

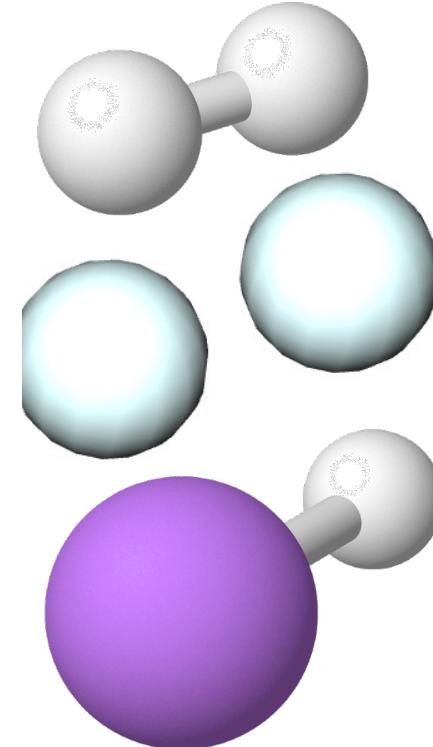
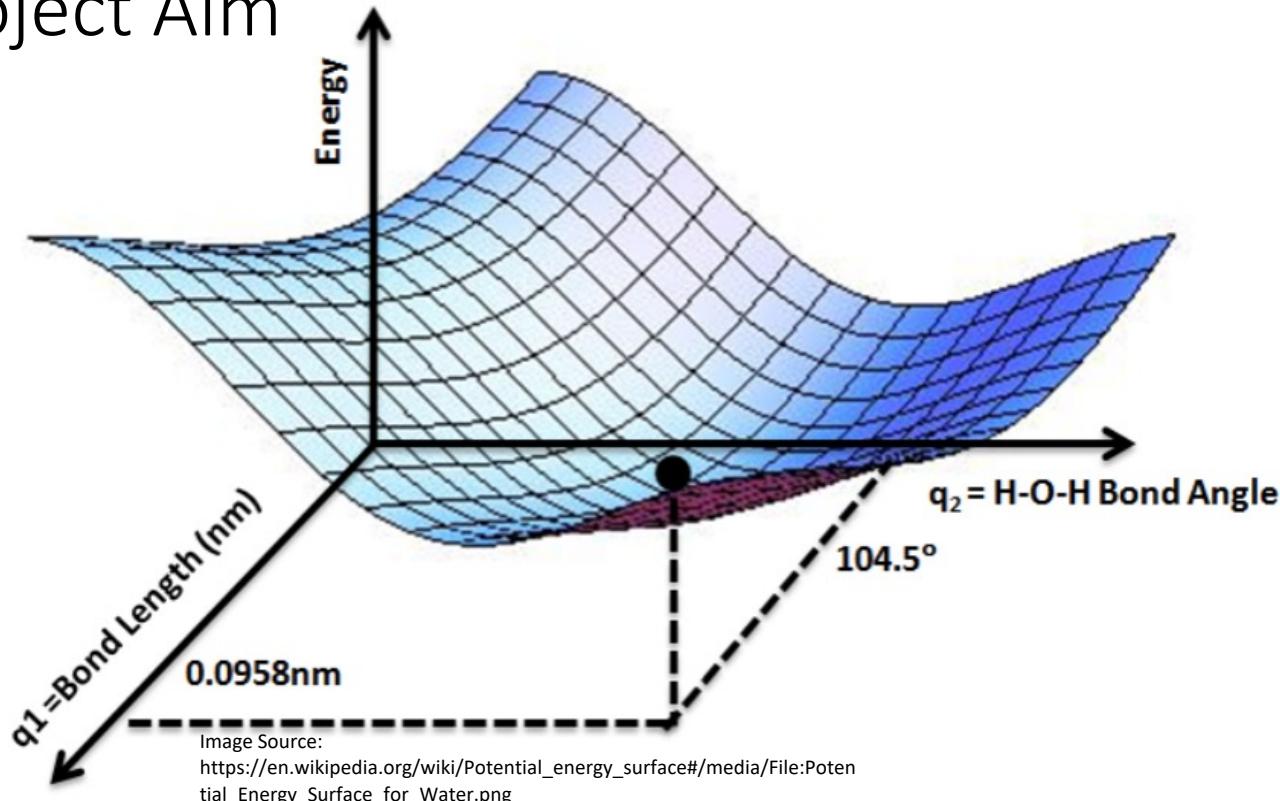
# Exploring the Potential Energy Surface of various Molecules with a Problem-Inspired Ansatz

QHack Open Hackathon 2022

21-25 Feb 2022

Team: Qanything

# Project Aim



- $\text{H}_2$ : Hydrogen molecule
- $\text{He}_2$ : Helium Dimer
- $\text{LiH}$ : Lithium Hydride

Aim: Explore Potential Energy Surface (PES) of  $\text{H}_2$ ,  $\text{He}_2$ , and  $\text{LiH}$ , 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

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

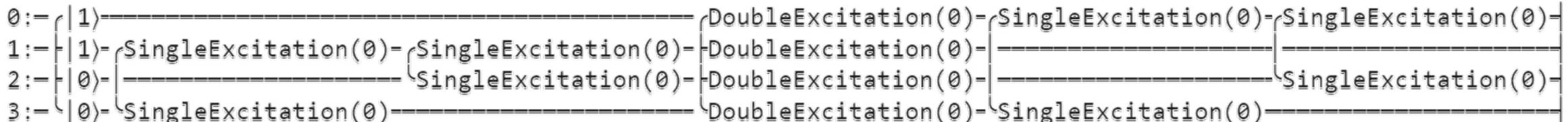
Singles                  Doubles                   $\theta$ : Parameters to Optimise

- 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 H<sub>2</sub>, requiring 4 qubits

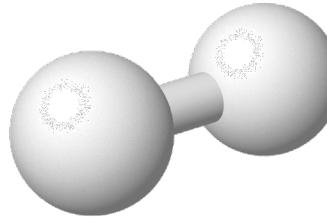
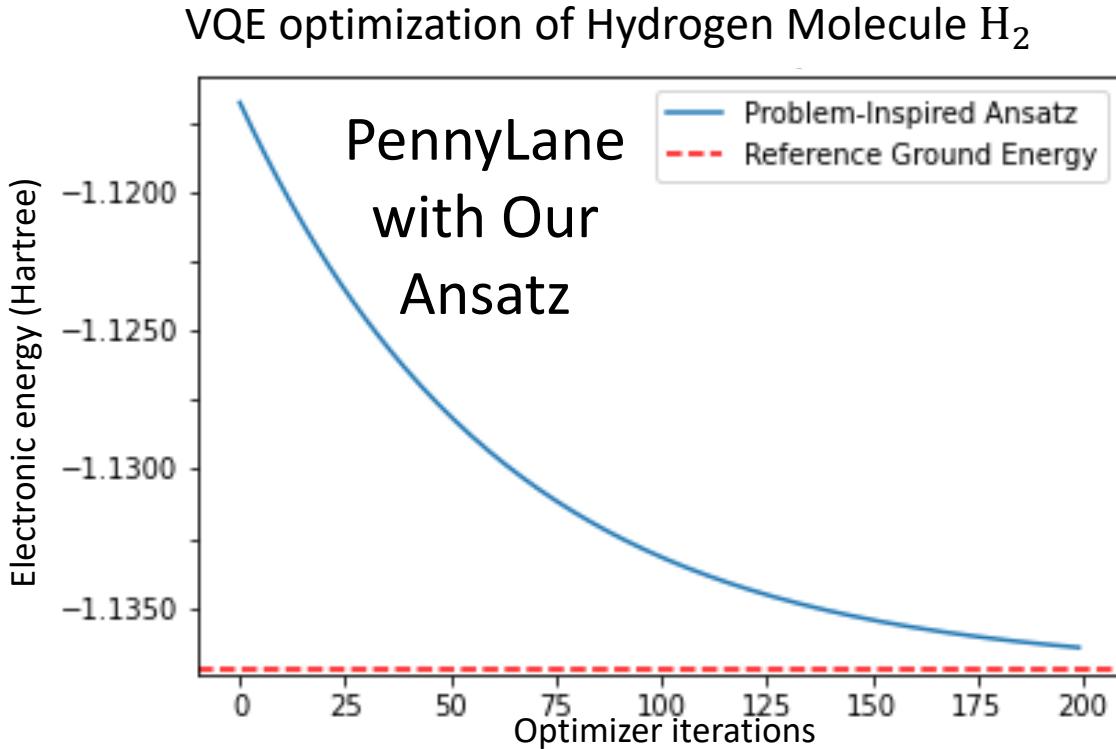
Measurement  
 $\langle \psi_{PI} | \hat{H} | \psi_{PI} \rangle$

