

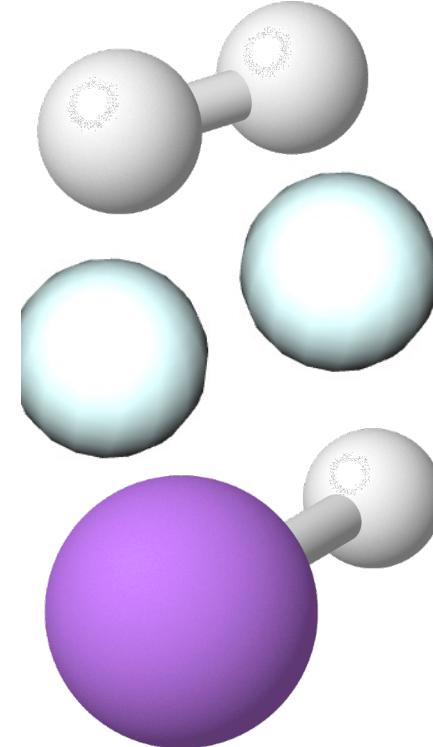
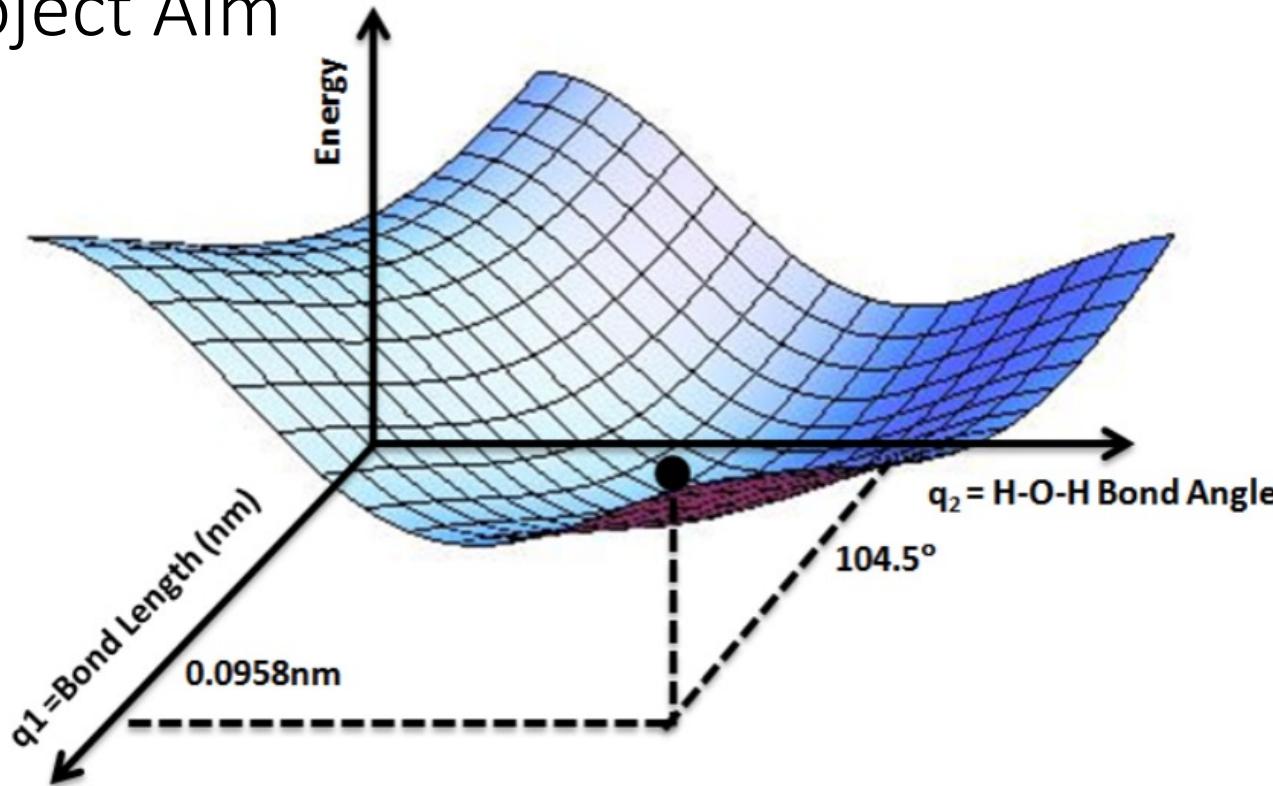
Exploring the Potential Energy Surface of various Molecules with a Problem-Inspired Ansatz

QHack 2022

26 Feb 2022

Team: Qanything

Project Aim



- H_2 : Hydrogen molecule
- He_2 : Helium Dimer
- LiH : Lithium Hydride

Aim: Explore Potential Energy Surface (PES) of H_2 , He_2 , and LiH , using Variational Quantum Eigensolver (VQE) with a Problem-Inspired Ansatz.

Motivation: PES enables us to study molecular properties, such as the equilibrium molecular bond lengths.

Objectives:

- We shall use PennyLane to build our problem-inspired ansatz and perform VQE optimization.
- We shall implement the IBMQ noise models and Mitig zero noise extrapolation and study how NISQ devices can affect the PES.
- We use QAMUY to cross check our results.

Molecular Hamiltonian and the Problem-Inspired Ansatz

$$\hat{H} = \sum_i c_i \sigma_i + \sum_{ij} c_{ij} \sigma_i \sigma_j + \sum_{ijk} c_{ijk} \sigma_i \sigma_j \sigma_k + \dots$$

- Molecular Hamiltonian is an energy operator consisting of all electrons and the nucleus of the molecule
- It can be decomposed as a linear combination of Pauli strings
- VQE can be used to find the minimum energy of the molecular Hamiltonian

Our Problem-
Inspired Ansatz

$$|\psi_{PI}\rangle = \prod_{\alpha} U_{\alpha}(\theta_{\alpha}) |1_1 \dots 1_n 0_{n-1} \dots 0_m\rangle$$

n : Number of electrons
 m : Number of molecular orbitals

Disentangled UCC

$$U_{\alpha}(\theta_{\alpha}) \in \{U_{i,k}(\theta_{i,k}), U_{ij,kl}(\theta_{ij,kl})\}$$

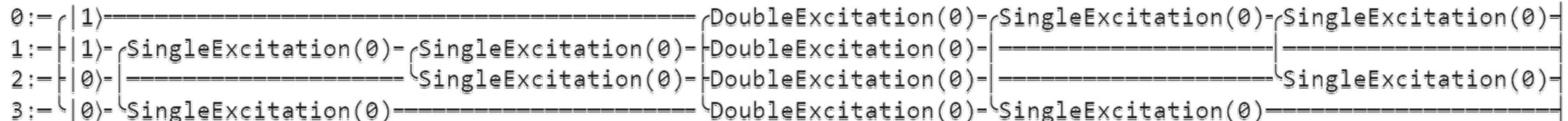
Singles Doubles θ : Parameters to Optimise

- We used the Disentangled UCC, a problem-inspired ansatz
- It consists of singles and doubles excitation operators applied to the Hartree-Fock state.
- As an example, shown below is the Disentangled UCC ansatz for H₂, requiring 4 qubits

Measurement
 $\langle \psi_{PI} | \hat{H} | \psi_{PI} \rangle$

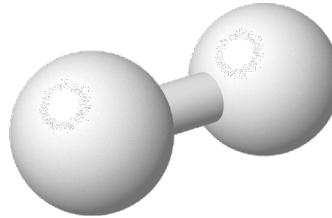
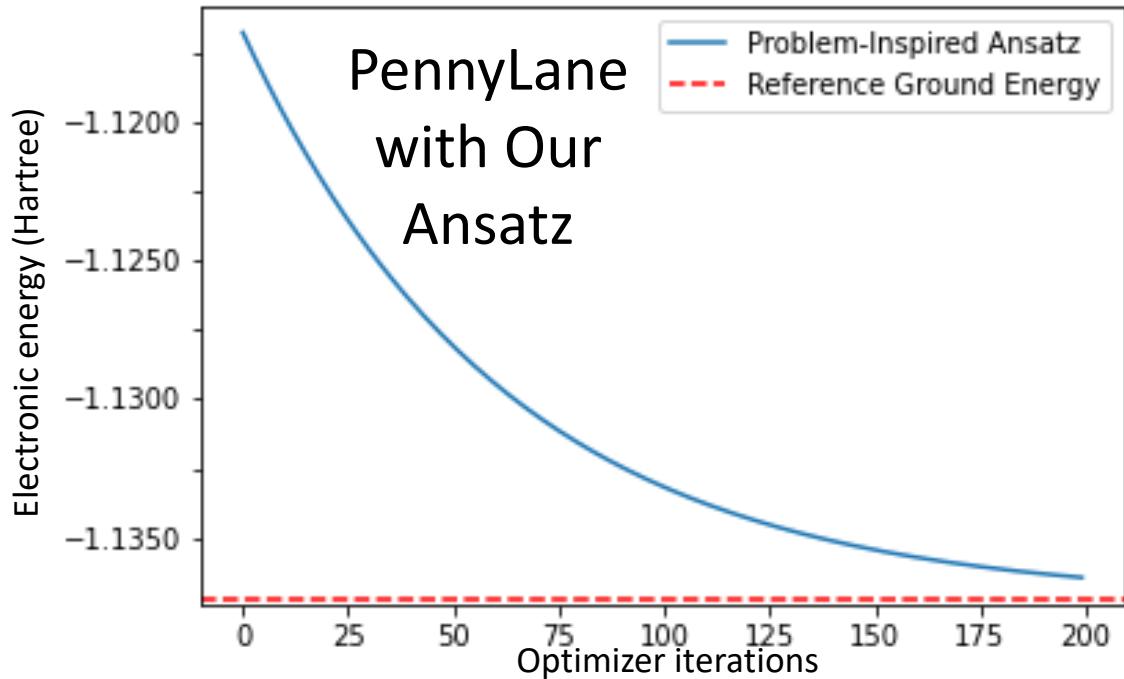
Hartree-Fock state

