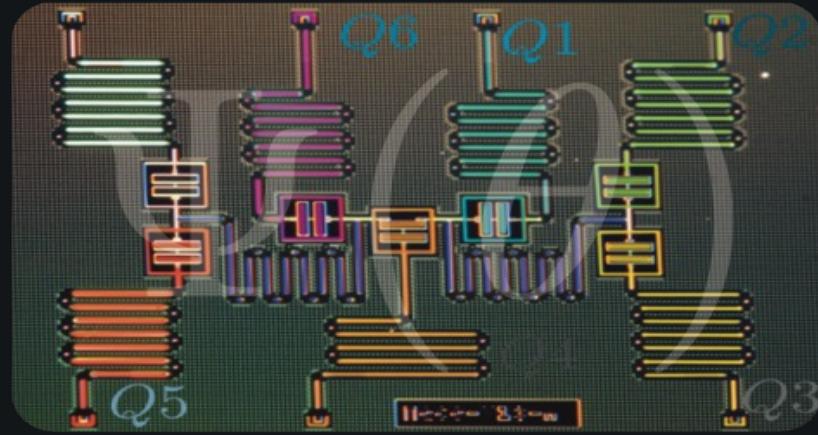


# Quantum Chemistry Calculations



Excited states of LiH (4 qubits) in IBMQ 20 qubit Poughkeepsie Hardware

How can we test/implement these algorithms ?



Qiskit takes care for the full implementation of hybrid quantum/classical algorithms for different applications and problems.

# Introducing the new Qiskit applications



[...] We're rearranging the framework's original “elements” — Terra, Aer, Ignis, and Aqua — into **more-focused application modules** that target specific user groups, and plug into the tools used by experts in different domains. [...] [2021]

