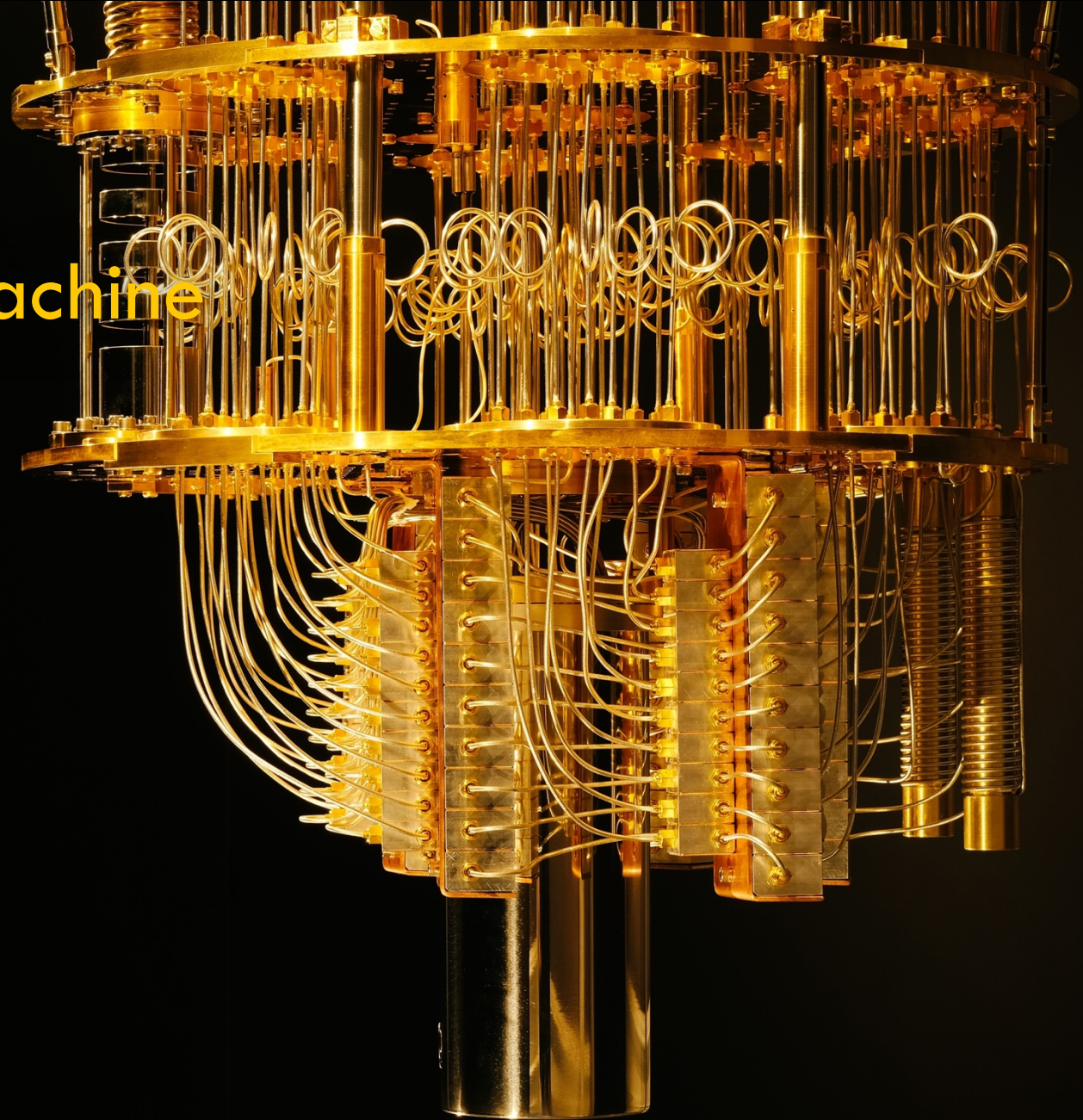


# Quantum Computation for Machine Learning, AI, and Optimization

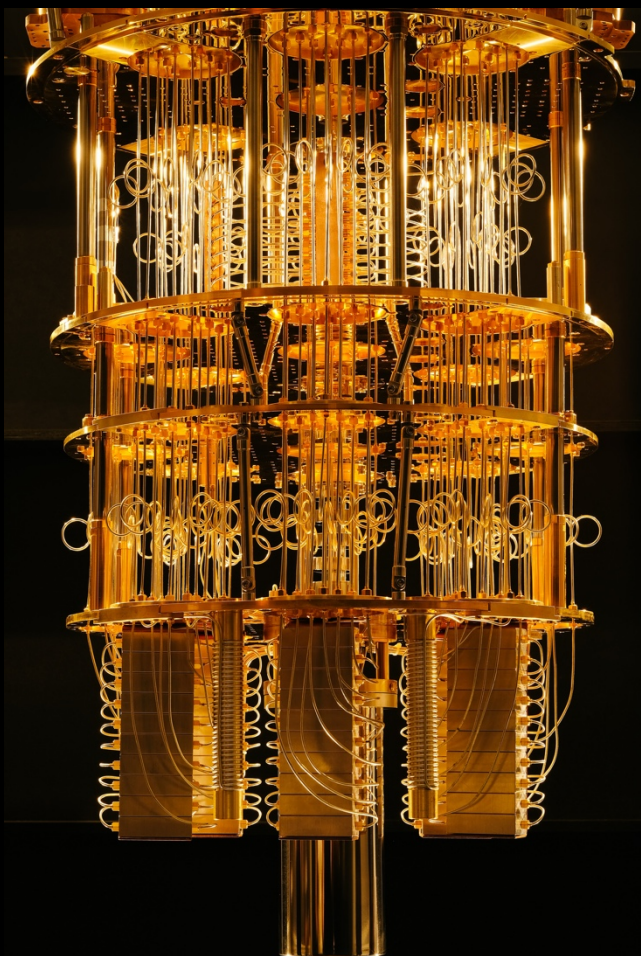
**Zlatko K. Minev, Ph.D.**

**IBM Quantum @ TJ Watson**



# Experimental Superconducting Quantum Computing

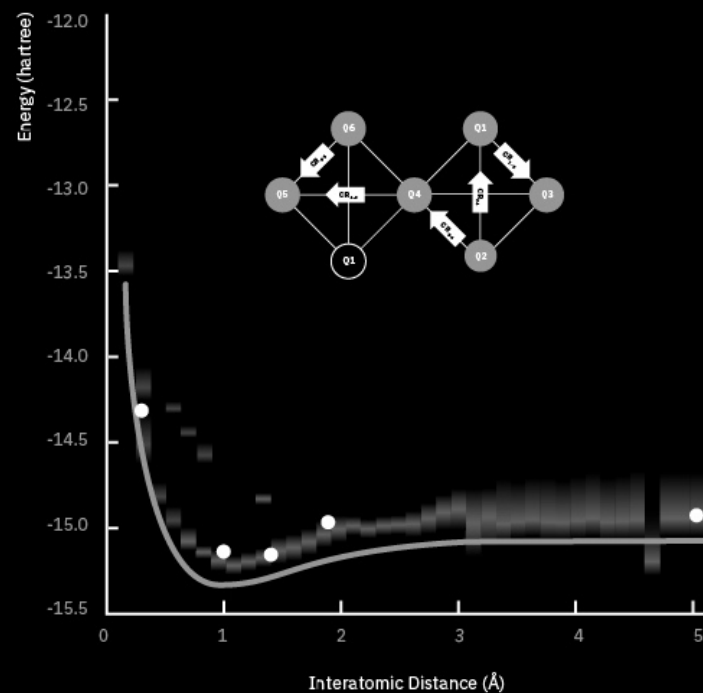
## Hardware



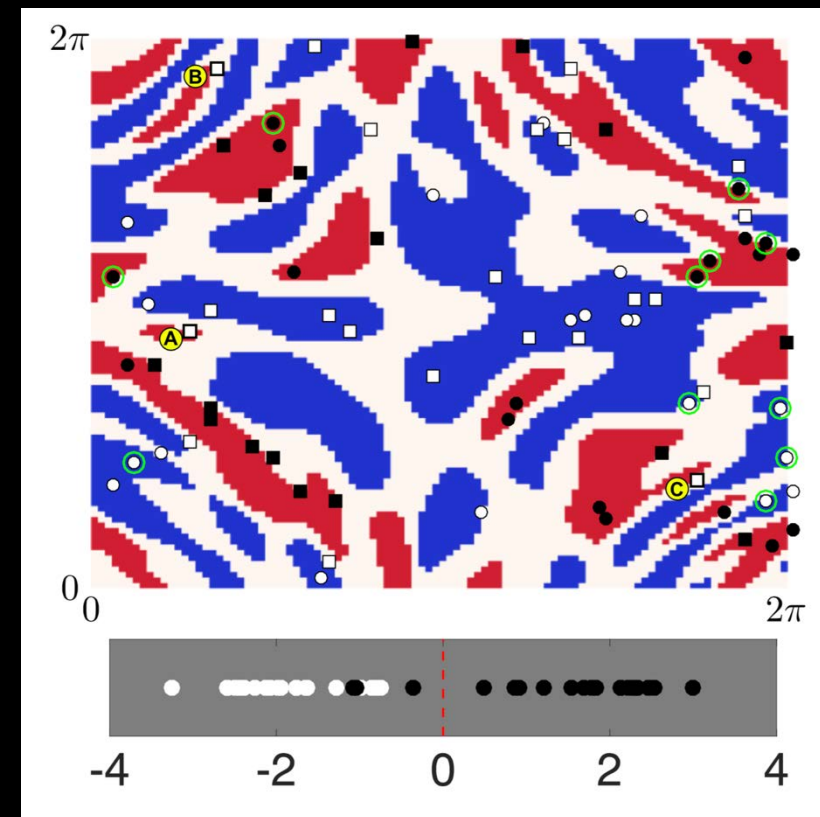
## Chemistry



Beryllium hydride ( $\text{BeH}_2$ ):



