Scott N. Genin, PhD
Head of Materials Discovery

scott.genin@otilumionics.com
www.otilumionics.com

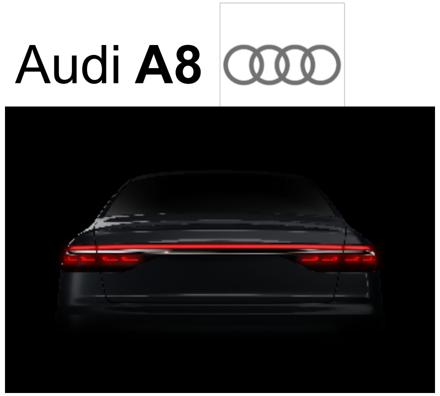
Quantum Chemistry on Quantum Annealers

March 2019

OTI Lumionics

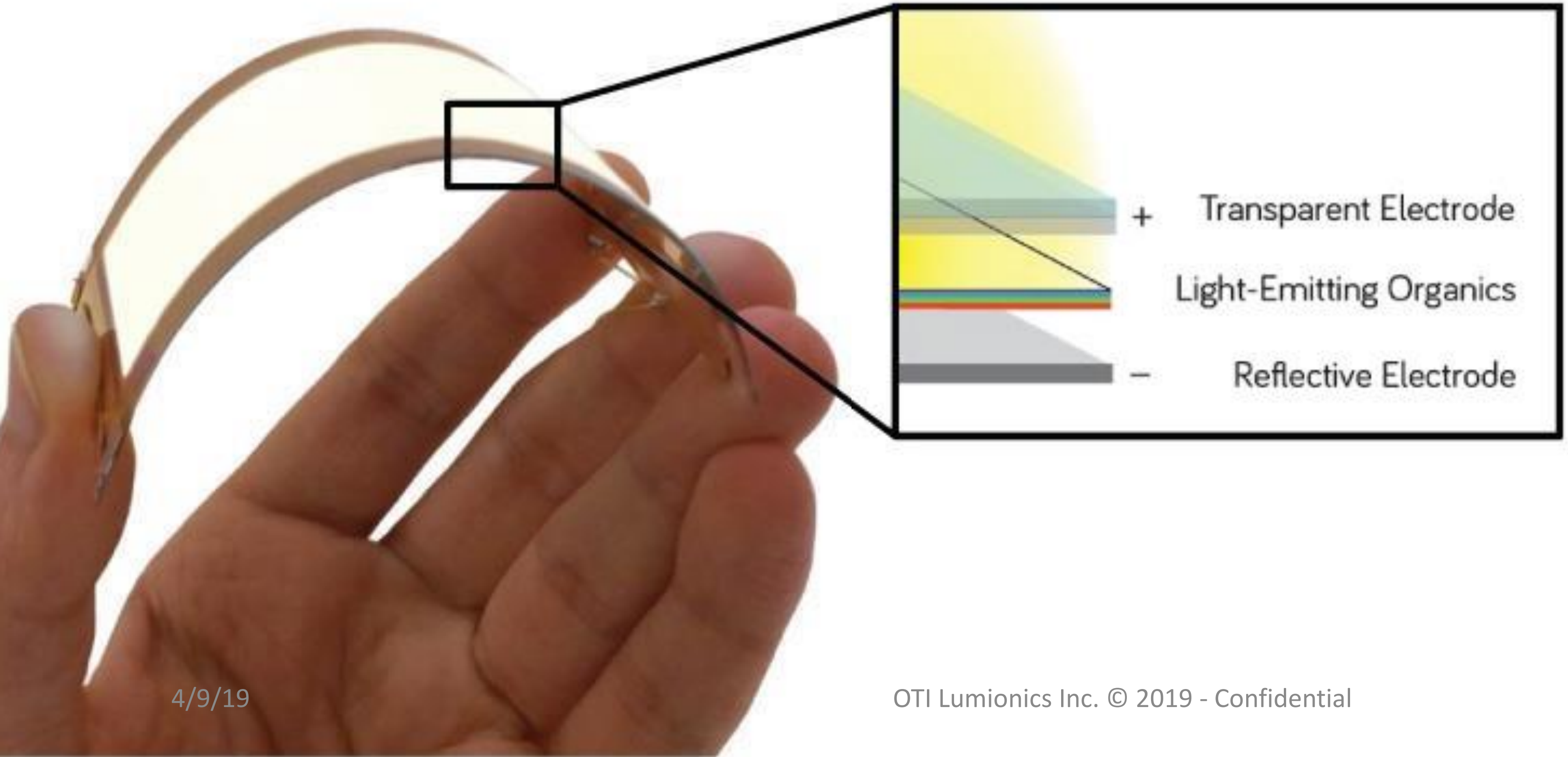
What We Do
Materials Discovery

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

OTI

Materials Discovery → Quantum Simulations → Synthesis → Validation → Production Testing → Materials Discovery

OTI

Detailed Specifications

MP Ready Materials

Tool Builders

Canon, TOKKI, COHERENT, Sunic, APPLIED MATERIALS, ULVAC, TEL

Panel Makers

SAMSUNG DISPLAY, Visionox, JOLED, LG Display, EDO 和辉光电, BOE, 华星光电 CSOT, TIANMA, JDI Japan Display Inc.

