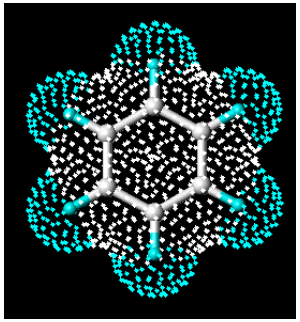
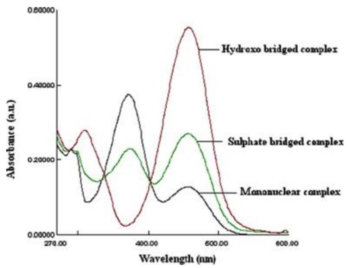
Quantum Computers and Quantum Chemistry

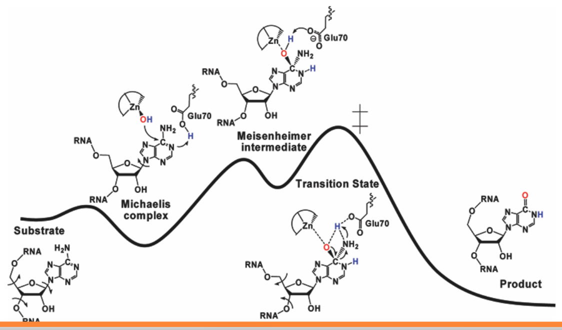


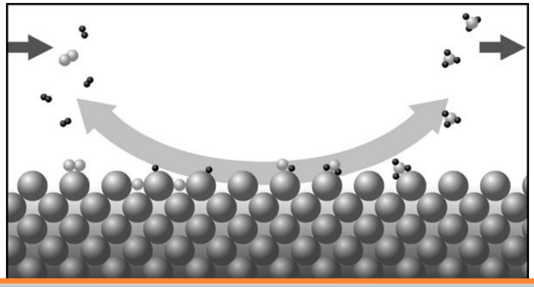
Jarrod McClean
Aspuru-Guzik Group
Harvard University

Promises of Quantum Chemistry

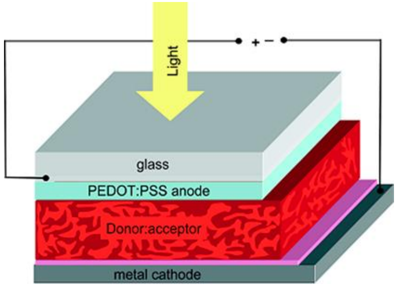
Understanding

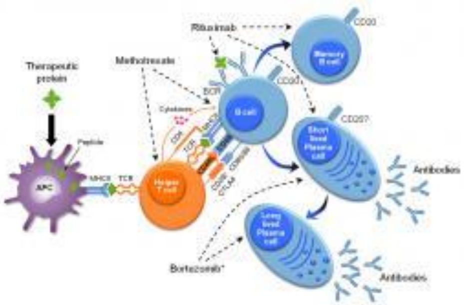






Control

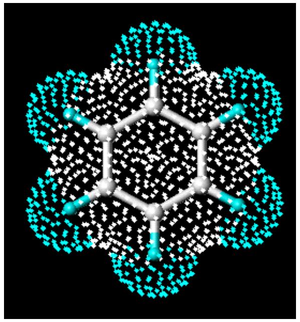




The Electronic Structure Problem

"The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

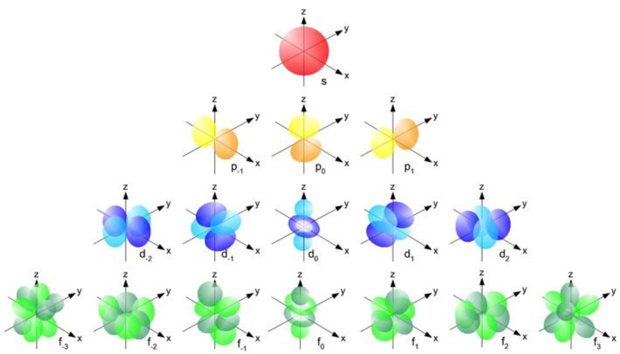
-Paul Dirac

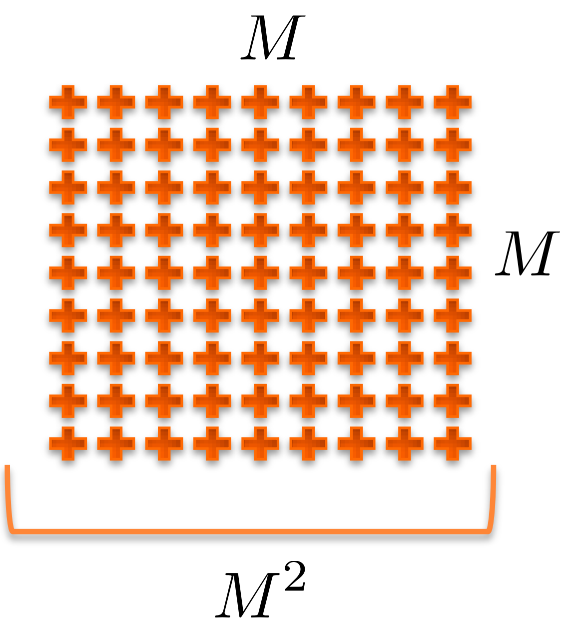


↔

$$\mathcal{H}\left|\psi\right\rangle = E\left|\psi\right\rangle$$

WHAT'S SO "COMPLICATED"?





$$D = M^N$$

$$M = 100$$
$$N = 80$$

$$D = 100^{80} = 10^{160}$$

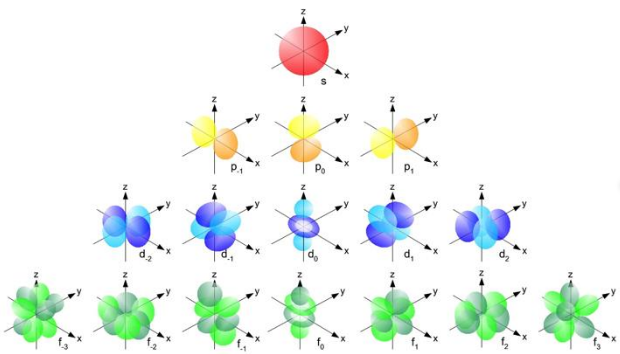
Electrons:

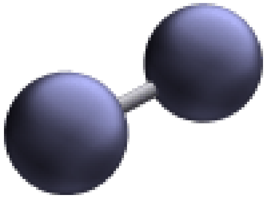
$$D = \begin{pmatrix} M \\ N_\alpha \end{pmatrix} \begin{pmatrix} M \\ N_\beta \end{pmatrix}$$

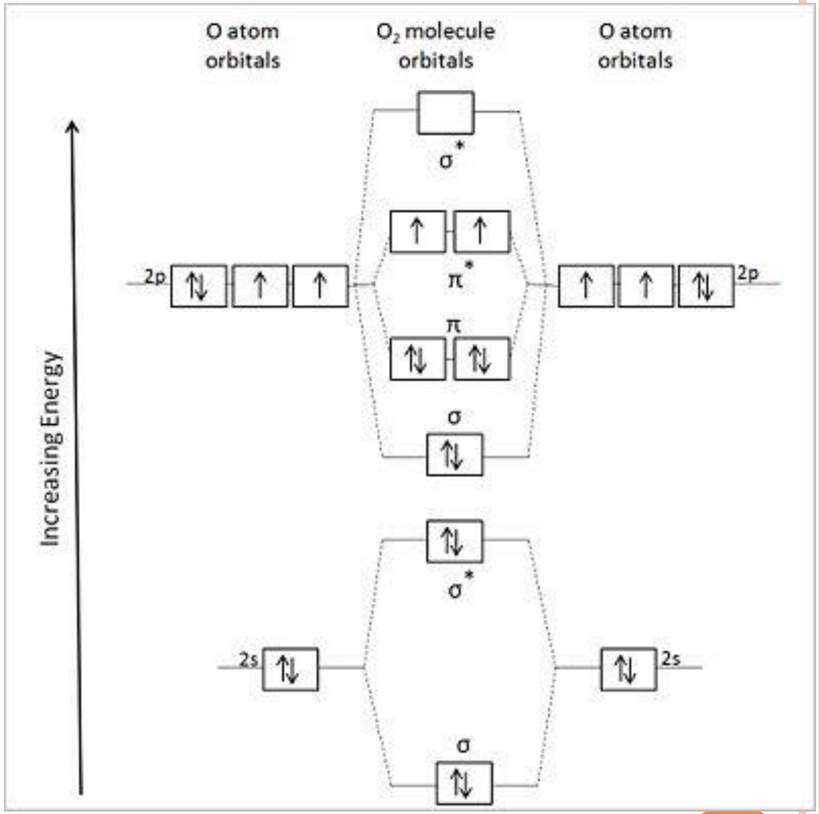
One mole
10^{23}

Particles in universe
10^{80}

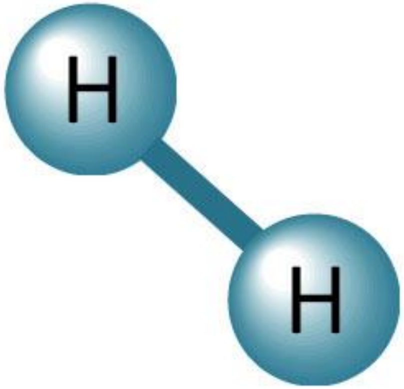