PennyLane Quantum Circuit for H₂



Performing VQE Energy Optimisation using PennyLane

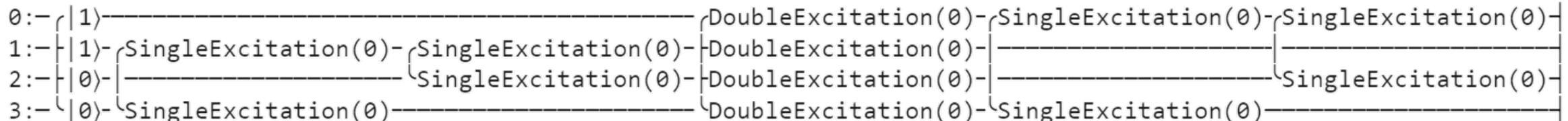
VQE optimization of Hydrogen Molecule H_2



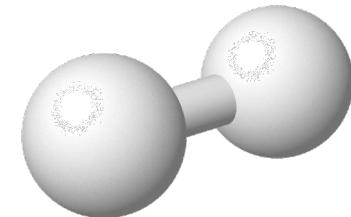
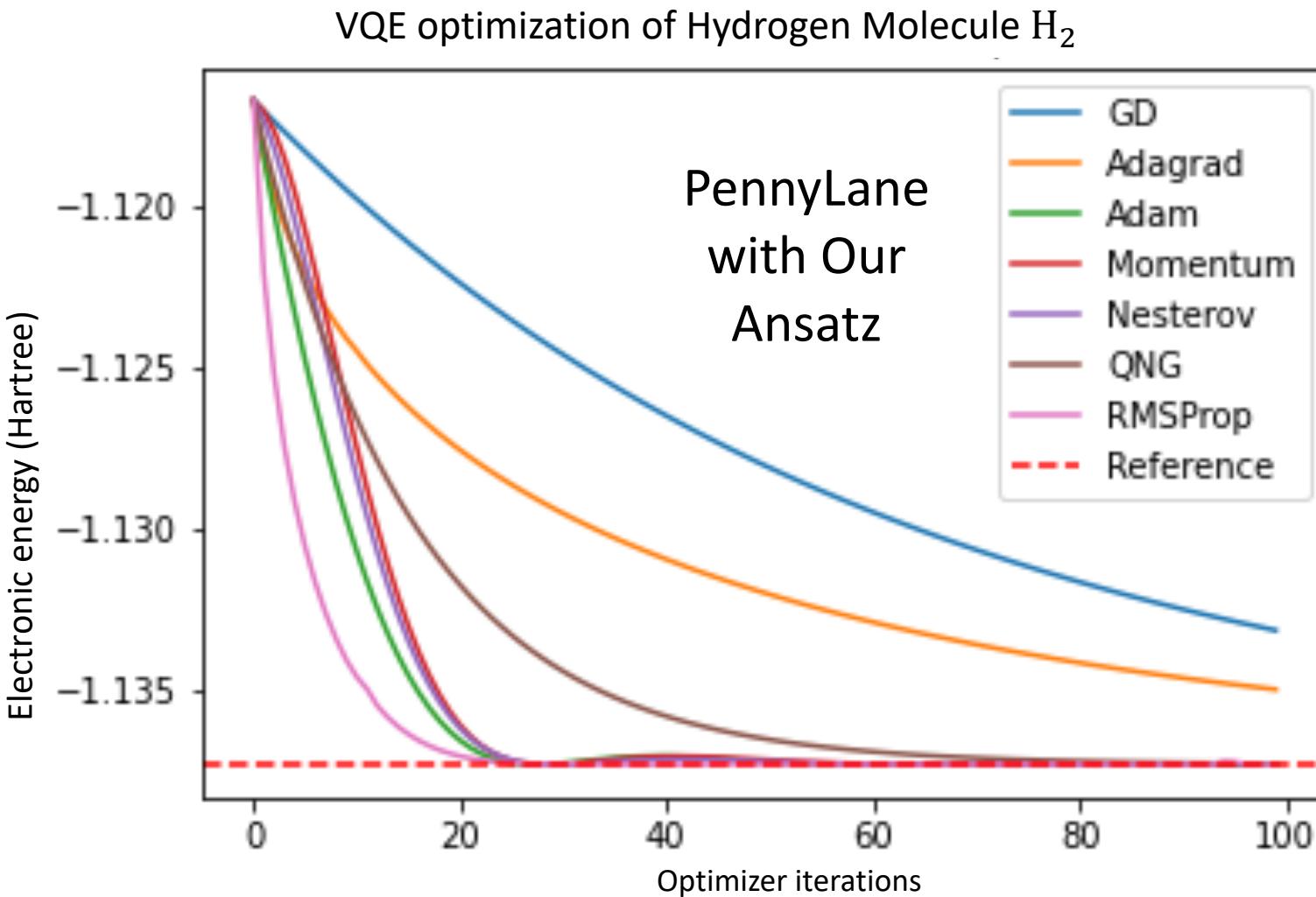
H_2 : Hydrogen molecule

Bond length:
 $r = 1.4$ Bohr

- Parameters are Optimized using Gradient Descent with Default Settings
- No. of Electrons: 2
No. of Qubits: 4
No. of Pauli Strings (to measure): 15
No. of Single Excitations Rotations Gate : 4
No. of Double Excitations Rotations Gate : 1
Total No. of Excitations Parameter: 5



Benchmarking Using PennyLane Built-in Classical Optimizer



H₂: Hydrogen molecule

Bond length:
r = 1.4 Bohr

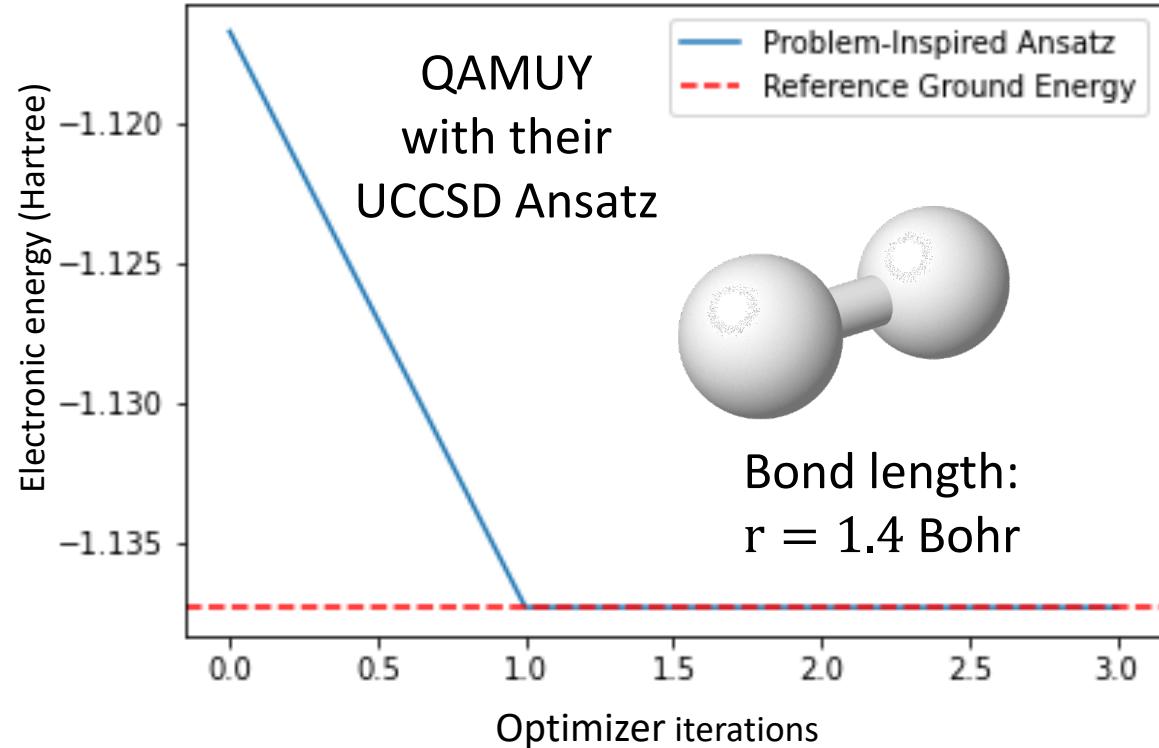
We tested the various optimizers available in PennyLane applied to H₂ using our Disentangled UCC ansatz and ranked them according to their accuracy.