## Machine Learning



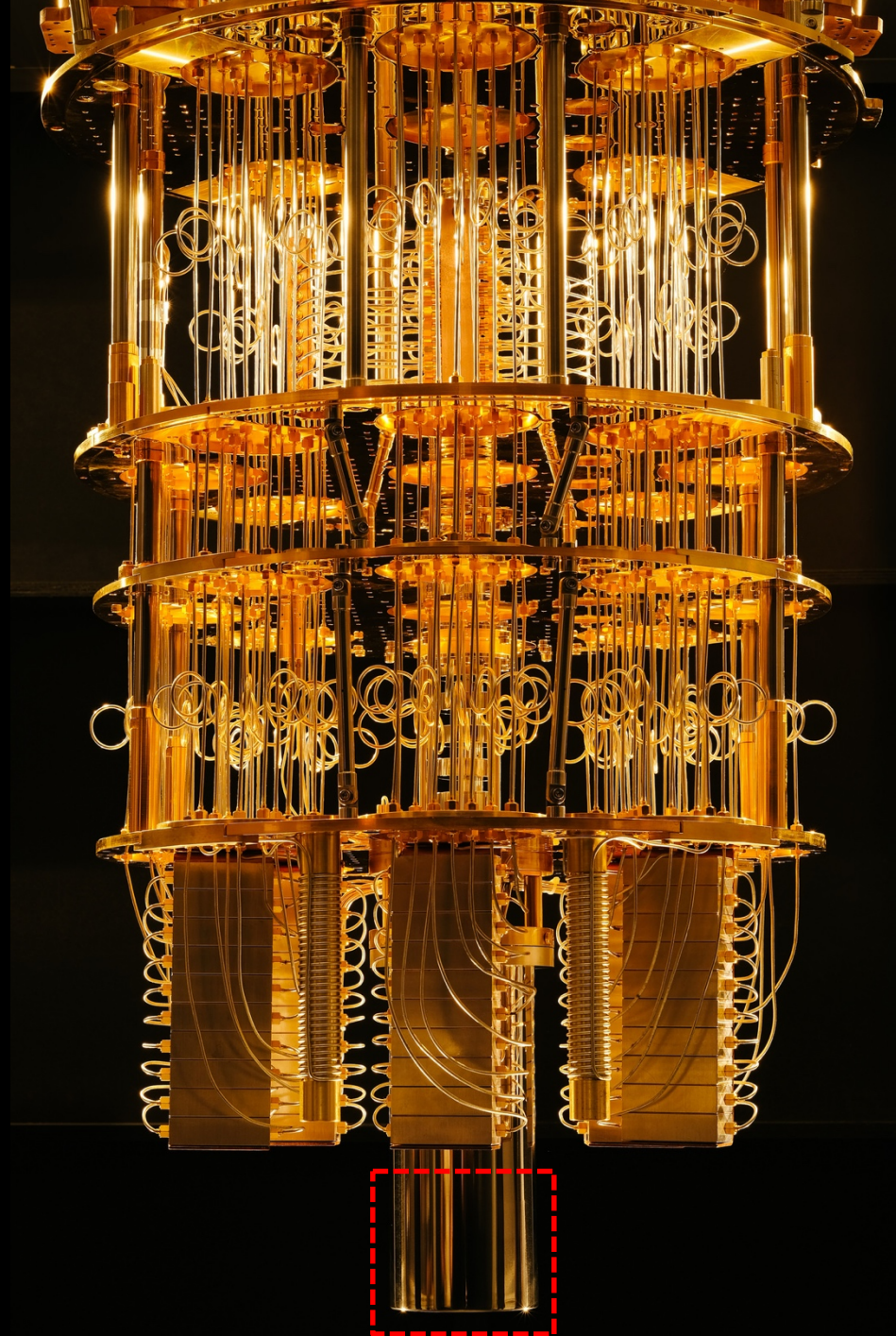
# **Cloud-based quantum computing**

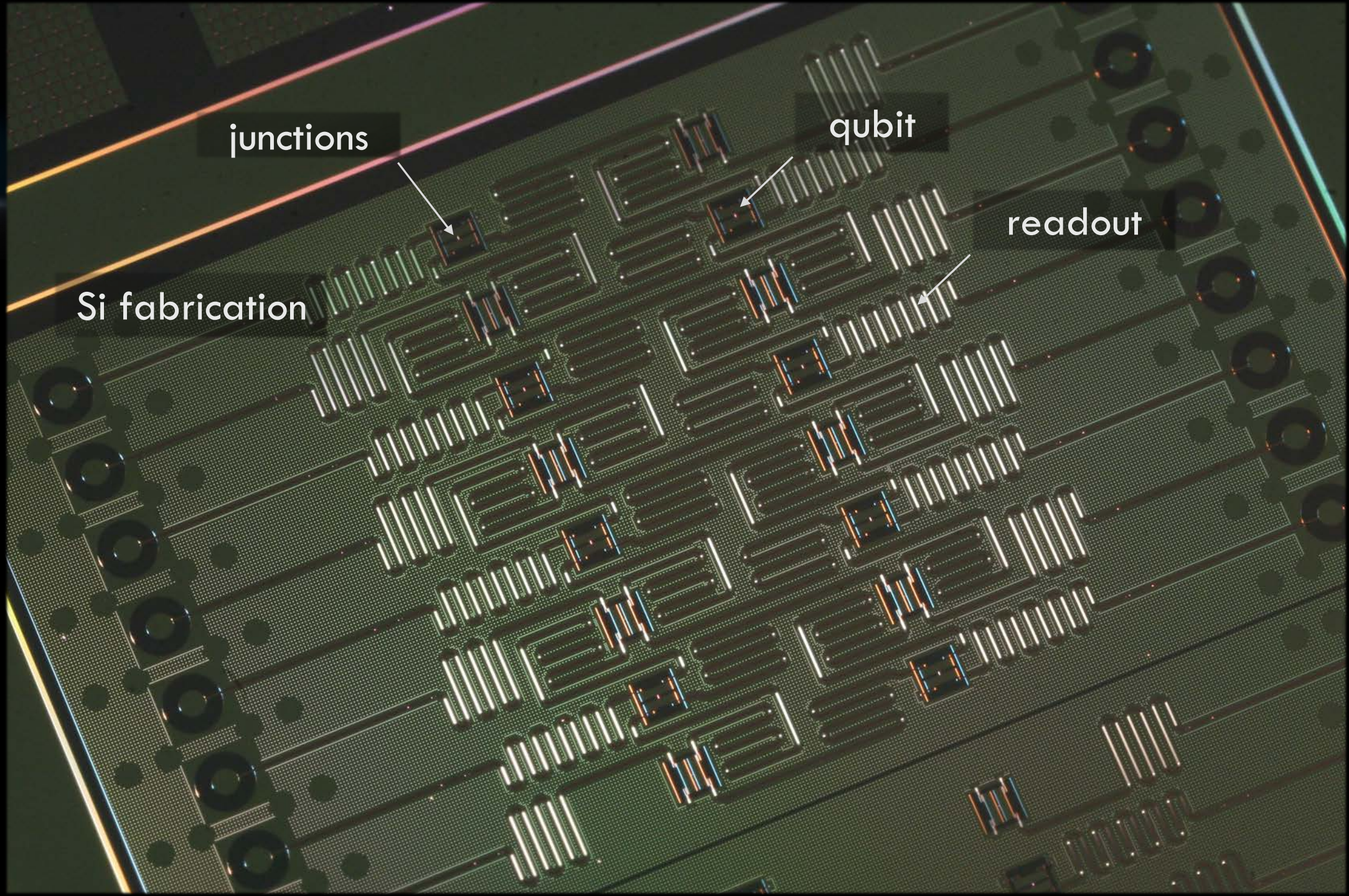
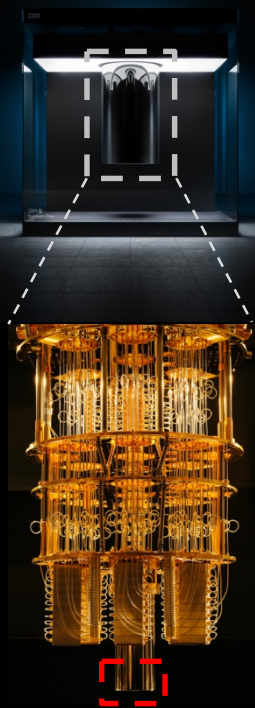
**What does today's hardware look like?**