Traditional Solution

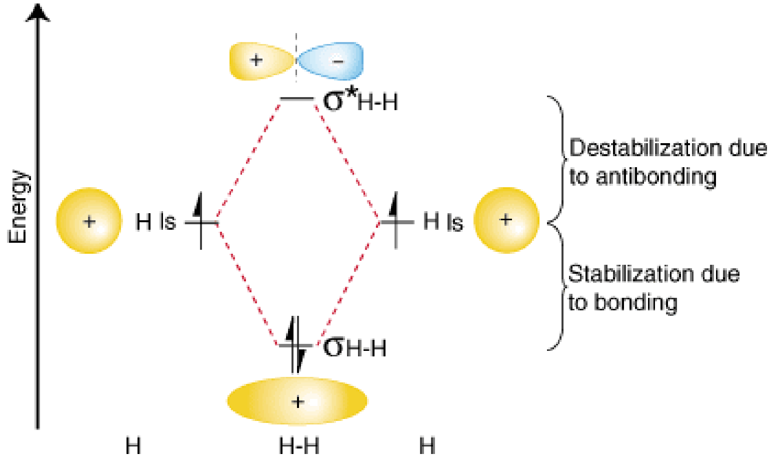






TRADITIONAL CHALLENGES





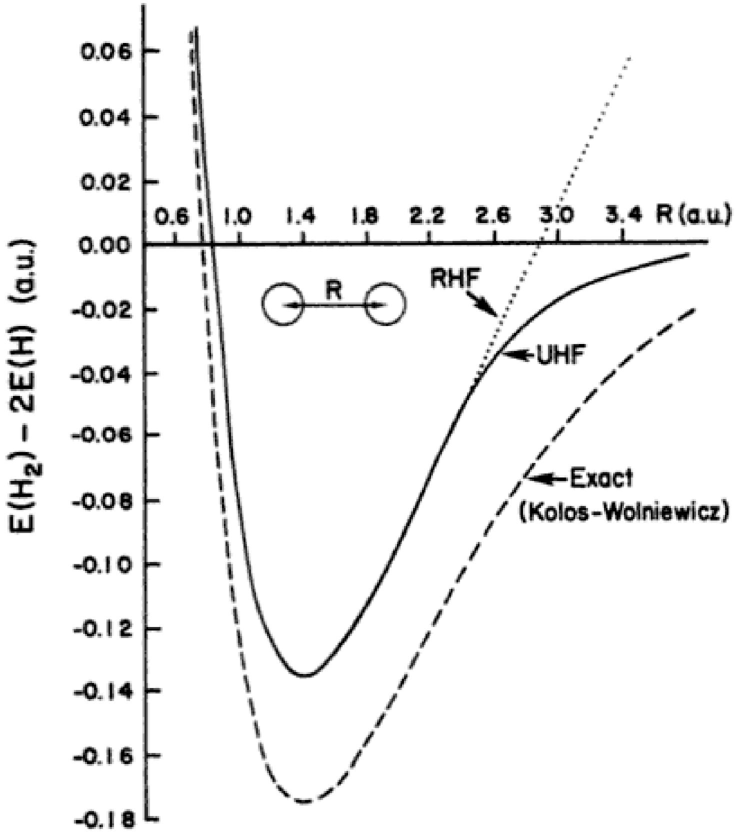
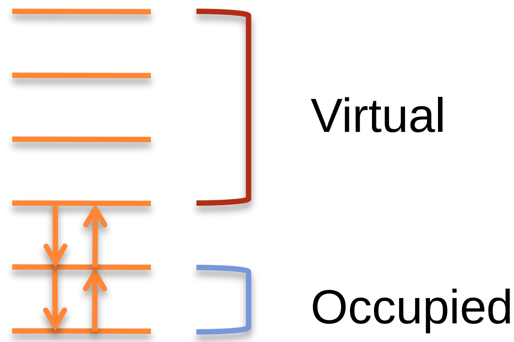
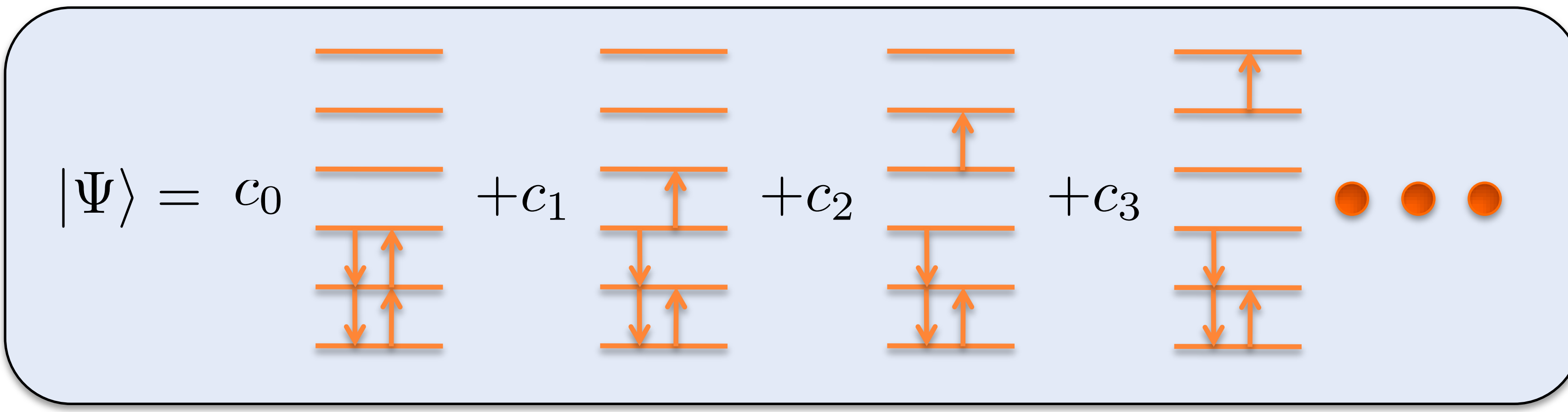


Figure 3.19 6-31G** potential energy curves for H_2.