Optimiser Ranking:

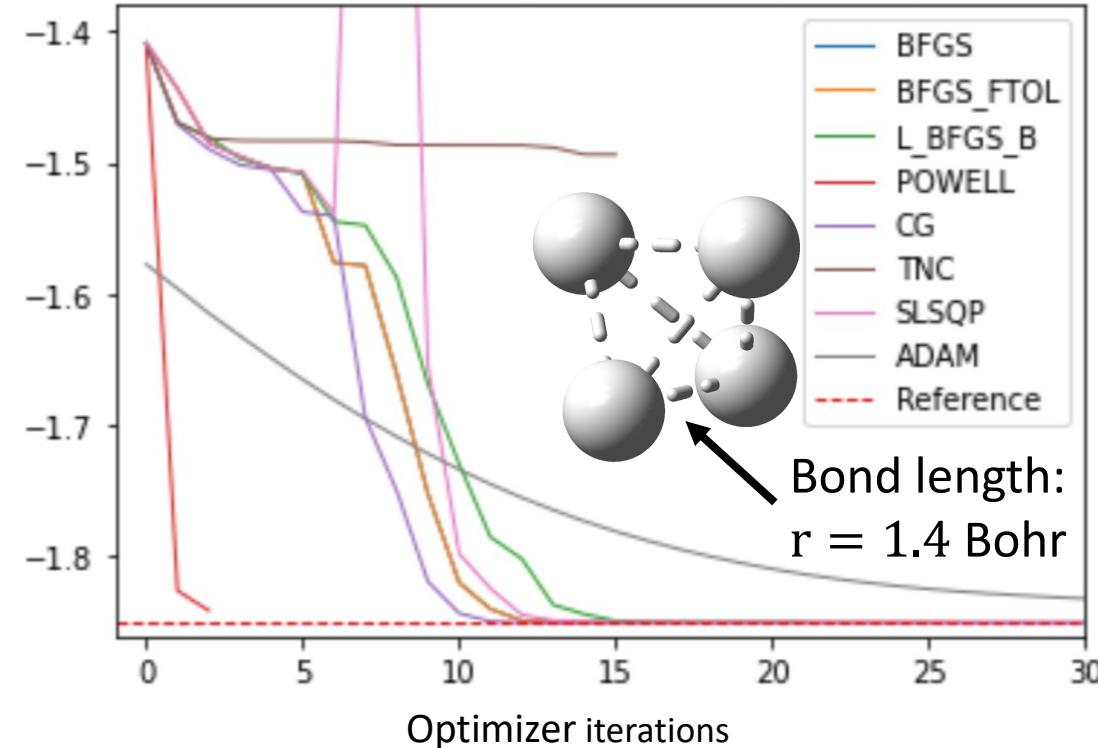
1. RMSProp
2. Adam
3. Nesterov
4. Momentum
5. QNG
6. Adagrad
7. Gradient Descent

Implementing VQE on H₂ and Tetra Hydrogen H₄ with QAMUY

VQE optimization of H₂ in QAMUY
(BFGS Only)



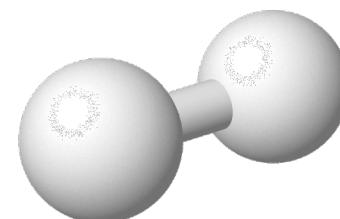
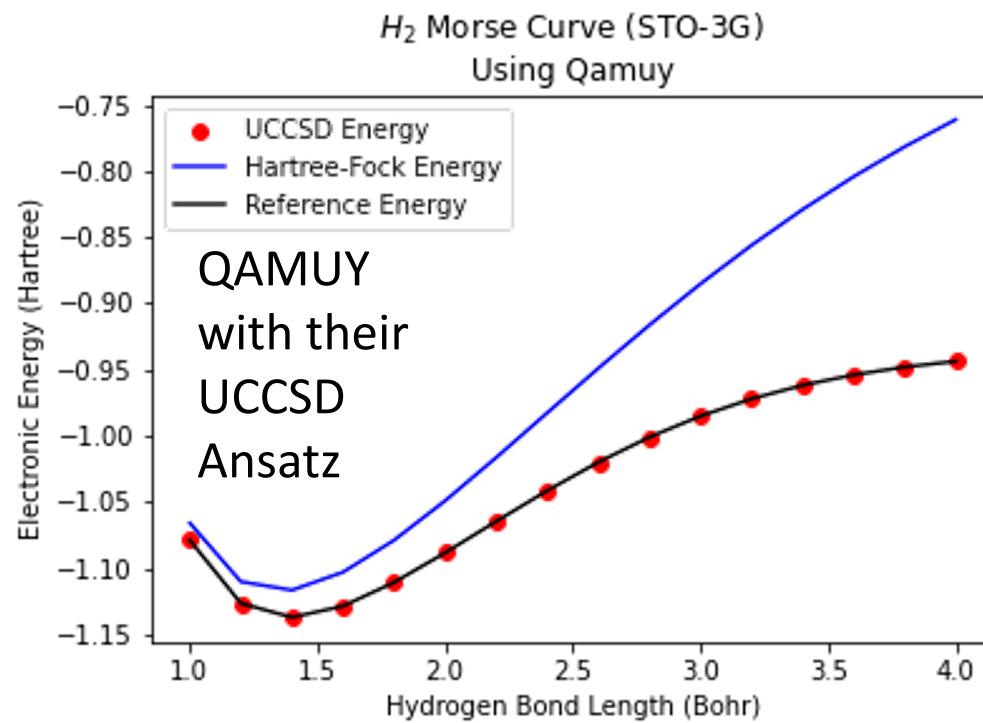
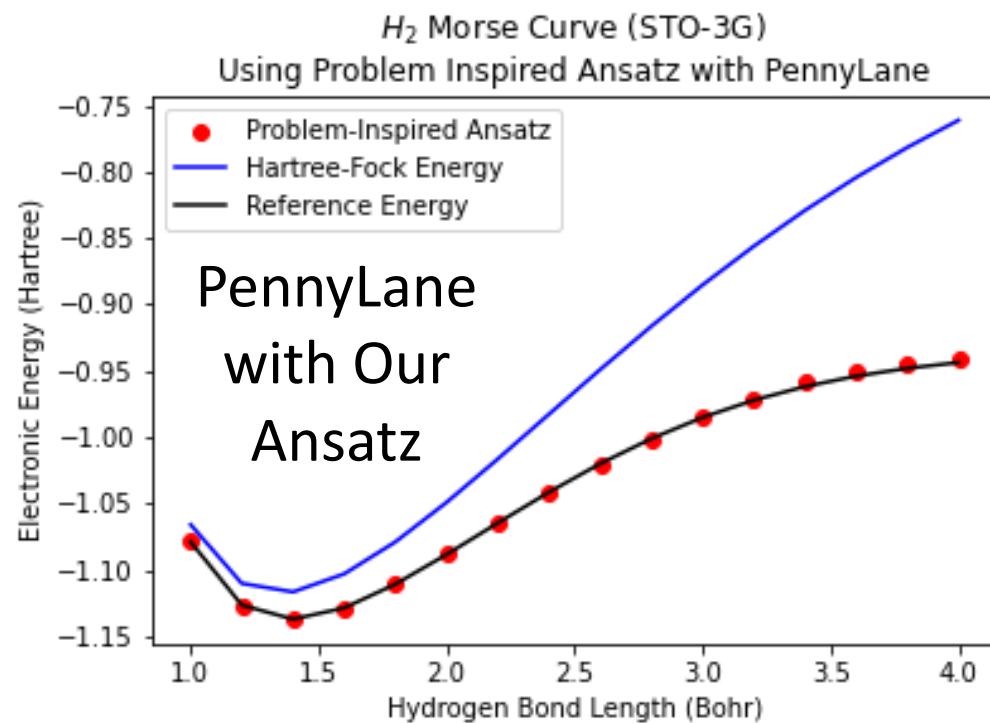
VQE Optimisation of Tetra Hydrogen H₄ Various in QAMUY (Various Optimisers)



QAMUY with their UCCSD Ansatz

The optimizers from QAMUY were able to provide accurate results with quick convergence