# Qiskit Nature

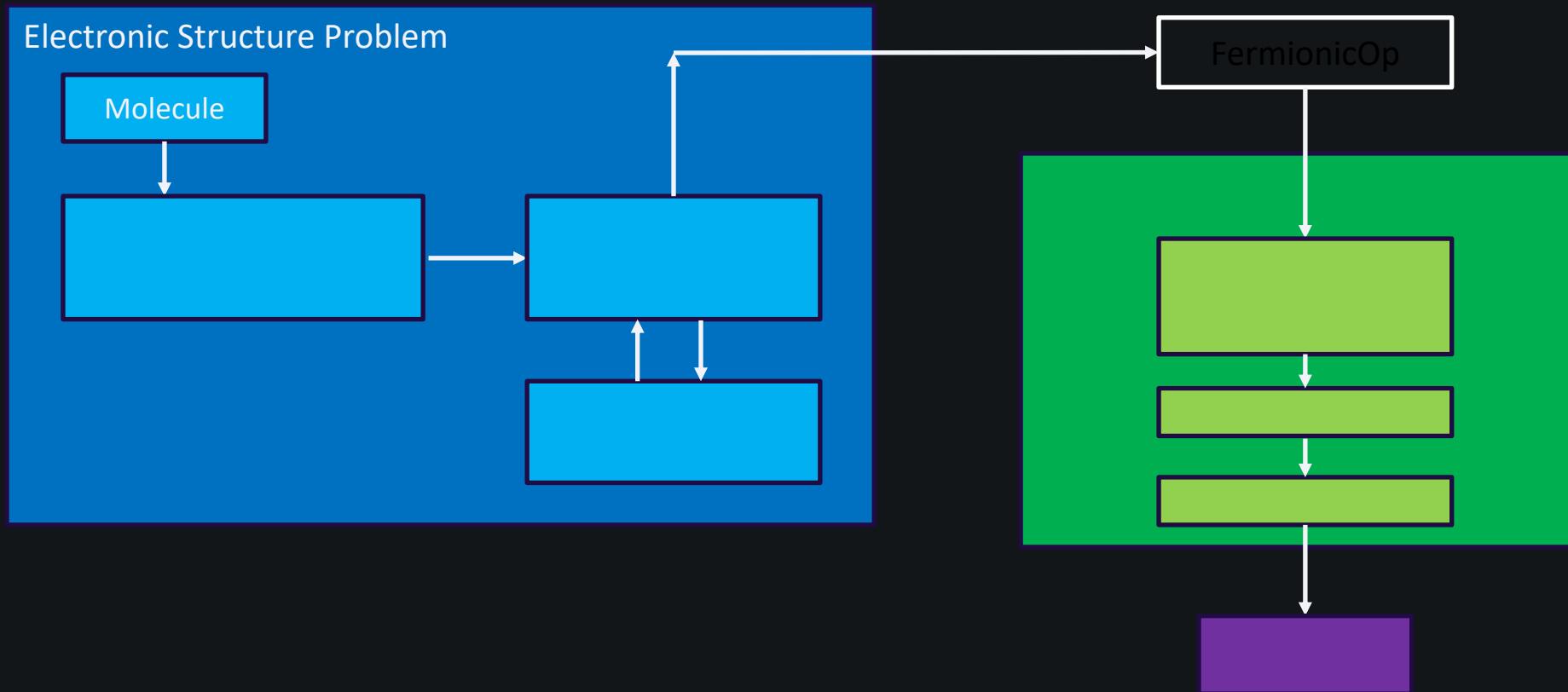


## Qiskit Nature aims in

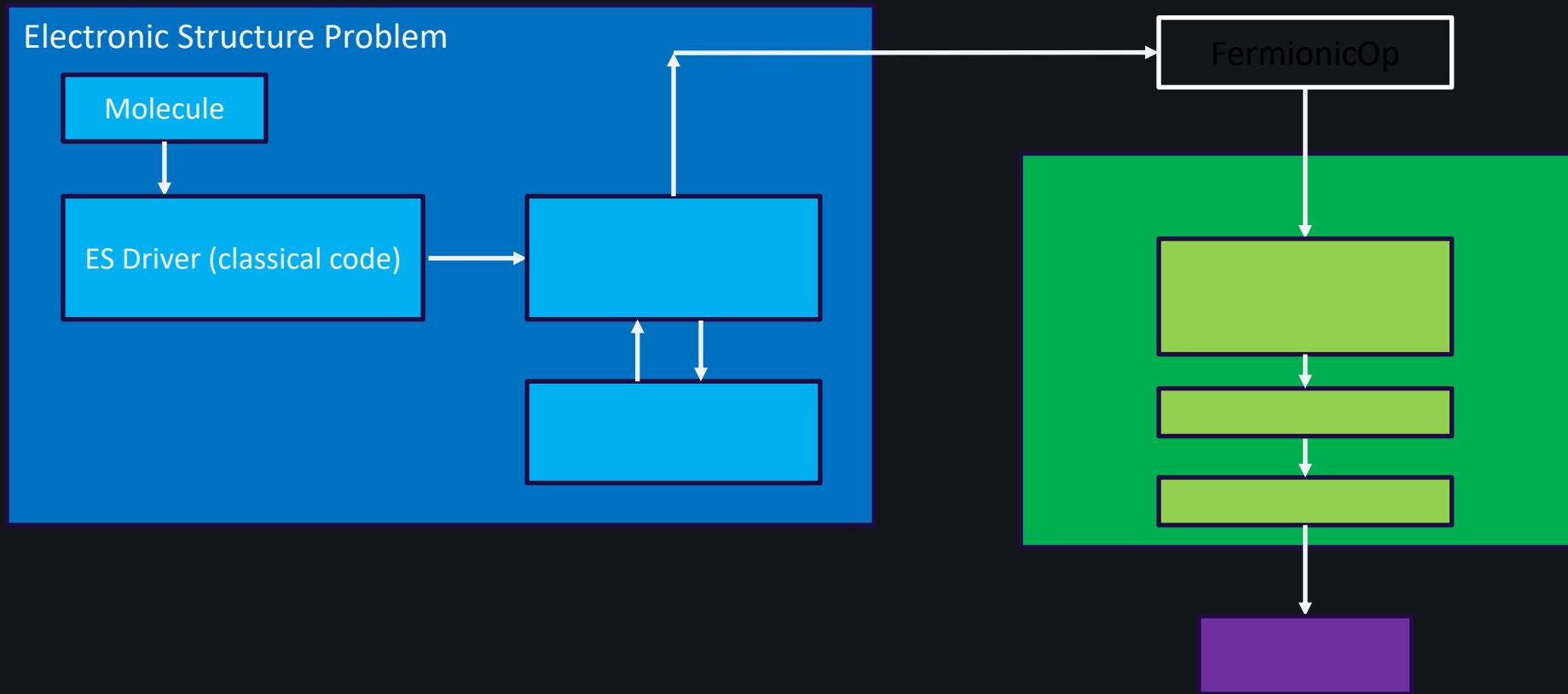
- Bridging the gap between natural sciences and quantum simulation
- Allowing researchers to model problems originated from natural sciences using a quantum computer.

**Qiskit Nature was designed with modularity and extensibility in mind without loosing the applicability to real world applications.**

