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Simulating Electronic Structure on Noisy Quantum Hardware: From Gate to Annealing Models

September 2018

OTI Lumionics

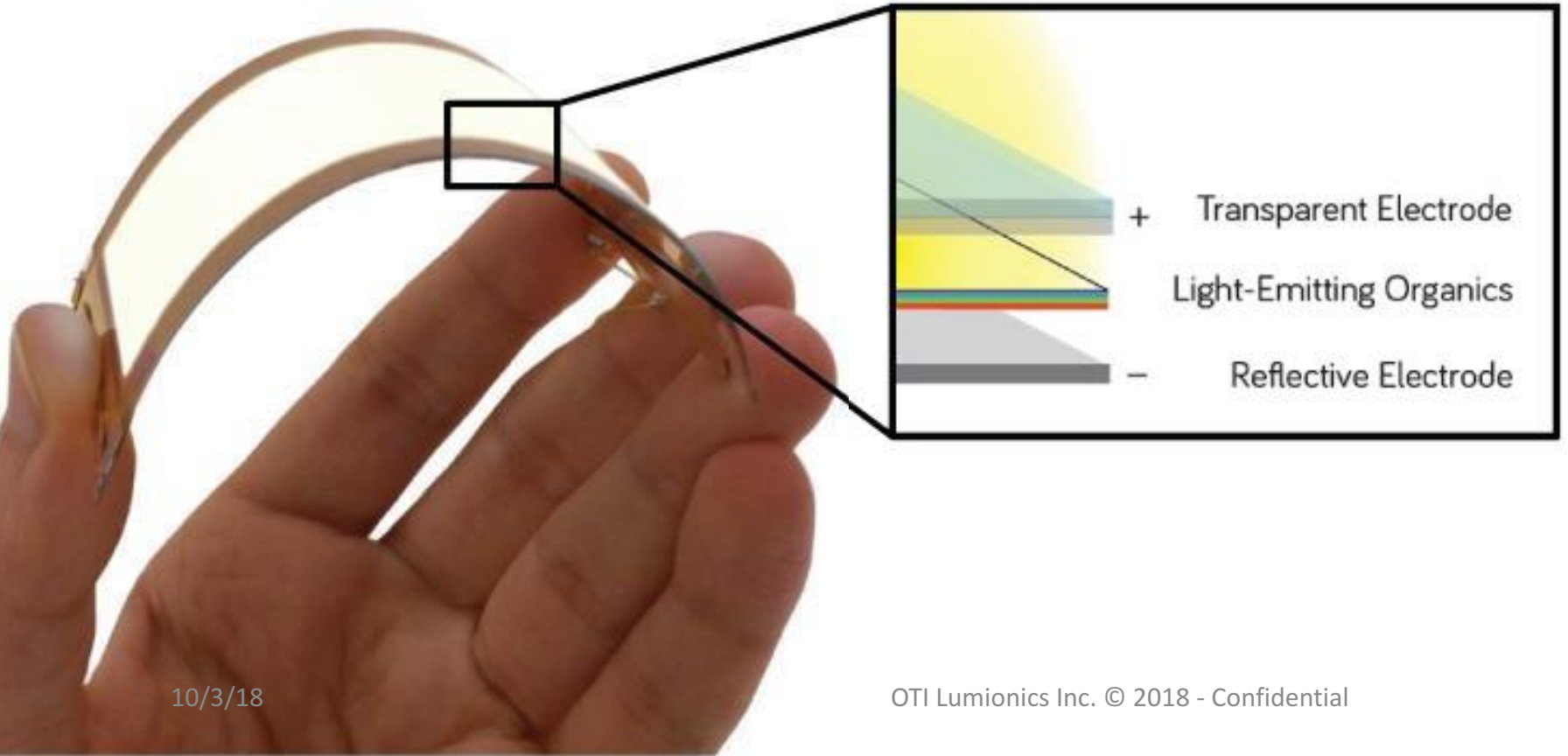
What We Do

Materials Discovery

Developing advanced materials to solve large scale industrial problems for displays + lighting

Organic Light Emitting Diode (OLED)

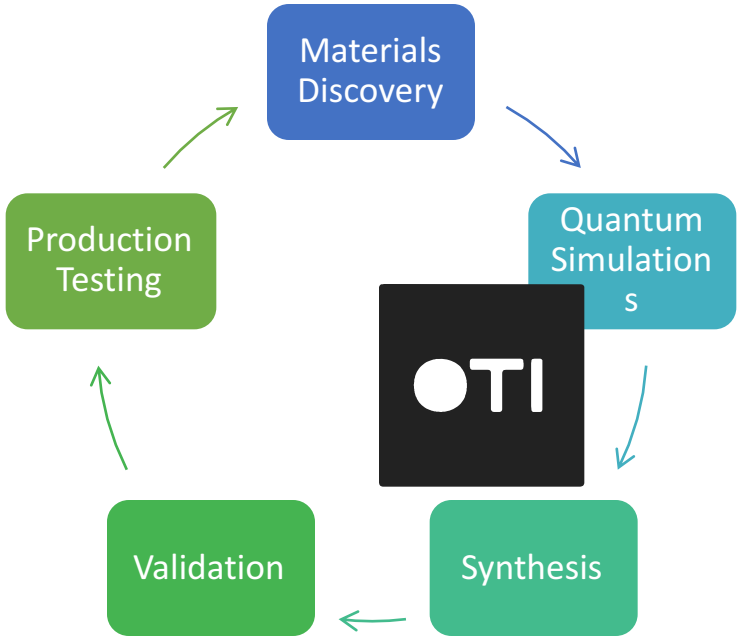
Light from organic pigments sandwiched between electrodes