Potential Energy Surface for H_2 using Exact Quantum Simulator

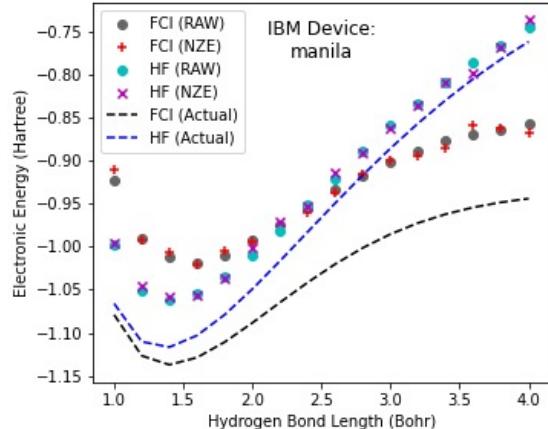


Bond lengths:
 $r = 1.0$ to 4.0 Bohr

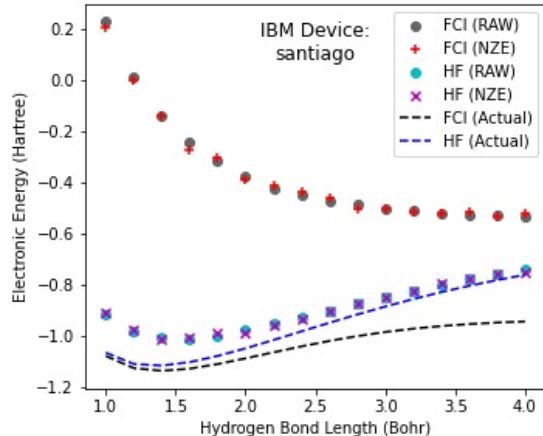
Potential Energy Surface for H₂ using IBMQ Device Noise Models

Open providers

Best performing

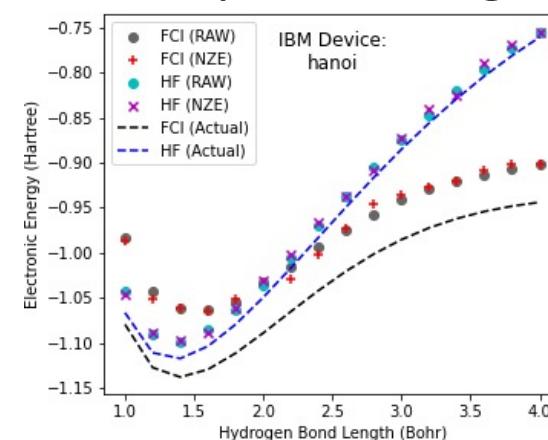


Worst performing

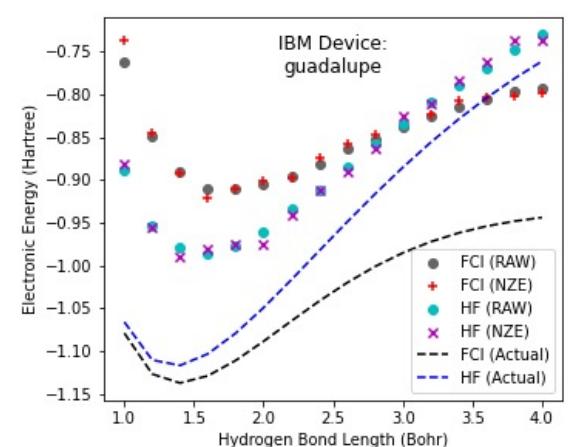


Paid providers

Best performing



Worst performing



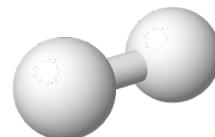
Legend

GREY Dots: Our Optimised Problem Inspired Ansatz

+: Problem Inspired Ansatz w/ Mitiq Zero Noise Extrapolation

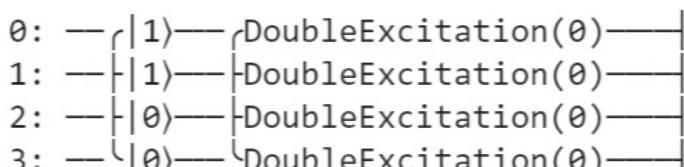
CYAN Dots: Hartree-Fock (HF) State Only

X: HF w/ Mitiq Zero Noise Extrapolation



Bond lengths:
r = 1.0 to 4.0 Bohr

Actual Quantum
Circuit Implemented:



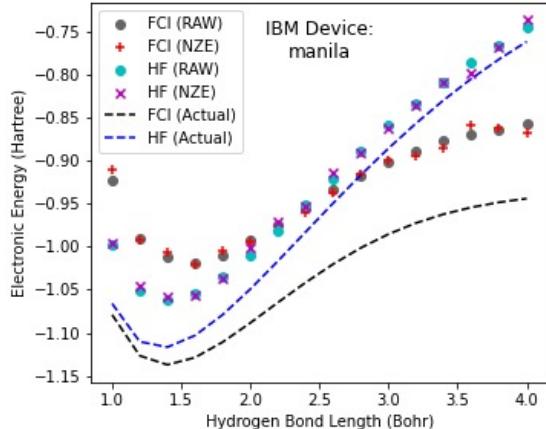
- Note: From the plots, our implementation of Mitiq as an error mitigation technique did not appear to help with improving the accuracy of our results. (???)

- Turns out for H₂, the only gate that contributes to PES is Double Excitations.
- We remove all Singles Excitations from quantum circuit to reduce circuit noise.
- All Noise model obtained from IBMQ Device backends
- Number of Shots Per Pauli String Expectation: 20,000

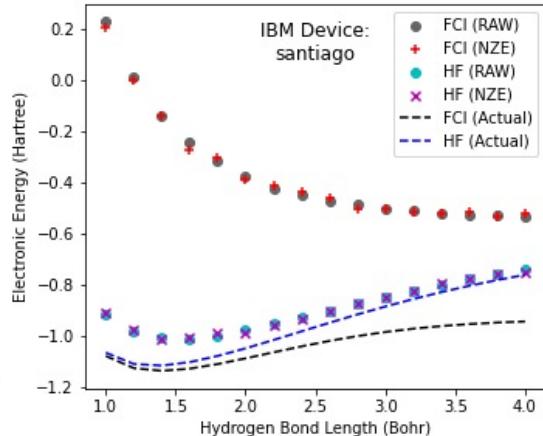
Potential Energy Surface for H₂ using various IBMQ Device Noise Models