Beyond the mean Field

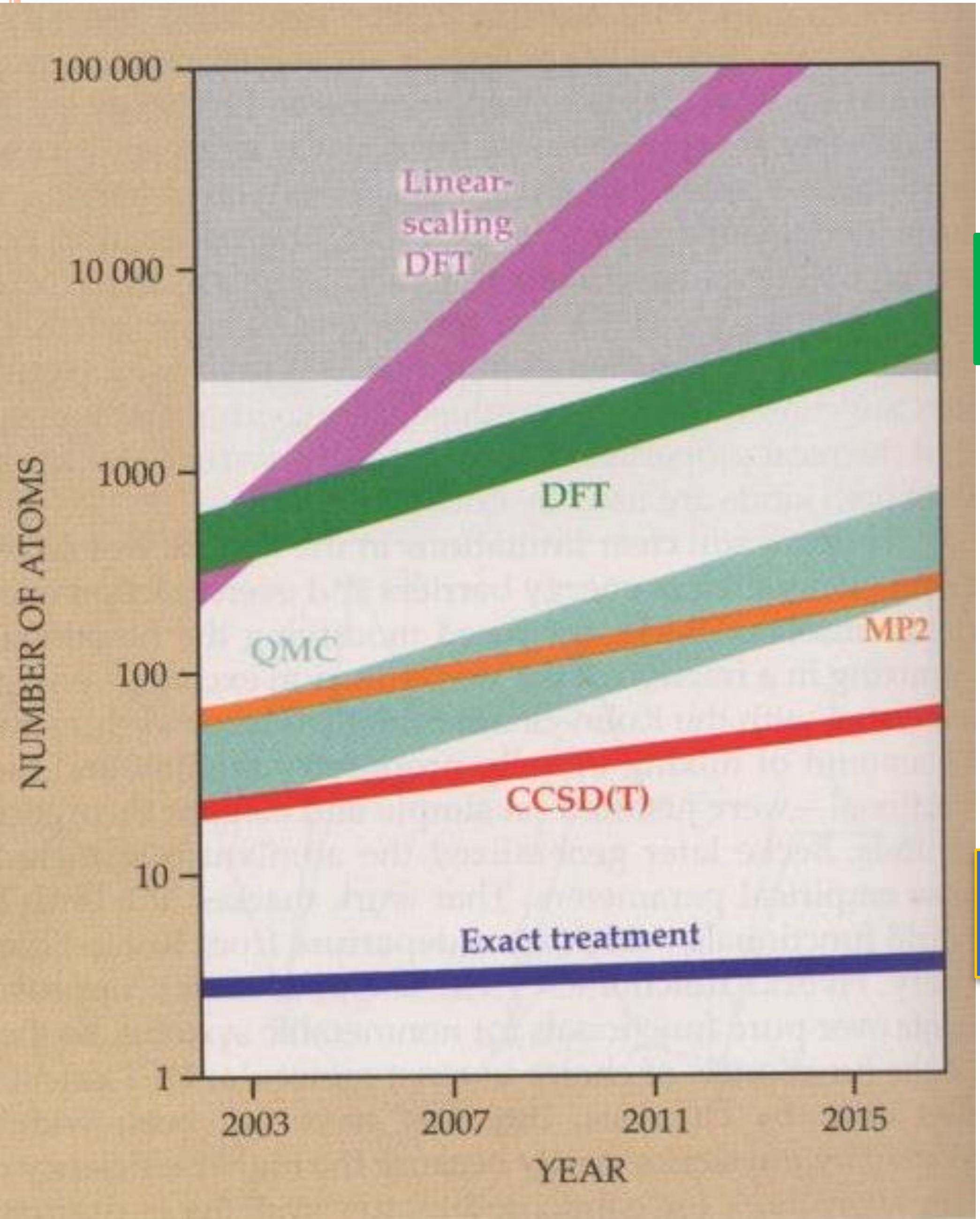




$$|\Psi\rangle = c_0\,|111100\ldots0\rangle + c_1\,|111010\ldots0\rangle + \ldots$$

$$|\Psi\rangle = \sum_{i_1 i_2 \ldots i_N} c^{i_1 i_2 \ldots i_N} |i_1 i_2 \ldots i_N\rangle$$

ALTERNATIVES



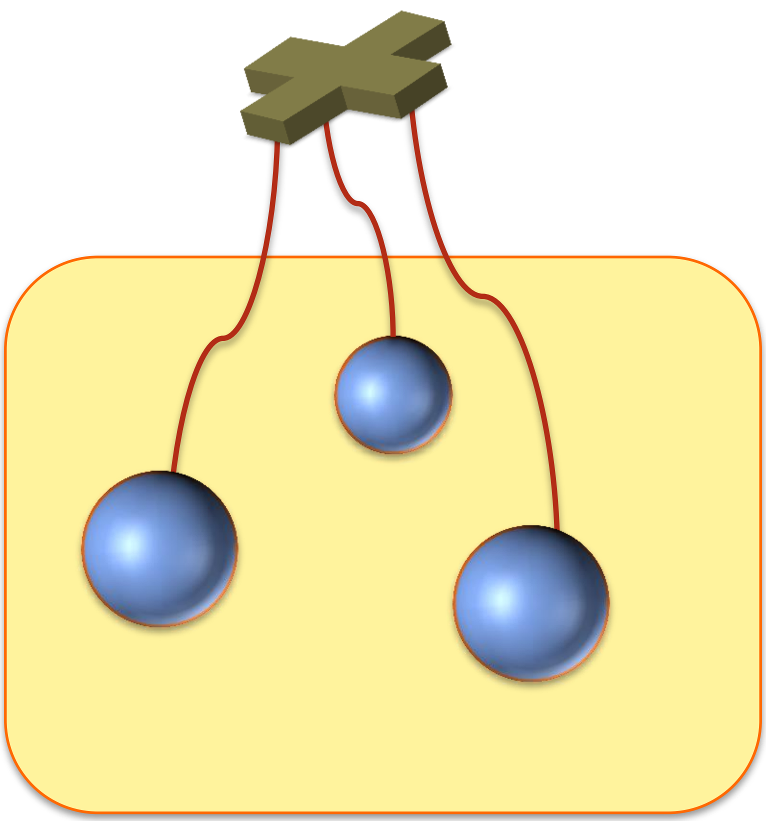
DFT: Errors in transition states, Charge transfer excitations, anions,…

Full Configuration Interaction: Exact (within a basis)

M. Head-Gordon, M. Artacho, ***Physics Today*** 4 (2008)

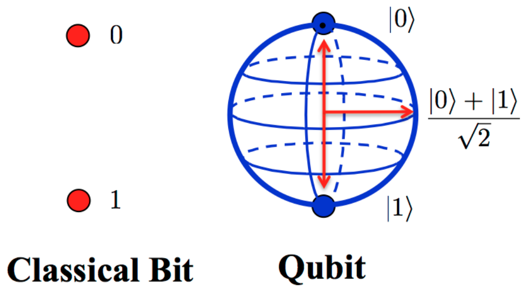
Quantum Marionette

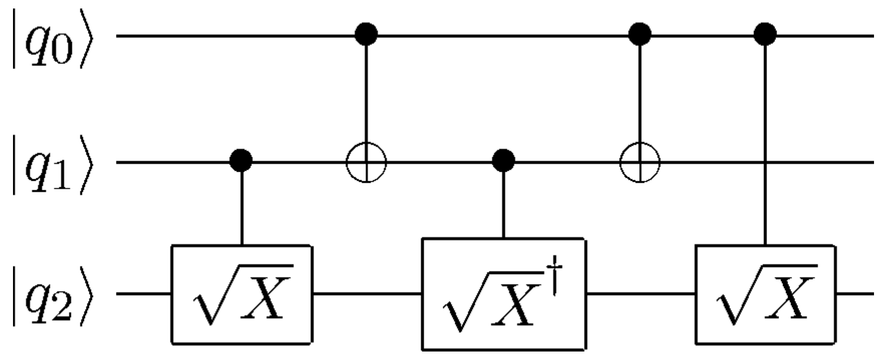
Engineer Hamiltonian → Let system naturally explore quantum space → Measure interesting parts of the system