OEMs

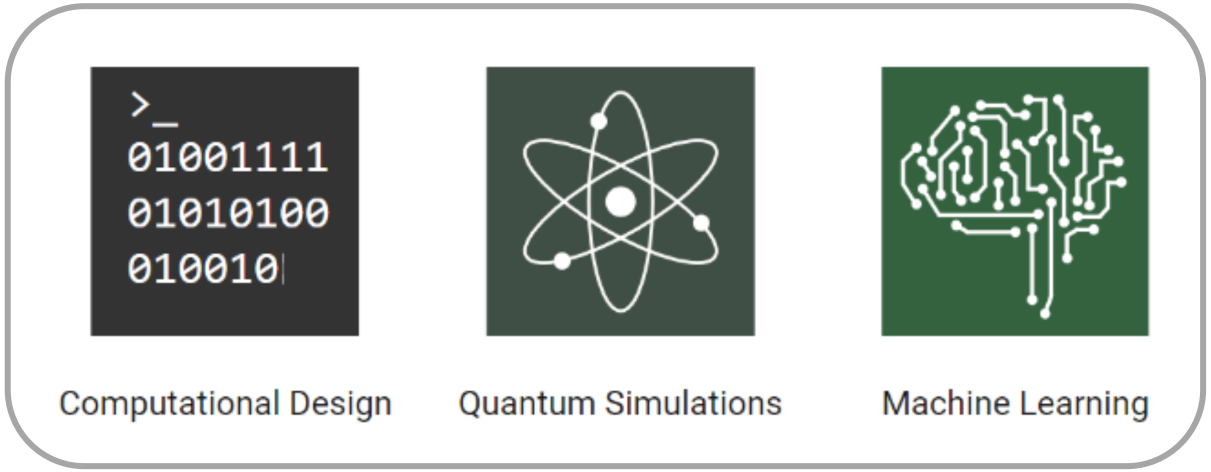
SAMSUNG, LG, hp, Google, HUAWEI, Microsoft, lenovo

Our Materials Discovery Platform

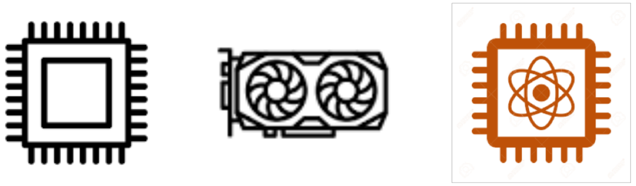
Advanced computation + simulation + ML/AI

Properties

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



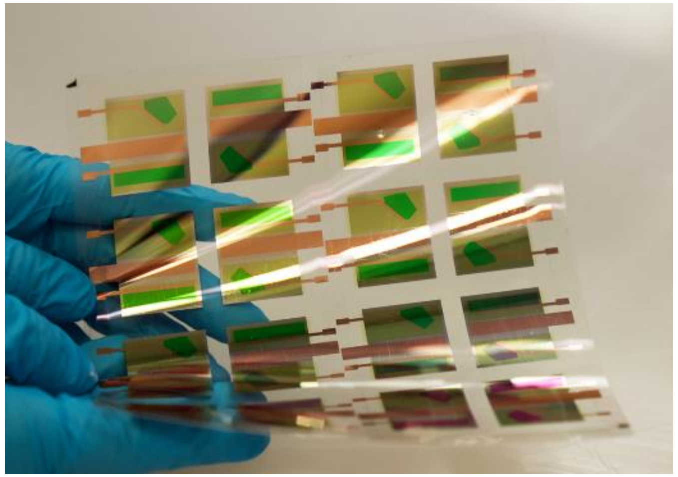
Structure

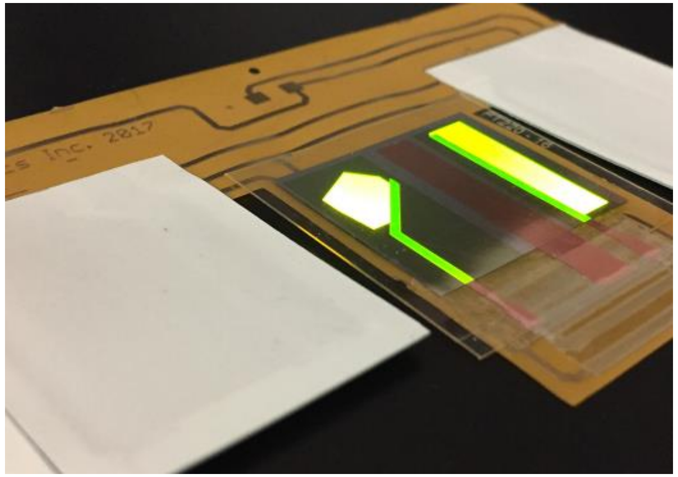


CPU GPU QPU (Quantum Processing Unit)

Example: Aerelight for Print™

Flexible OLED module for print + packaging



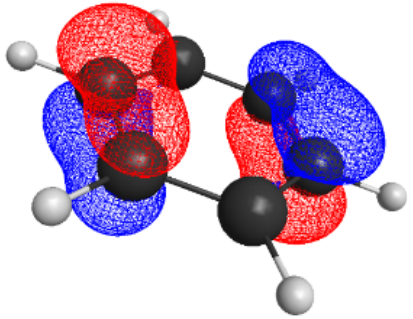


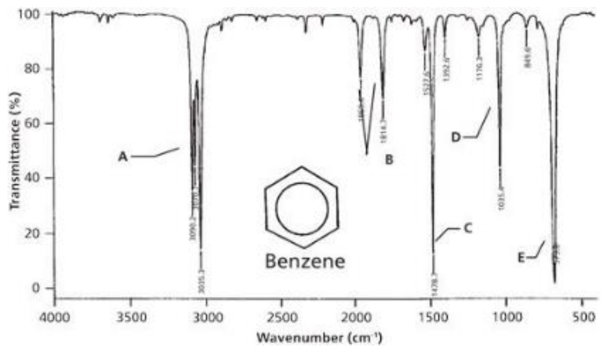
Example: ConducTorr™ for Transparent Display