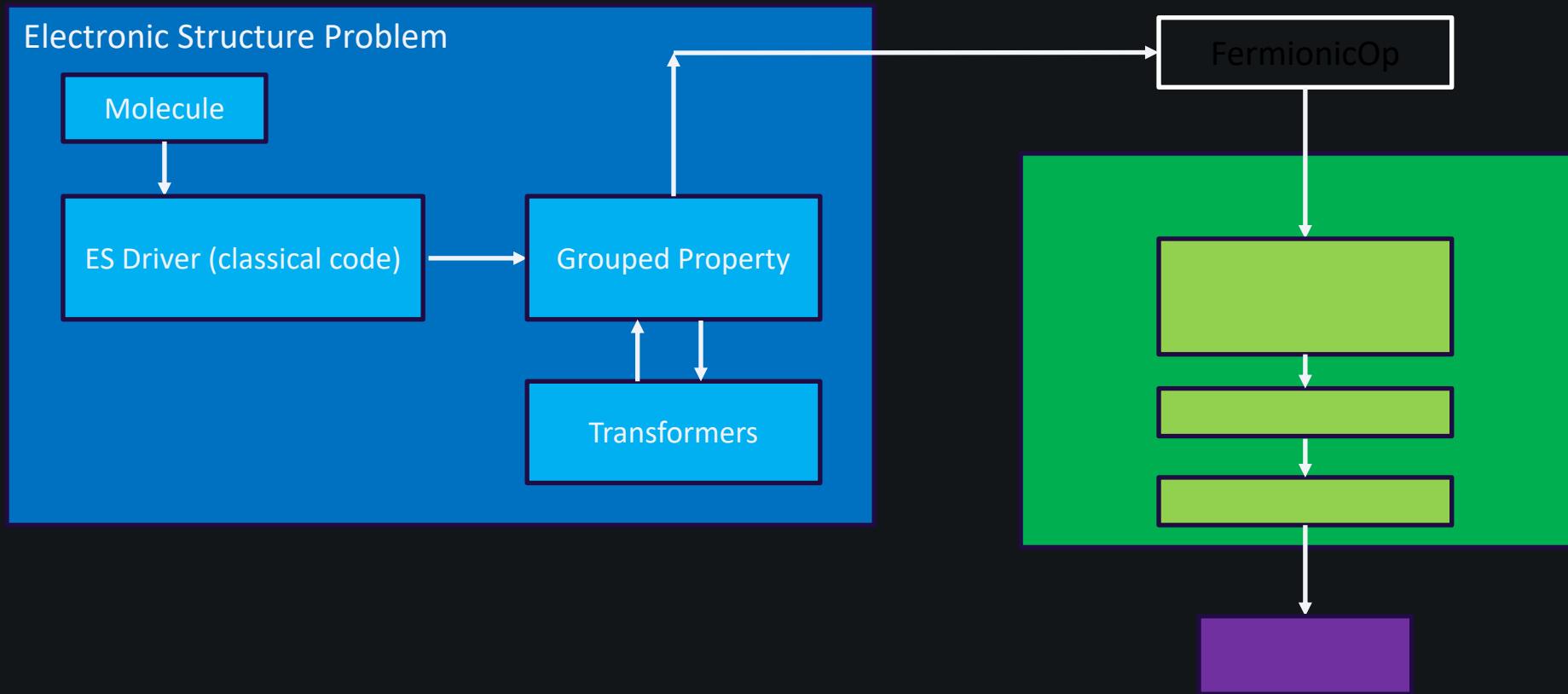
# Qiskit Nature Structure



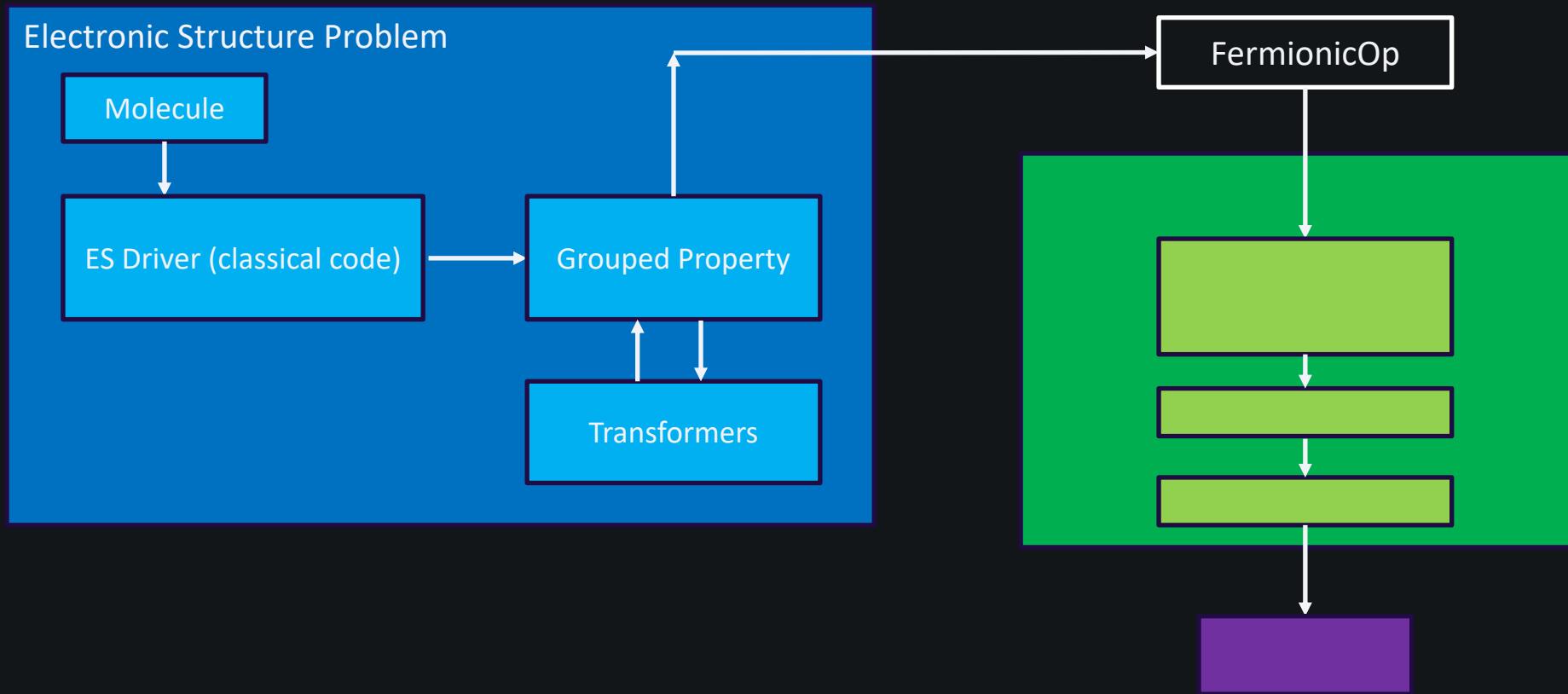
# Qiskit Nature Structure



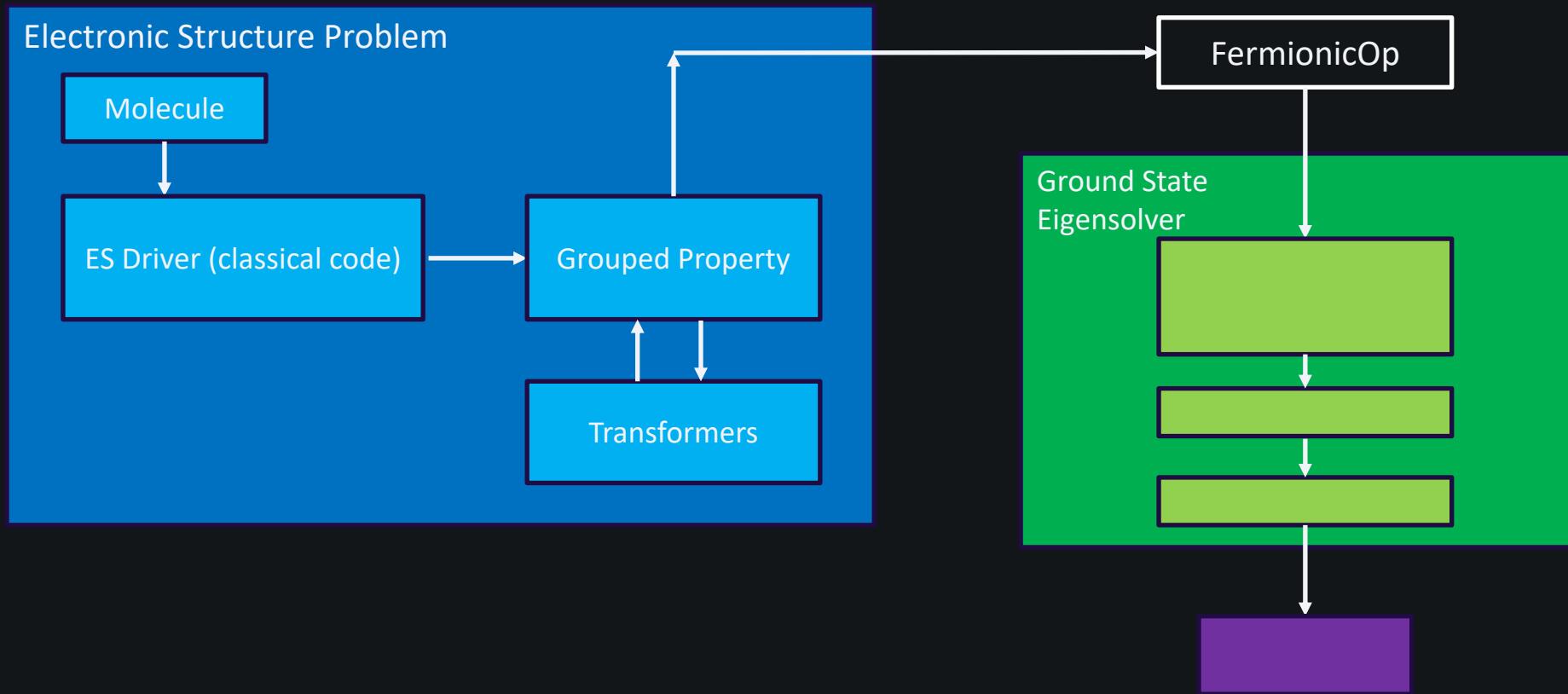