$c^{i_1 i_2 \ldots i_N}$

Quantum Computing Notation





$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

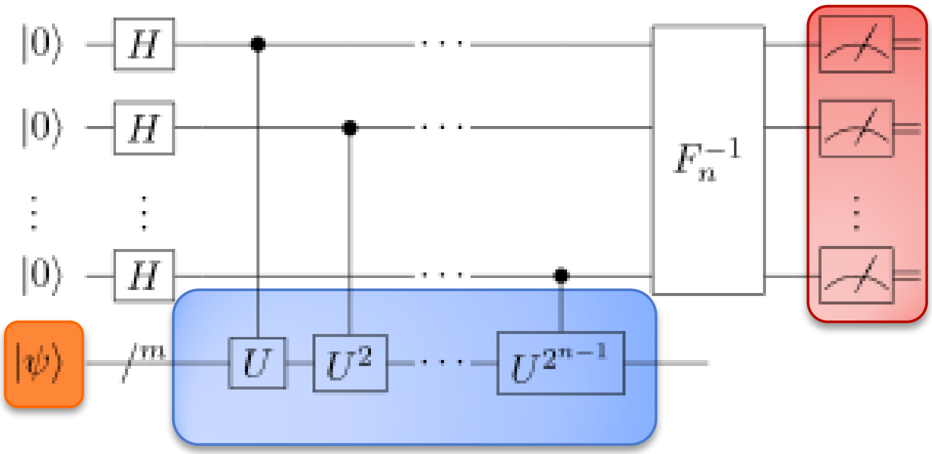
$$|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$X = \text{NOT} = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$X|0\rangle = |1\rangle$$

$$X|1\rangle = |0\rangle$$

Quantum Phase Estimation



$$U = e^{-iH\delta t}$$

$$H = \sum_\alpha H_\alpha$$

Prep $|\psi\rangle$ → Evolution → Measurement → $\{|\Psi_i\rangle, E_i\}$

Classical: $O(M^N)$

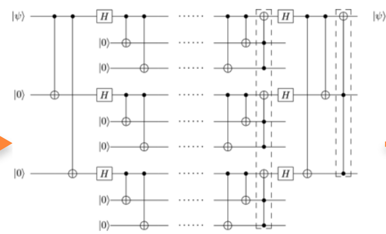
Quantum: $O(M^5)$

Challenge: Coherence time

Aspuru-Guzik, Dutoi, Love, Head-Gordon, *Science* 309, 1704–1707 (2005).

A New Co-design Perspective

Currently: Given a task, design quantum circuit (or computer) to perform it.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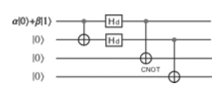
Problem: General or optimal solution can require millions of gates.

Alternative: Given a task and the current architecture, find the best solution possible.

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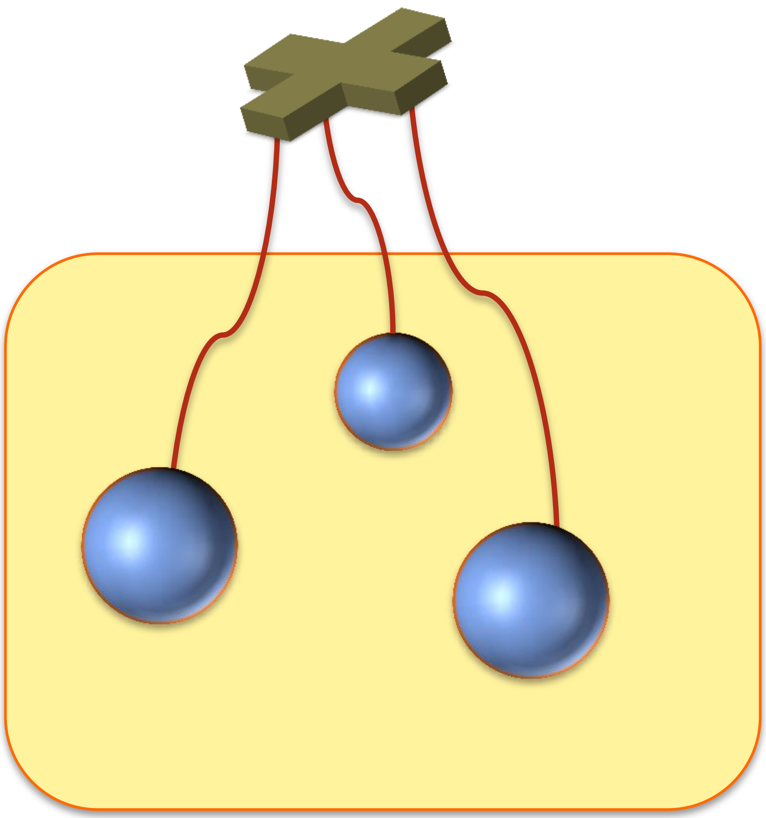
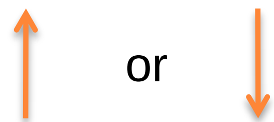
Peruzzo†, **McClean†**, Shadbolt, Yung, Zhou, Love, Aspuru-Guzik, O'Brien. *Nature Communications*, 5 (4213):1– 7, 2014.
† Equal Contribution by authors

Easy Task For A Quantum Computer





$$\langle \sigma_i^z \rangle \qquad \langle \sigma_1^z \sigma_2^z \ldots . \sigma_n^z \rangle$$

- Efficient to perform on any prepared quantum state
- In general, it may be very hard to calculate this expectation value for classically for some states