# Commercial cloud service

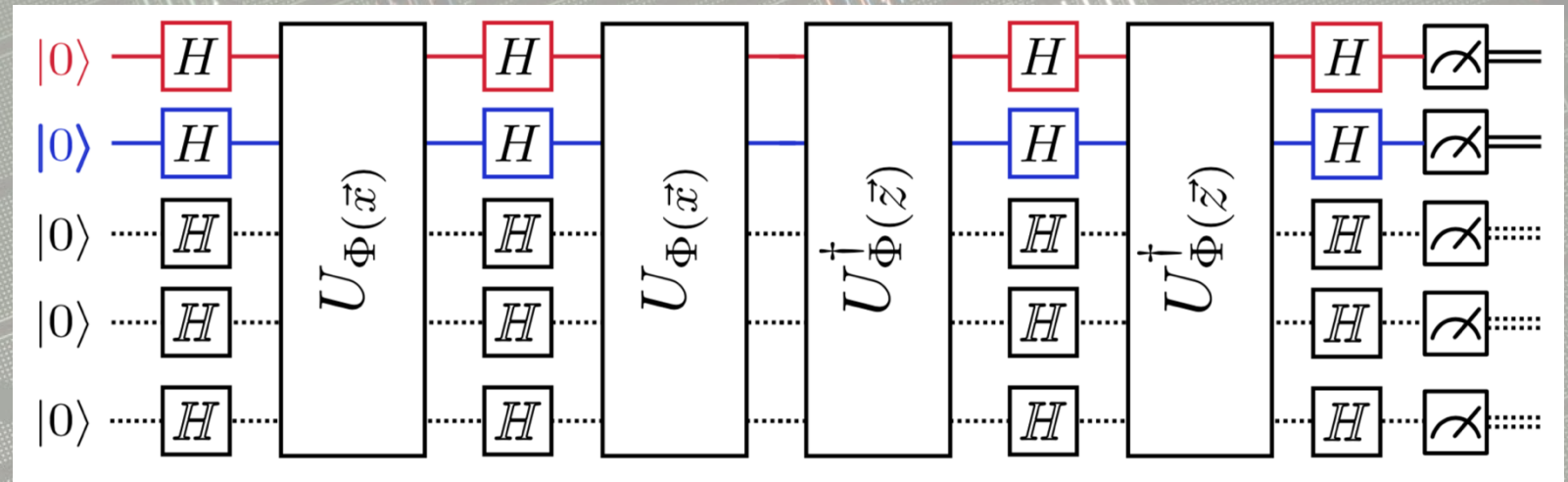
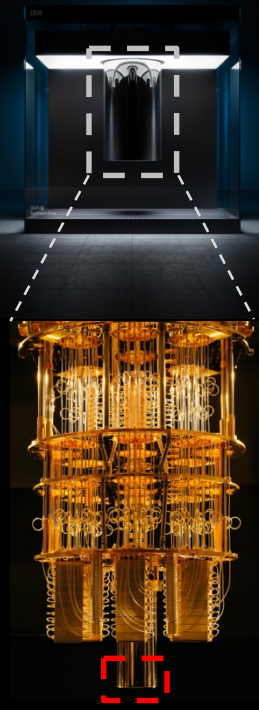


IBM Q  
System One





# From chip to algorithm



# Quantum Applications

# Possible application areas for quantum computing

We believe the following areas might be useful to explore for the early applications of quantum computing:

## Chemistry

Material design, oil and gas, drug discovery

## Artificial Intelligence

Classification, machine learning, linear algebra

## Optimization

Portfolio optimization, scenario analysis, pricing



LETTER

**LETTER**

**Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets**

Y. Kanda<sup>1\*</sup>, Antonio Mezzacapo<sup>1\*</sup>, Kristan Temme<sup>1</sup>, Maika Takita<sup>1</sup>, Markus Brink<sup>1</sup>, Jerry M. Chow<sup>1</sup> & Jay M. Gambetta<sup>1,2</sup>

Quantum computers can be used to address electronic-structure problems in materials science and condensed matter physics, interacting fermionic problems, and existing high-performance numerical methods for problems numerically intractable with the size of the system. Following the computational approach of the quantum eigensolver, this algorithm can produce extremely accurate energy estimates for quantum chemistry<sup>2,3,5,8</sup>, it applies stringent requirements to the coherence of the quantum hardware. An alternative approach is to use quantum optimization problems (VQEs) where they were introduced in quantum chemistry<sup>4,11</sup> and in quantum chemistry<sup>16,17</sup> and in quantum chemistry<sup>18</sup>. Ritz's variational principle to prepare approximate ground states that depend on a set of parameters, the energy is then estimated by minimizing the energy of the trial states. A new set of improved variational trial states that depend on a set of parameters, the energy is then estimated by minimizing the energy of the trial states. A new set of improved variational trial states that depend on a set of parameters, the energy is then estimated by minimizing the energy of the trial states.

# Hardware-enabled quantum computing for small molecules

Abhinav Kandala<sup>1\*</sup>, Antonio Mezzacapo<sup>1\*</sup>, Kristan Temme<sup>1</sup>, Armin Vaezi<sup>1</sup>, David K. S. *et al.*

Quantum computers can be used to address electronic-structure problems and problems in materials science and condensed matter physics that can be formulated as interacting fermionic problems, problems which stretch the limits of existing high-performance computers<sup>1</sup>. Finding exact solutions to such problems numerically has a computational cost that scales exponentially with the size of the system, and Monte Carlo methods are unsuitable owing to the fermionic sign problem. These limitations of classical computational methods have made solving even few-atom electronic-structure problems interesting for implementation using medium-sized quantum computers. Yet experimental implementations have so far been restricted to molecules involving only hydrogen and helium<sup>2–8</sup>. Here we demonstrate the experimental optimization of Hamiltonian problems with up to six qubits and more than one hundred Pauli terms, determining the ground-state energy for molecules of increasing size, up to BeH<sub>2</sub>. We achieve this result by variational quantum eigensolver (vqe) specifically to the problem of finding the ground state of fermionic Hamiltonians<sup>9</sup> and a robust method for preparing trial states that are tailored specifically to the problem of increasing size, up to BeH<sub>2</sub>. We demonstrate the flexibility of the vqe in an external magnetic field in our experiments and compare the results with noise. Our method

problem using the quantum phase estimation algorithm<sup>15</sup>. Although this algorithm can produce extremely accurate energy estimates for quantum chemistry<sup>2,3,5,8</sup>, it applies stringent requirements on the coherence of the quantum hardware.

An alternative approach is to use quantum optimizers, which have been previously demonstrated utility, for example, for combinatorial problems<sup>16,17</sup> and in quantum chemistry as variational quantum eigensolvers (VQEs) where they were introduced to reduce the number of qubits on quantum hardware<sup>4,18,19</sup>. The VQEs are approximations to the exact solution of the quantum computer.

An alternative to the VQE approach is the quantum eigensolver (QES) which has been previously demonstrated for quantum chemistry problems [19]. The QES uses the coherence requirements of the VQE to prepare a trial state and its energy. In this approach, the quantum computer is used to prepare a trial state and its energy. The advantage of the QES is that it can prepare a trial state with a new set of improved parameters. The advantage of a QES over classical simulation methods is that it can prepare trial states that are not amenable to efficient classical numerics. The QES approach realized in experiments has so far been limited to a small number of parameters. The QES approach realized in experiments has so far been limited to a small number of parameters. The QES approach realized in experiments has so far been limited to a small number of parameters.