# Qiskit Nature Structure



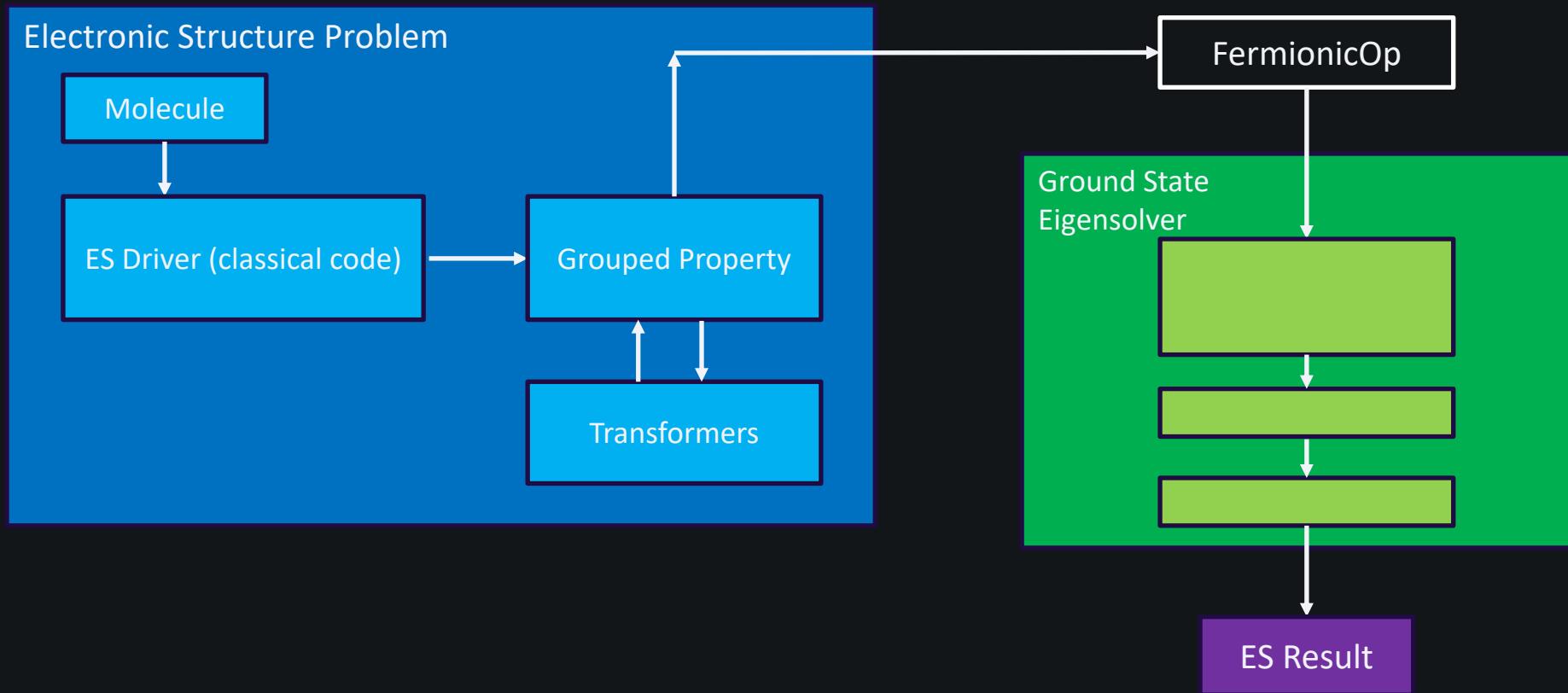
# Qiskit Nature Structure



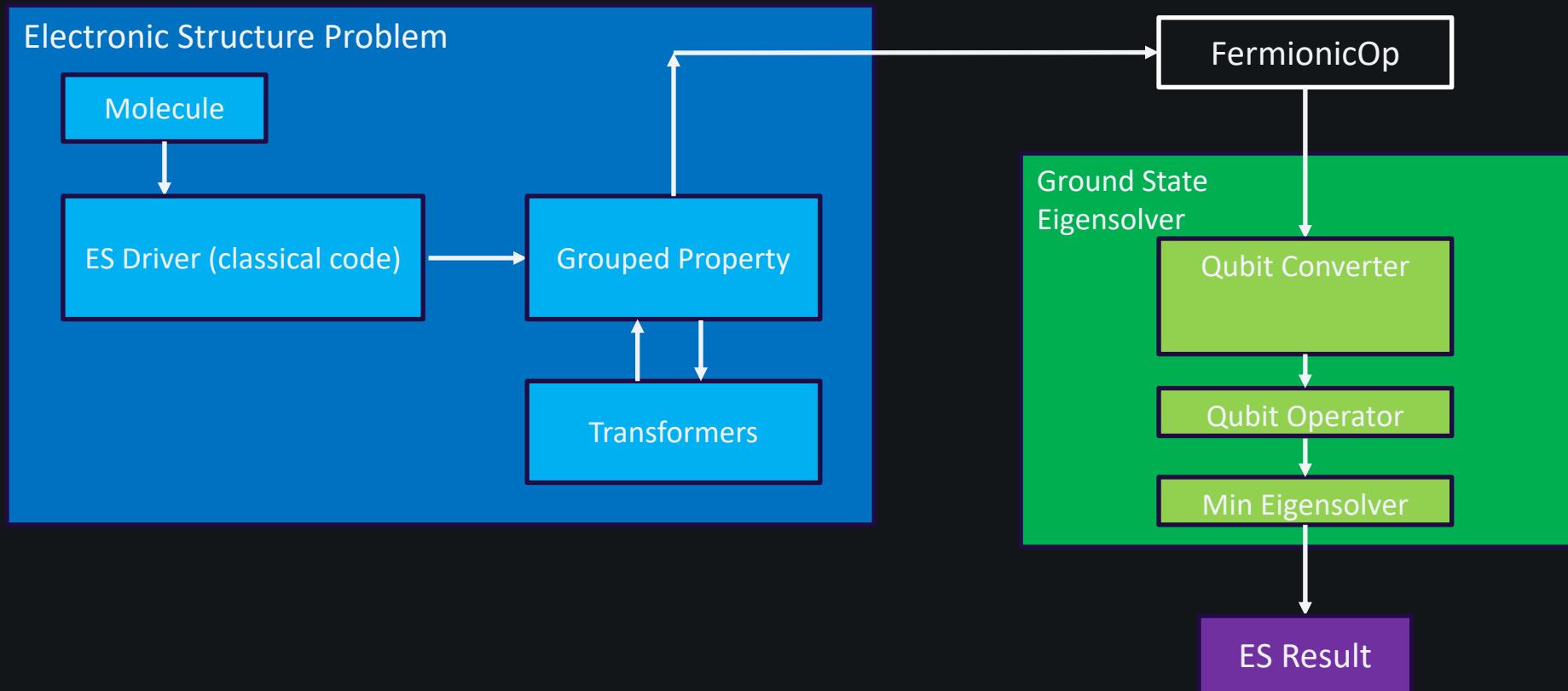
# Qiskit Nature Structure



# Qiskit Nature Structure



# Qiskit Nature Structure



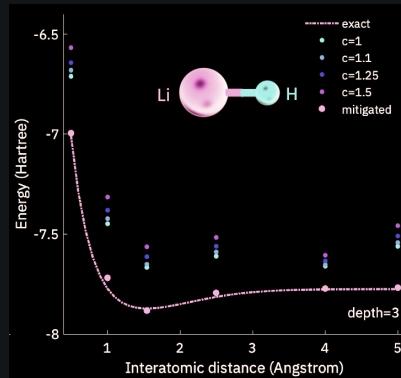
Qiskit Nature uses algorithms that leverage Qiskit Runtime...