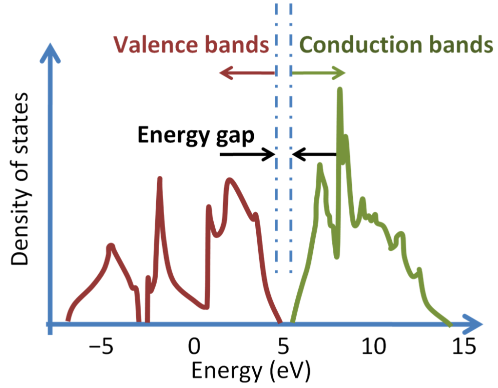
Automotive Demonstration

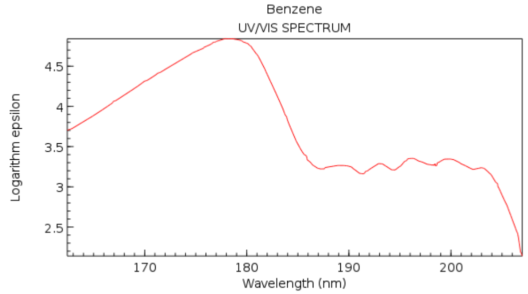
Quantum Chemistry

Why do we care?

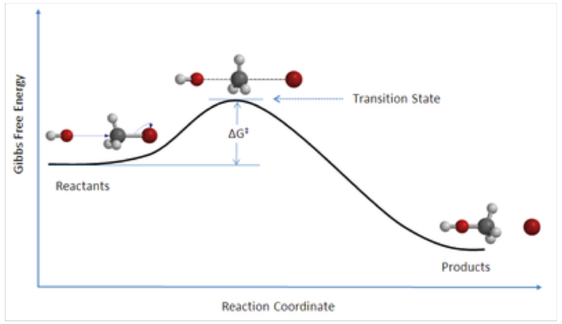








NIST Chemistry WebBook (https://webbook.nist.gov/chemistry)



Understanding and prediction of the Structure -> Property relationship

Overview of Quantum Chemistry on a Quantum Computer

$H = \sum_{ij} C_i^j a_j^\dagger a_i + \sum_{ijkl} C_{ij}^{kl} a_k^\dagger a_l^\dagger a_j a_i$

Generate a fermionic Hamiltonian

$H = \sum \hat{P}_i$

Transform into spin basis (function of Pauli Operators)

$|\psi(\theta)\rangle = \exp\left(\hat{T} - \hat{T}^\dagger\right) |\psi_0\rangle$

Construct Ansatz (UCC)

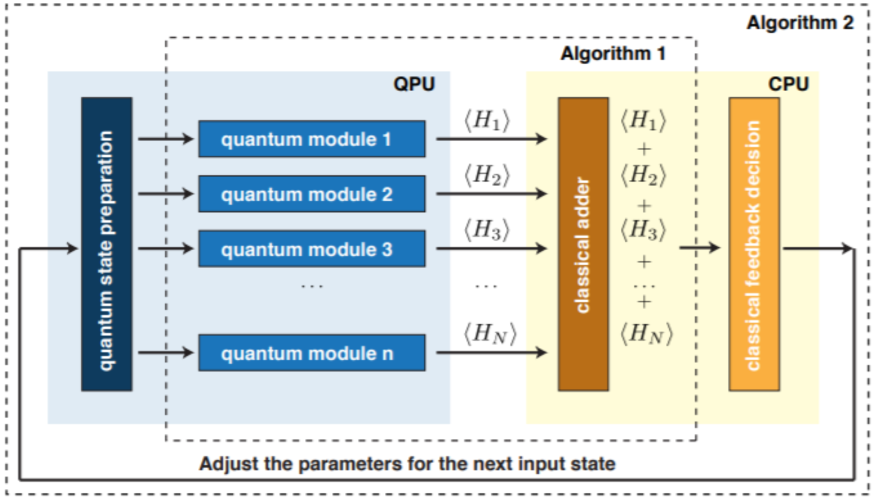
$\hat{T} = \hat{T}_1 + \hat{T}_2 + \cdots$

$$\hat{T}_1 = \sum_{ij} C_i^j a_j^\dagger a_i \qquad \hat{T}_2 = \sum_{ijkl} C_{ij}^{kl} a_k^\dagger a_l^\dagger a_j a_i$$