Organic Pigments

Closed Loop Development with Customer Feedback

In-house end-to-end testing from materials discovery up to production testing



Detailed Specifications

MP Ready Materials

Tool Builders

Panel Makers

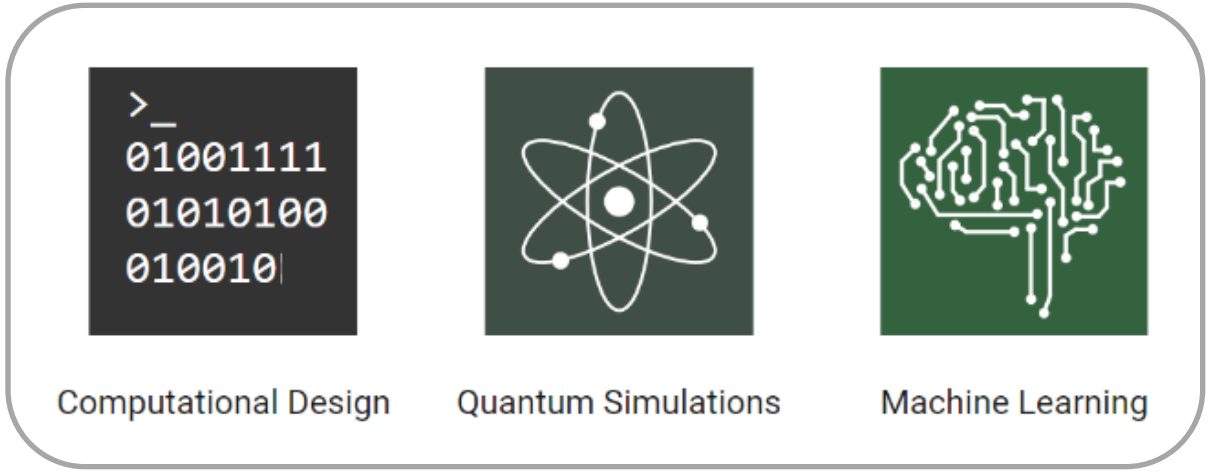
OEMs

Our Materials Discovery Platform

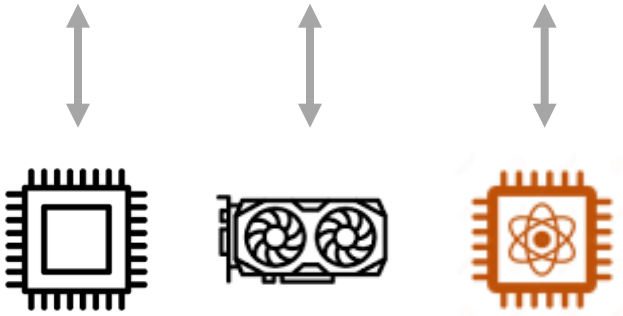
Advanced computation + simulation + ML/AI

Properties

- Vapor pressure
- Optical constants
- Electronic structure
- Film forming
- Crystallinity
- Etc.

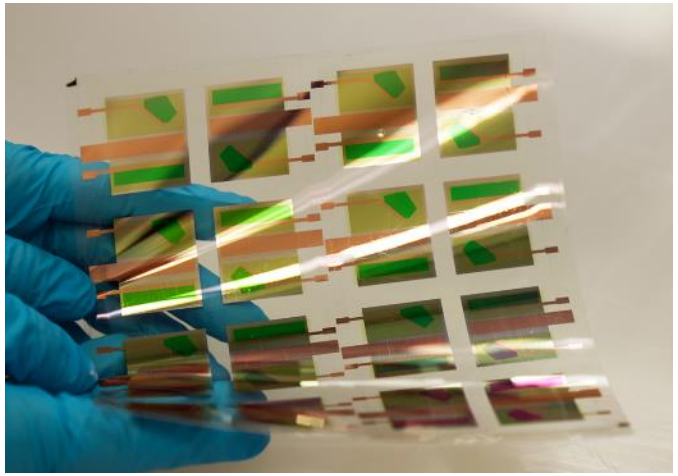
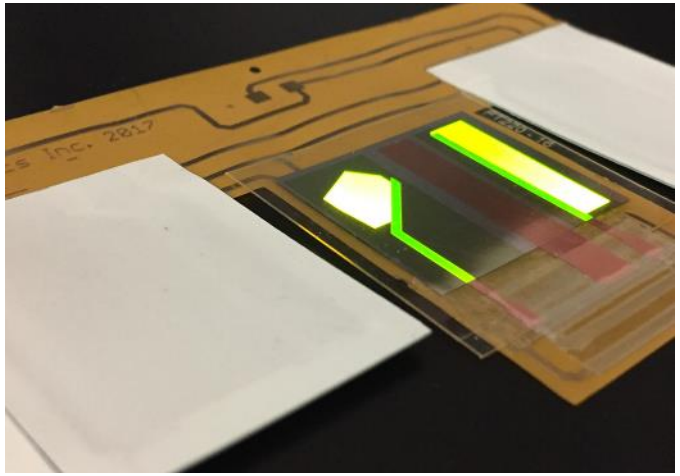


Structure



Example: Aerelight for Print™

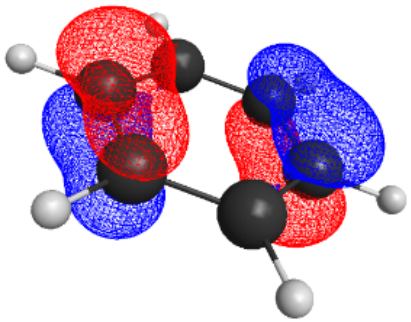
Flexible OLED module for print + packaging