Hartree-Fock state

PennyLane Quantum Circuit for H<sub>2</sub>



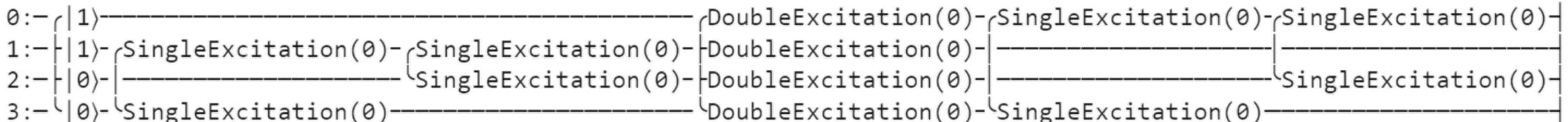
# Performing VQE Energy Optimisation using PennyLane



H<sub>2</sub>: Hydrogen molecule

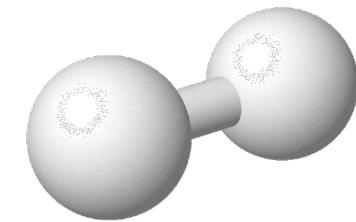
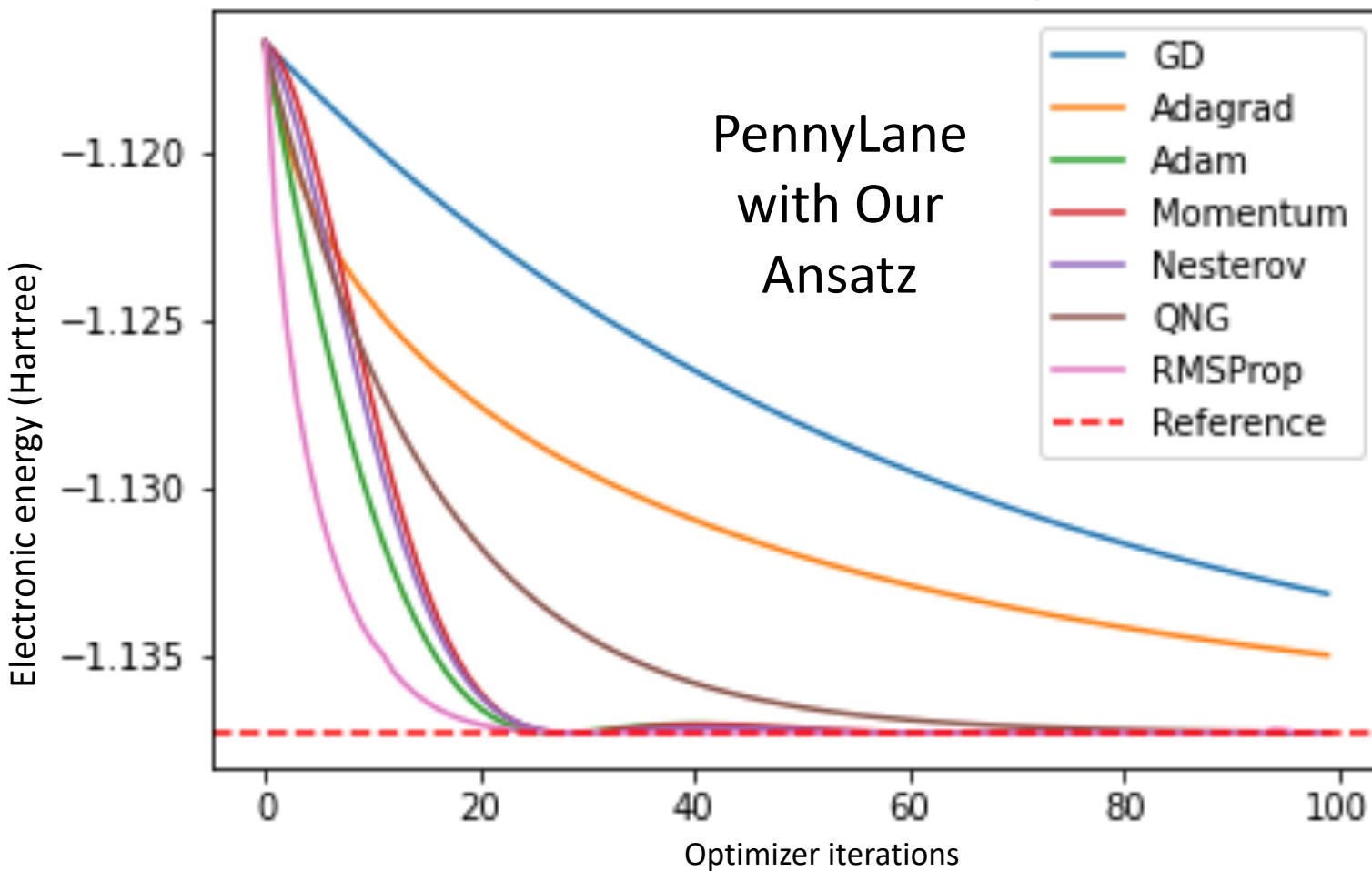
Bond length:  
r = 1.4 Bohr

- 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 Optimizers

VQE optimization of Hydrogen Molecule  $H_2$



$H_2$ : Hydrogen molecule

Bond length:  
 $r = 1.4$  Bohr

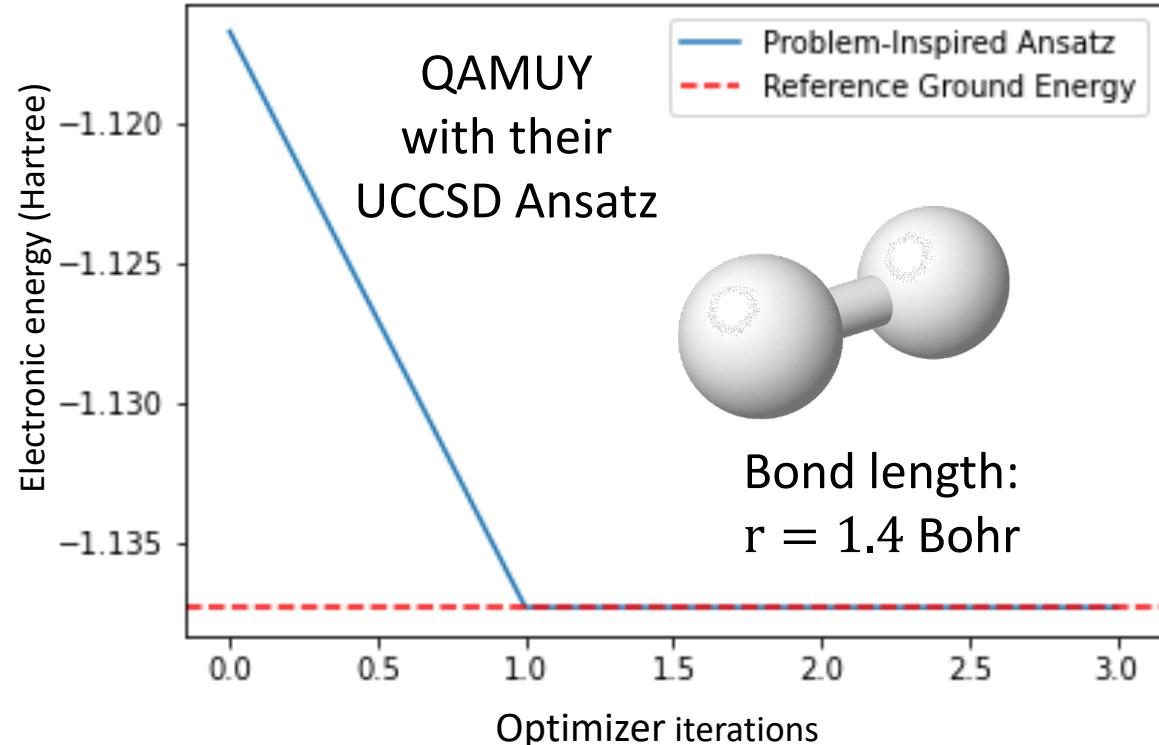
We tested the various optimizers available in PennyLane applied to  $H_2$  using our Disentangled UCC ansatz and ranked them according to their accuracy.