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 of the ith Pauli word

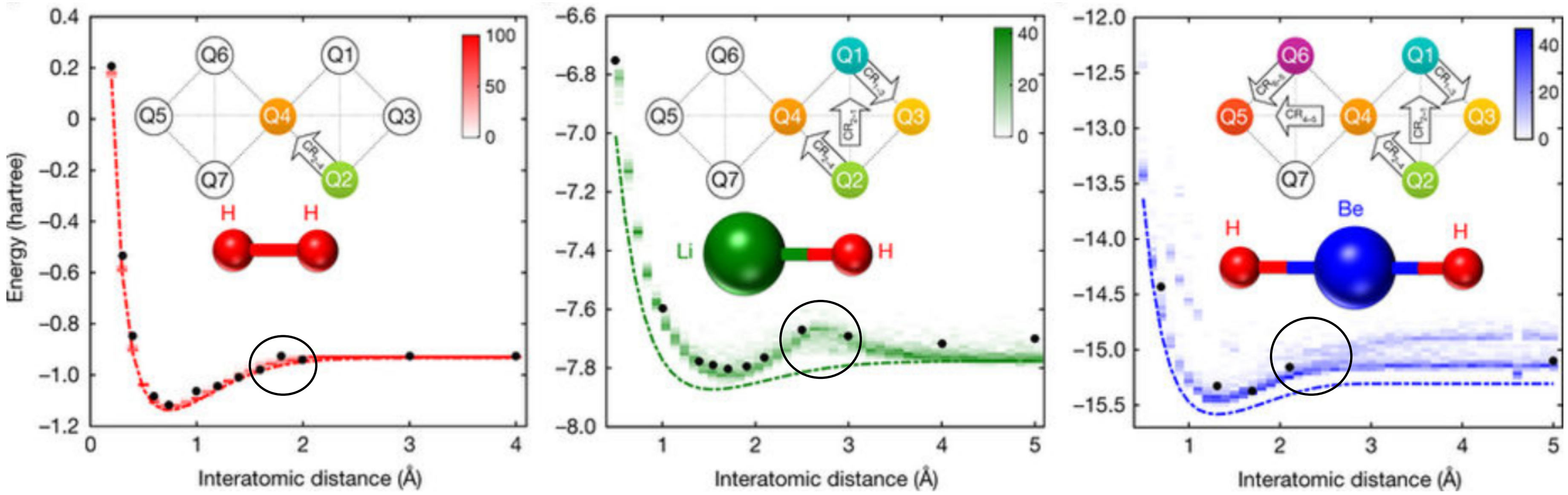


With serial processing, time scales linearly with number of Pauli words

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

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

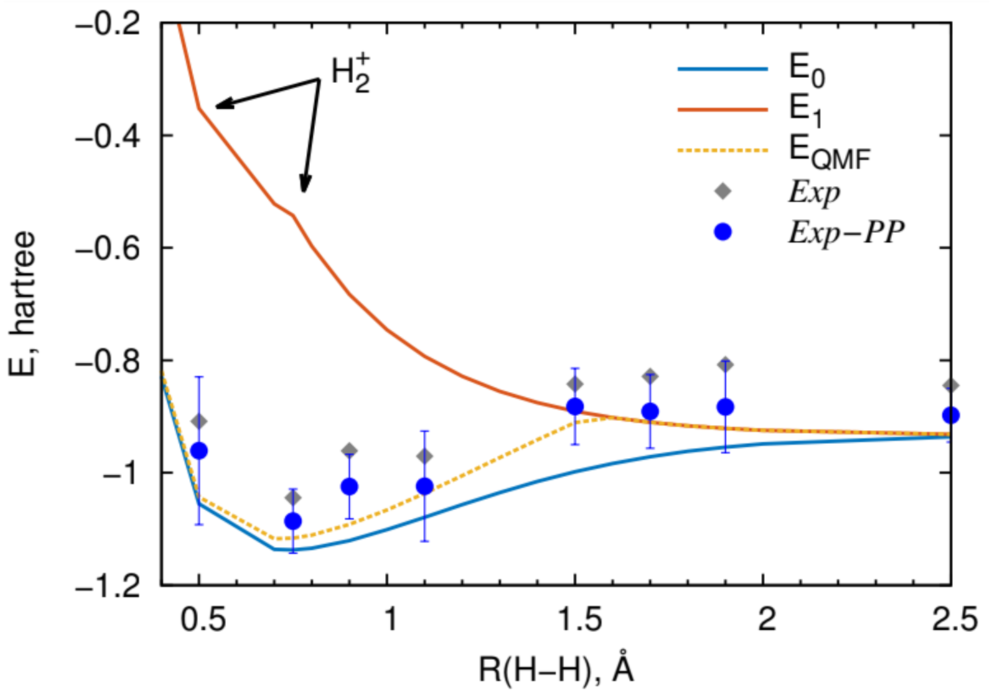
Hidden Consequences

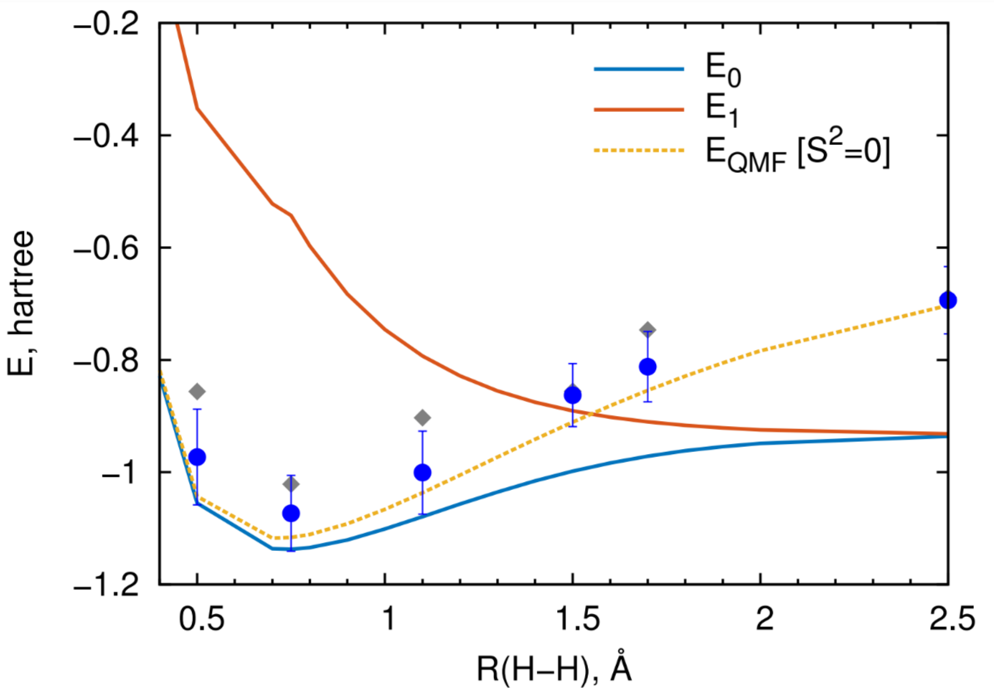


Is this “kink” a hardware problem or theory problem?

