

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

QHack 2022

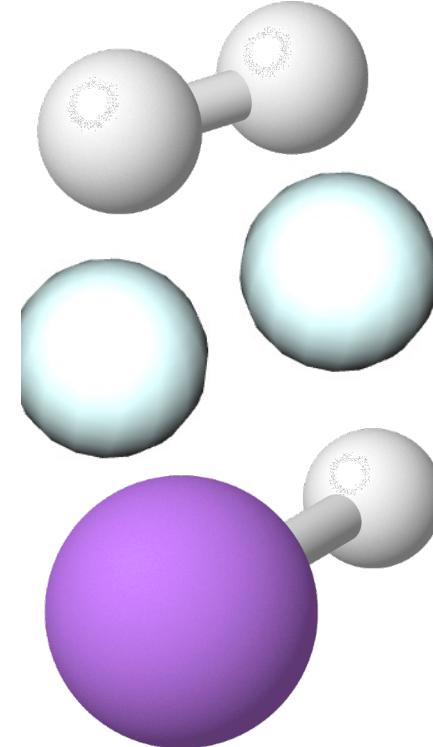
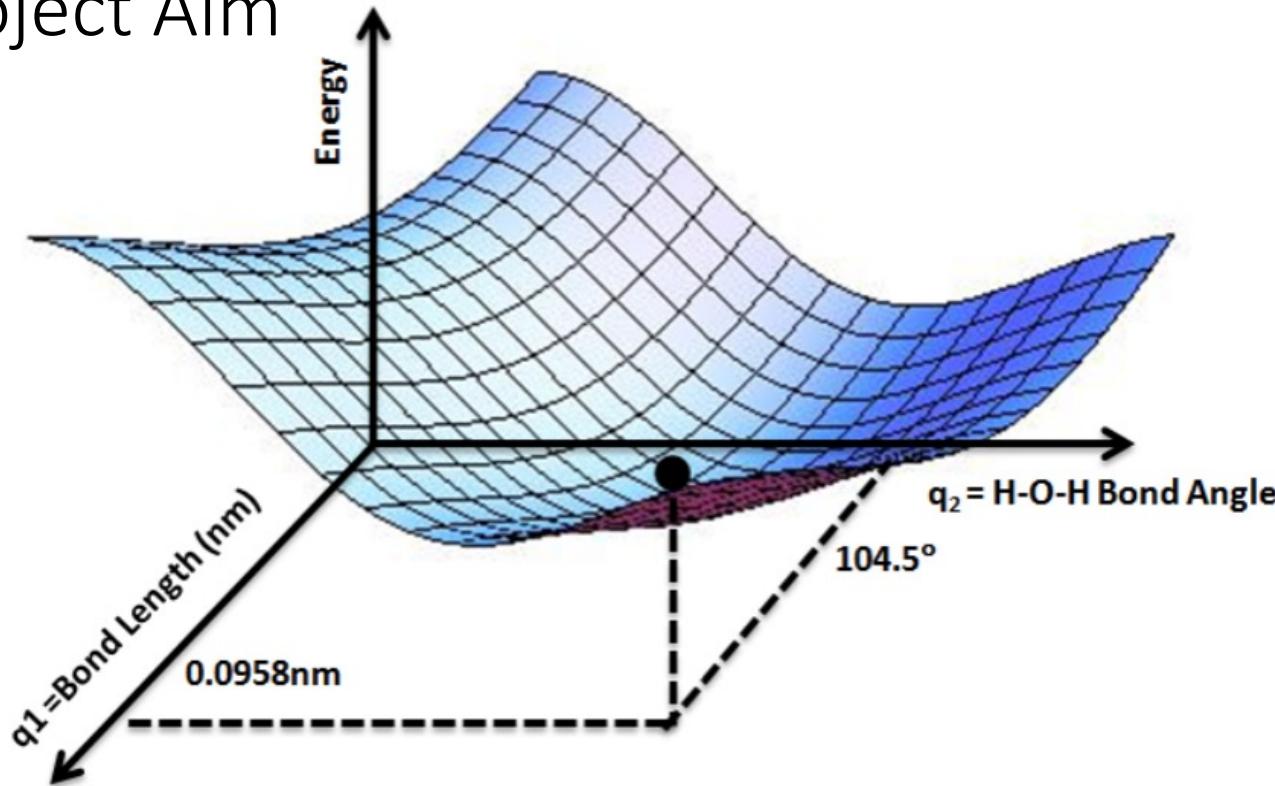
26 Feb 2022