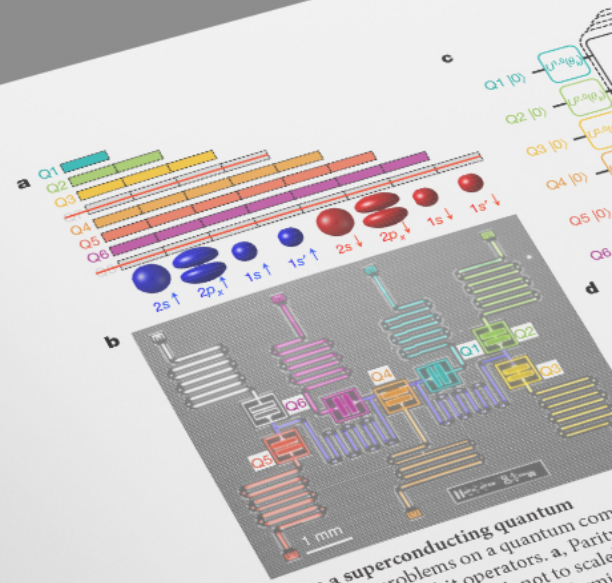
The VQE approach realized in experiments has so far been limited by different factors. Typically, a unitary coupled cluster ansatz for the trial state is considered<sup>6,7</sup>, which has a number of parameters that scales quartically with the number of spin orbitals that are considered in the single- and double-excitation approximation. Furthermore, when implementing the unitary coupled cluster ansatz on a quantum computer, Trotterization errors need to be accounted for<sup>19-21</sup>. Here we introduce and implement a hardware-efficient ansatz preparation for a VQE, whereby trial states are parameterized by quantum gates that are tailored to the physical states for small electronic-structure problems and viability of such trial states for quantum processor to perform optimizations of the molecular energies of  $H_2$ ,  $LiH$  and  $BeH_2$ , and extend its application to a superconducting quantum model in an external magnetic field. The device used in the experiments is a superconducting quantum transmon qubit<sup>22</sup>. The device is a six fixed-frequency transmon qubit, where it is thermally anchored to its

the state  $|00\dots 0\rangle$ , applying  $d$  entanglers  $U_{\text{ENT}}$  that all rotations, giving

$$= \prod_{q=1}^N [U^{q,d}(\theta)] \times U_{\text{ENT}} \times \prod_{q=1}^N [U^{q,d}(\theta)]$$

$$|\Phi(\theta)\rangle = \prod_{q=1}^N [U^{q,d}(\theta)] \times U_{\text{ENT}} \times \prod_{q=1}^N [U^{q,d}(\theta)] |00 \dots 0\rangle$$

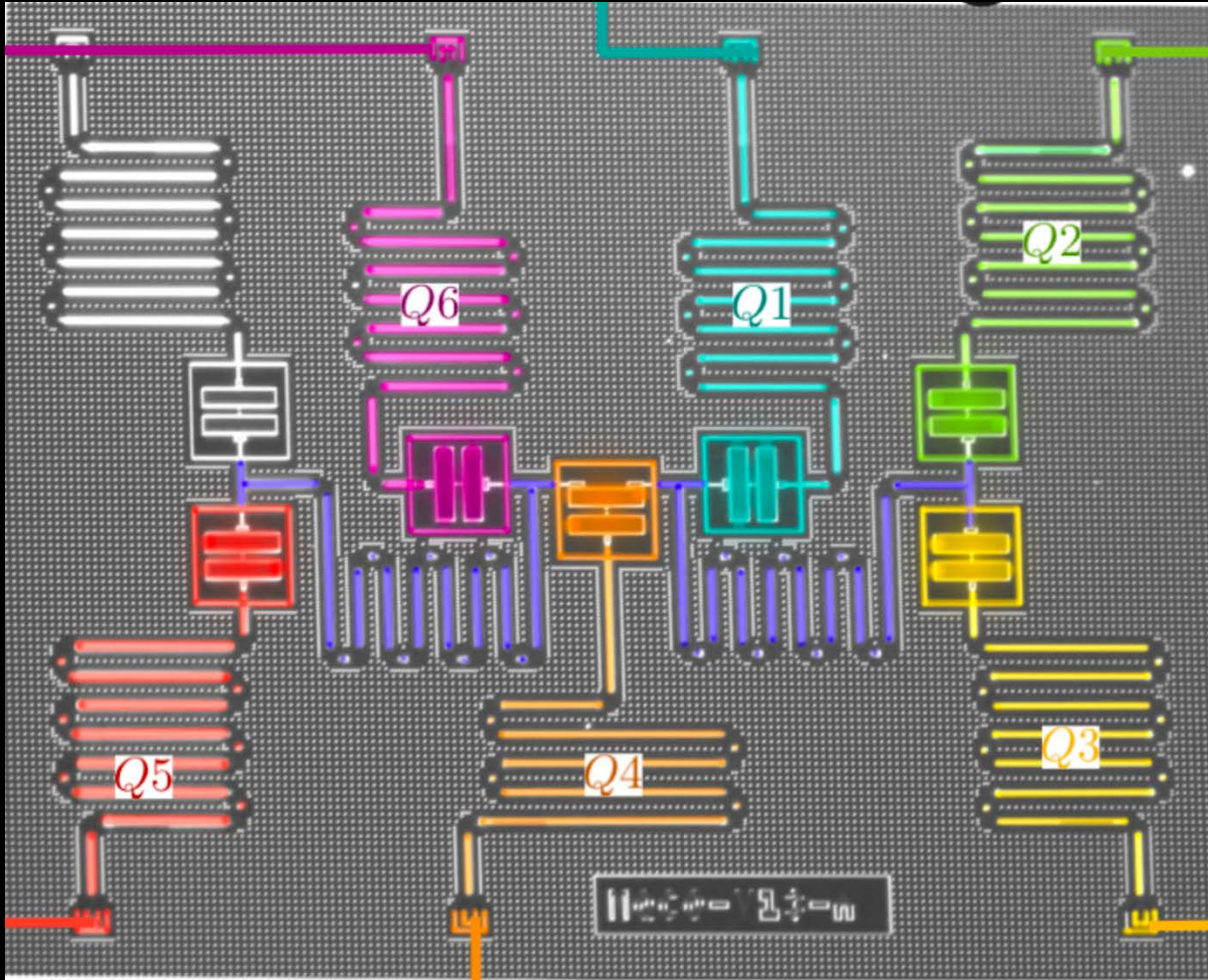
Because the qubits are all initialized in set of Z rotations of  $U^{q,0}(\theta)$  is not independent angles  
 $p = N(3d + 2)$  and the individual coupling time  $\tau$  and the numerical simulations indicate  
 numerical simulations indicated that the entanglement obtained for fixed-phase entangled states as variational parameters. Our results rely on the accurate implementation of  $U_{\text{ENT}}$  that can be used with any unitary coupling gate in contrast to unitary gates that reduce the fidelity quantum gates through the basis of a theoretical model of the entanglers  $U_{\text{ENT}}^{\text{theoretical}}$ . The resonance gates<sup>23</sup>, S gates, and the minimum number of minimal gates required for a given algorithm.



**Figure 1 | Quantum chemistry on a superconducting quantum processor.** Solving problems on a quantum computer relies on mappings between fermionic and qubit operators. **a**, Parity mapping of eight spin orbitals (drawn in blue and red, not to scale) to six qubits owing to fermion parity symmetries. The length of the bars indicate the spin orbitals that are encoded in each qubit. **b**, False-colour micrograph of the superconducting quantum processor with transmon qubits. These qubits are coupled via two coplanar waveguide resonators (violet) and have individual coplanar waveguide