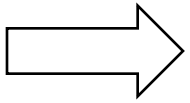



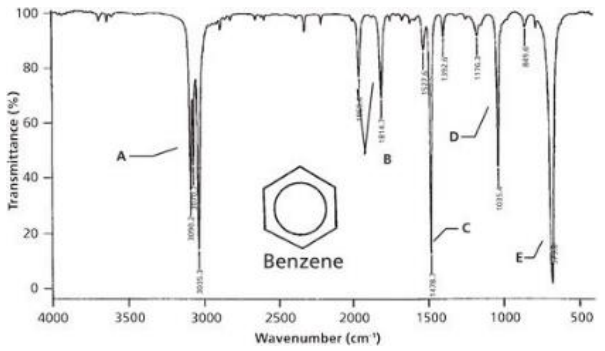


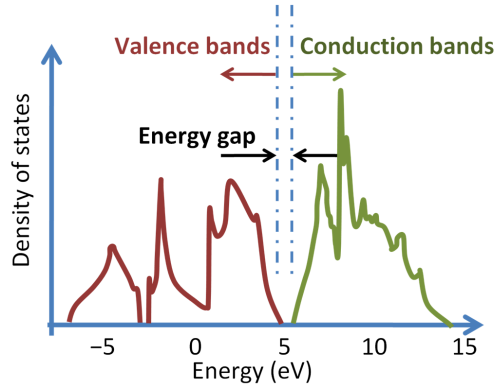
Quantum Chemistry

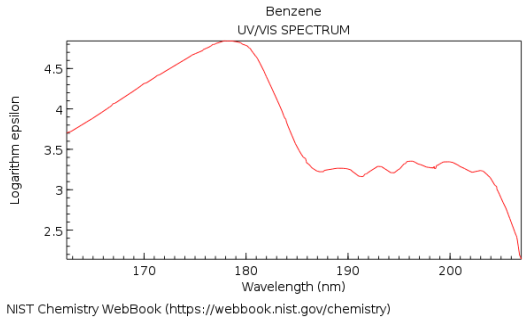
Why do we care?

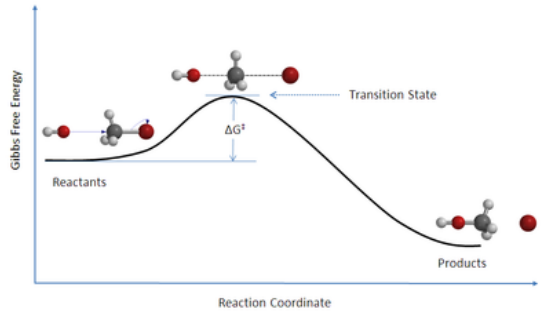








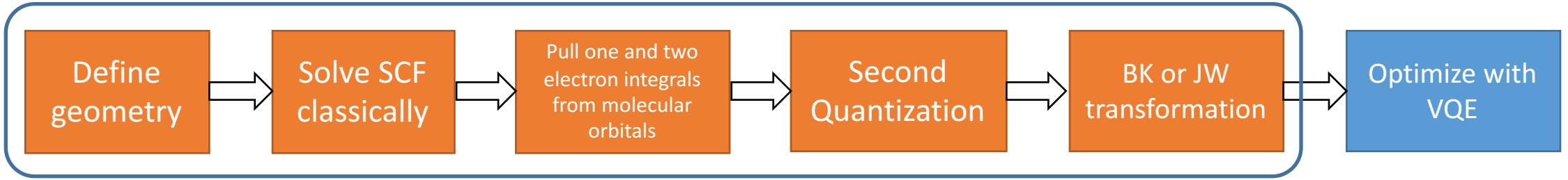




Understanding and prediction of the Structure -> Property relationship

Current Model of Quantum Chemistry on universal QPUs

Some not so good news



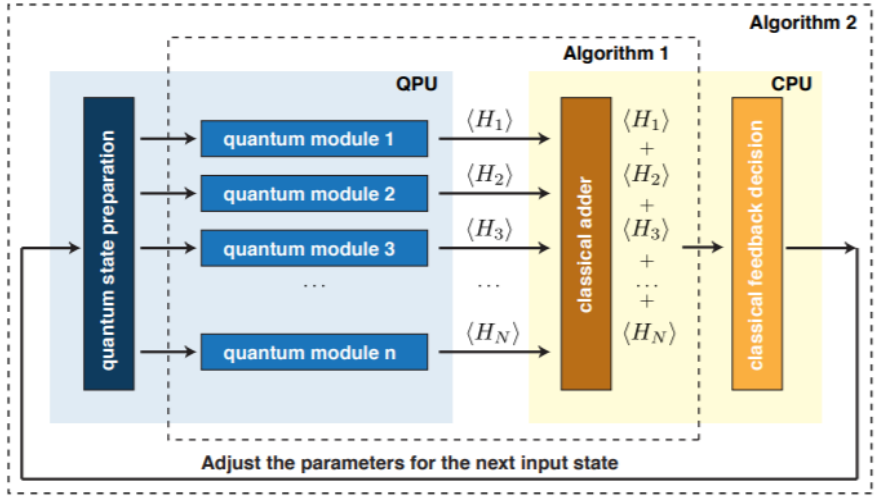
All of this done on a classical computer… lots of work

The hope is to surpass the HF wavefunction/orbitals on a quantum computer

Variational Quantum Eigensolver

$$\hat{H} = \sum \hat{P}_i$$ Where $\hat{P}_i = \prod \sigma_j^n$, *n* = {x,y,z} & *j* = qubit index

$$E_0 \leq \sum \langle \Psi_i | \hat{P}_i | \Psi_i \rangle$$ Where Ψ is wavefunction



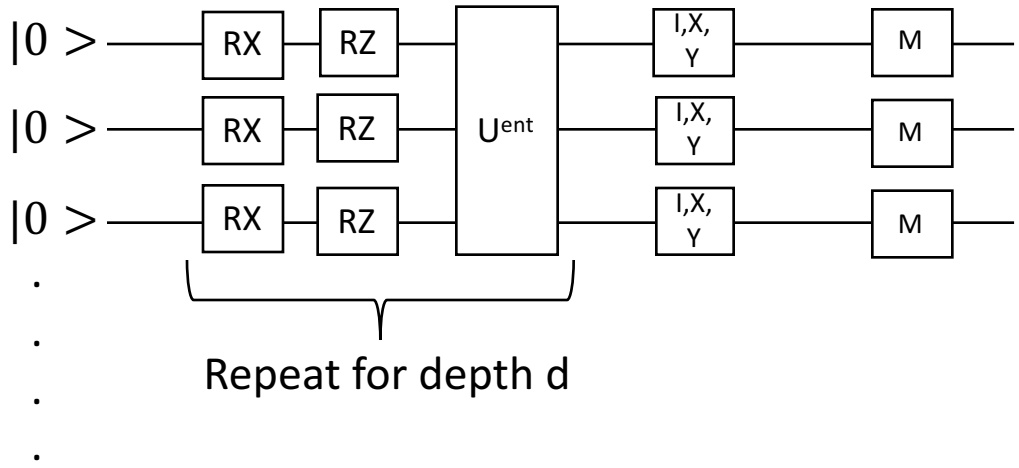
*Peruzzo *et al.* Nat. Comm. 5 (2014)