Variational Basics

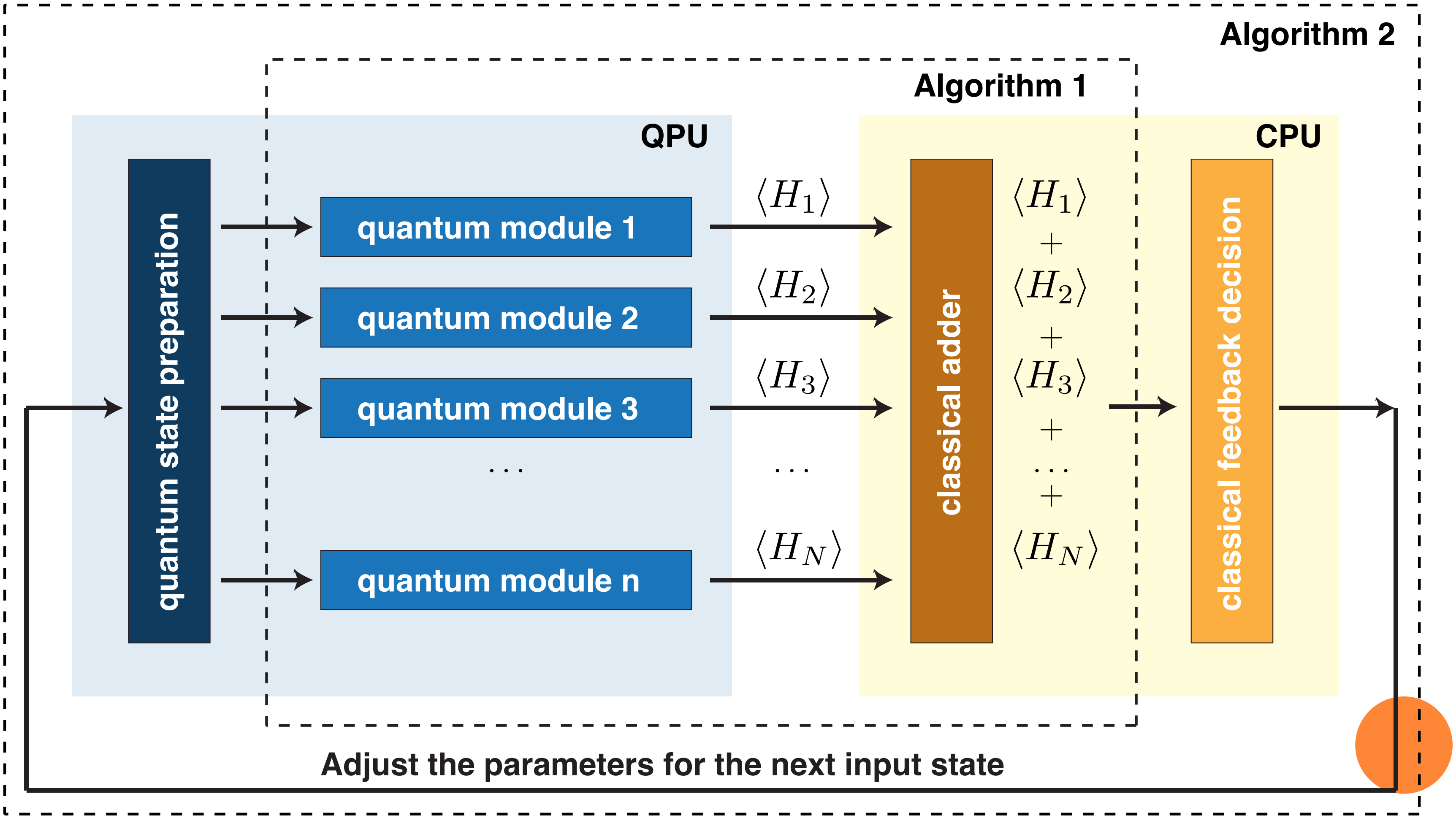
Variational Formulation: $$\underset{|\psi\rangle}{\operatorname{argmin}} \frac{\langle\psi| \mathcal{H} |\psi\rangle}{\langle\psi|\psi\rangle}.$$

Can write a Hermitian Hamiltonian as: $$\mathcal{H} = h^i_\alpha \sigma^i_\alpha + h^{ij}_{\alpha\beta}\sigma^i_\alpha \sigma^j_\beta + h^{ijk}_{\alpha\beta\gamma}\sigma^i_\alpha \sigma^j_\beta \sigma^k_\gamma + \ldots$$

By Linearity: $$\langle\psi| \mathcal{H} |\psi\rangle \equiv \langle\mathcal{H}\rangle = \mathcal{H} = h^i_\alpha \langle\sigma^i_\alpha\rangle + h^{ij}_{\alpha\beta} \langle\sigma^i_\alpha \sigma^j_\beta\rangle + h^{ijk}_{\alpha\beta\gamma} \langle\sigma^i_\alpha \sigma^j_\beta \sigma^k_\gamma\rangle + \ldots$$

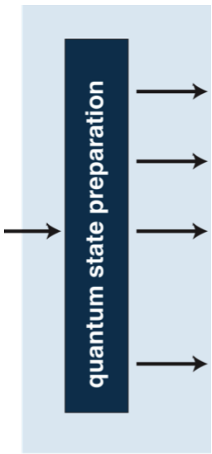
Easy for a Quantum Computer: $\langle\sigma^i_\alpha \sigma^j_\beta \sigma^k_\gamma \ldots\rangle$ → Easy for a Classical Computer: $+, \times \to \langle H\rangle$

Computational Algorithm



Quantum Hardware State Ansatz

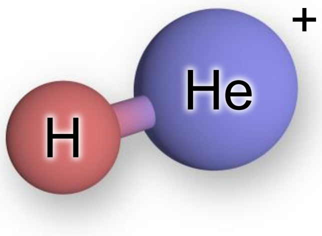
Any Quantum Device with “knobs”