Team Members:

- Chee Chong Hian (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 (Proofreading)

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

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

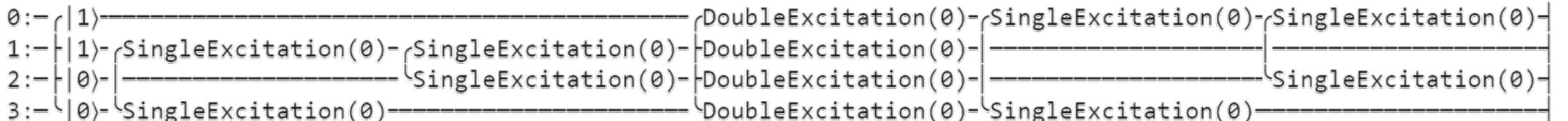
Singles

Doubles

θ : Parameters to Optimise

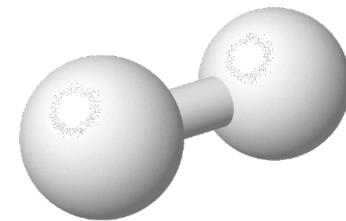
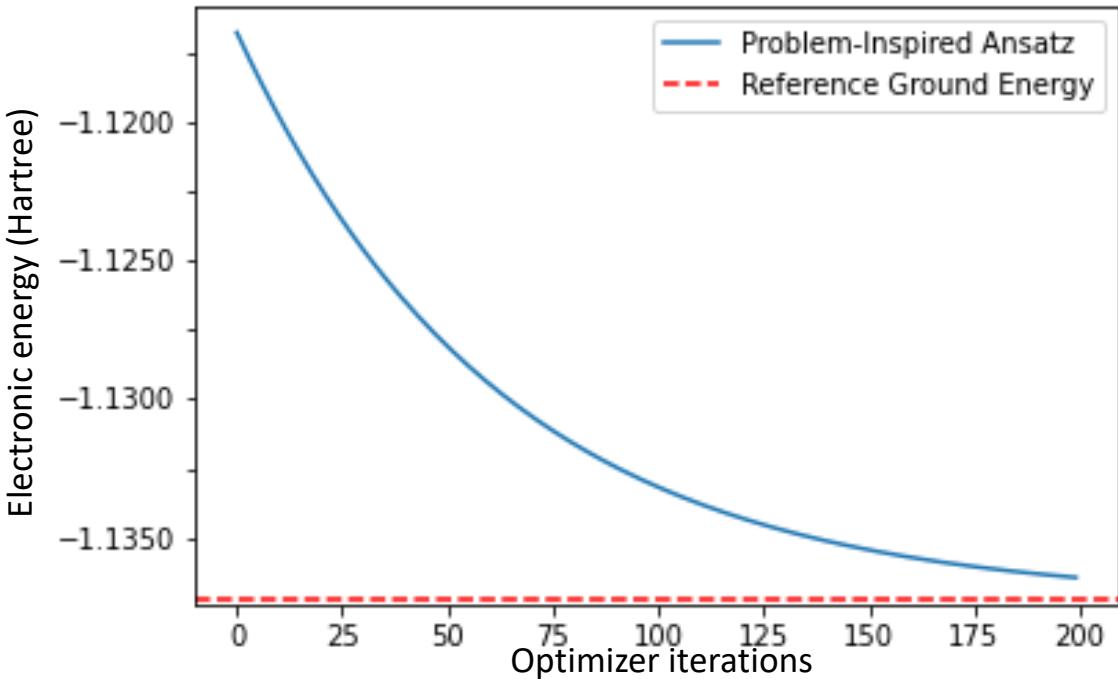
- We used the Disentangled UCC, a problem-inspired ansatz
- It consists of singles and doubles excitation operators applied to the Hartree-Fock state.
- As an example, shown below is the Disentangled UCC ansatz for H₂, requiring 4 qubits