With serial processing, time scales linearly with number of Pauli words

BK transformation generates $O(N^4)$ Pauli words

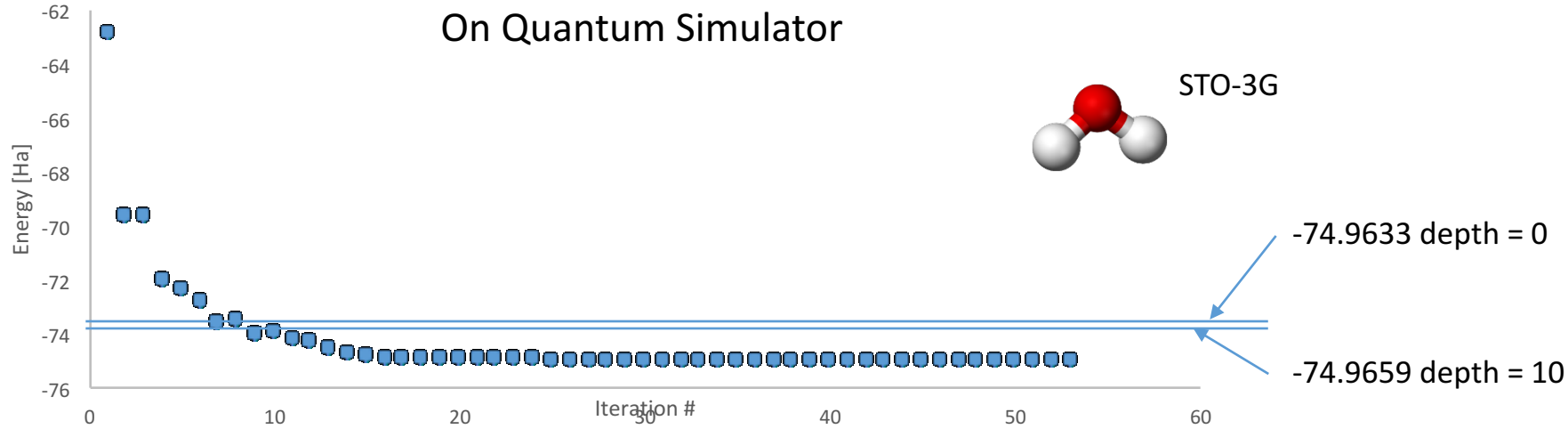
Ansatz Construction – Conventional Wisdom

UCC and Variational



- To get close to FCI, often depth >30
- 2-qubit operators > 10 = too much error on QPU (19Q-Acorn)
- UCC is not rigorous solution of ES, but a problem that is difficult for a classical computer to solve