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

Unitary Coupled Cluster

Quantum computers cannot directly encode

$$U = \exp(T_1 + T_2 + \cdots)$$

$$\Big\downarrow \text{ Trotterized}$$

$$U \approx \left(\exp\left(\frac{T_1}{M}\right)\exp\left(\frac{T_2}{M}\right)\ldots\right)^M \quad M \geq 1$$

Even simplest fermionic operators are lengthy combination of Pauli terms

$$a_5^\dagger a_4^\dagger a_3 a_2 - a_2^\dagger a_3^\dagger a_4 a_5$$
$$\rightarrow \frac{i}{8}(x_2 y_4 + z_1 x_2 z_3 y_4 - y_2 x_4 - z_1 y_2 z_3 x_4 - y_2 x_4 z_5 - z_1 y_2 z_3 x_4 z_5 + x_2 y_4 z_5 + z_1 x_2 z_3 y_4 z_5)$$

Lengthy combinations of Pauli terms increases quantum circuit depth

LiH/STO-6G, C. Hempel *et al*. *Phys. Rev. X* **8**, 031022 (2018)

Qubit Coupled Cluster Method

$$\Psi(\tau,\omega) = \hat{U}(\tau)|\omega\rangle$$

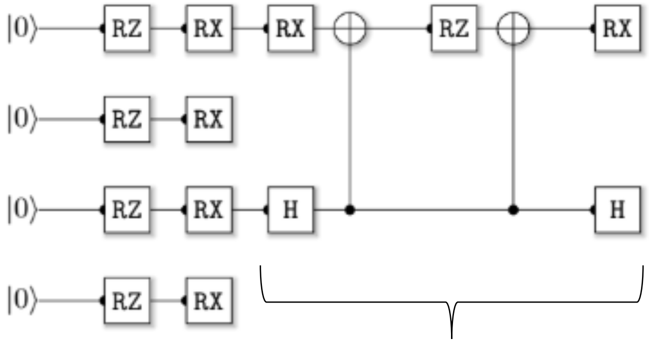
General form of qubit methods

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

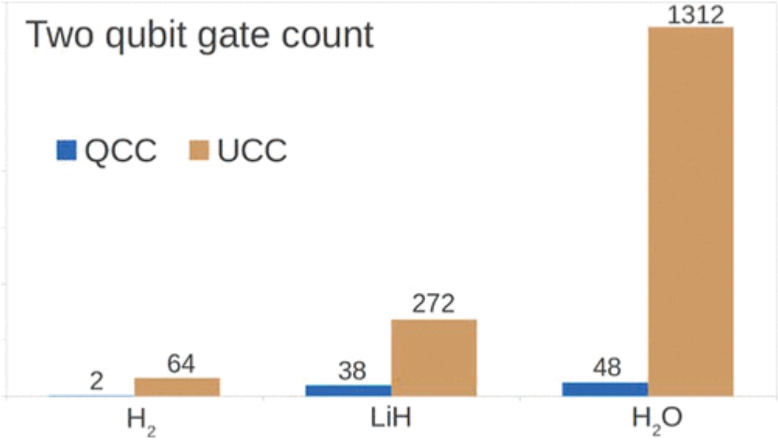
$\hat{P}$ is Pauli word entanglers

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

Variational search for ground state

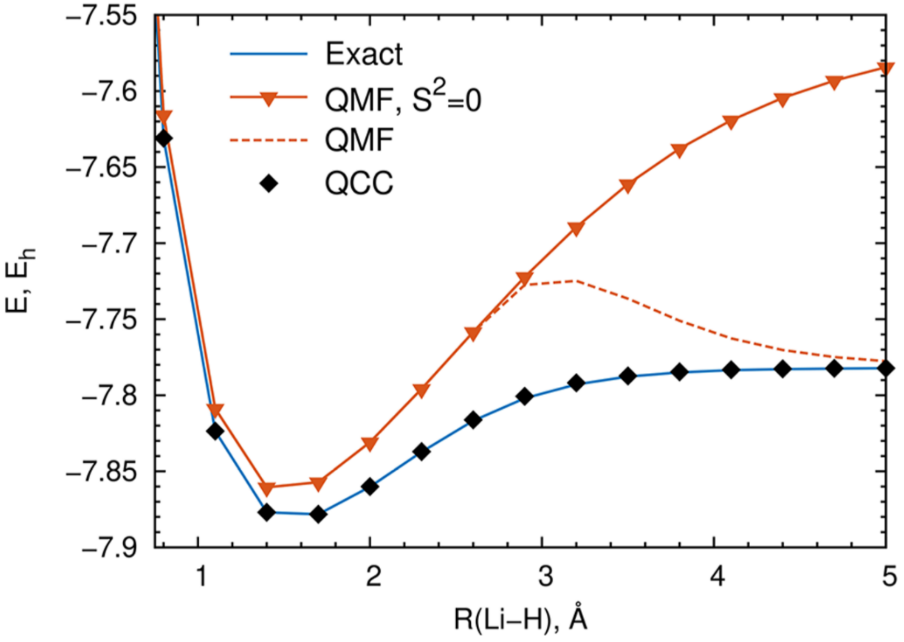


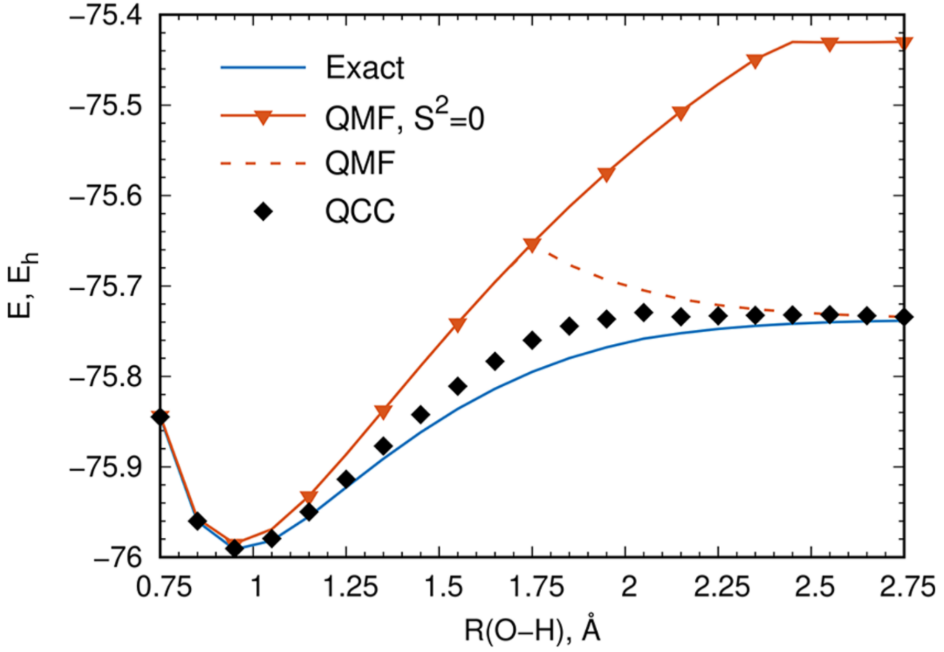
$\hat{P} = y_0 x_2$



https://pubs.acs.org/doi/abs/10.1021/acs.jctc.8b00932

PES Curve for LiH & H_2O





Quantum Chemistry on Quantum Annealers

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)

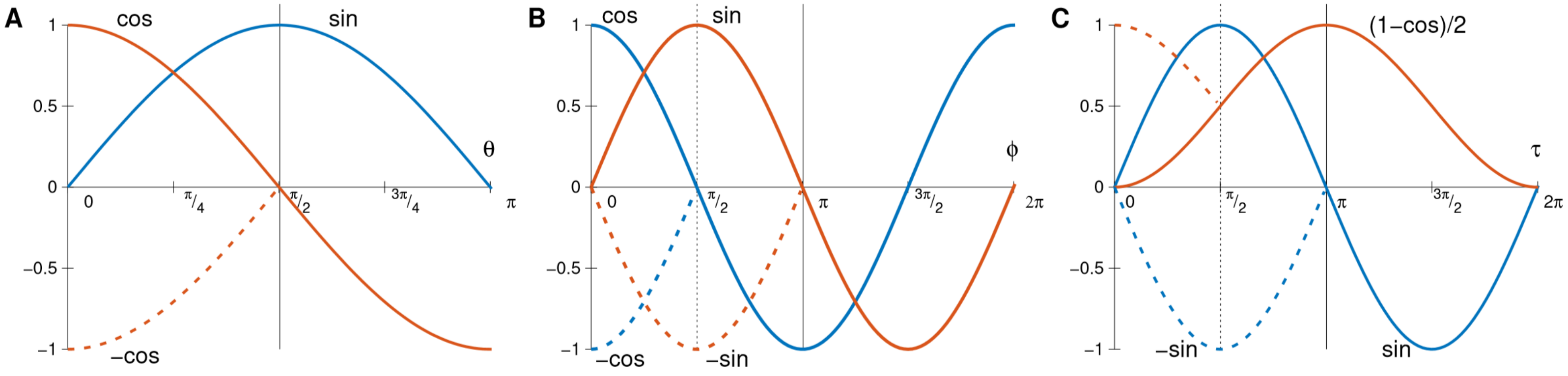
We have developed a quantum solver for quantum chemistry on a quantum annealer

Qubit Transformation and Domain Folding

$\theta \in [0, \frac{\pi}{2})$

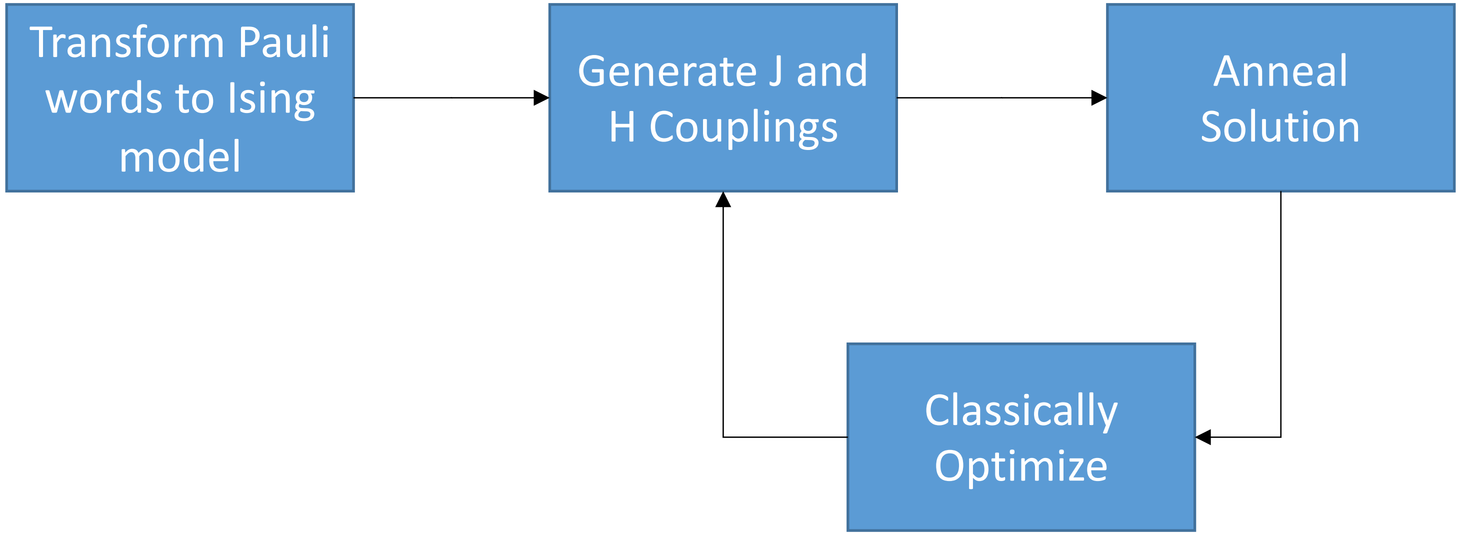
$\varphi \in [0, \pi)$ or $[0, \frac{\pi}{2})$