#### Optimiser Ranking:

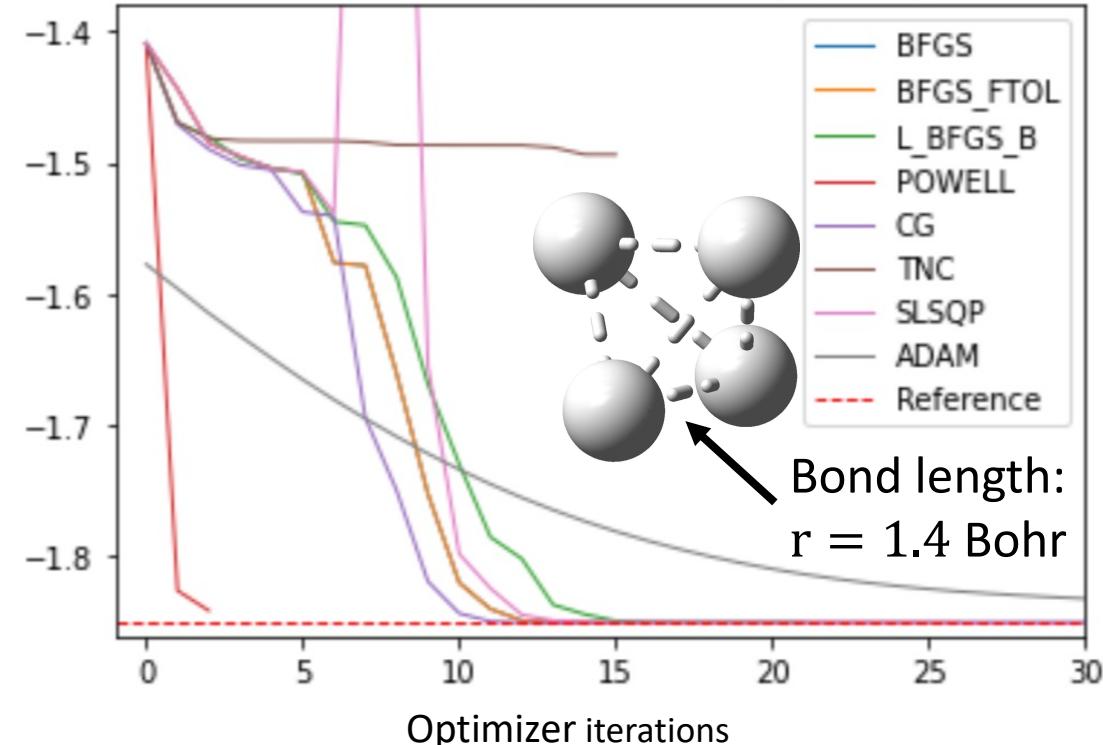
1. RMSProp
2. Adam
3. Nesterov
4. Momentum
5. QNG
6. Adagrad
7. Gradient Descent

# Implementing VQE on H<sub>2</sub> and Tetra Hydrogen H<sub>4</sub> with QAMUY

VQE optimization of H<sub>2</sub> in QAMUY  
(BFGS Only)

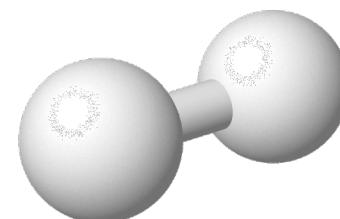
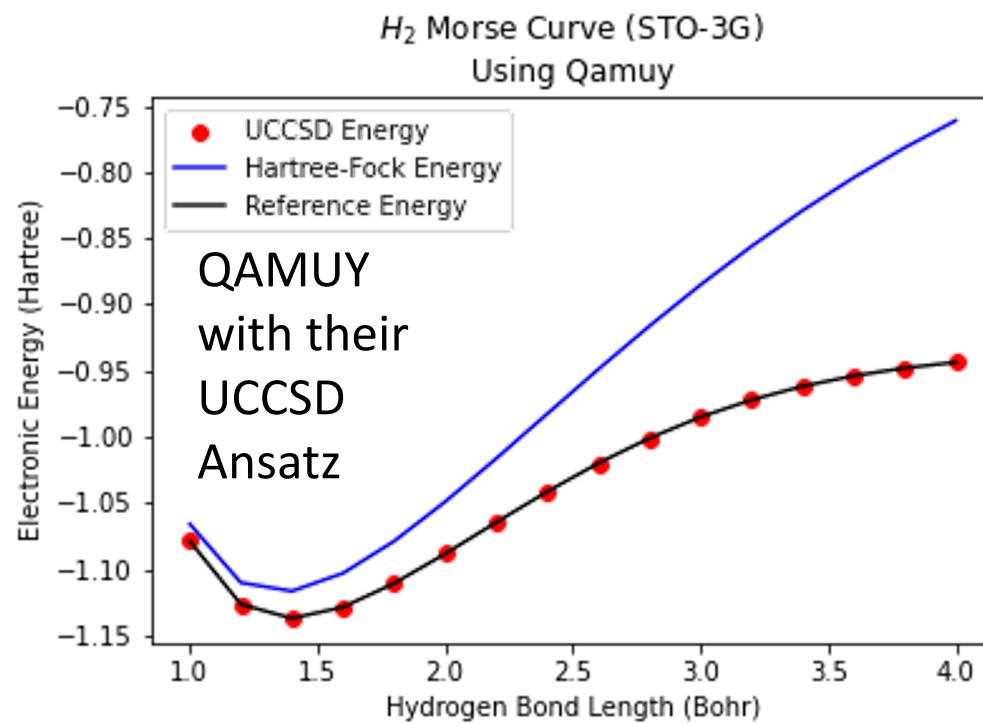
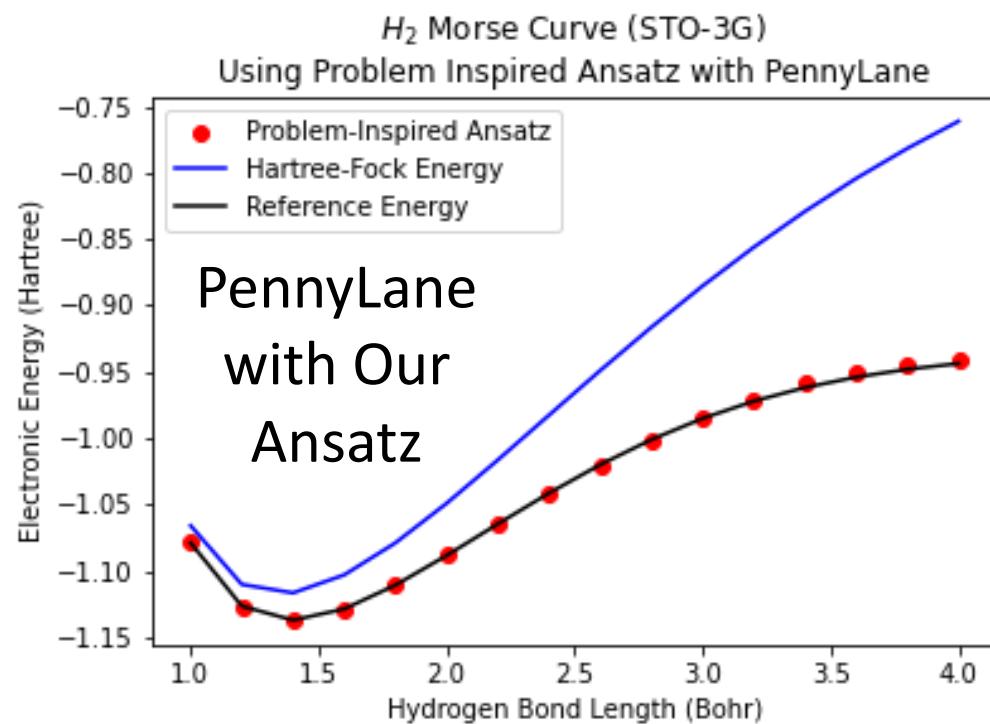


VQE Optimisation of Tetra Hydrogen H<sub>4</sub> Various in QAMUY (Various Optimisers)



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

# Potential Energy Surface for $\text{H}_2$ using Exact Quantum Simulator

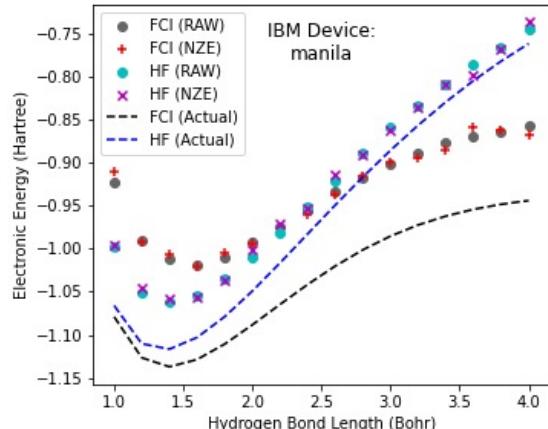


Bond lengths:  
 $r = 1.0$  to  $4.0$  Bohr

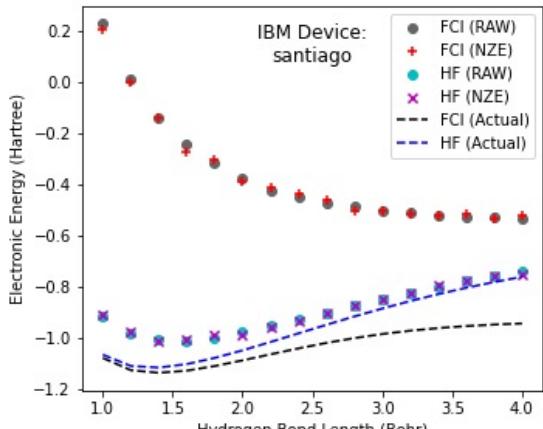
# Potential Energy Surface for H<sub>2</sub> using various IBMQ Device Noise Models