Hartree-Fock state



Performing VQE Energy Optimisation using PennyLane

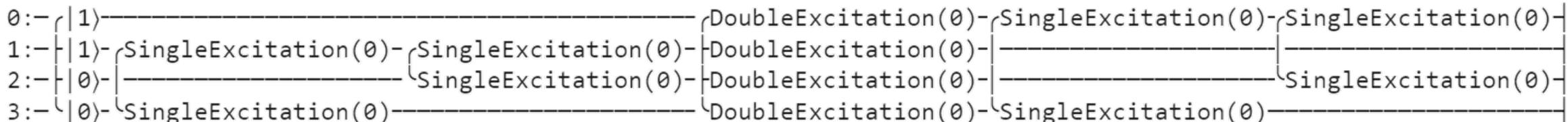
VQE optimization of Hydrogen Molecule H_2



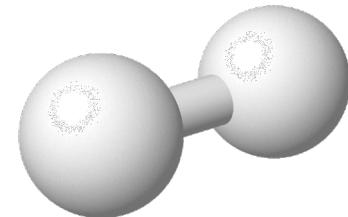
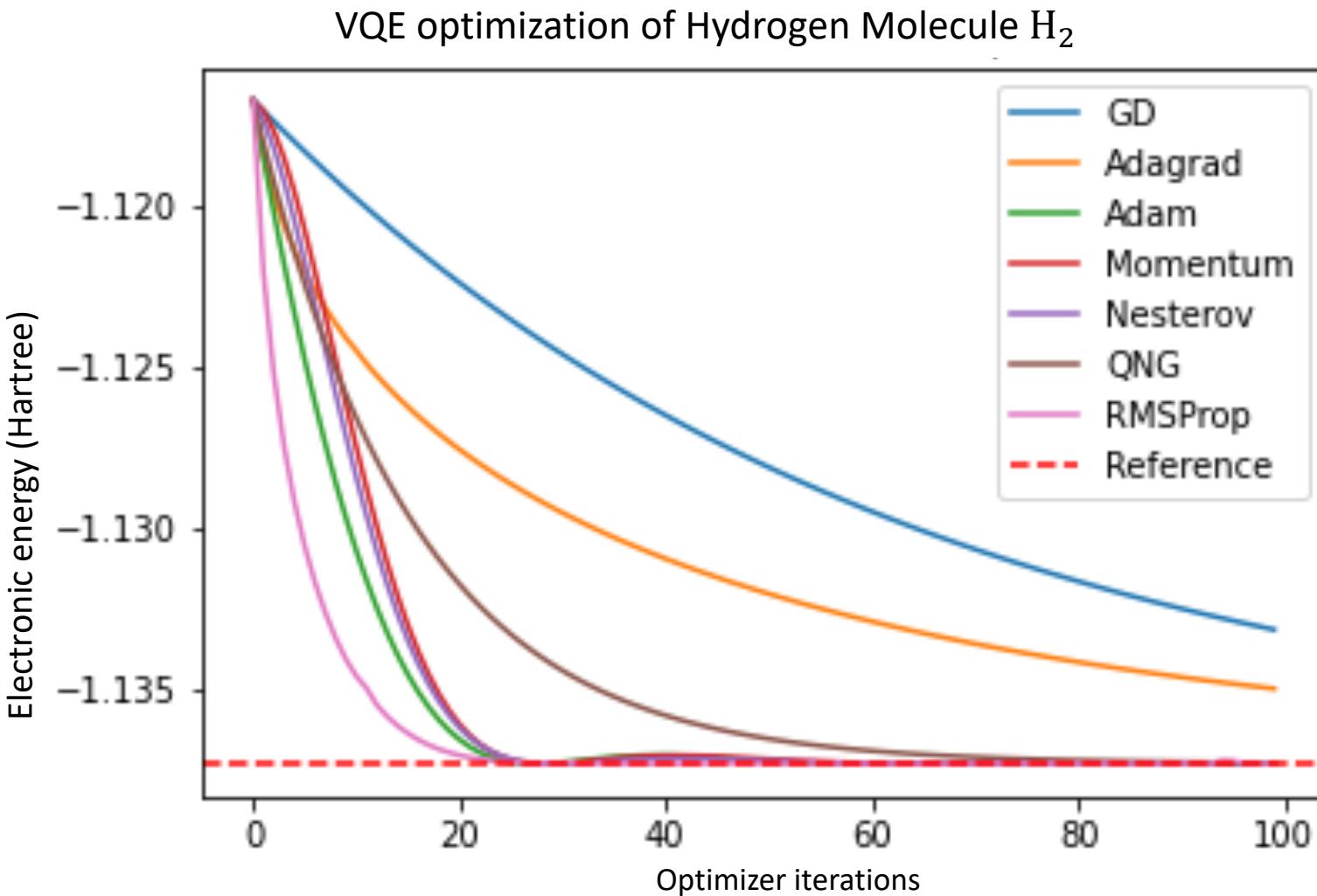
H_2 : Hydrogen molecule

