Quantum Chemistry on Quantum Annealers
March 2019
Developing advanced materials to solve large scale industrial problems for displays + lighting
Organic Light Emitting Diode (OLED)

Light from organic pigments sandwiched between electrodes
Closed Loop Development with Customer Feedback
In-house end-to-end testing from materials discovery up to production testing

Materials Discovery

Production Testing

Quantum Simulations

Validation

Synthesis

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

Computational Design  Quantum Simulations  Machine Learning

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?

Understanding and prediction of the Structure -> Property relationship
Overview of Quantum Chemistry on a Quantum Computer

\[ H = \sum_{ij} C_{ij}^l a_j^\dagger a_i + \sum_{ijkl} C_{ijkl}^k a_k^\dagger a_l^\dagger a_j a_i \]

\[ H = \sum \hat{P}_i \]

\[ |\psi(\theta)\rangle = \exp(\hat{T} - \hat{T}^\dagger) |\psi_0\rangle \]

\[ \hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots \]

\[ \hat{T}_1 = \sum_{ij} C_{ij}^l a_j^\dagger a_i \]

\[ \hat{T}_2 = \sum_{ijkl} C_{ijkl}^k a_k^\dagger a_l^\dagger a_j a_i \]

Generate a fermionic Hamiltonian

Transform into spin basis (function of Pauli Operators)

Construct Ansatz (UCC)
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 \( \Psi \) 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 – H₂ on QPU

Broken symmetry GHF between 1.5 Å – 1.6 Å, as it transitions from singlet to triplet
Quantum computers cannot directly encode

\[
U = \exp(T_1 + T_2 + \cdots)
\]

Trotterized

\[
U \approx \left( \exp \left( \frac{T_1}{M} \right) \exp \left( \frac{T_2}{M} \right) \cdots \right)^M \quad M \geq 1
\]

Even simplest fermionic operators are lengthy combination of Pauli terms

\[
i a_5^+ a_4^+ a_3 a_2 - a_2^+ a_3^+ a_4 a_5
\to \frac{1}{8} (x_2 y_4 + z_1 x_2 z_3 y_4 - y_2 x_4 - z_1 y_2 z_3 x_4 - y_2 x_4 z_5 - z_1 y_2 z_3 x_4 z_5 + x_2 y_4 z_5 + z_1 x_2 z_3 y_4 z_5)
\]

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

\[ \hat{U}(\tau) = \prod_k^N \exp \left( i \tau_k \hat{P}_k \right) \]

\( \hat{P} \) is Pauli word entanglers

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

Variational search for ground state

https://pubs.acs.org/doi/abs/10.1021/acs.jctc.8b00932
PES Curve for LiH & H₂O
Quantum Chemistry on Quantum Annealers

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

IBM Q (20 qubits)

D-Wave 2000Q (2048 qubits)

Annealer is suitable for solving binary optimization problems (not applicable for quantum chemistry)
Qubit Transformation and Domain Folding

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

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

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

\[ z_i \rightarrow \cos \theta_i \]

\[ x_i \rightarrow \cos \varphi_i \sin \theta_i \]

\[ y_i \rightarrow \sin \varphi_i \sin \theta_i \]
Solution on Quantum Annealer

Transform Pauli words to Ising model → Generate J and H Couplings → Anneal Solution → Classically Optimize
PES Curves Solved on Quantum Annealer
Benefit of the use of the annealer
Where Are We Today

Started to test industrial problems

Current state-of-the-art quantum simulations (IBM, Nature 549, 242–246)

Industrial relevant size materials

We are here!

7 qubits (BeH₂)
14 qubits (H₂O)
70 qubits (phenyl)
128 qubits (LiQ)
264 qubits (BCP)
500 qubits (Alq₃)
10,000 qubits (vinyl polymer)

We have demonstrated industrial relevant size simulations on quantum hardware

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