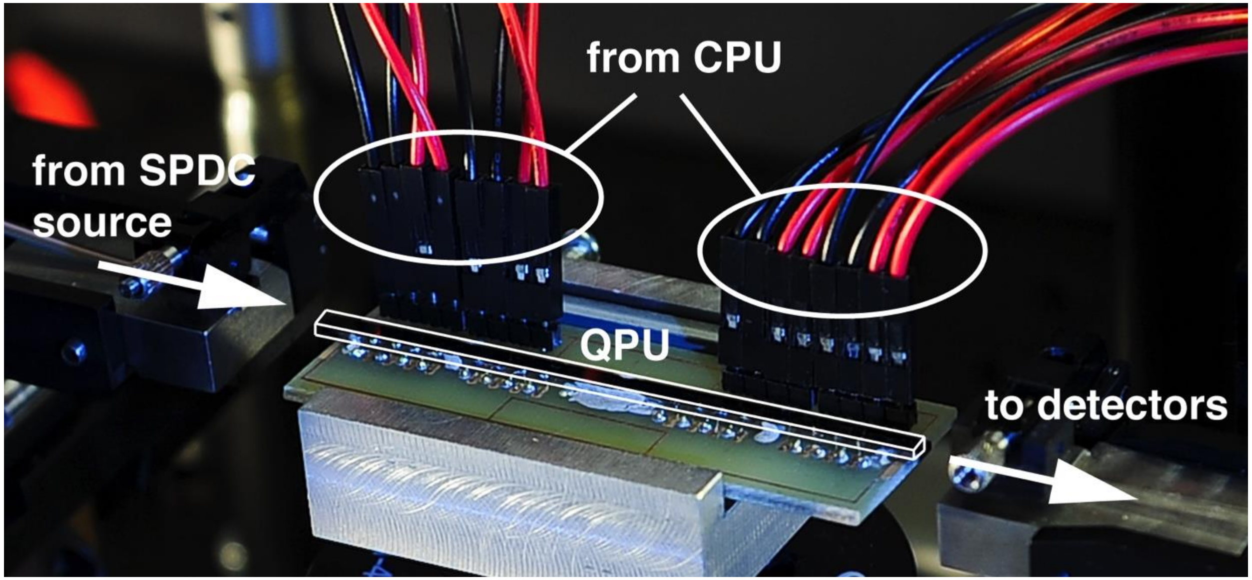


$$= |\Psi(\{\theta_i\})\rangle$$

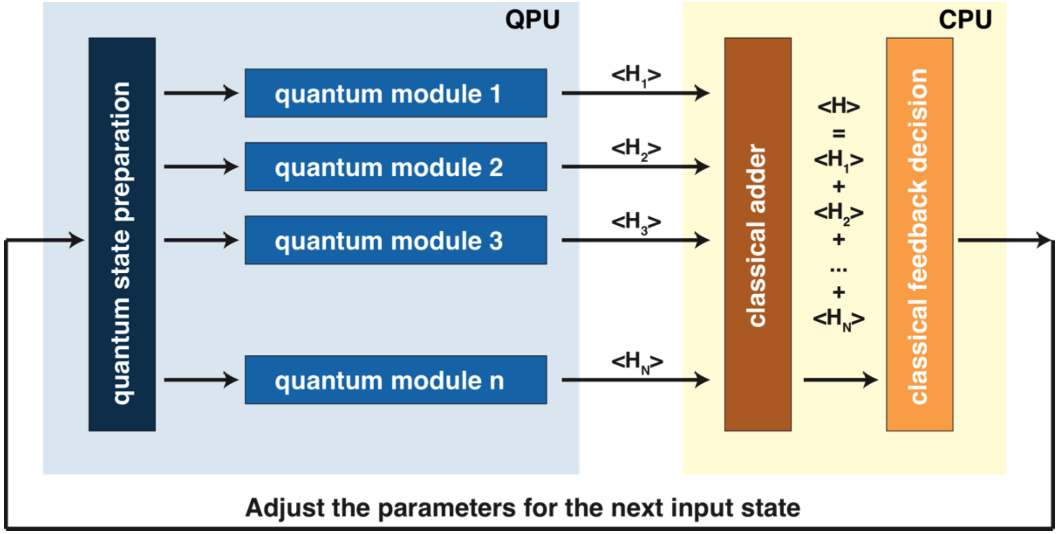
Advantages:
- Use the complexity of your device to your advantage
- Always satisfies a variational principle
- Coherence time requirements are set by the device, not algorithm