On Quantum Simulator

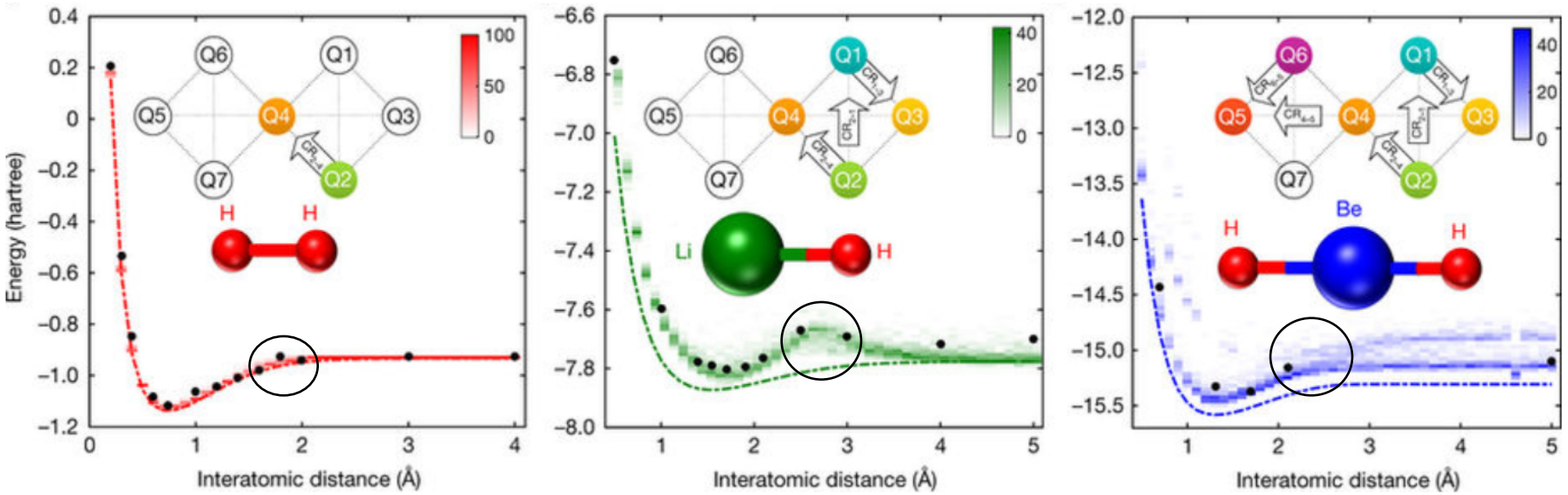


STO-3G

-74.9633 depth = 0

-74.9659 depth = 10

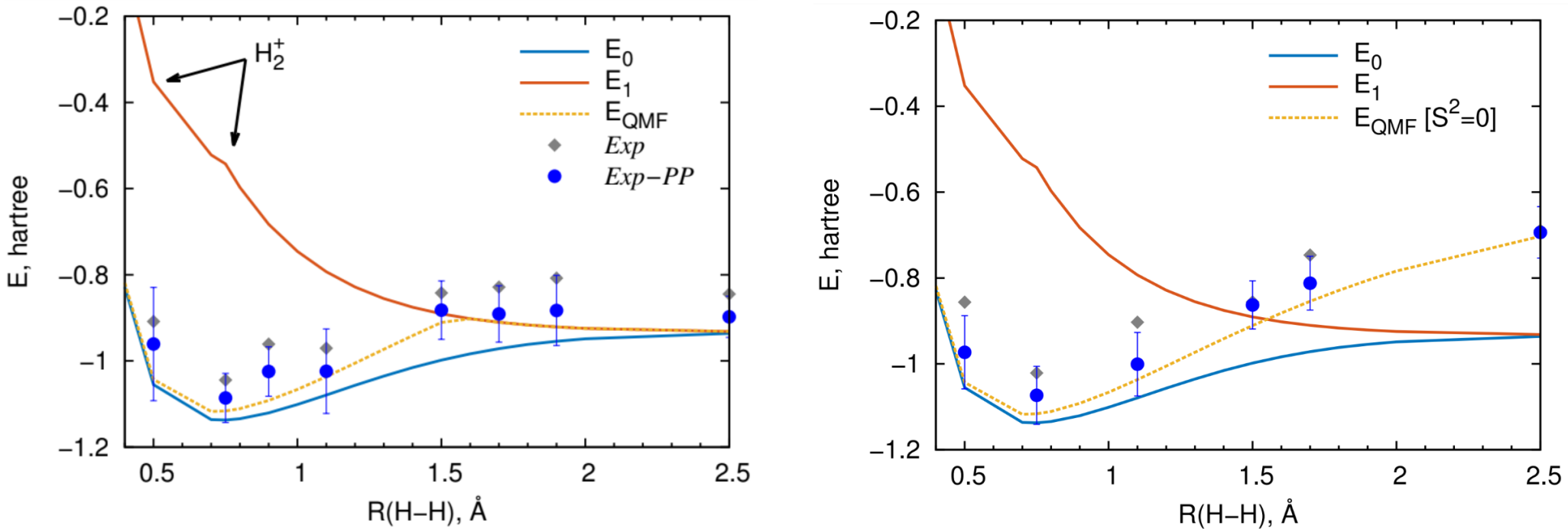
Hidden Consequences



Is this “kink” a hardware problem or theory problem?

Kandala *et al.* (2017) Nature 549, 242-246

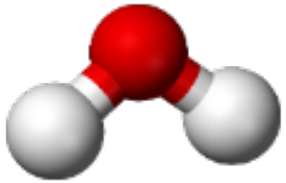
Broken Symmetry Transition – H_2 on QPU



Broken symmetry GHF between 1.5 A – 1.6 A, as it transitions from singlet to triplet

Our Innovation: Error Correction

Reduces error in finale solution by reducing noise



Water Simulated on QPU arXiv:[1806.00461]

Nosie filter removes random bit flips based on incorrect electron numbers and spin

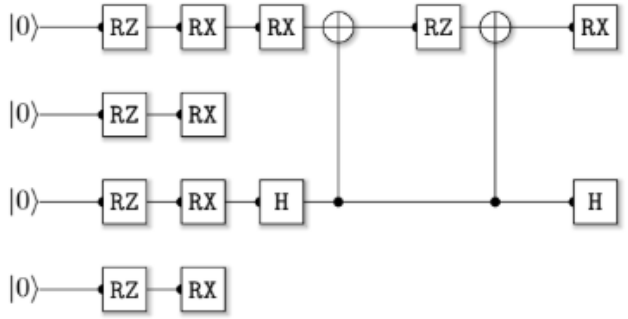
UCC vs. QCC

$\Psi(\tau, \omega) = \hat{U}(\tau)|\omega\rangle$ General form of CC methods

$\hat{U}(\tau) = \prod_{k}^{N} \exp\left(\frac{i\tau_k \hat{P}_k}{2}\right)$ $\hat{P}$ is Pauli word entanglers

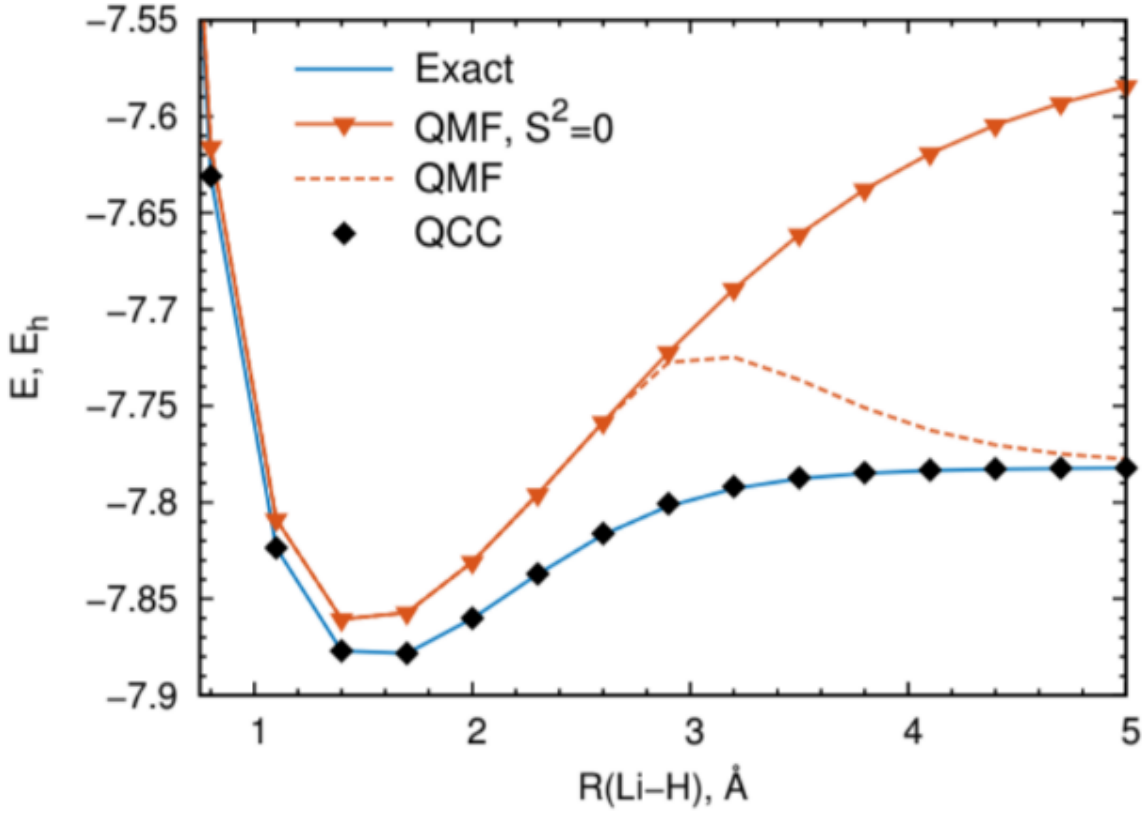
$E(\tau, \omega) = \langle\omega|U(\tau)^{\dagger}\hat{H}U(\tau)|\omega\rangle$