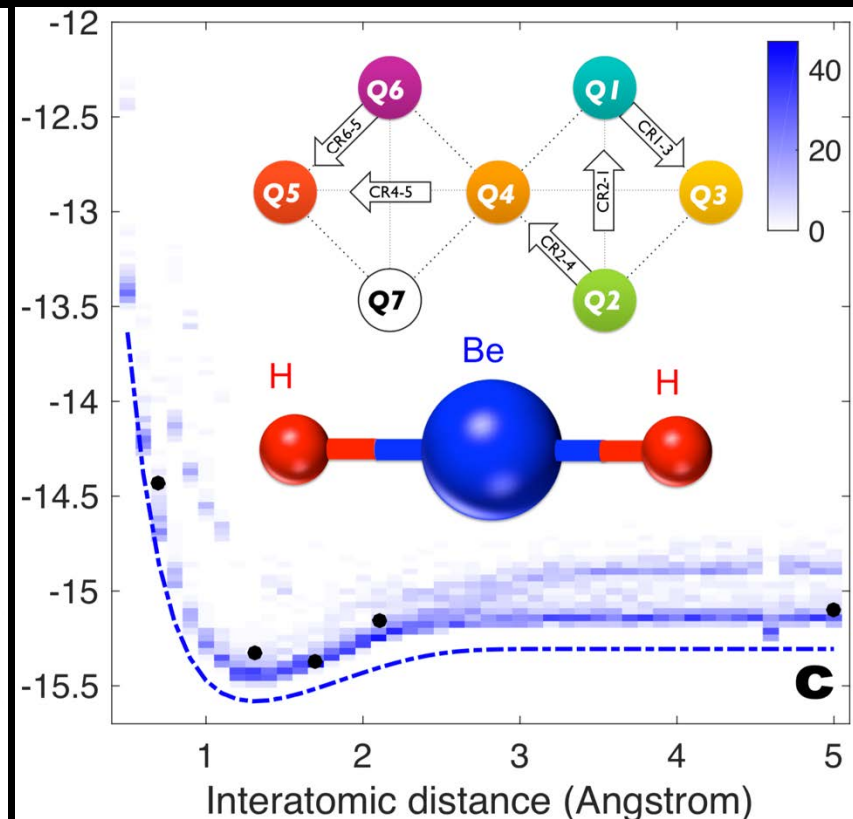
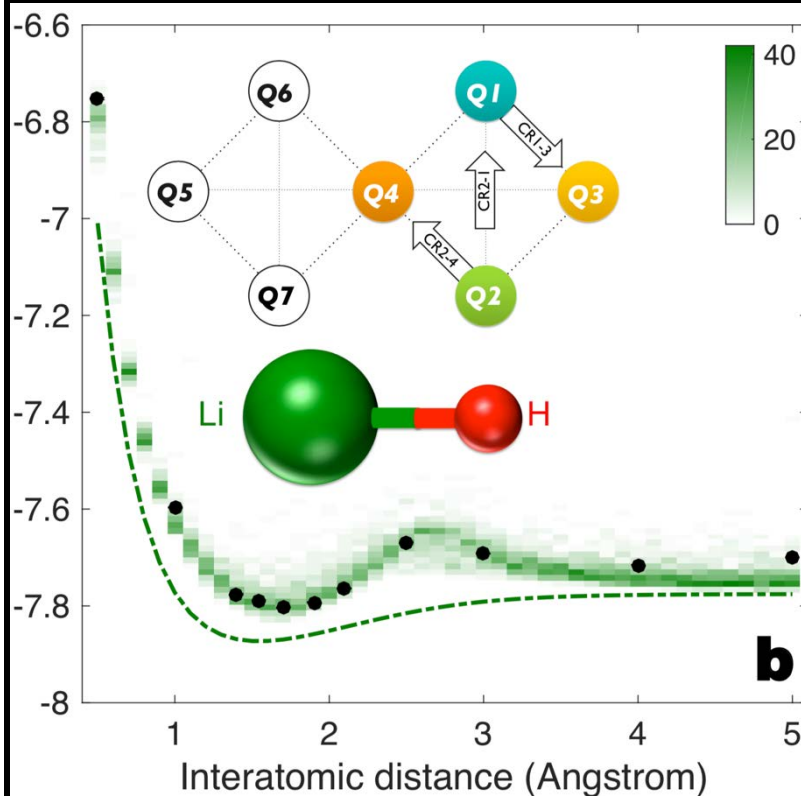
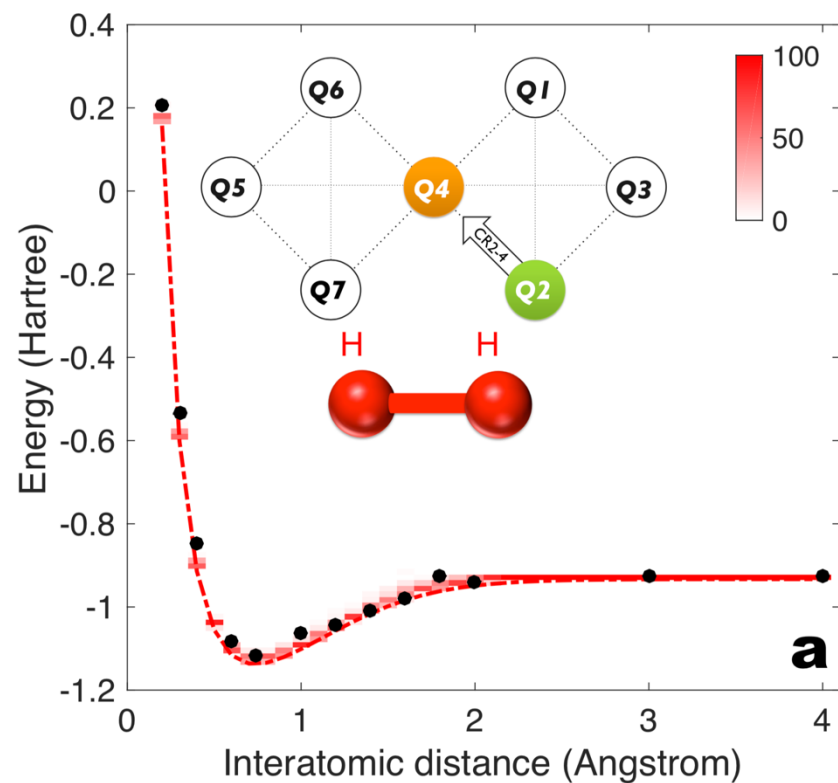
# Experimental Results