Open Providers

Best performing

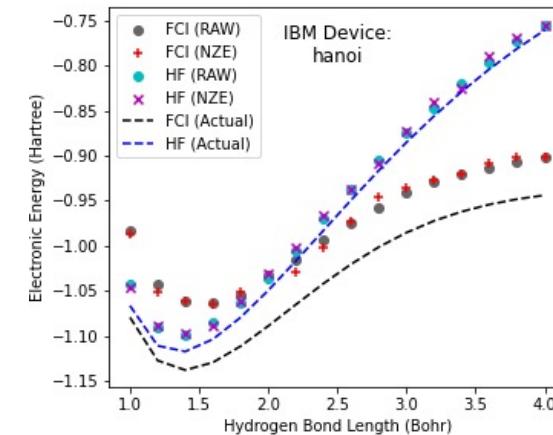


Worst performing

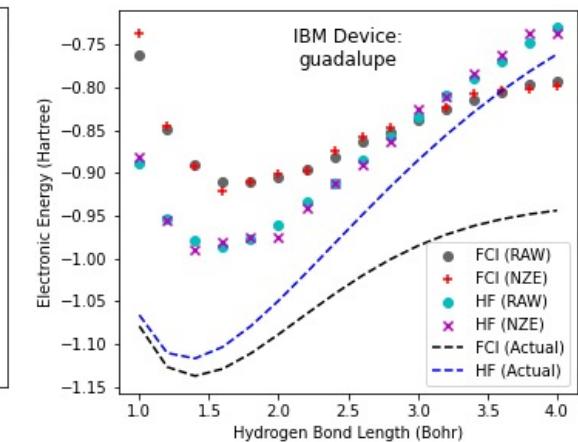


Exclusive Providers

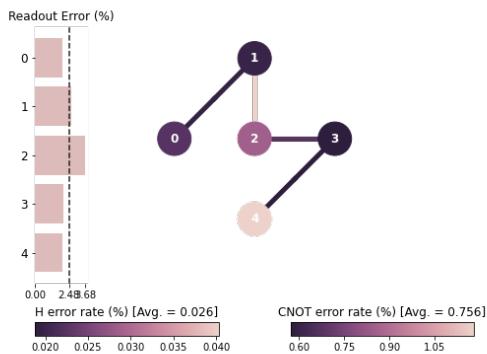
Best performing



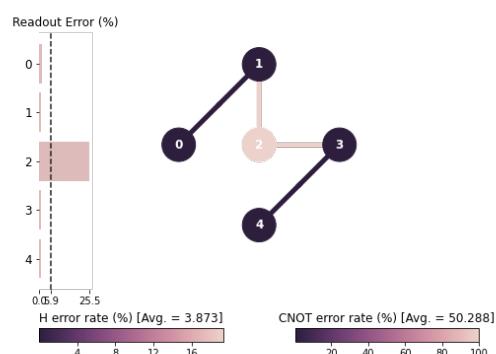
Worst performing



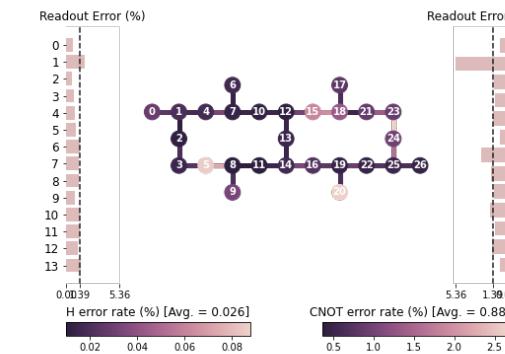
ibmq_manila Error Map



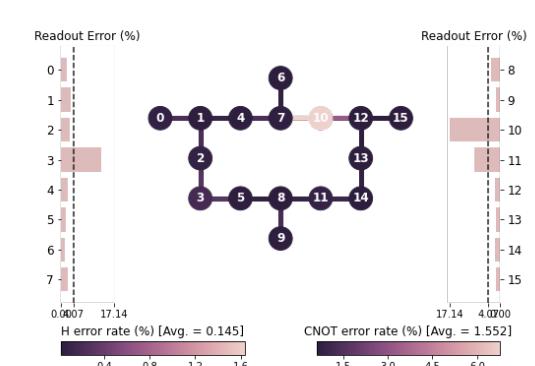
ibmq_santiago Error Map



ibmq_hanoi Error Map



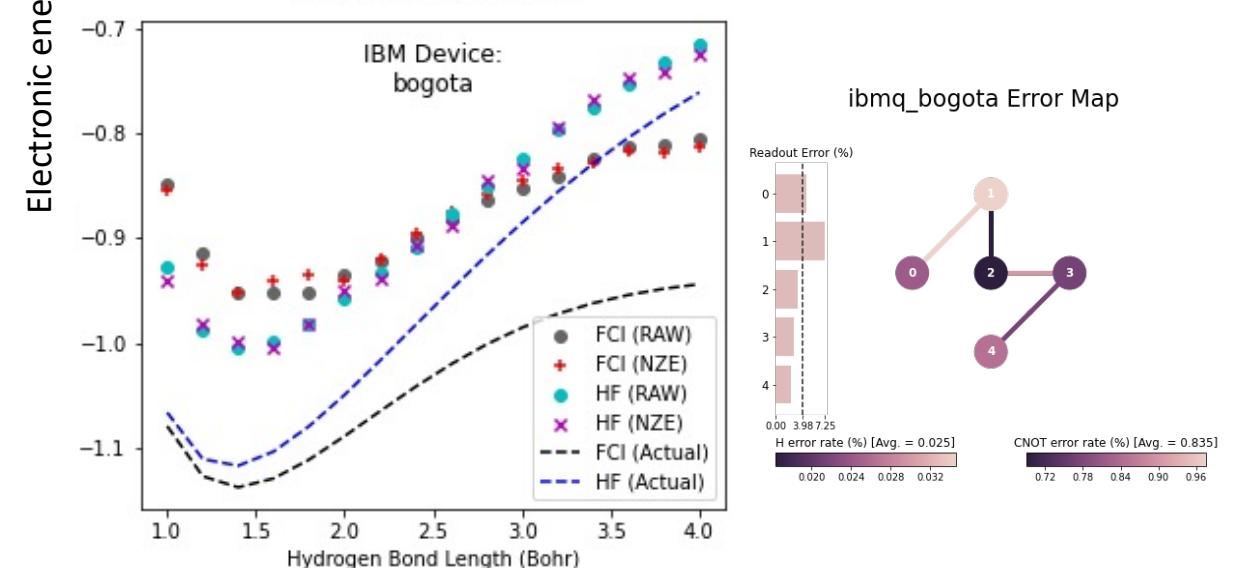
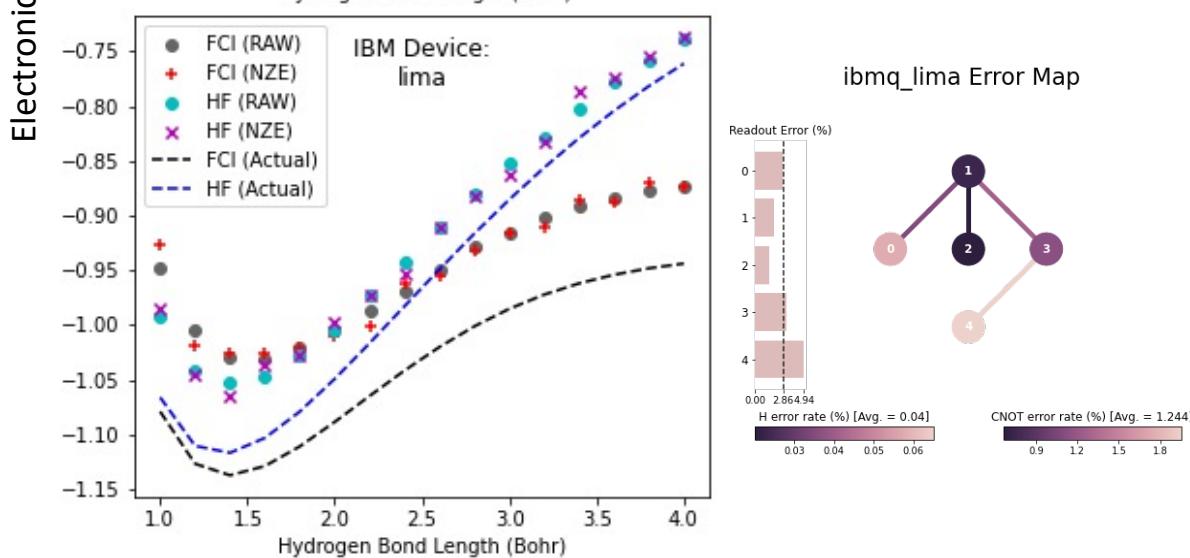
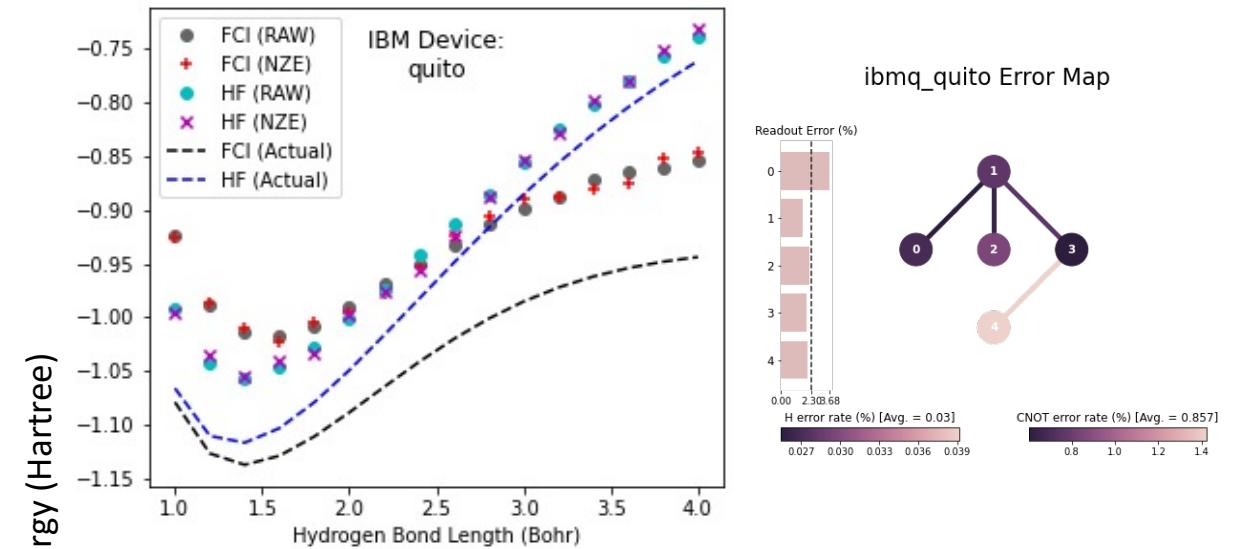
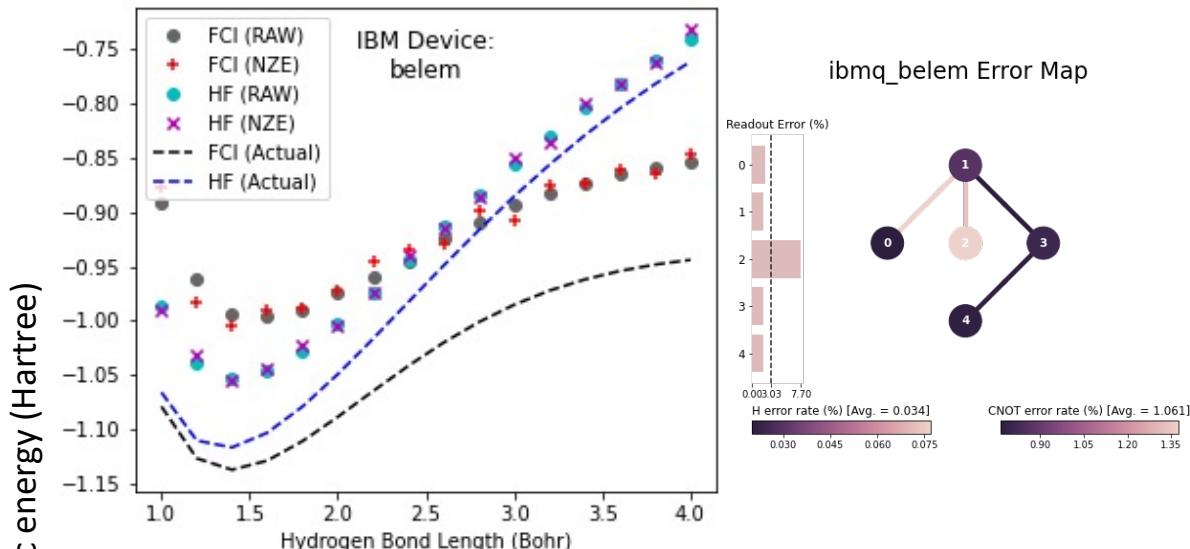
ibmq_guadalupe Error Map