QCC is closed form opposed to UCC which is not



Example Ansatz for QCC

PES Curve for LiH



Our Innovation: Quantum Adiabatic Solver

Enables quantum chemistry to be run on annealer

Universal Gate

IBM Q (20 qubits)

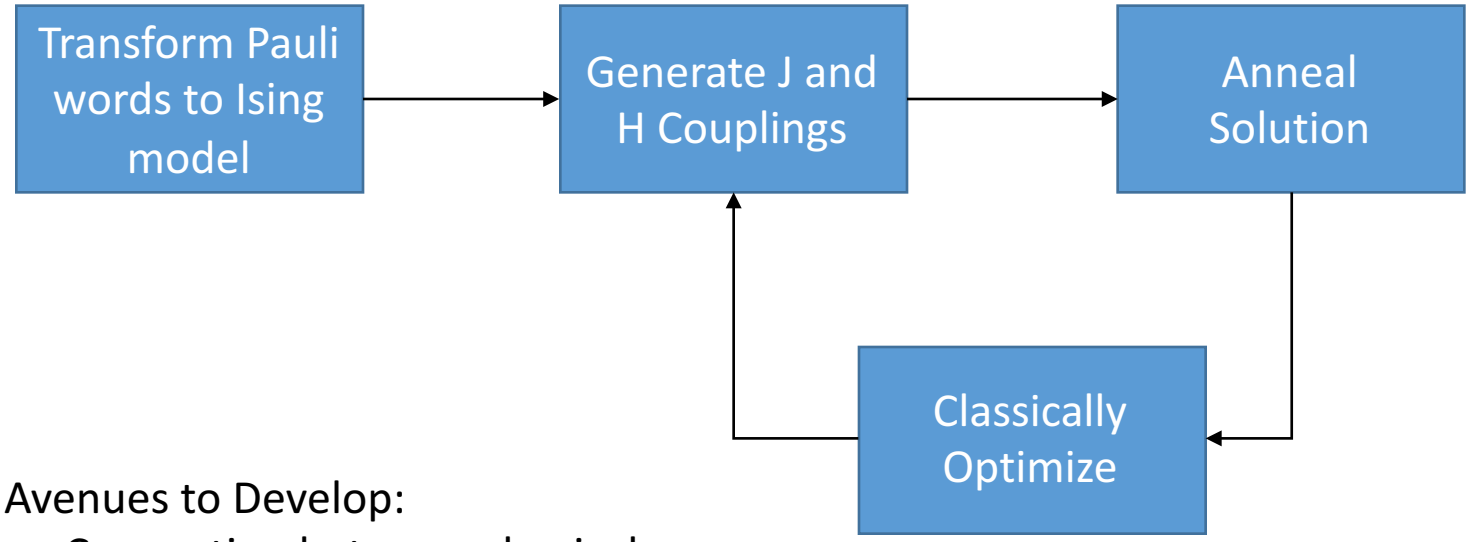
Quantum Annealer

D-Wave 2000Q (2048 qubits)

← Annealer is suitable for solving binary optimization problems
(not applicable for quantum chemistry)