# Qiskit Runtime

IBM Quantum

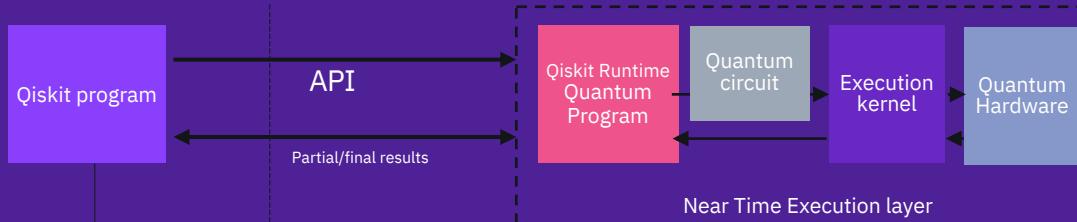
Computing the binding curve of LiH with error mitigation requires running **4.8 billion quantum circuits**.

The circuit repetition time governs the program runtime determined by the type of the quantum hardware.



Circuit repetition time	Program runtime
5 microsecond	7 hours
5 millisecond	290 days

## Increasing efficiently – *Qiskit Runtime*



An user submits a **program** which produces **circuits**, and after can be **call/execute** it in the **Quantum Program Runtime**

Now the tight loop can execute without returning to the queue.

This model improved CLOPS from ~200 – 1.4K

Qiskit Runtime 4.0X  
Algorithm 1.8X  
System Software 1.5X  
Control Systems 4.2X  
Device Fidelities 2.8X  
**Total 120x improvement on QPU speed**



Keep in mind there are also chemistry related applications in near term quantum computers beyond electronic structure...

# Beyond Electronic Structure

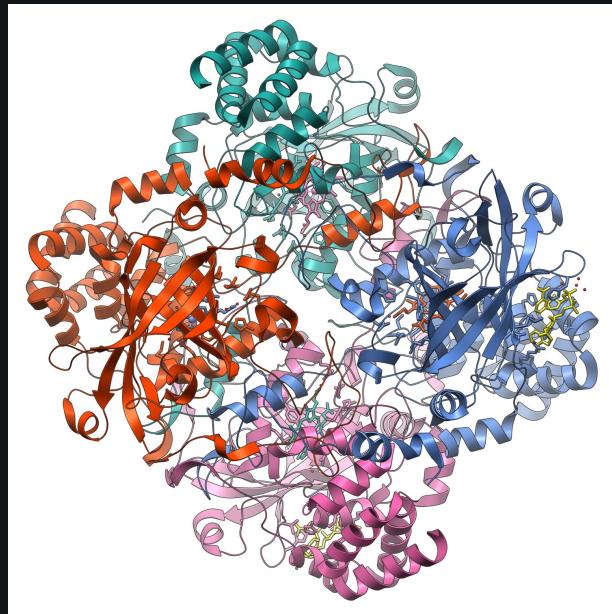
# Protein Folding Problem

## The Levinthal's Paradox

If a protein were to attain its correctly folded configuration by sequentially sampling all the possible conformations, it would require a time **longer than the age of the universe** to arrive at its correct native conformation.

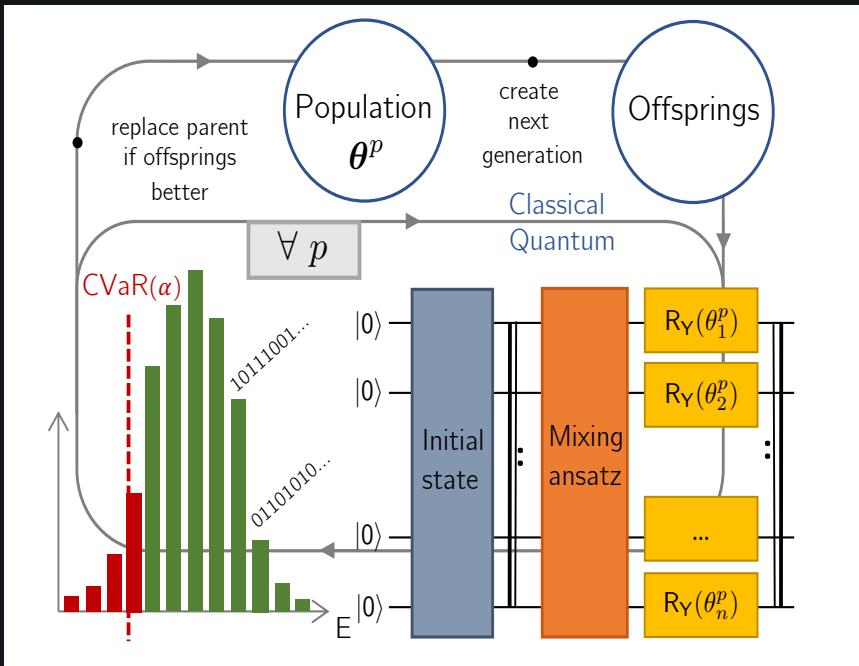
The "**paradox**" is that most small proteins fold spontaneously on a millisecond or even microsecond time scale