## Open Providers

### Best performing

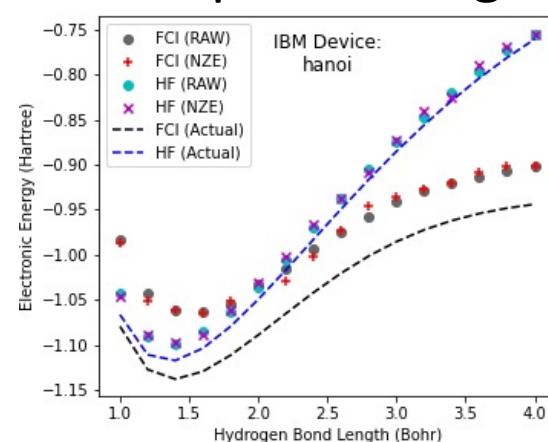


### Worst performing

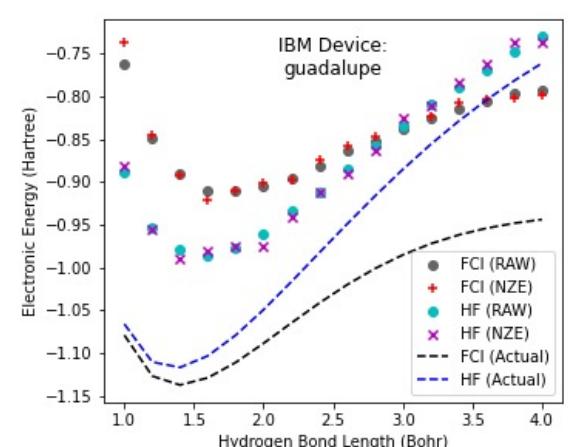


## Exclusive providers

### Best performing



### Worst performing



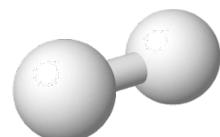
## Legend

**GREY Dots:** Our Optimised Problem Inspired Ansatz

**+**: Problem Inspired Ansatz w/ Mitiq Zero Noise Extrapolation

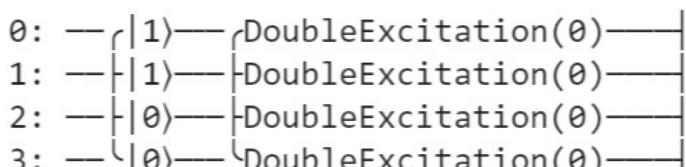
**CYAN Dots:** Hartree-Fock (HF) State Only

**X** : HF w/ Mitiq Zero Noise Extrapolation



Bond lengths:  
r = 1.0 to 4.0 Bohr

Actual Quantum  
Circuit Implemented:



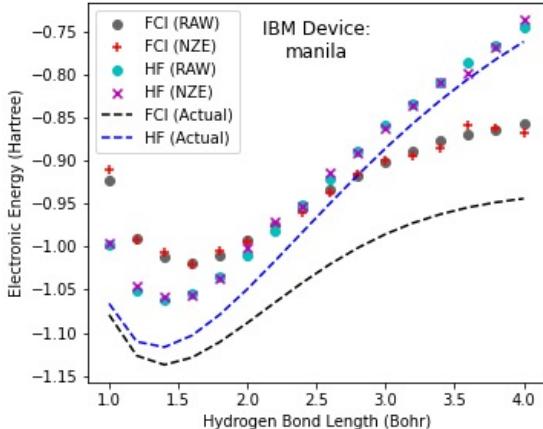
- Note: From the plots, our implementation of Mitiq as an error mitigation technique did not appear to help with improving the accuracy of our results. (???)

- Turns out for H<sub>2</sub>, 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

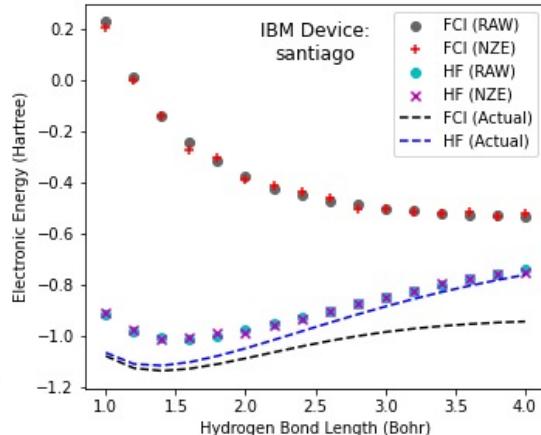
# Potential Energy Surface for H<sub>2</sub> using various IBMQ Device Noise Models