$\tau \in [0, \pi)$ or $[0, \frac{\pi}{2})$

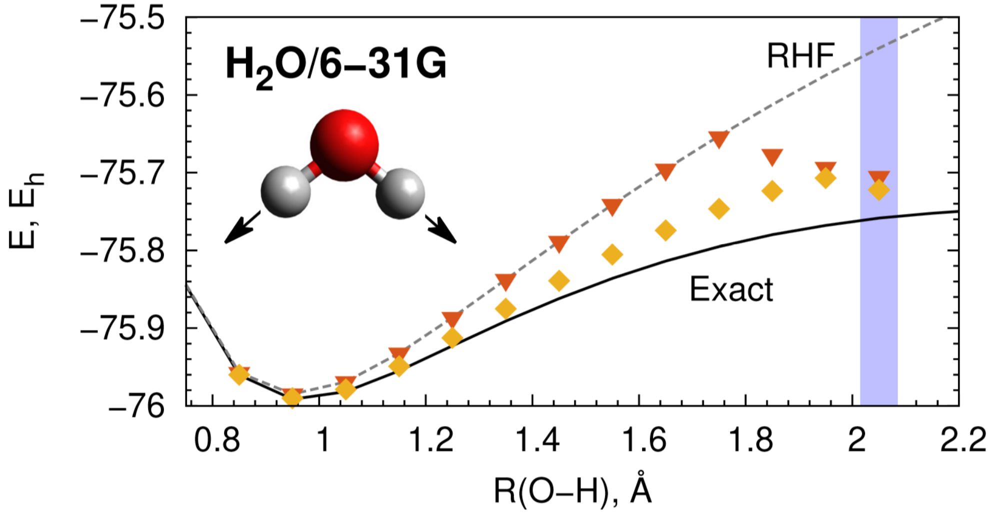


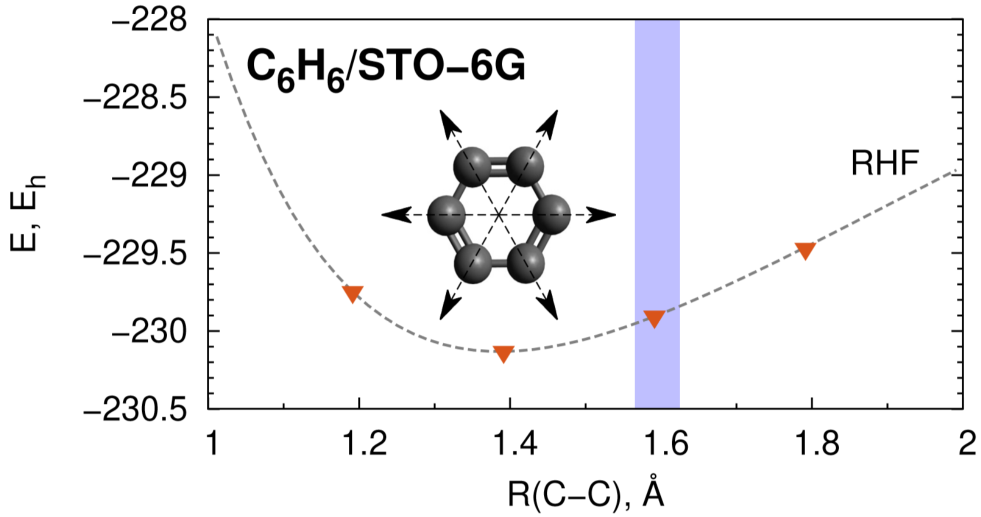
$$z_i \rightarrow \cos\theta_i$$
$$x_i \rightarrow \cos\varphi_i \sin\theta_i$$
$$y_i \rightarrow \sin\varphi_i \sin\theta_i$$