Computing the ground state energy for small molecules



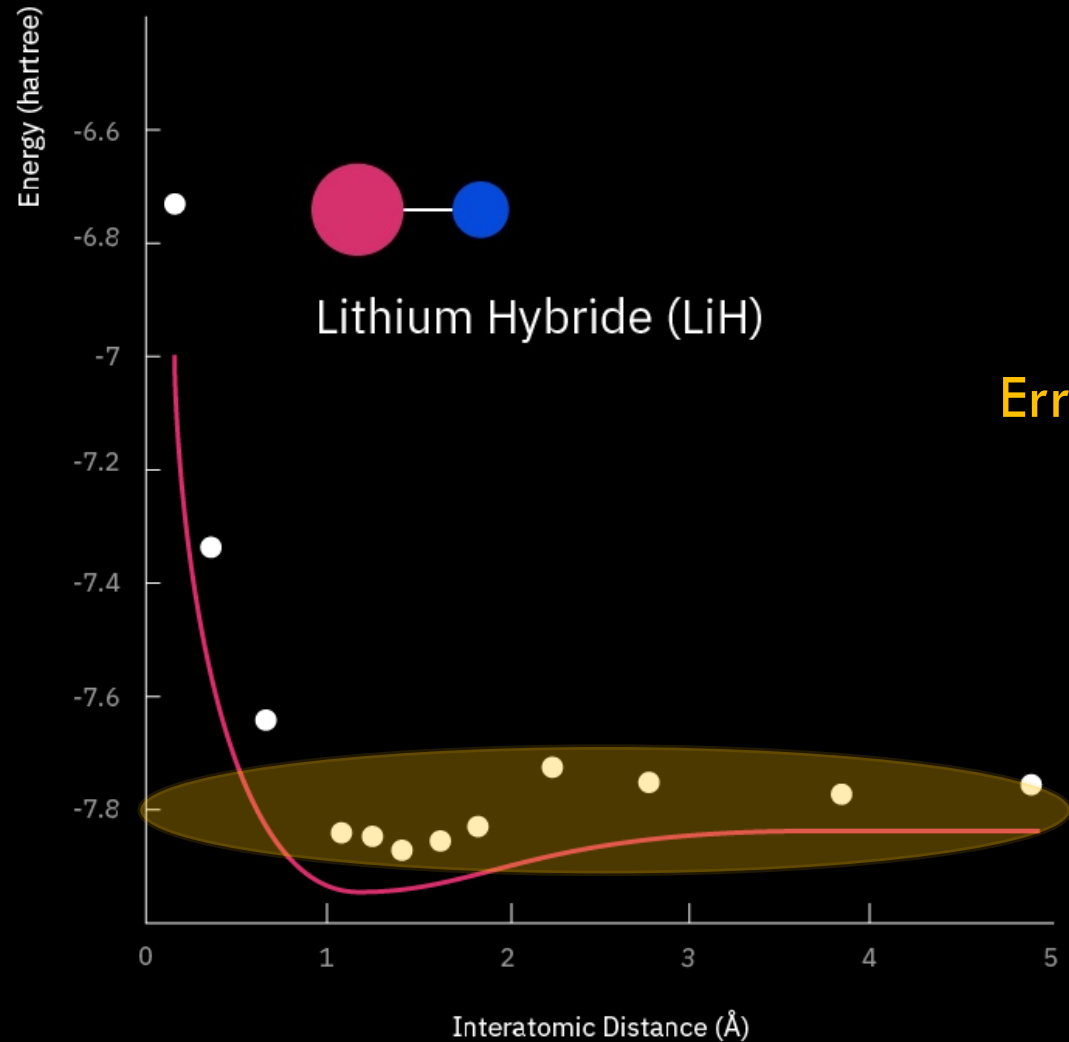
# Experimental Results

Computing the ground state energy for small molecules

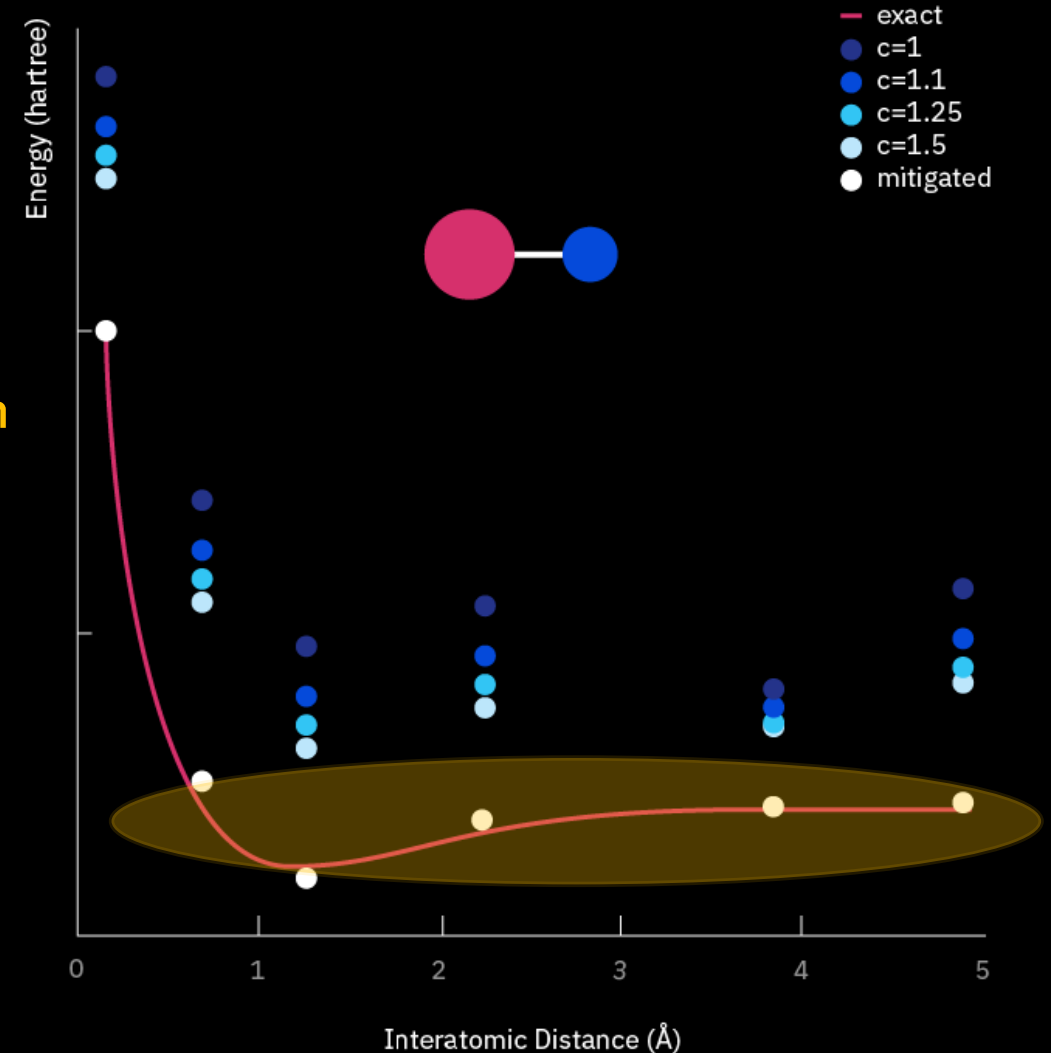


# Error mitigation: improving accuracy

Recovering correct result in the presence of noise



Error mitigation



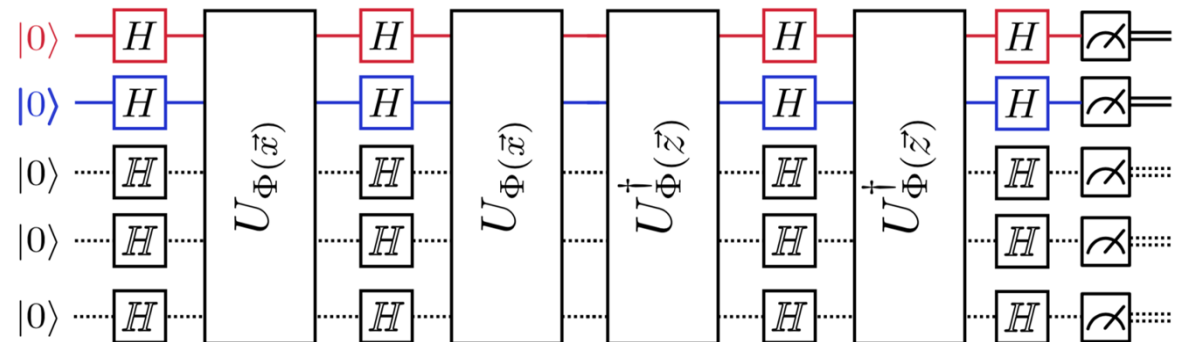
# **Quantum Machine Learning**

**Example: Support Vector Machines (SVM)**

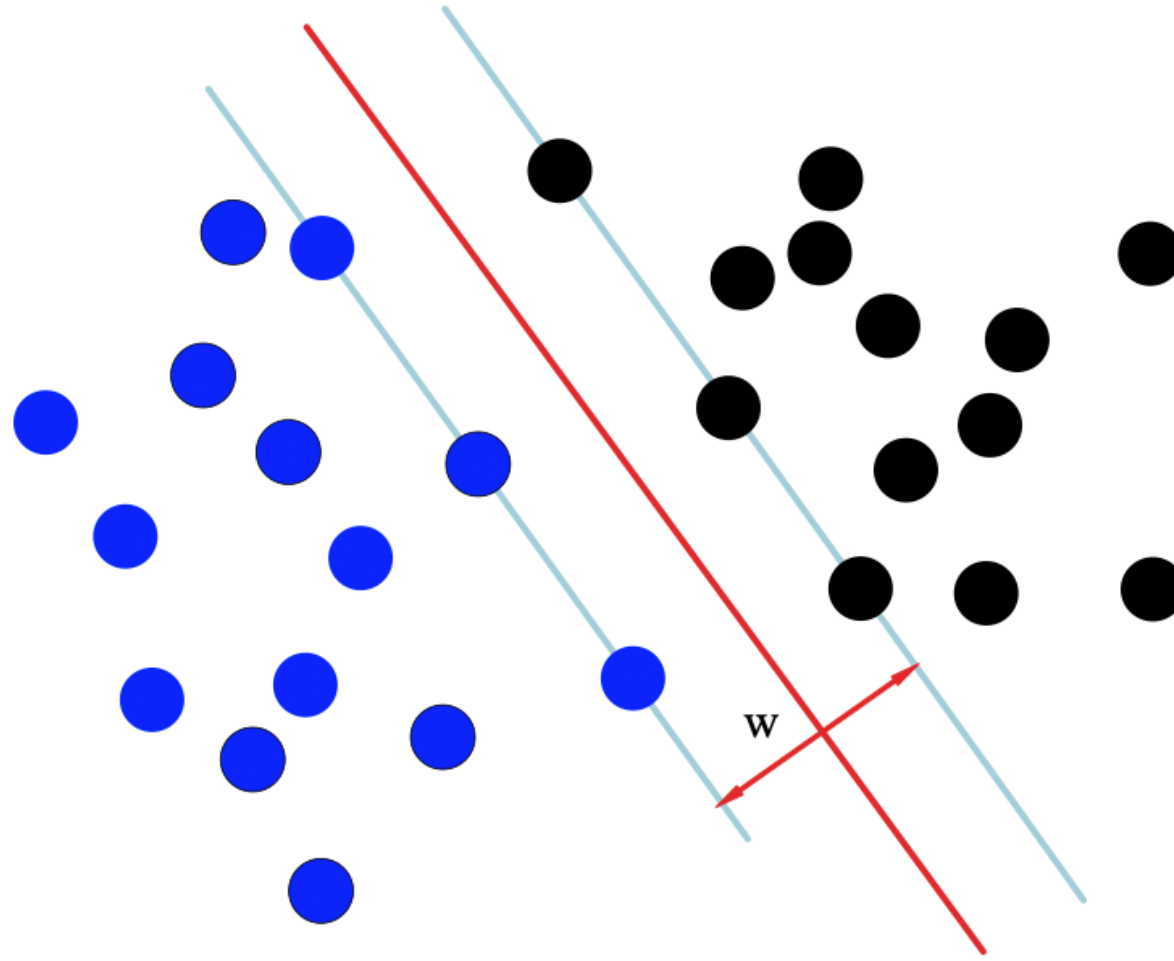


Classical vector  $\vec{x}$  is encoded into the exponentially-large quantum state space.