Bond length:
 $r = 1.4$ Bohr

- Parameters are Optimized using Gradient Descent Using Default Settings



Benchmarking Using PennyLane Built-in Classical Optimizer



H₂: Hydrogen molecule

Bond length:
r = 1.4 Bohr

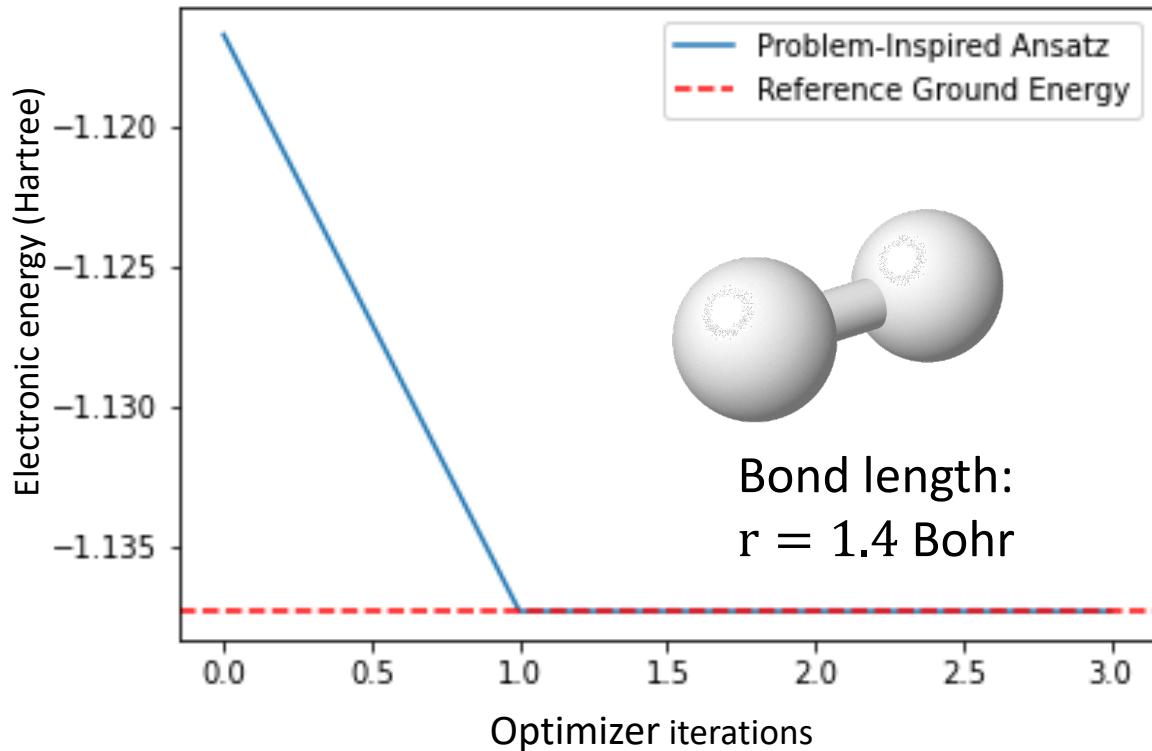
We tested the various optimizers available in PennyLane applied to H₂ using our Disentangled UCC ansatz and ranked them according to their accuracy.