Solution on Quantum Annealer

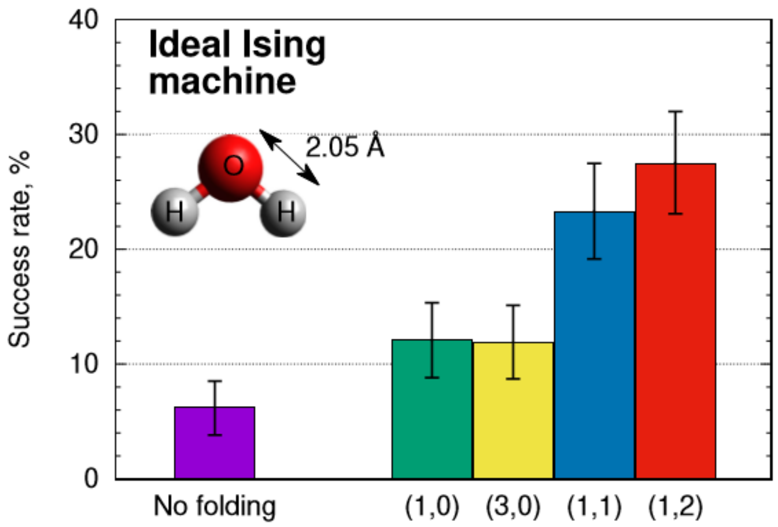


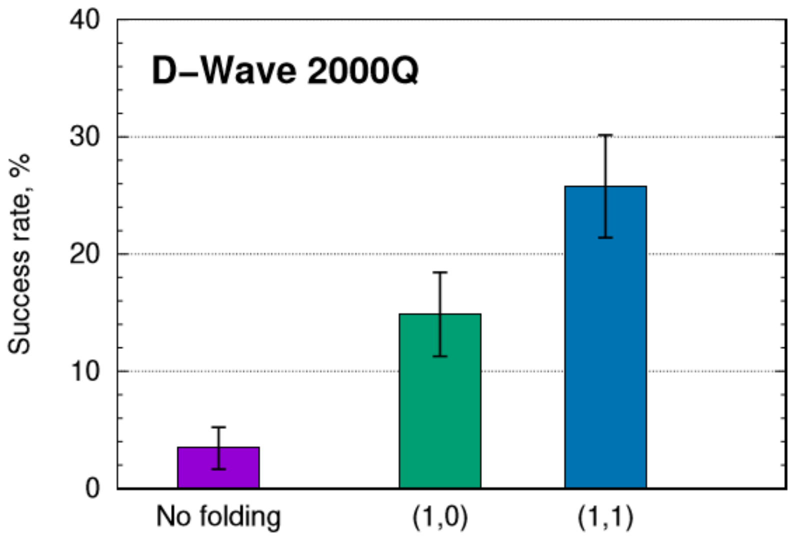
PES Curves Solved on Quantum Annealer





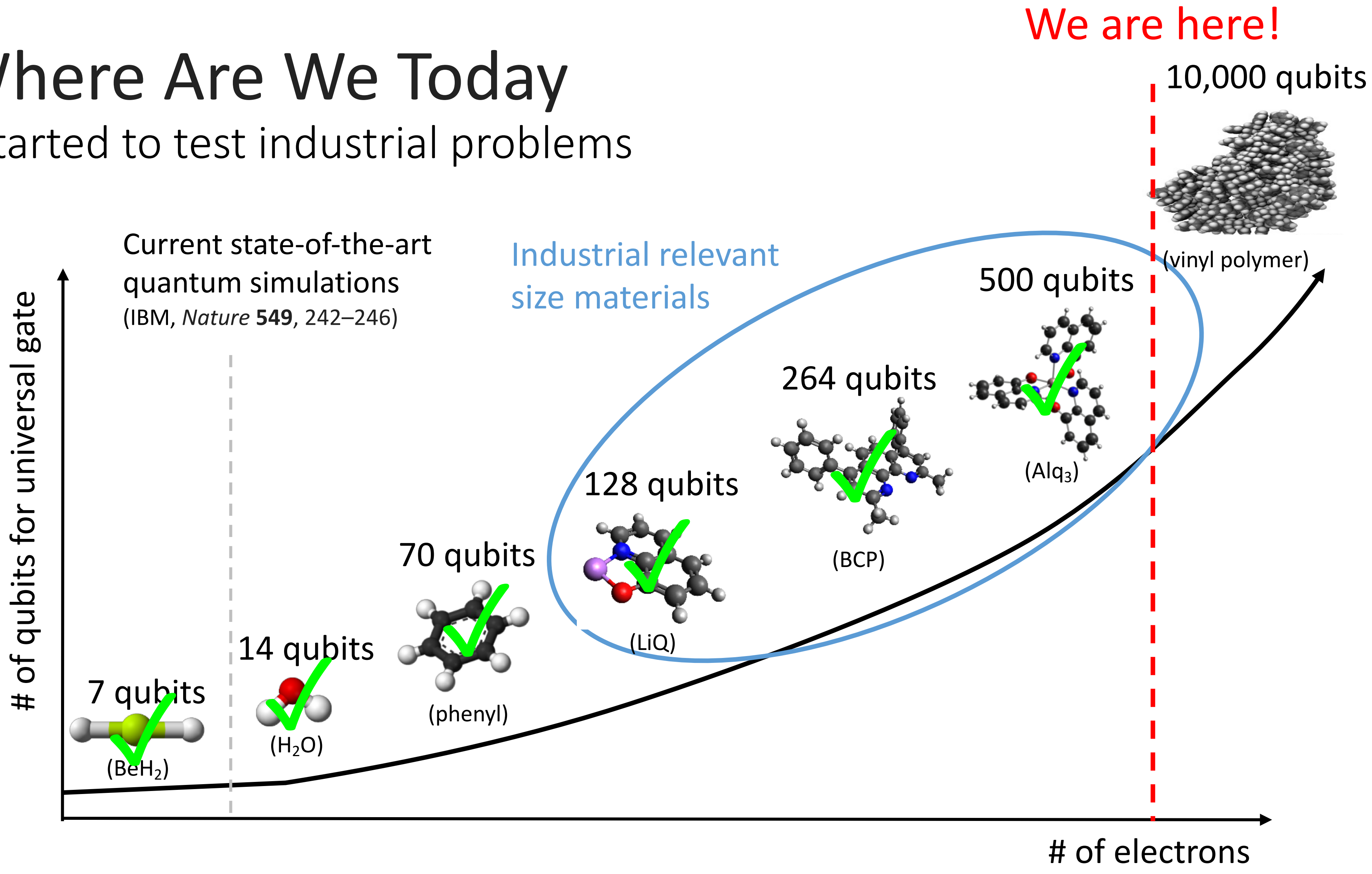
Benefit of the use of the annealer





Where Are We Today

Started to test industrial problems



We have demonstrated industrial relevant size simulations on quantum hardware