Simulated IBM Quantum Devices Noise Map

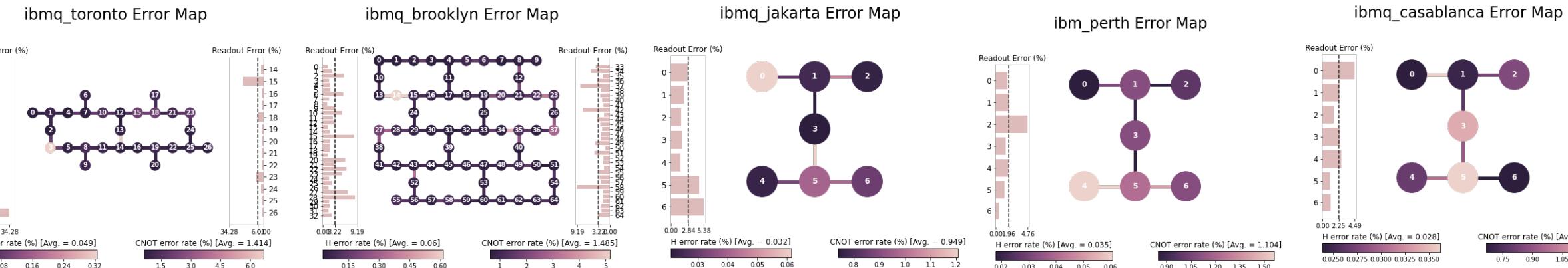
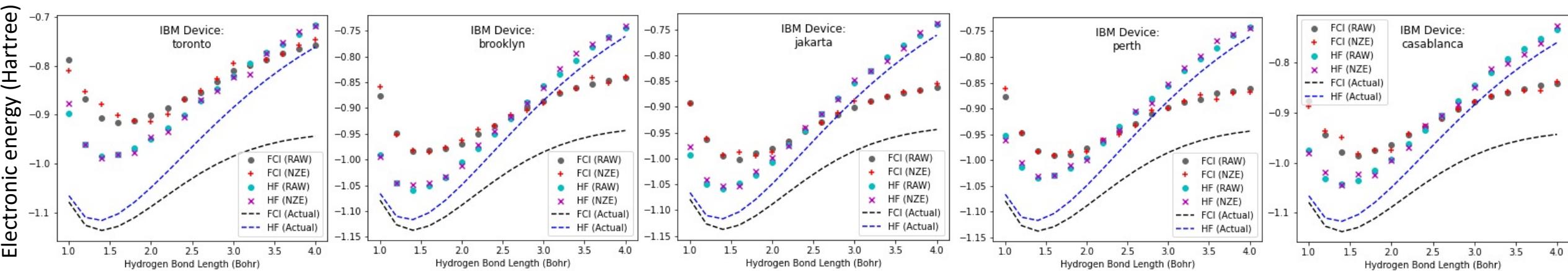
Potential Energy Surface for H₂ using various IBMQ Device Noise Models

Other Open Providers



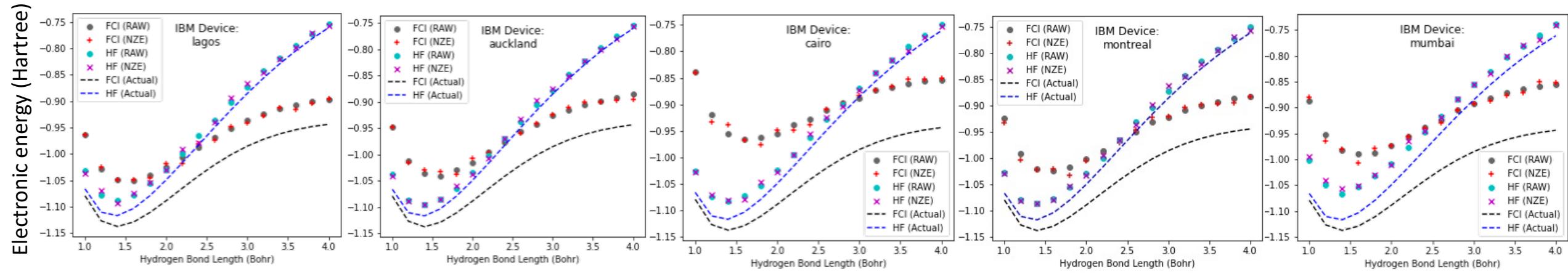
Potential Energy Surface for H₂ using various IBMQ Device Noise Models