Optimiser Ranking:

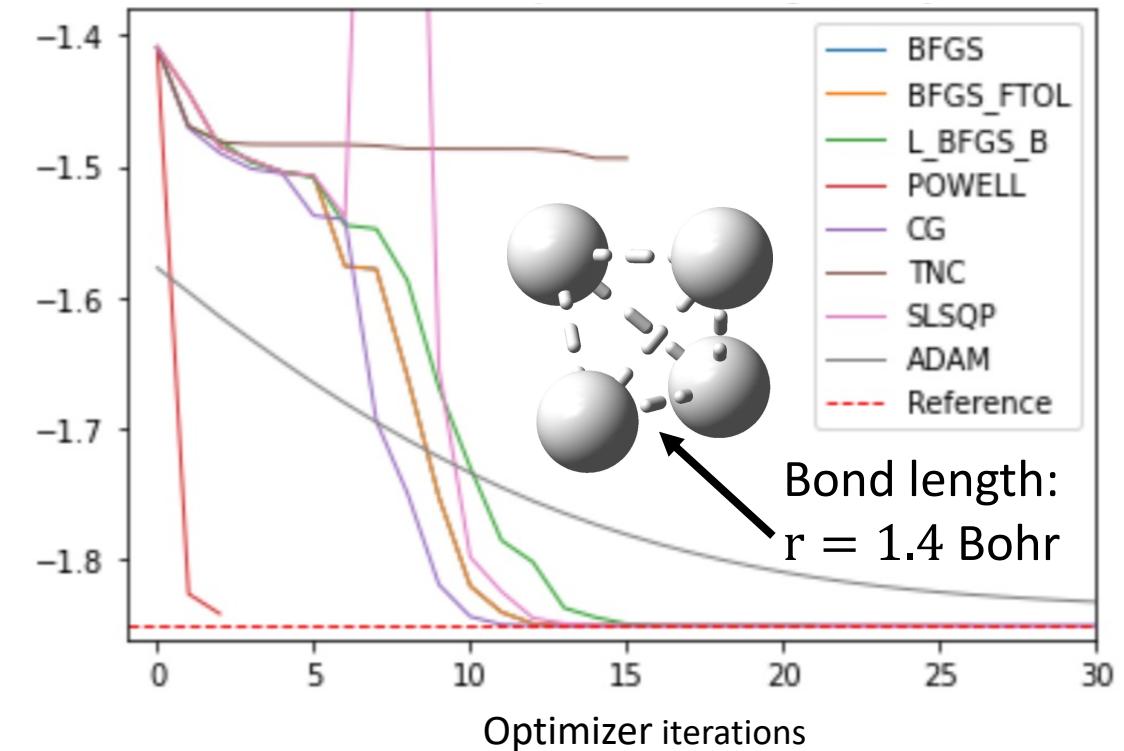
1. RMSProp
2. Adam
3. Nesterov
4. Momentum
5. QNG
6. Adagrad
7. Gradient Descent

(Bonus) Implementing VQE H₂ and Tetra Hydrogen H₄ with QAMUY using their UCCSD Ansatz

VQE optimization of H₂ in QAMUY
(BFGS Only)