What if we were able to sample **all possible configurations** and evaluate then in **single experiment**



# Protein Folding Algorithm

## Hybrid Quantum/Classical Algorithm



### Model

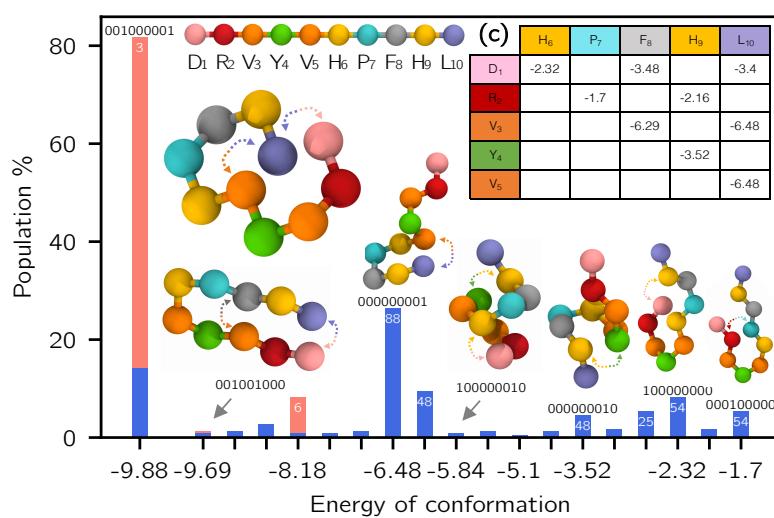
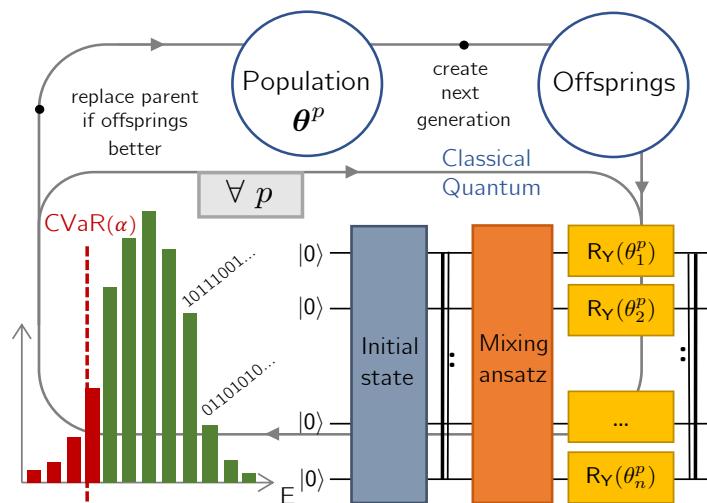
- Coarse grained model
- Hamiltonian encoding configurations and interactions
- Respect to all physical constraints of the problem

### Algorithm

- Enhanced hybrid quantum/classical algorithm for optimization problems (CVaR-VQE)
- Differential Evolution (genetic algorithm) for classical optimization