We have developed a quantum solver for quantum chemistry on a quantum annealer

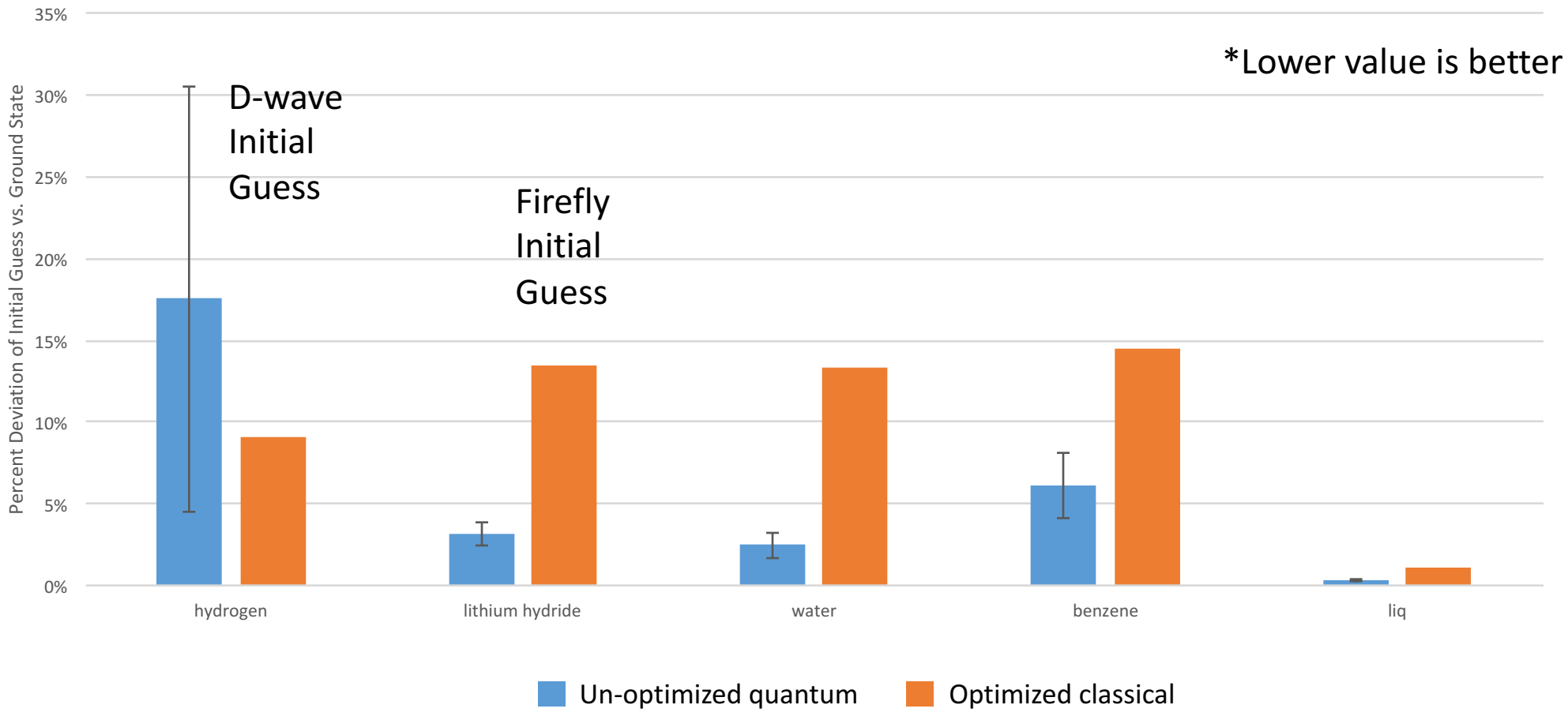
Solution on Quantum Annealer



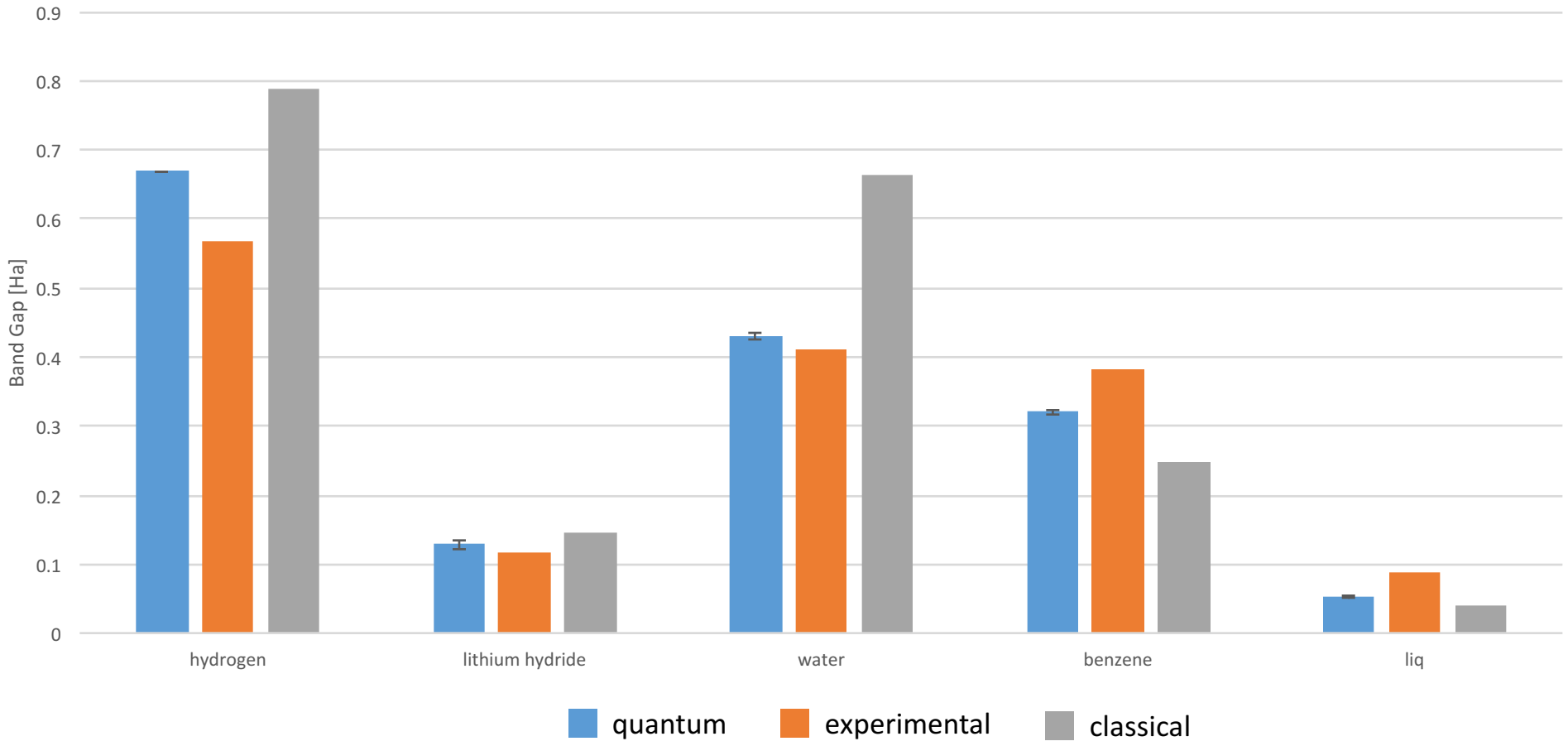
Avenues to Develop:

- Connection between classical and quantum optimization
- Frequency when to queue the D-wave