Quantum short depth circuits as classifiers



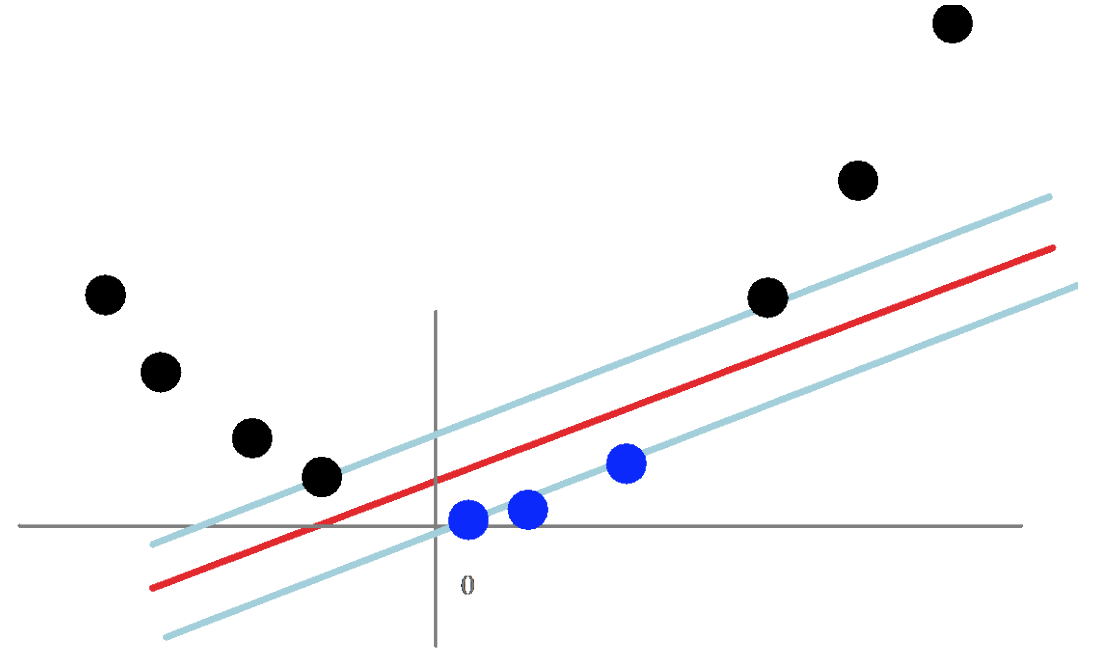
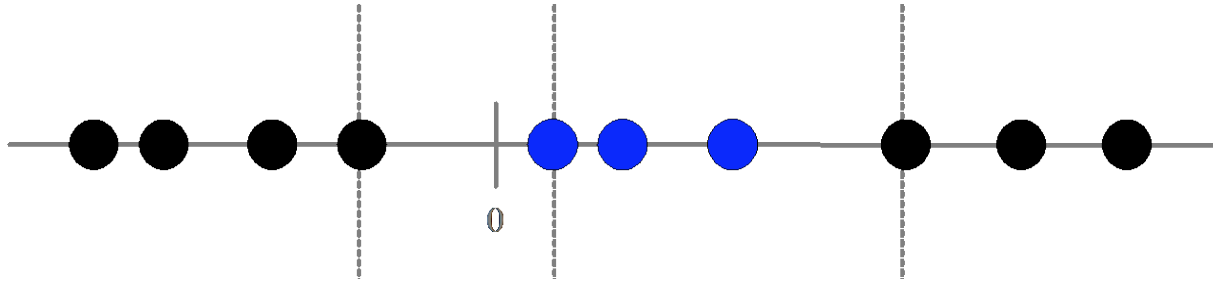
# Classical Computing: SVM Classification



# Classical Computing: Feature Space

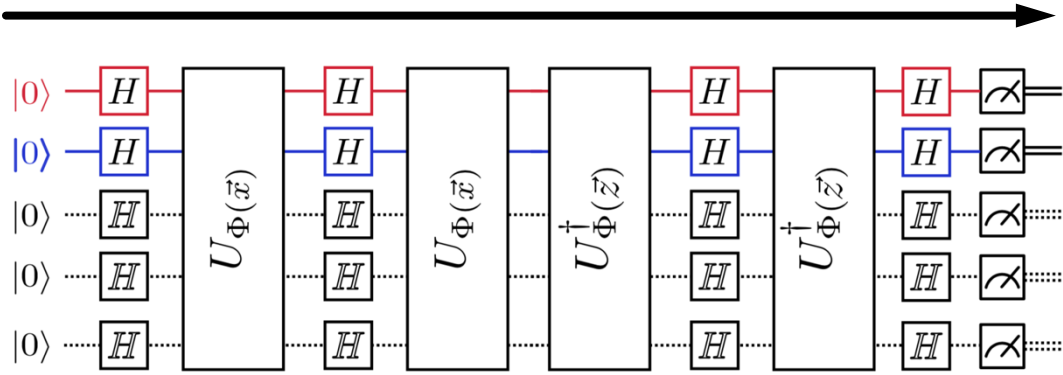
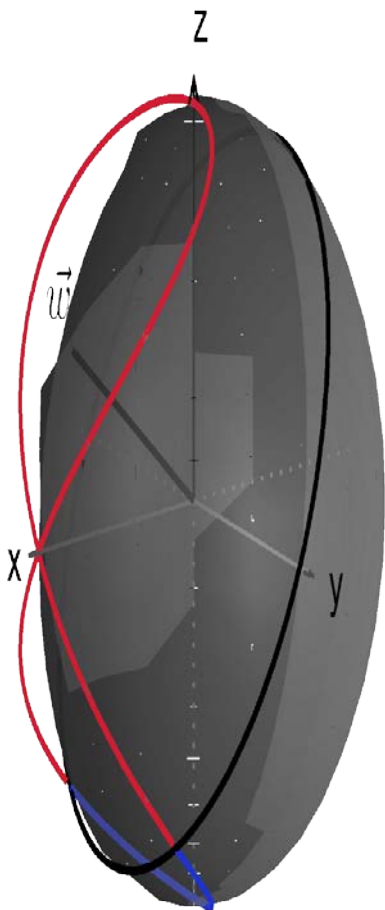
Data that is *not* linearly separable may become linearly separable by increasing dimensionality.