## Open Providers

### Best performing

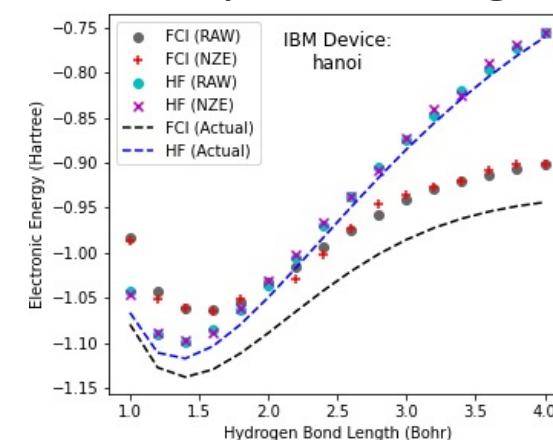


### Worst performing

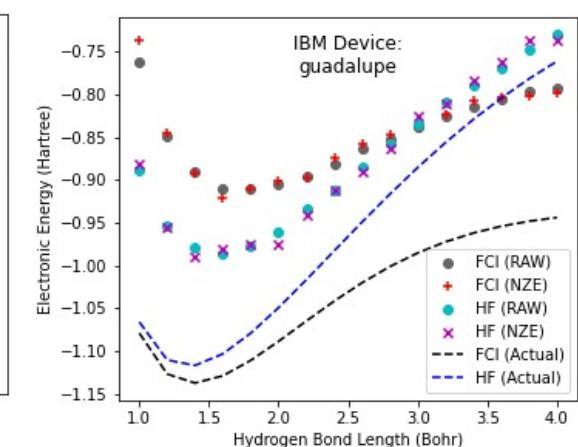


## Exclusive Providers

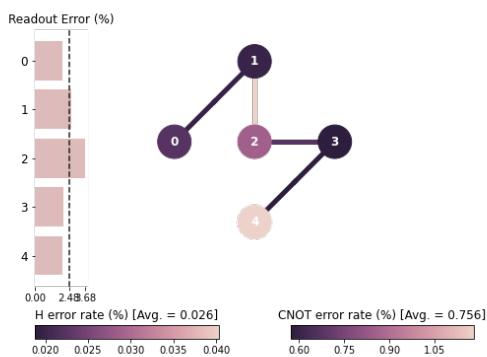
### Best performing



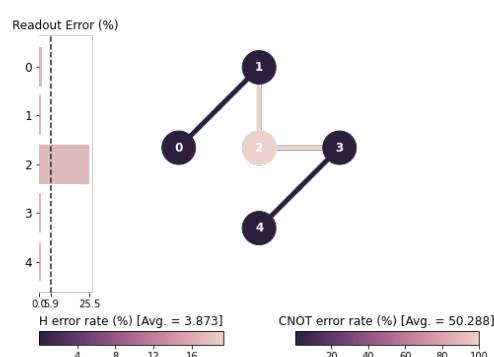
### Worst performing



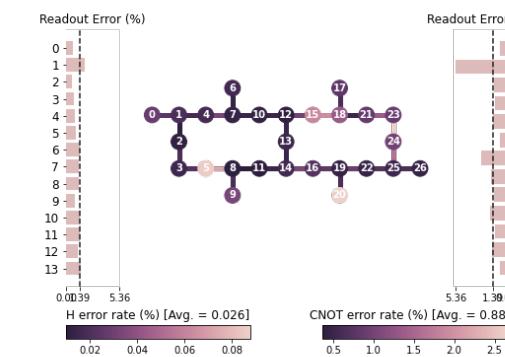
ibmq\_manila Error Map



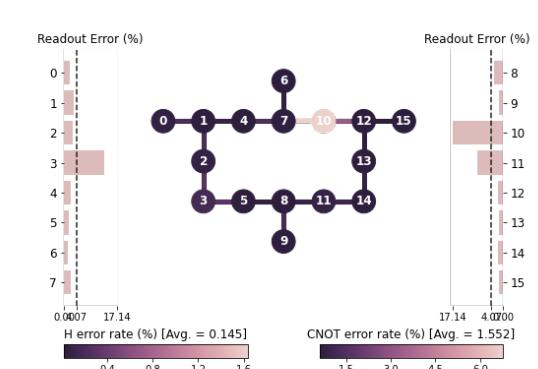
ibmq\_santiago Error Map



ibmq\_hanoi Error Map



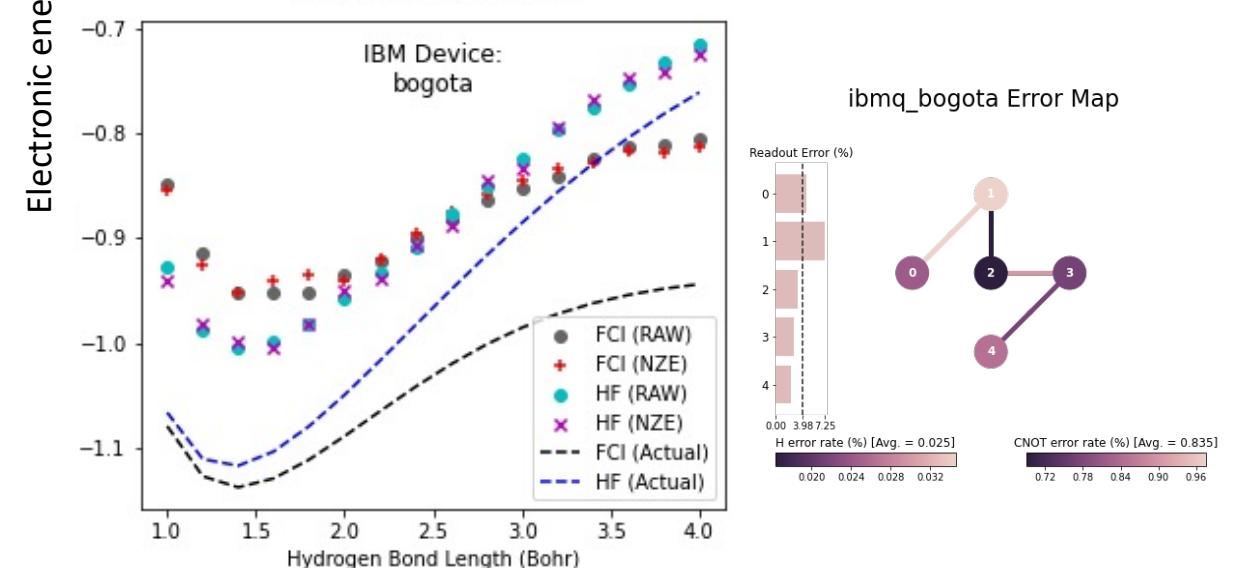
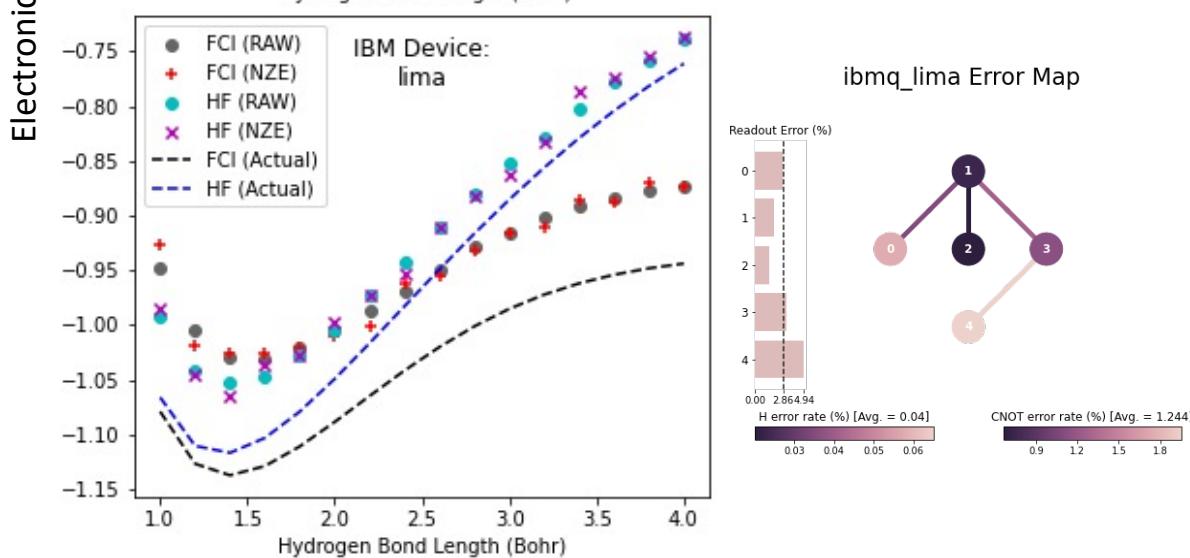
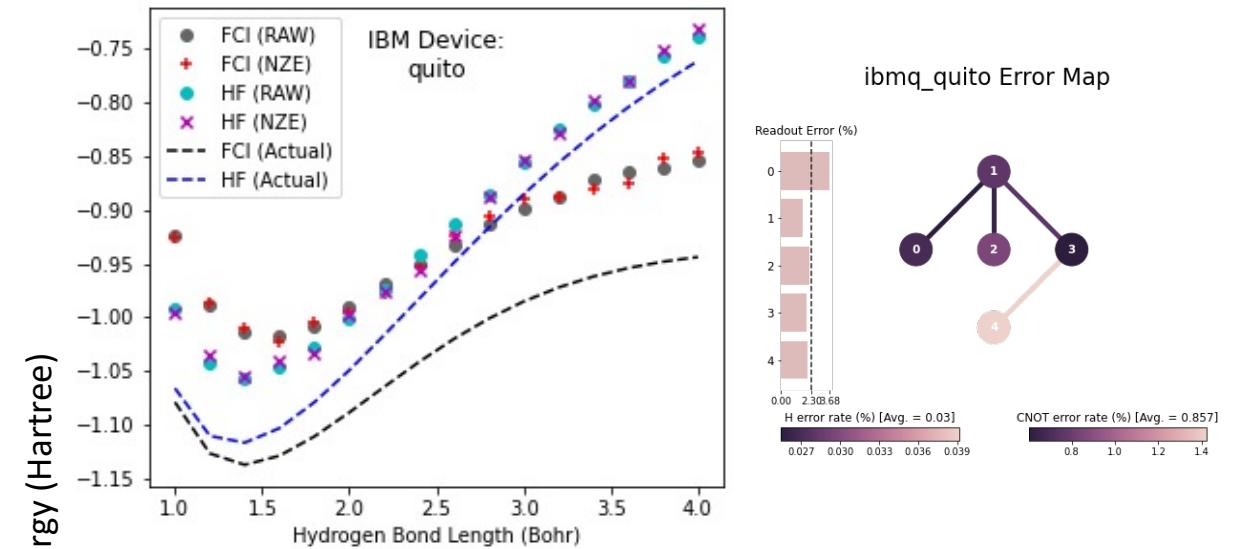
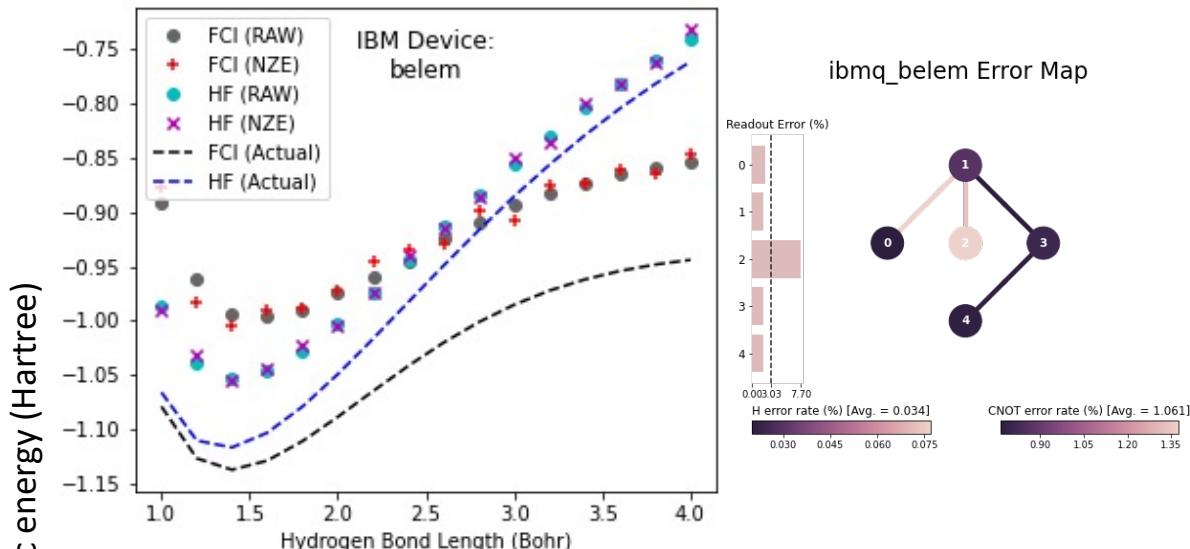
ibmq\_guadalupe Error Map