First Iteration Deviation: Quantum vs. Classical

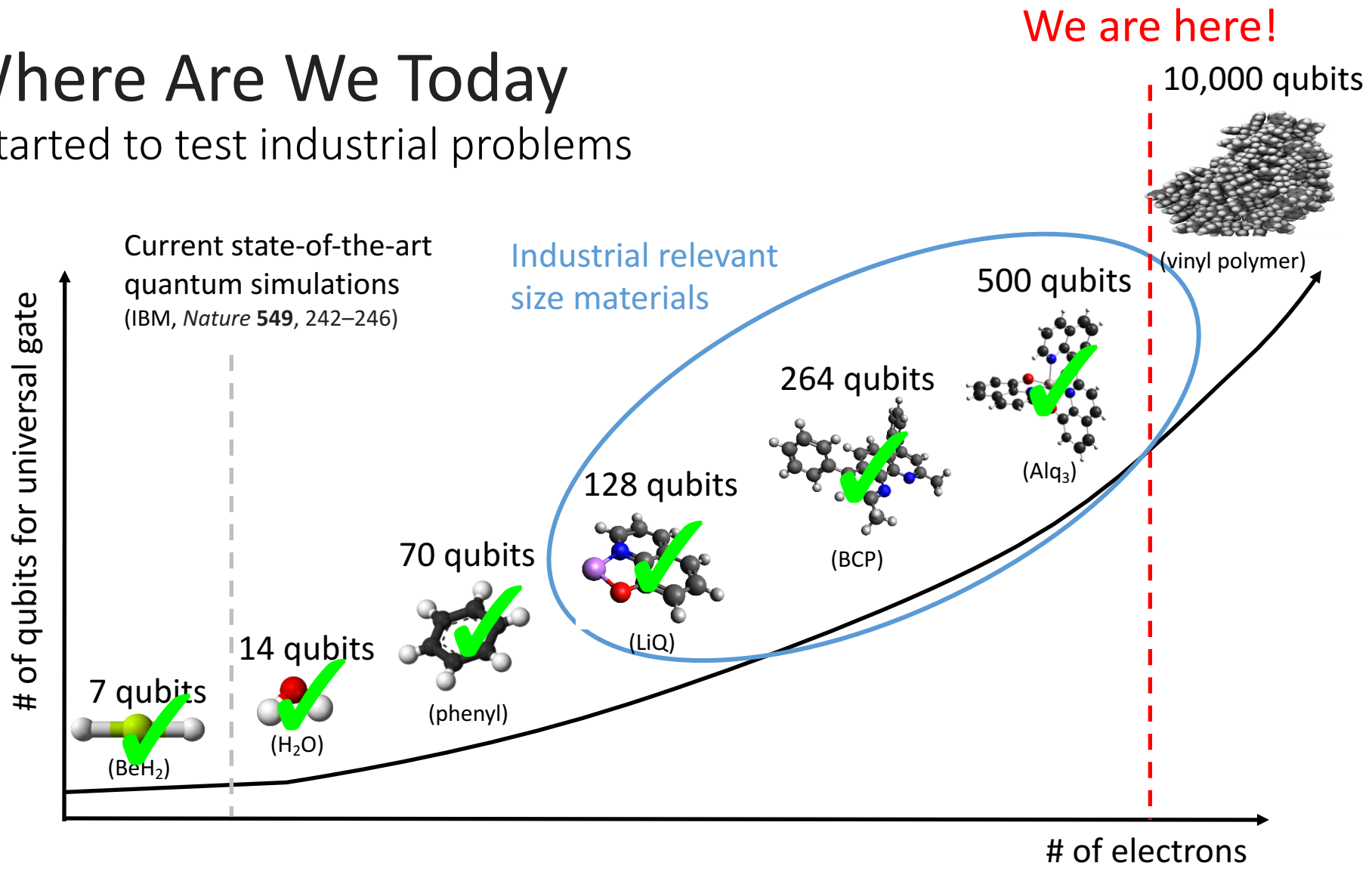


Simulation of Band Gap: Quantum vs Classical



Where Are We Today

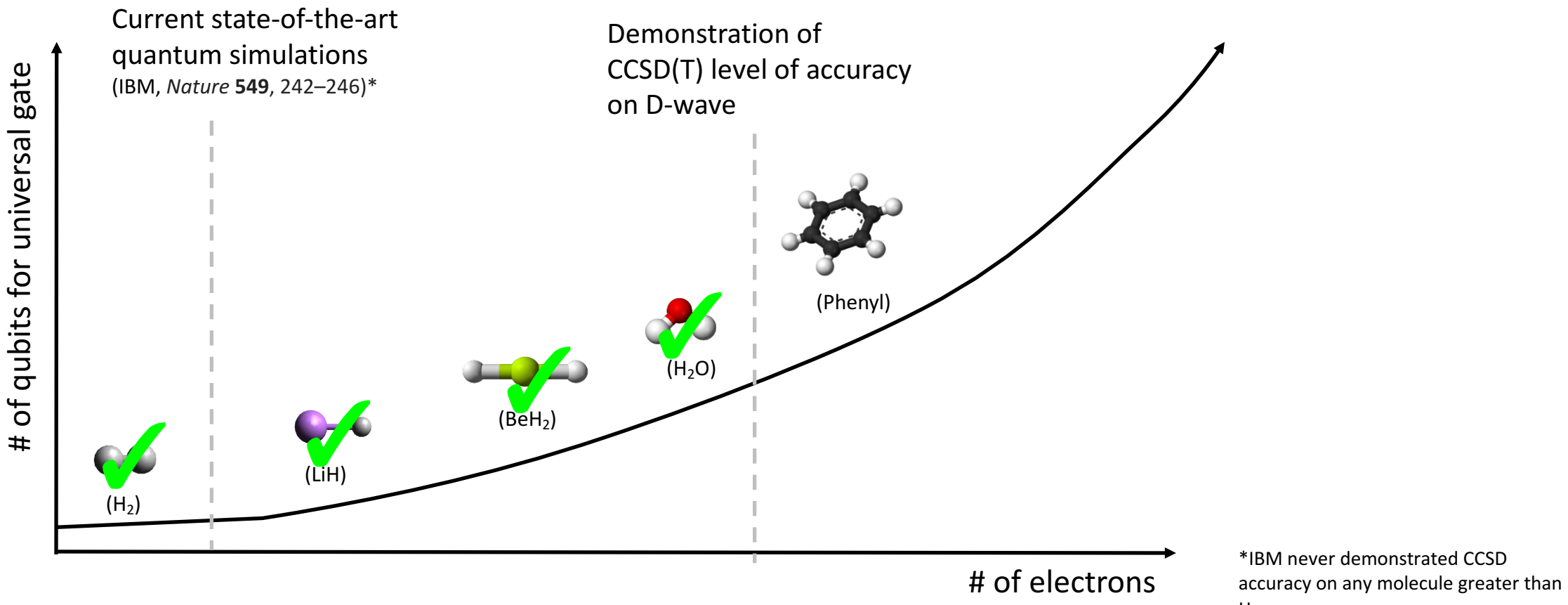
Started to test industrial problems



We have demonstrated industrial relevant size simulations on quantum hardware

Quantum Computing R&D

CCSD Demonstrated on Quantum Hardware



*IBM never demonstrated CCSD accuracy on any molecule greater than H_2

Energies obtained for small molecules on hardware higher in accuracy than IBM