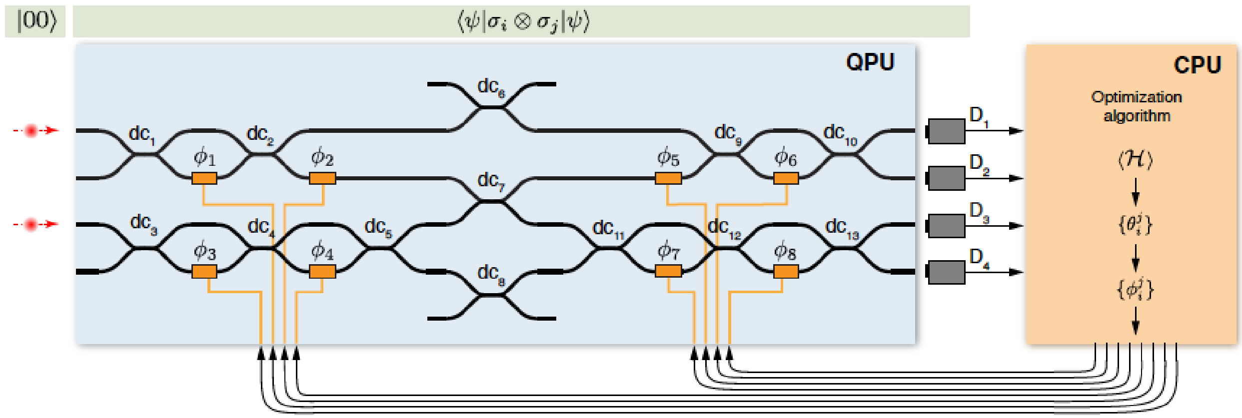
Model System



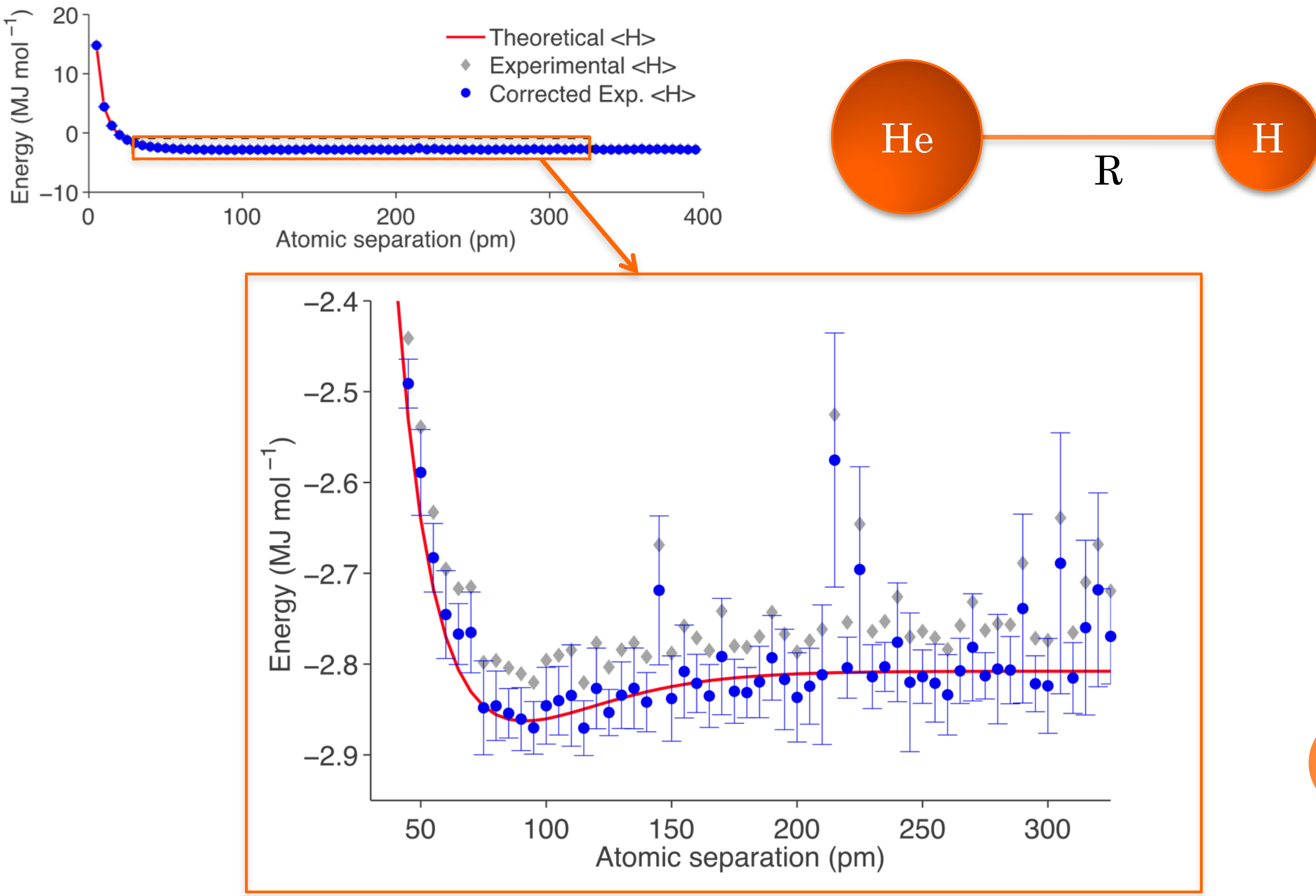


Physical Implementation

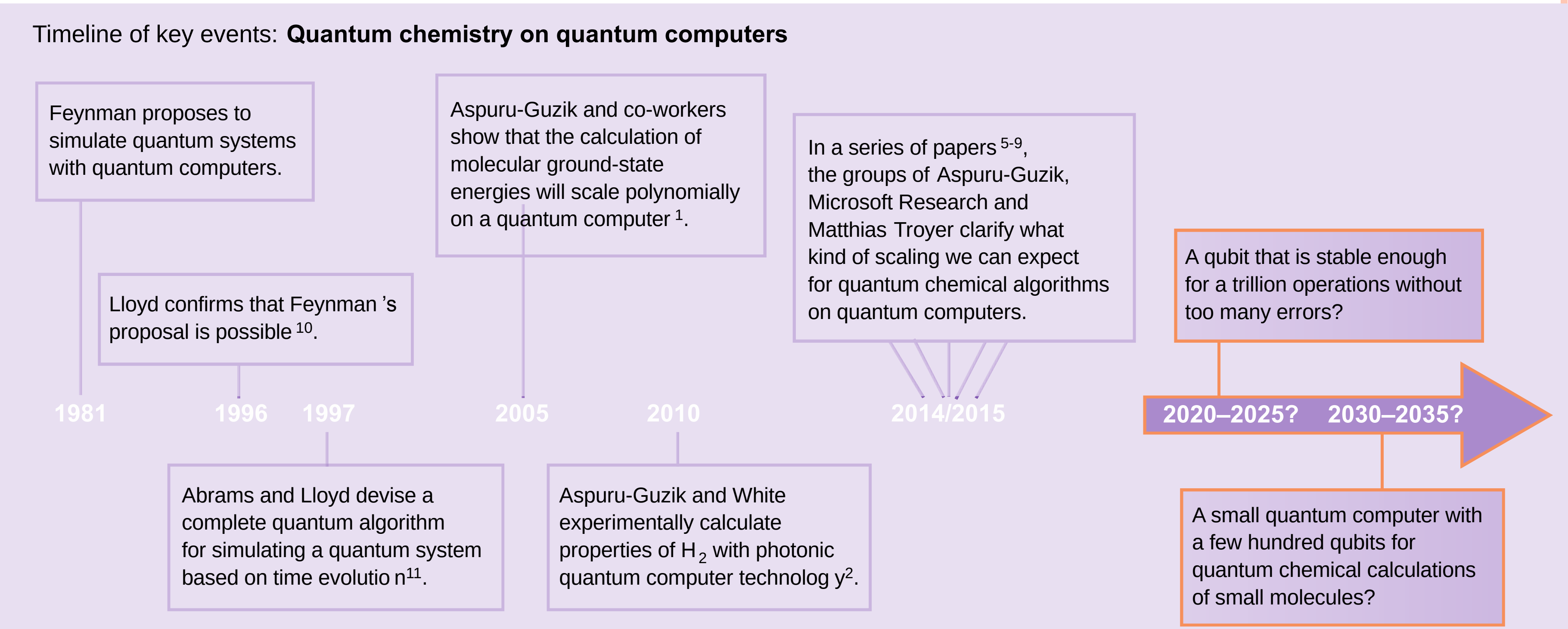




Experimental Electronic Curve



Quantum Computation Is Approaching



Mueck, *Nature Chemistry 7, 361–363 (2015)*

Summary

•Quantum computers offer a new route forwards to understanding and predicting the properties of chemical and material systems

•Considering both the problem and the available architecture offers a new way to utilize available quantum resources today

•A small scale implementation has been built and tested on quantum hardware

•Quantum software as well as quantum hardware is being pursued in industry, national labs, and academia and may be here sooner than we thought

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