Non-linear classification at cost of dimensionality

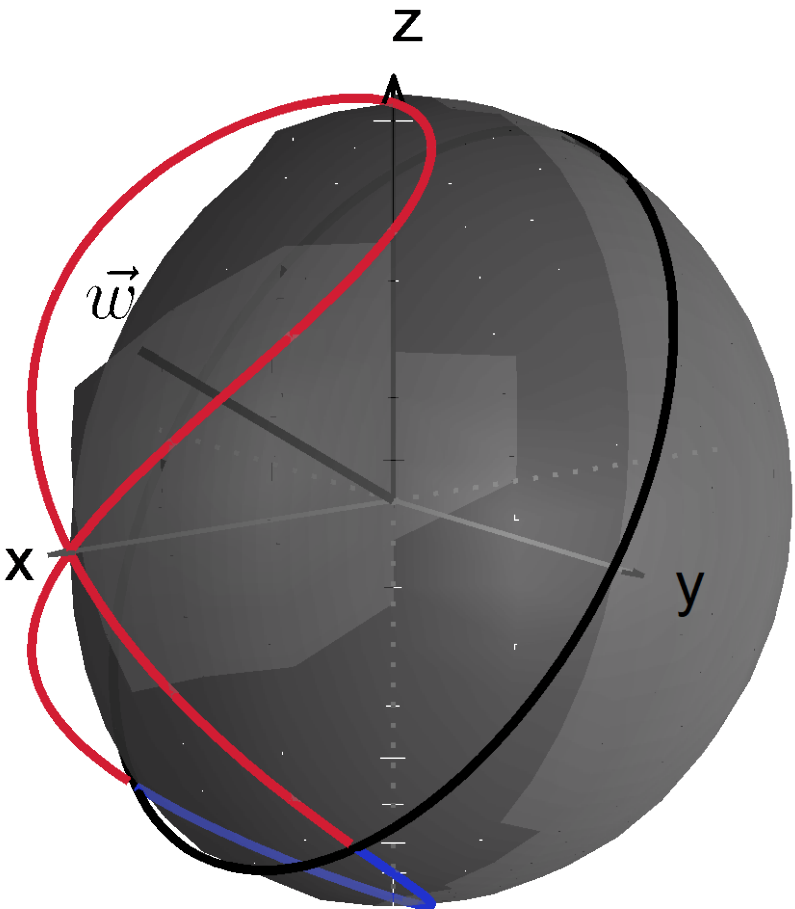


# Quantum-Enhanced Feature Space

Classical Classified Data

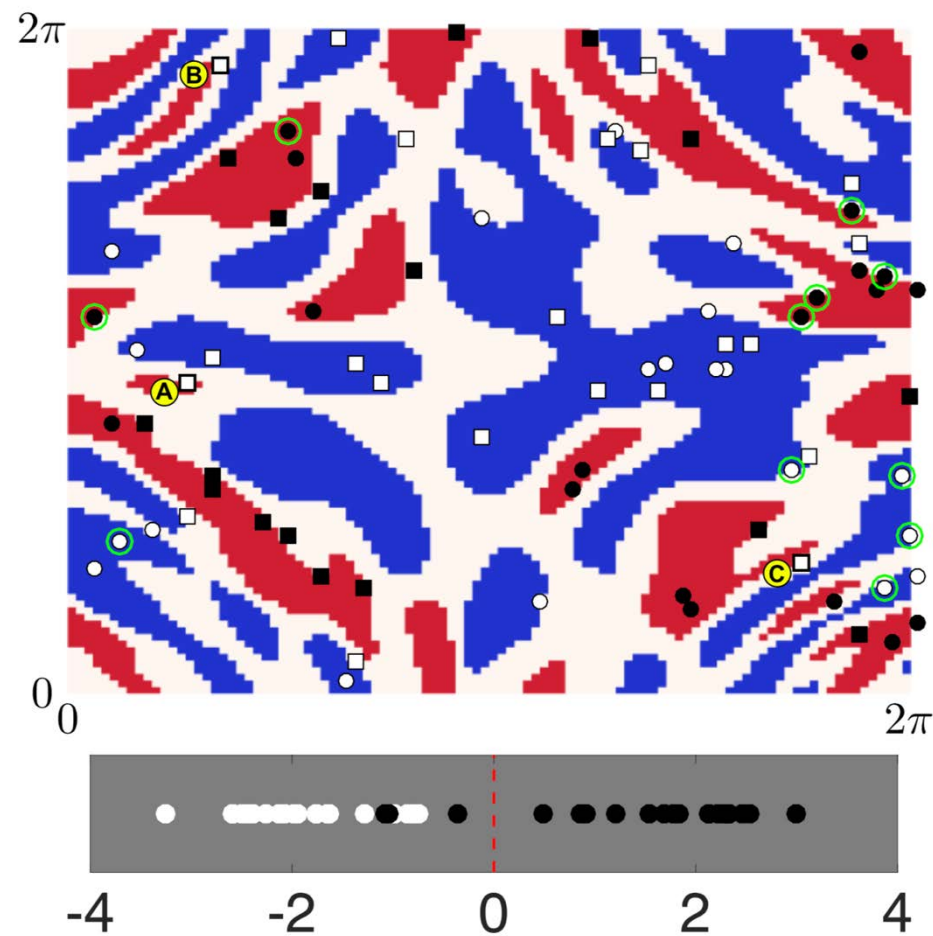


Quantum state space

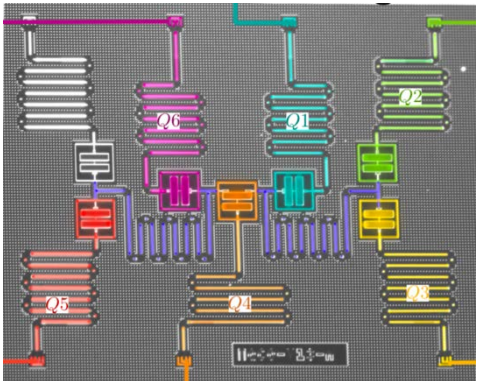
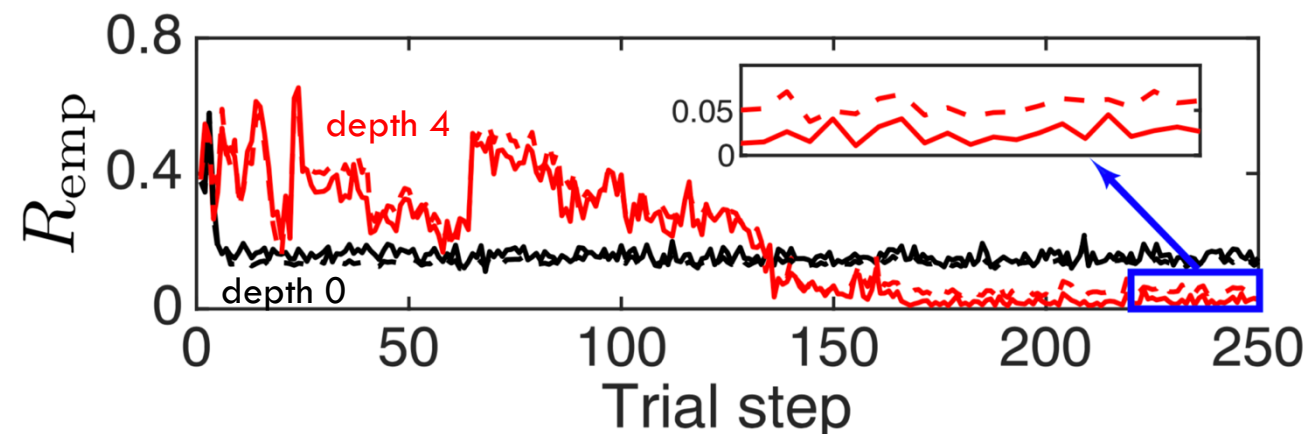


# Quantum-Enhanced Feature Space

Classical Classified Data



Training classifier in quantum state space

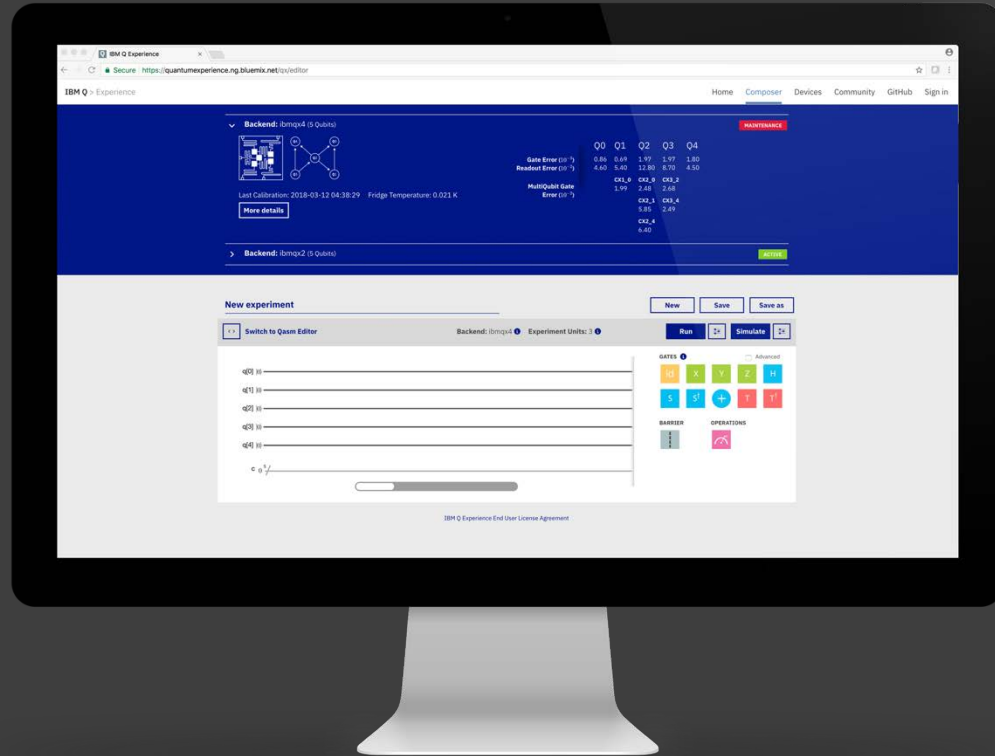


**How to start using quantum computers?**

**Qiskit**

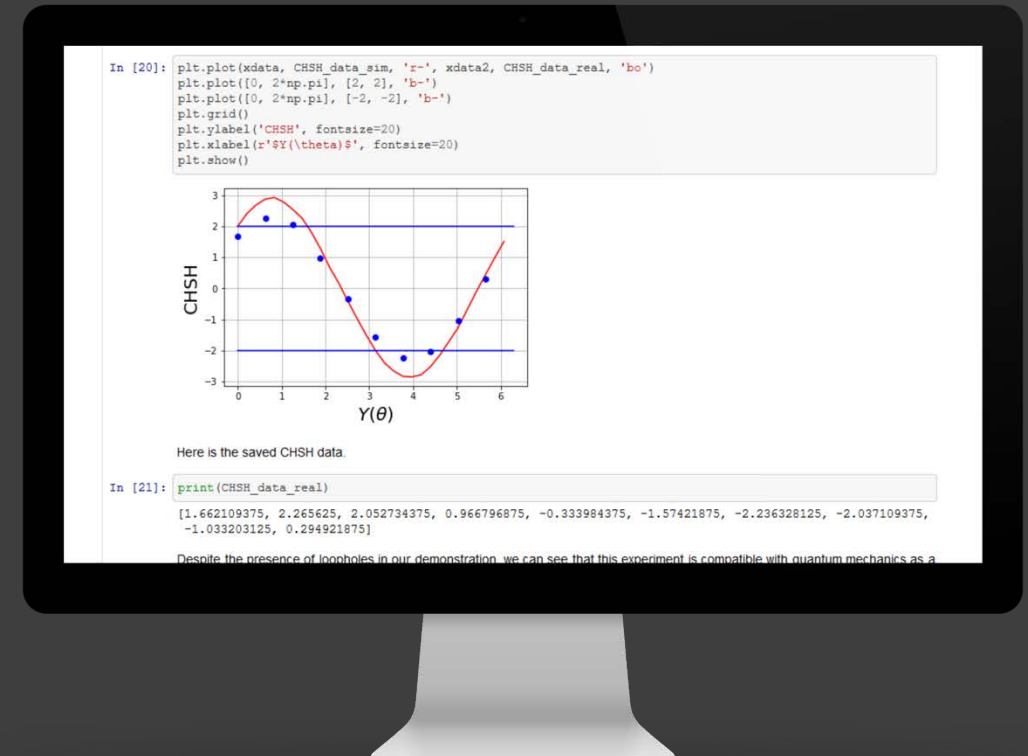
# Quantum Community

## IBM Q Experience



- Open to public for research and education
- Access via IBM Cloud

## QISKit.org



Software kit for short depth quantum circuits and building near term applications and experiments on quantum computers.

# Quantum Computing

IBM Technical Presentation

Thank you!

Zlatko K. Minev, Ph.D.