## Simulated IBM Quantum Devices Noise Map

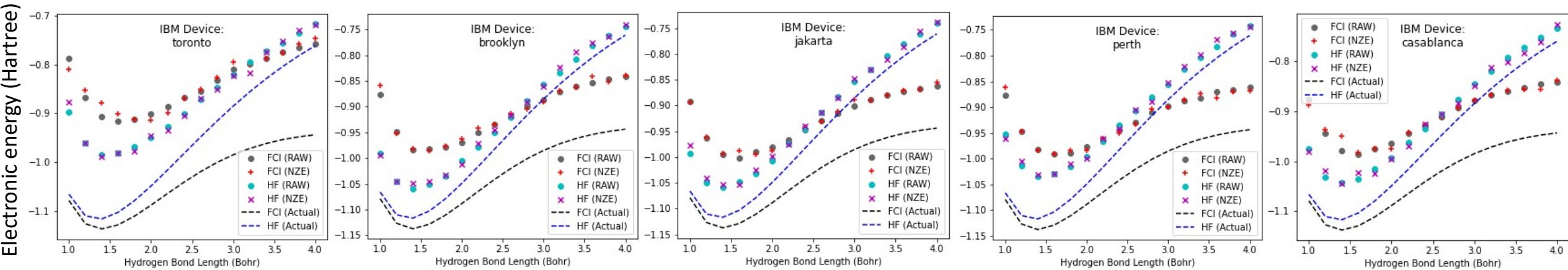
# Potential Energy Surface for H<sub>2</sub> using various IBMQ Device Noise Models