Other Exclusive Providers

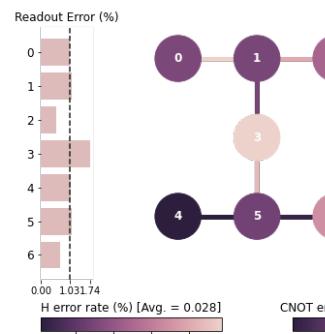


Potential Energy Surface for H₂ using various IBMQ Device Noise Models

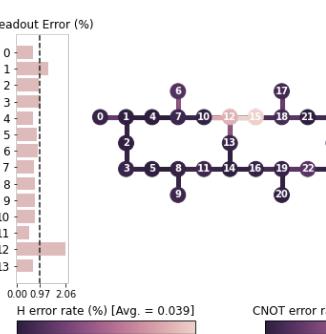
Other Exclusive Providers



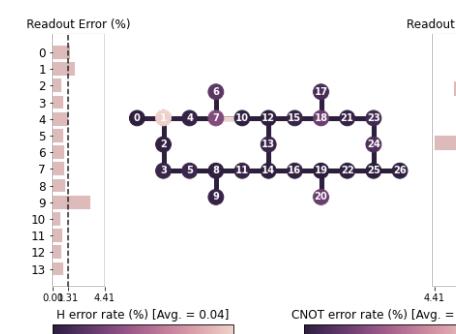
ibm_lagos Error Map



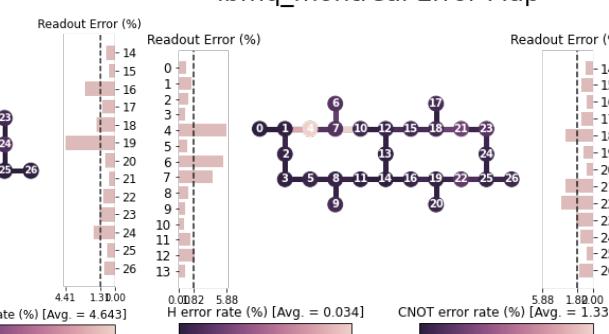
ibm_auckland Error Map



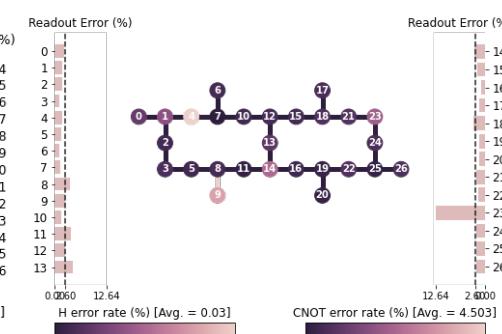
ibm_cairo Error Map



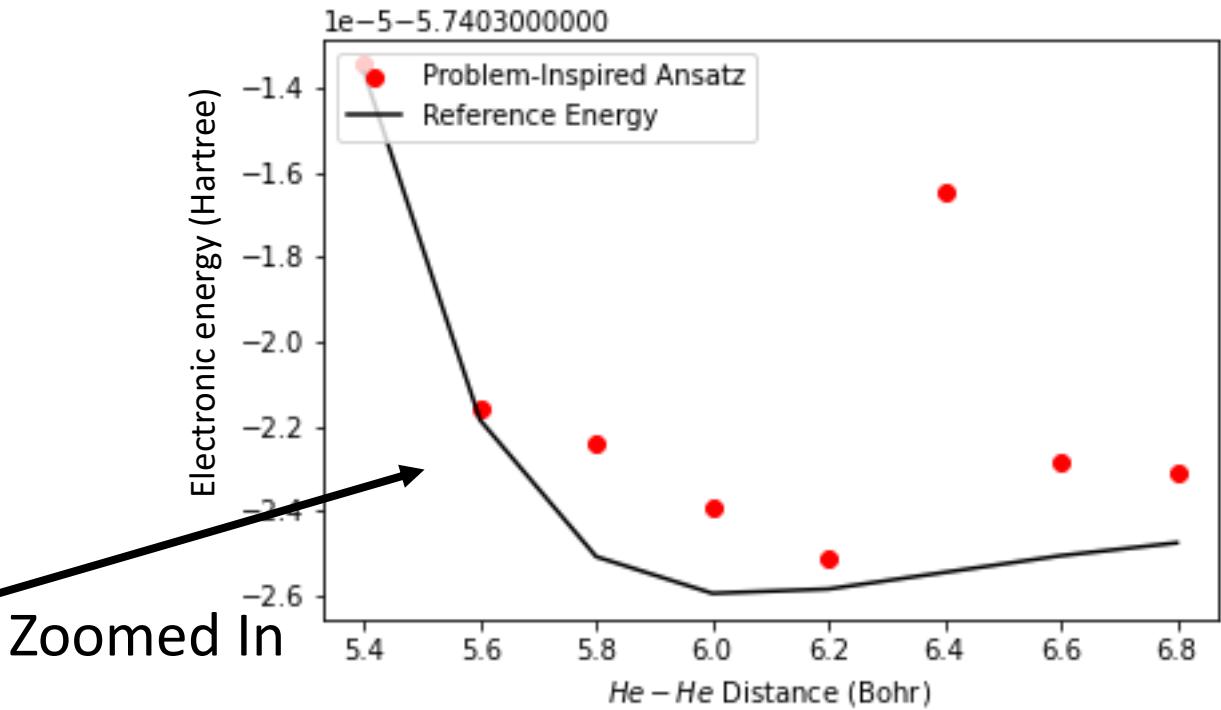
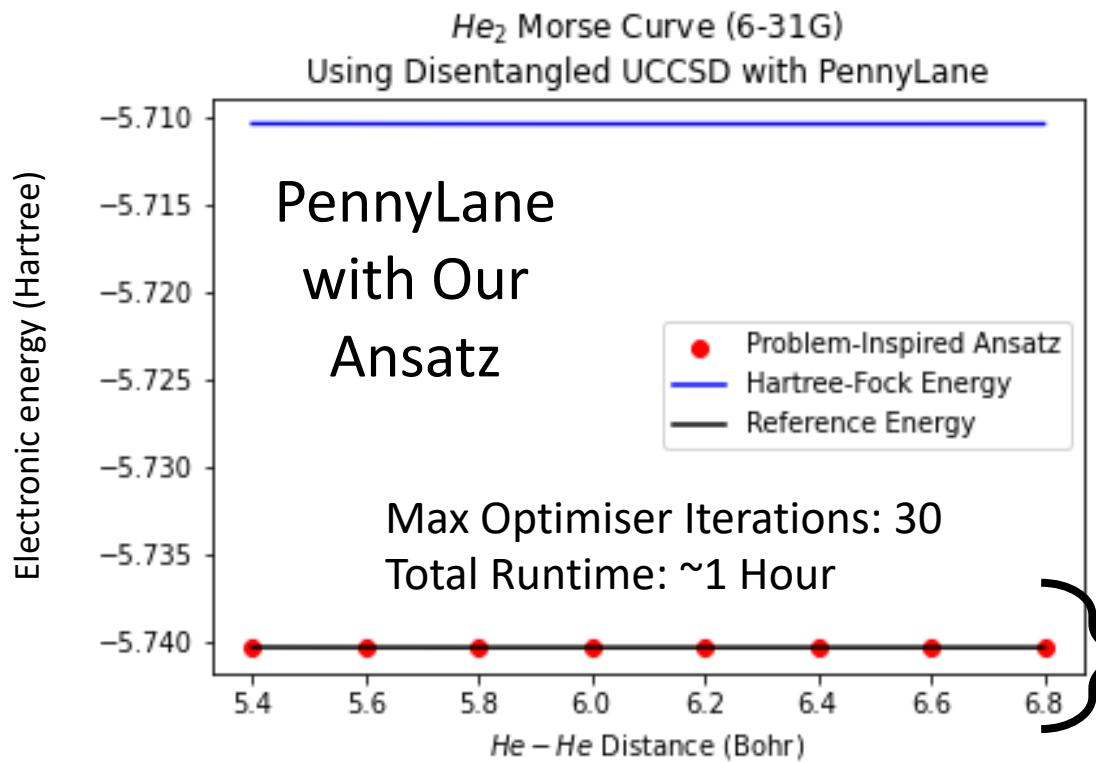
ibmq_montreal Error Map



ibmq_mumbai Error Map



Potential Energy Surface for He_2 using Exact Quantum simulator

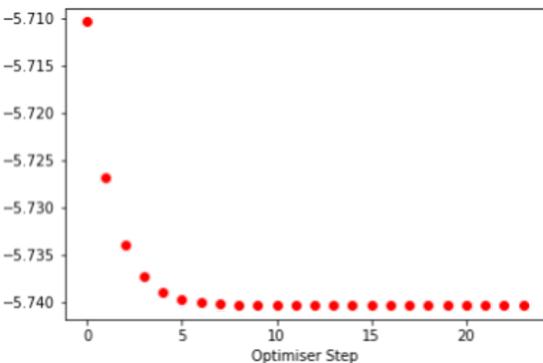


No. of Electrons: 4
No. of Qubits: 8
No. of Pauli Strings (to measure): 185
No. of Single Excitations Rotation Gate: 16
No. of Double Excitations Rotations Gate: 36
Total No. of Excitations Rotation Parameter: 52
Hartree-Fock State: $|1\ 1\ 1\ 1\ 0\ 0\ 0\ 0\rangle$

Distance:
 $r = 5.4 \text{ to } 6.8 \text{ Bohr}$

Detailed description: This section provides technical details about the quantum circuit parameters used for the simulation. It includes the number of electrons (4), qubits (8), and various rotation gates required for the Pauli string measurements. The Hartree-Fock state is specified as $|1\ 1\ 1\ 1\ 0\ 0\ 0\ 0\rangle$. Below this, a diagram shows two light blue spheres representing helium atoms.