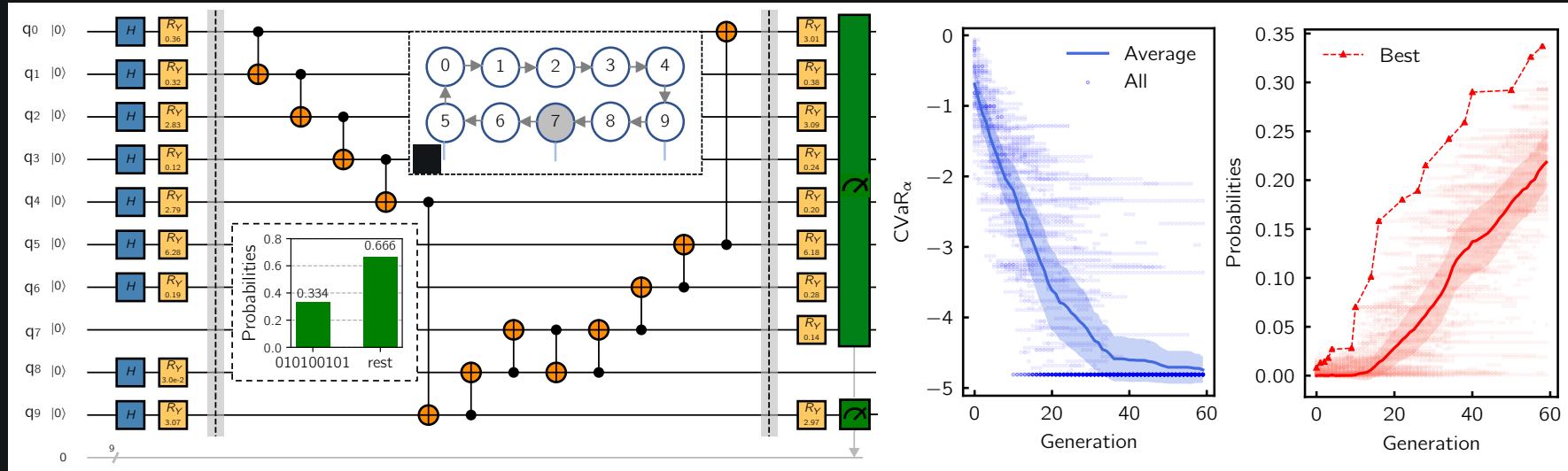
# Protein Folding Result

Simulation of Angiotensin peptide



**38 qubit** problem mapped to **22 qubit**

# Protein Folding Result

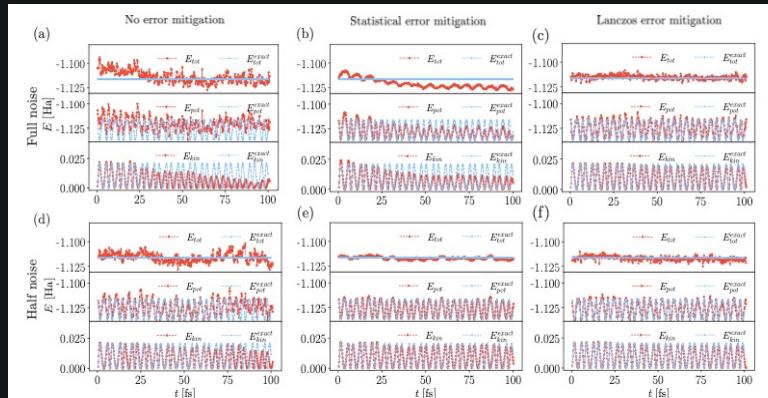
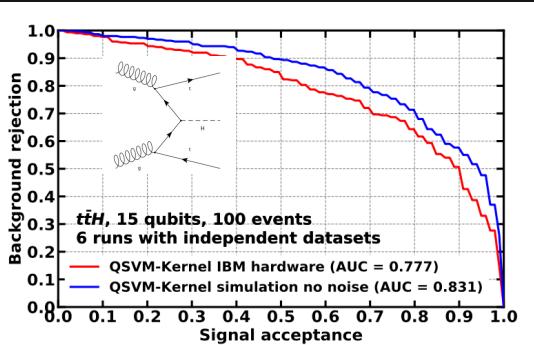


9 qubit neuropeptide simulated in IBM Q Poughkeepsie

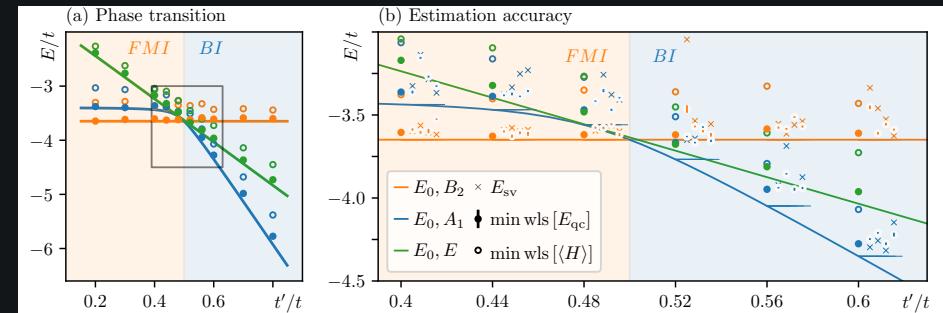
Protein Folding Problem is also available in the Qiskit Nature module!

# Other applications of near-term Quantum Computers

## Quantum Machine Learning for High Energy Physics

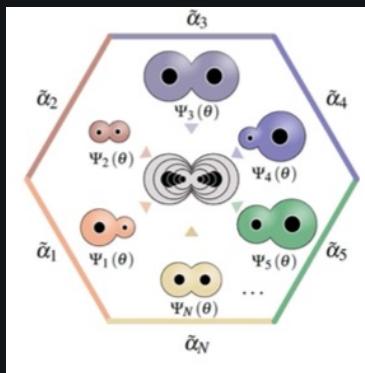


Molecular Dynamics simulations in a quantum computer

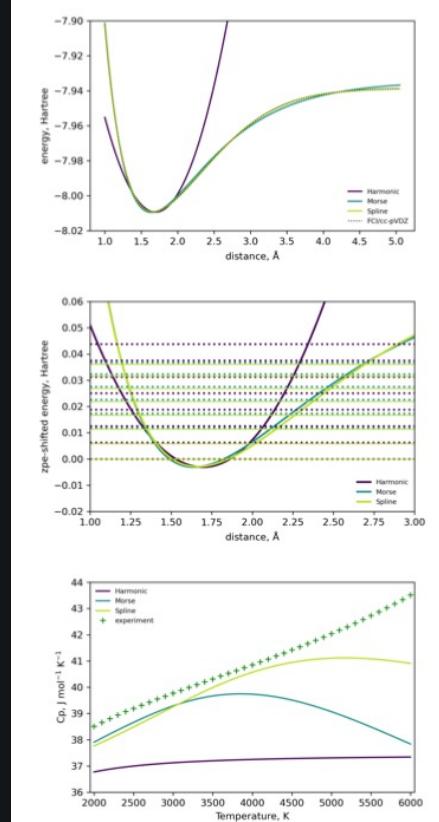


Ground State transitions in Fermi-Hubbard model

## Material Design



## Thermodynamic Observables in QC



# Take Home Messages

- Quantum Chemistry is important and there many challenges to overcome to simulate efficiently quantum computers
- Quantum Chemistry in the near term quantum computers relies on Hybrid Quantum Classical algorithms
- Methods to make solutions better exists, but this is an active field of research
- Qiskit Nature can be used to simulate chemical systems
- There are interesting problems also beyond electronic structure

Thank you