## Other Open Providers

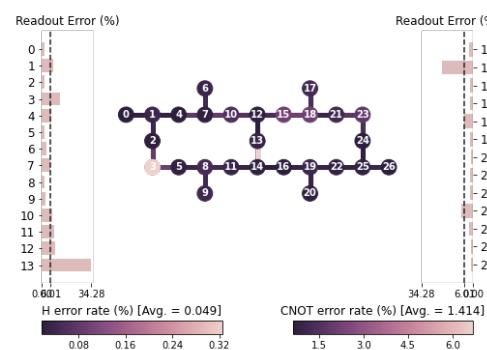


# Potential Energy Surface for H<sub>2</sub> using various IBMQ Device Noise Models

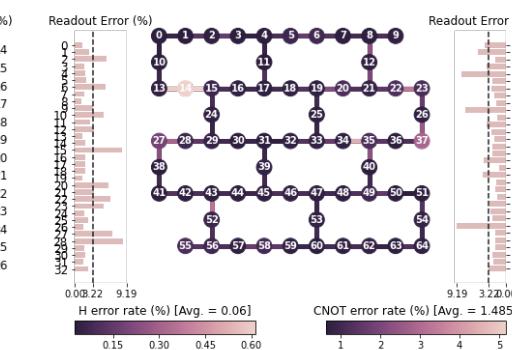
## Other Exclusive Providers



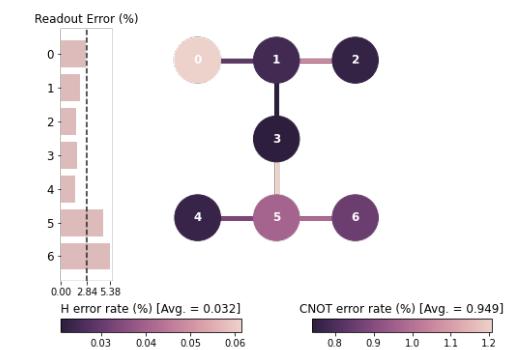
ibmq\_toronto Error Map



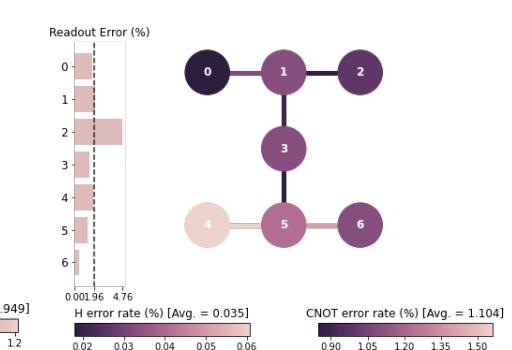
ibmq\_brooklyn Error Map



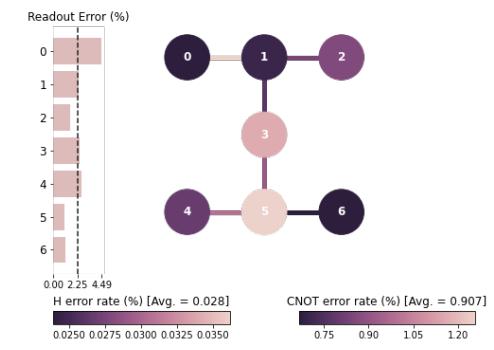
ibmq\_jakarta Error Map



ibm\_perth Error Map

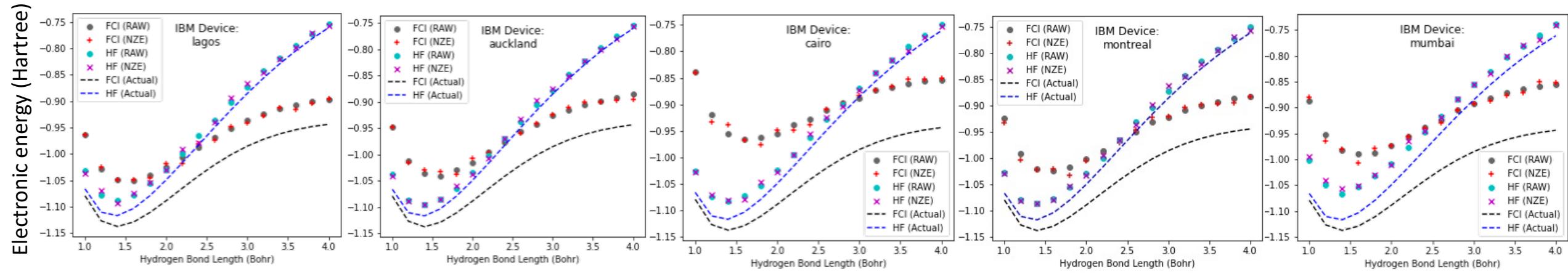


ibmq\_casablanca Error Map

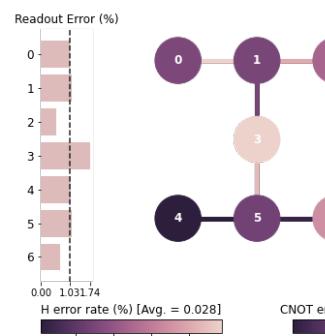


# Potential Energy Surface for H<sub>2</sub> using various IBMQ Device Noise Models

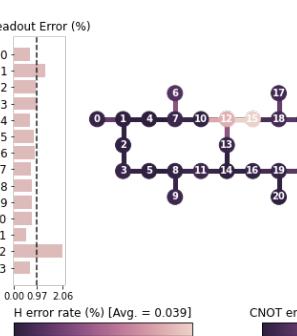
## Other Exclusive Providers



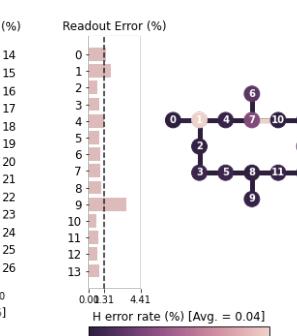
ibm\_lagos Error Map



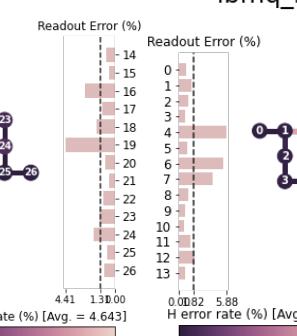
ibm\_auckland Error Map



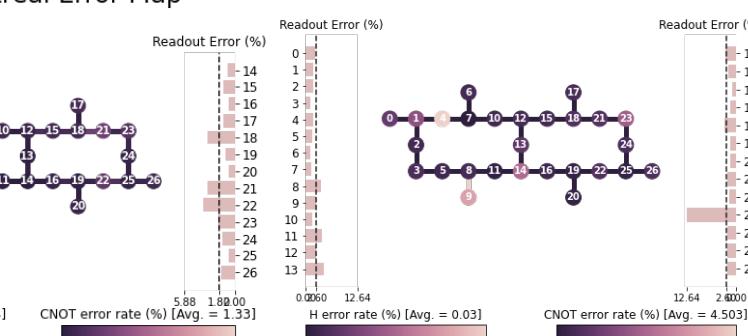
ibm\_cairo Error Map



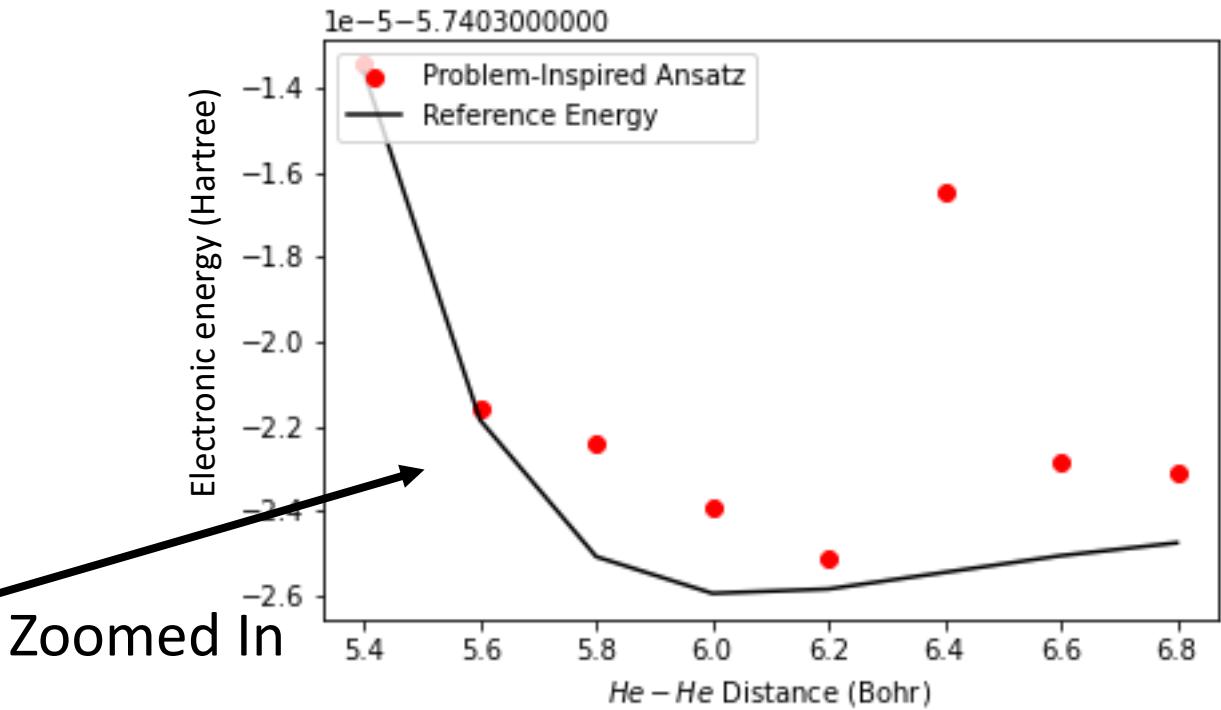
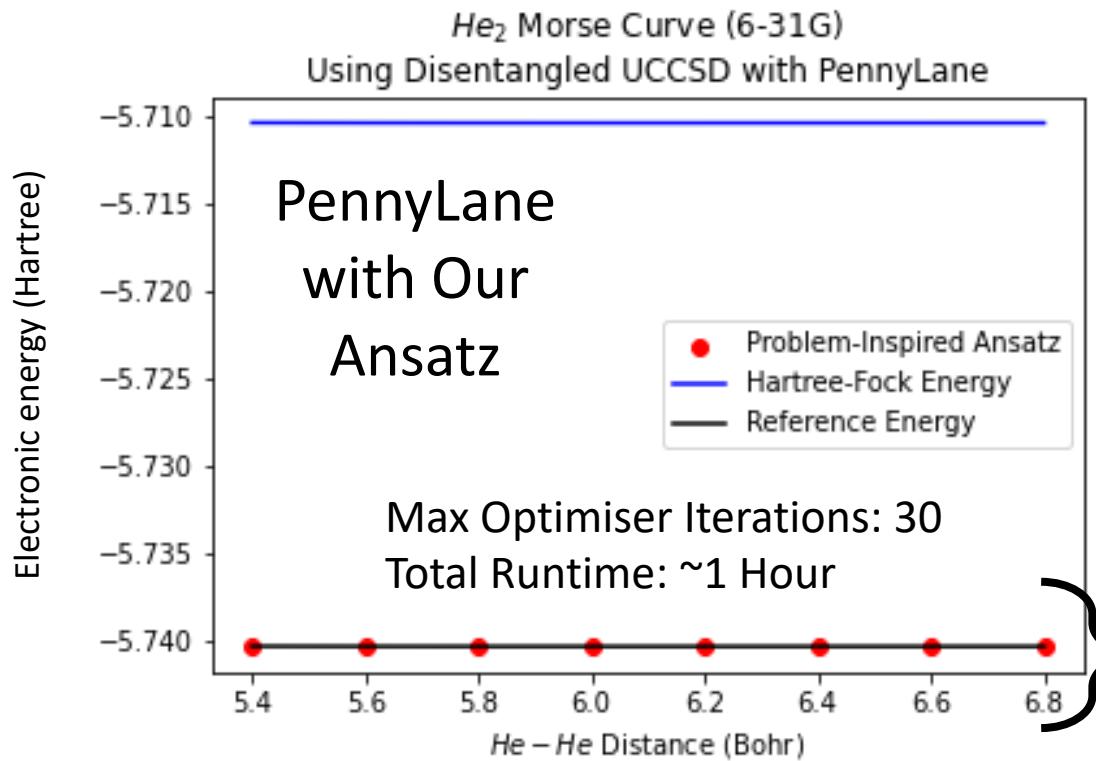
ibmq\_montreal Error Map



ibmq\_mumbai Error Map



# Potential Energy Surface for $\text{He}_2$ using Exact Quantum simulator

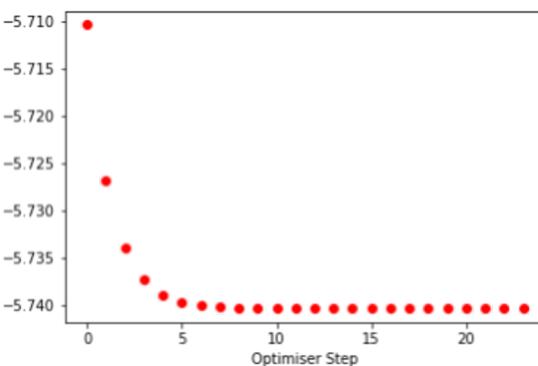


No. of Electrons: 4  
No. of Qubits: 8  
No. of Pauli Strings (to measure): 185  
No. of Single Excitations Rotation Gate: 16  
No. of Double Excitations Rotations Gate: 36  
Total No. of Excitations Rotation Parameter: 52  
Hartree-Fock State:  $|1\ 1\ 1\ 1\ 0\ 0\ 0\ 0\rangle$

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

A diagram showing two light blue spheres representing helium atoms, separated by a distance indicated by a vertical line between them.