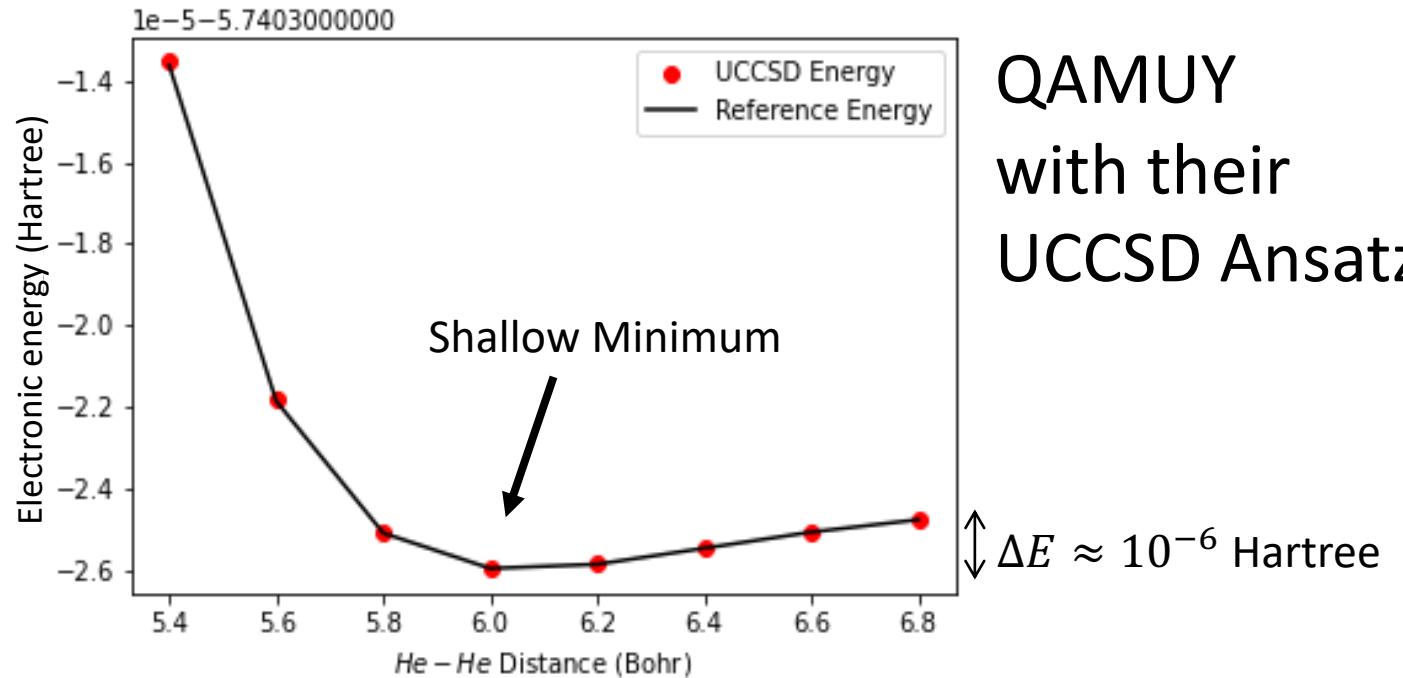
Energy Optimisation of He_2 @ 6Bohr



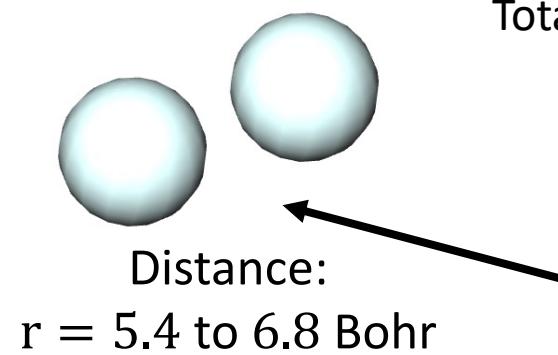
Note: Optimizers provided by PennyLane were unsuccessful in converging to the reference energy exactly in a limited number of steps (30 Iterations Max)

Potential Energy Surface for He_2 with QAMUY

He₂ Morse Curve (6-31G)



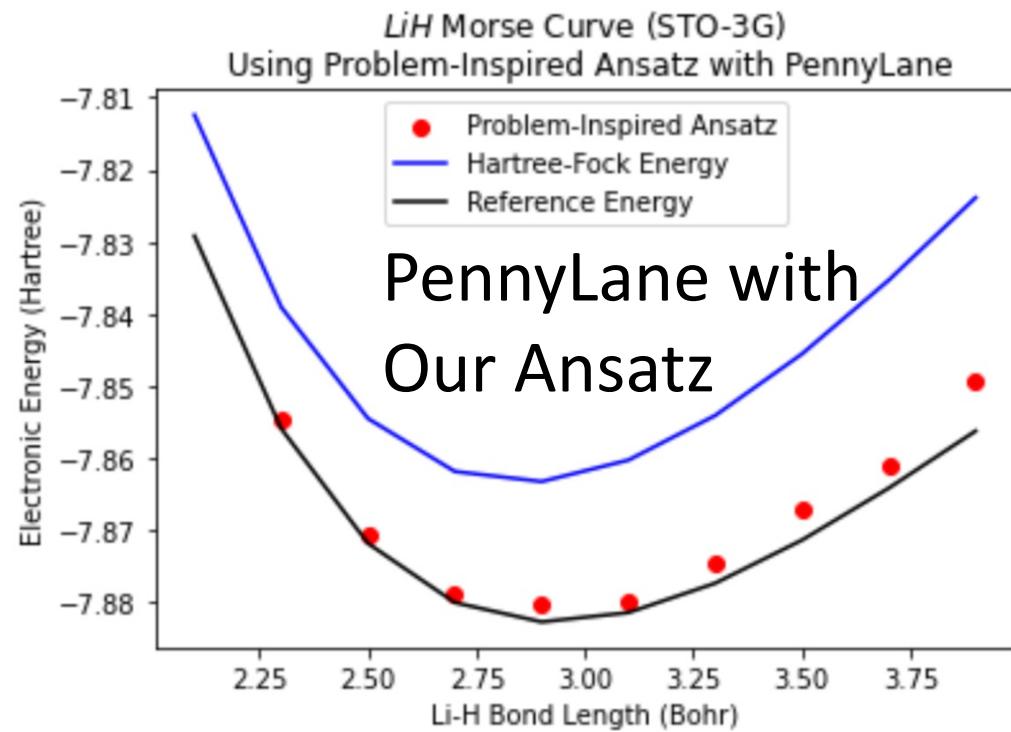
QAMUY
with their
UCCSD Ansatz



Total Runtime: ~5 min

There should be no Helium Bond as the
energy depth is too shallow to support
it

Potential Energy Surface for LiH using Exact Quantum simulator



No. of Electrons: 4

No. of Qubits: 12

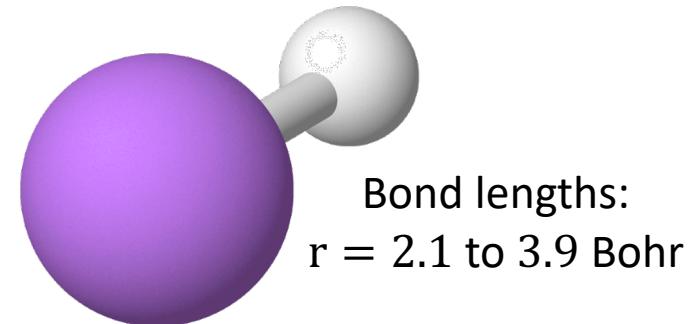
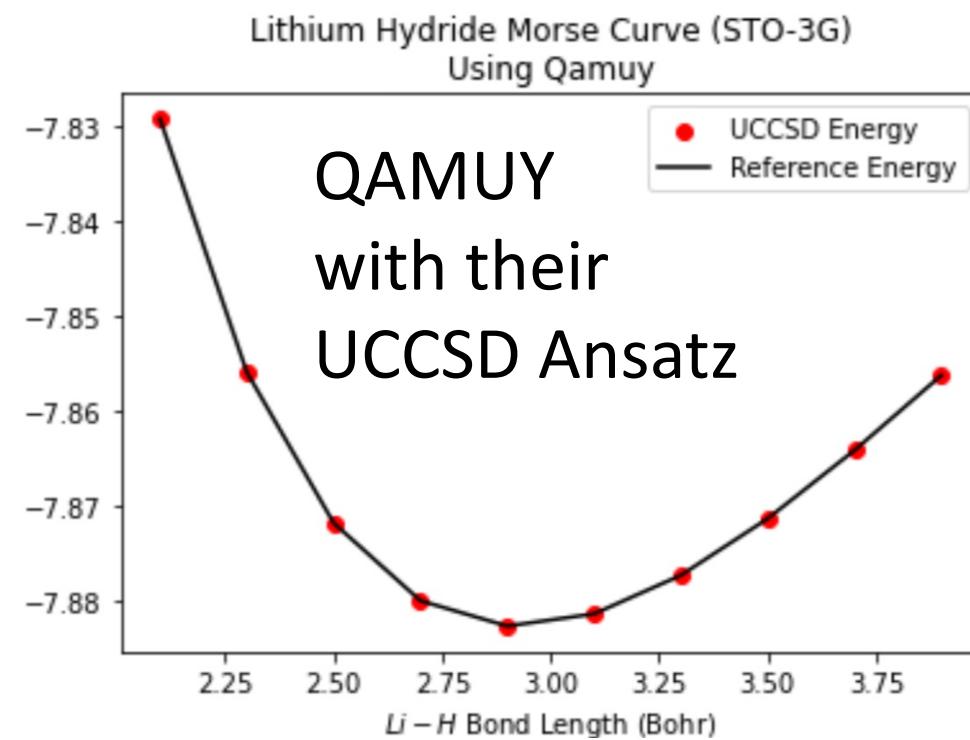
No. of Pauli Strings (to measure): 631

No. of Single Excitations Rotations Gate : 32

No. of Double Excitations Rotations Gate: 168

Total No. of Excitations Rotation Parameter: 200

Hartree-Fock State: $|1\ 1\ 1\ 1\ 0\ 0\ 0\ 0\ 0\ 0\ 0\ 0\rangle$



Contributing Members

Team Members (NUS, CQT):

- Chee Chong Hian (Main Lead, Coder, Curator)
- Benjamin Tan (Proofreading, Curator)
- Gan Beng Yee & Supanut Thanasilp (Tried in Running Our Quantum Circuit on Real IBM Devices, but it didn't work due to Technical Issues)
- Adrain Mak (Basic Proofreading, ASTAR)