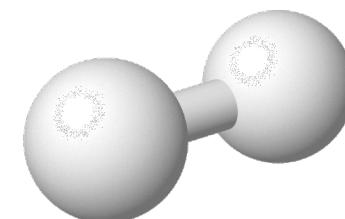
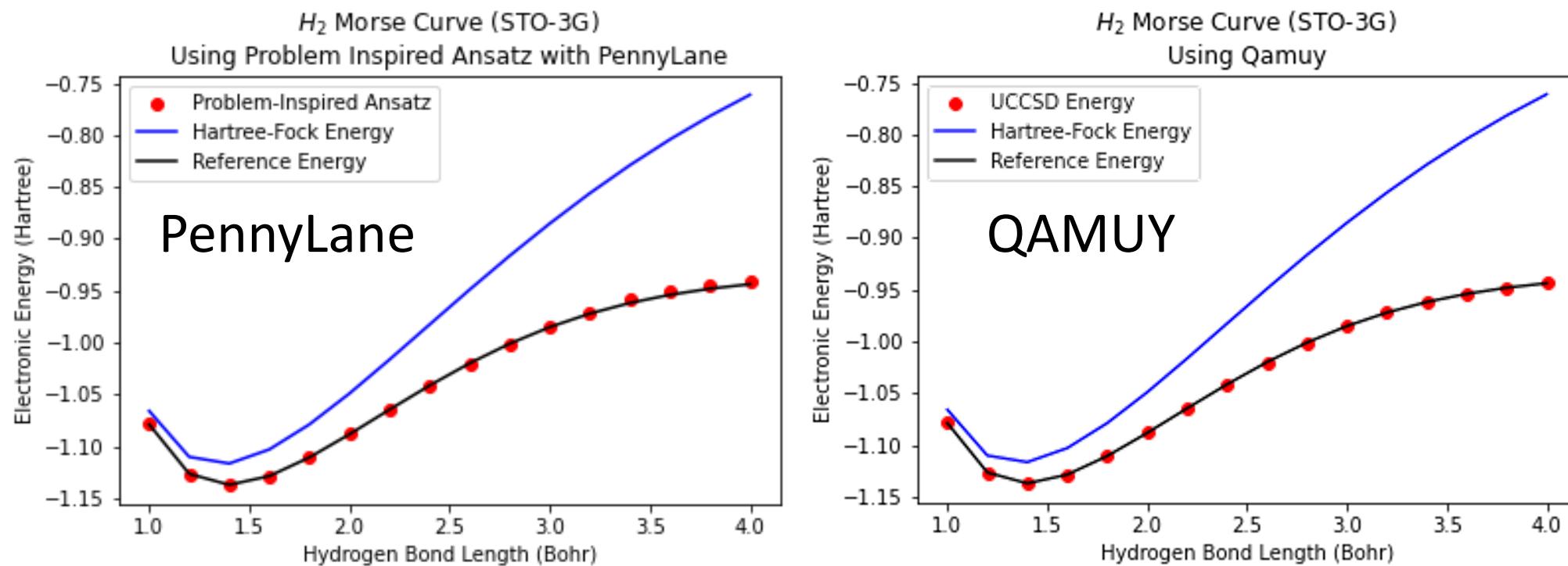


VQE Optimisation of Tetra Hydrogen H₄ Various
in QAMUY (Various Optimiser)