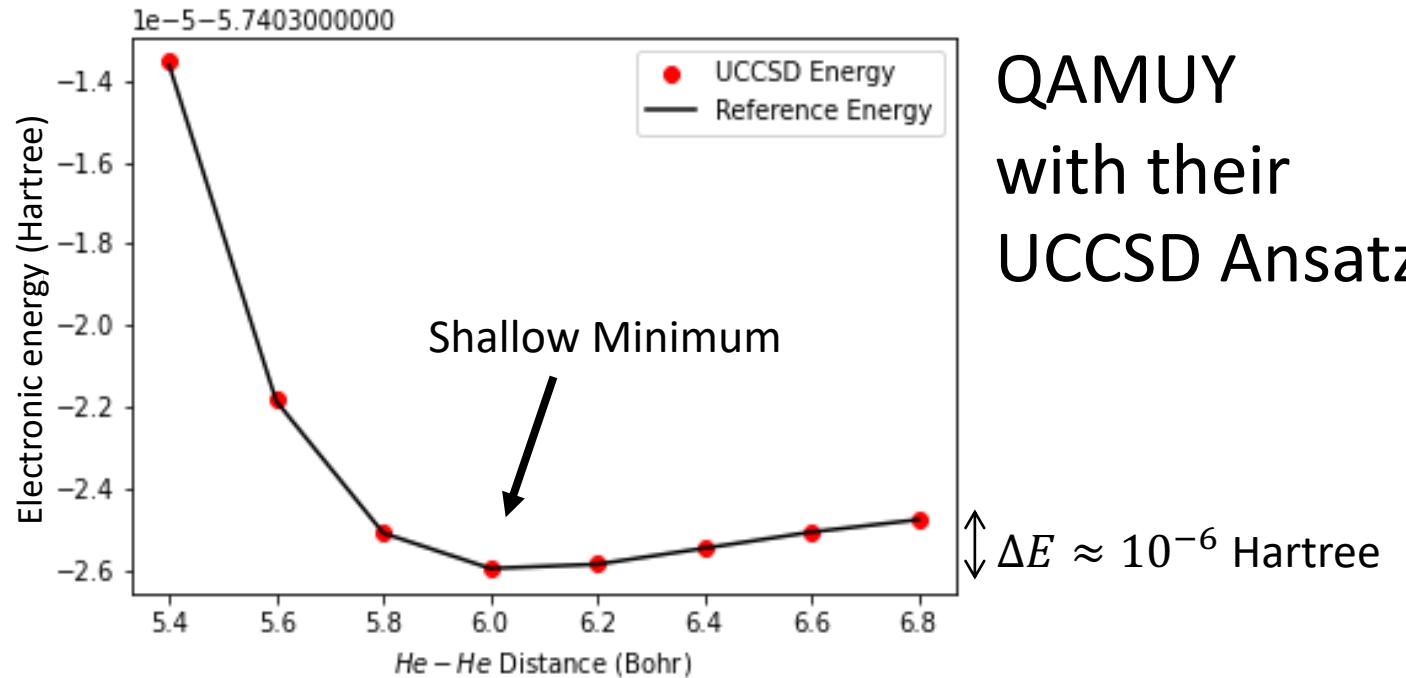
Energy Optimisation of  $\text{He}_2$  @ 6Bohr



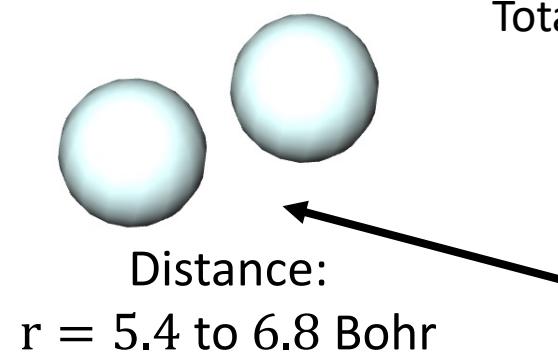
Note: Optimizers provided by PennyLane were unsuccessful in converging to the reference energy exactly in a limited number of steps (30 Iterations Max)

# Potential Energy Surface for $He_2$ with QAMUY

He<sub>2</sub> Morse Curve (6-31G)



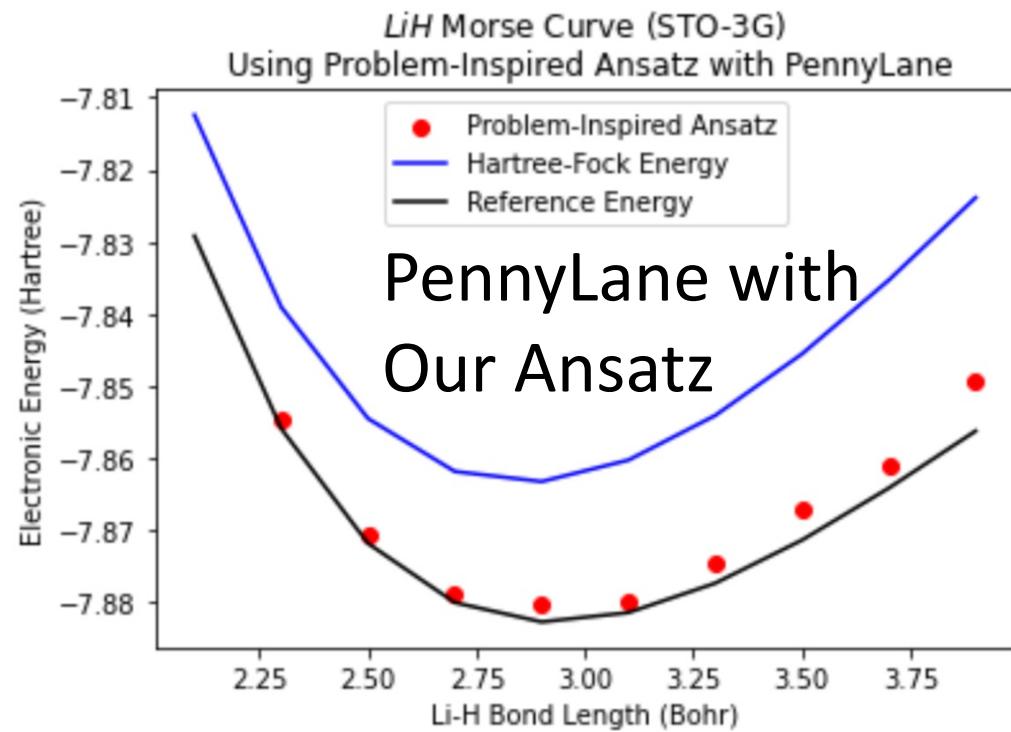
QAMUY  
with their  
UCCSD Ansatz



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

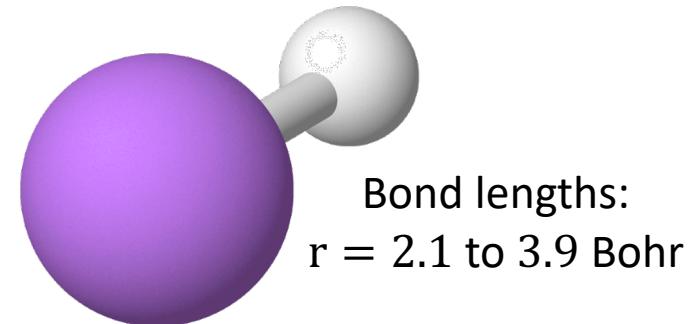
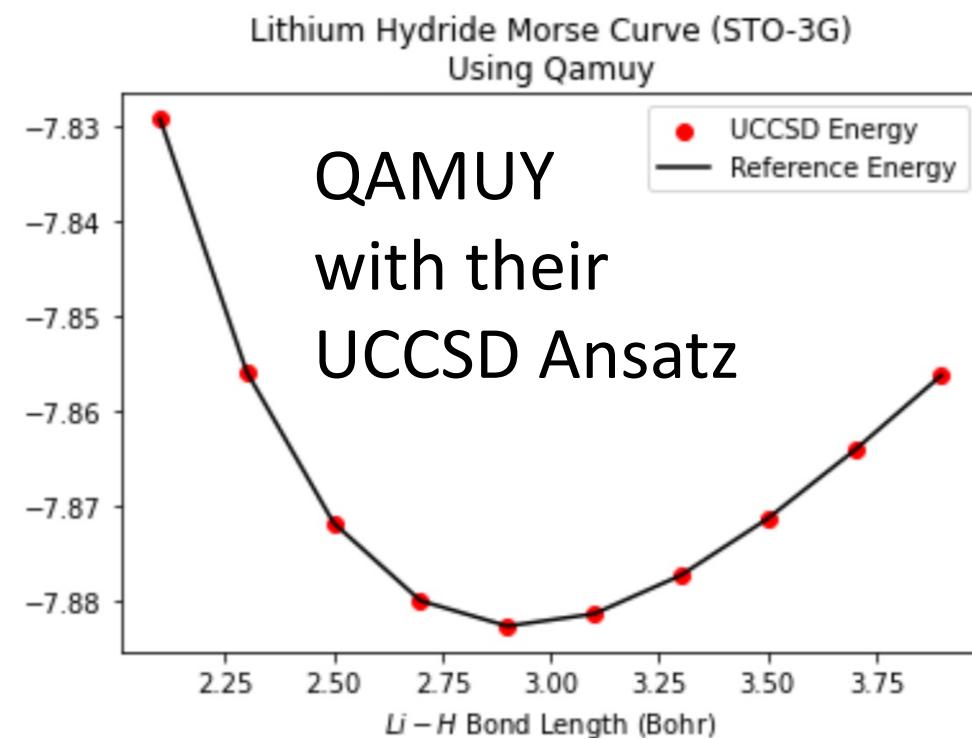
No. of Pauli Strings (to measure): 631

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, Assistant 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)