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

Potential Energy Surface for H_2 using Exact Quantum Simulator

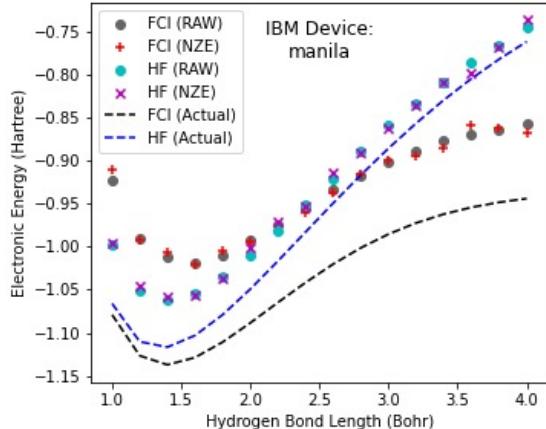


Bond lengths:
 $r = 1.0$ to 4.0 Bohr

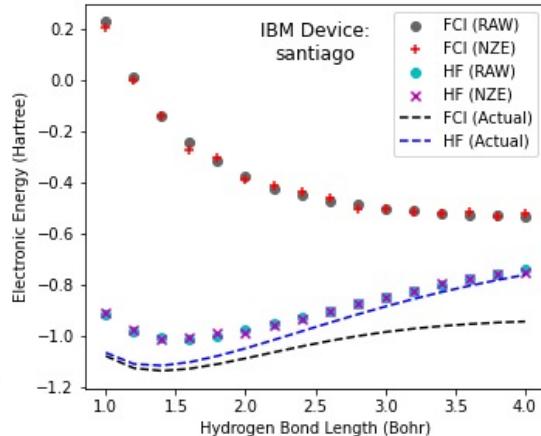
Potential Energy Surface for H₂ using IBMQ Device Noise Models

Open providers

Best performing

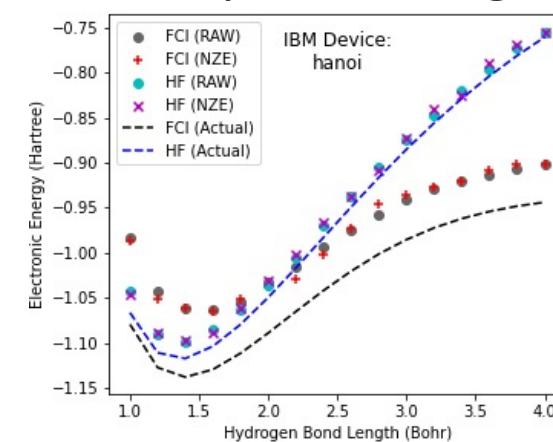


Worst performing

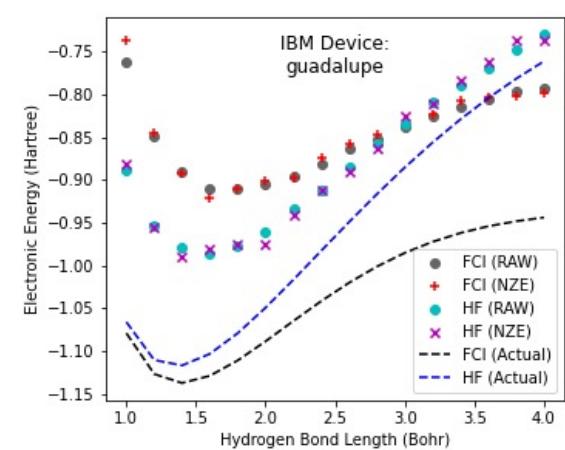


Paid providers

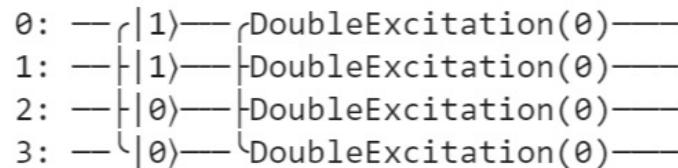
Best performing



Worst performing



Actual Quantum
Circuit Implemented:

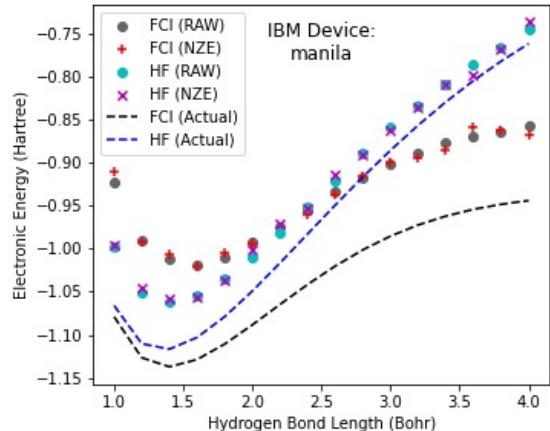


- Turns out for H₂, the only gate that contributes to PES is Double Excitations.
- We remove all Singles Excitations from quantum circuit to reduce circuit noise.
- All Noise model obtained from IBMQ Device backends
- Number of Shots Per Pauli String Expectation: 20,000
- Note: From the plots, our implementation of Mitig as an error mitigation technique did not appear to help with improving the accuracy of our results. (???)

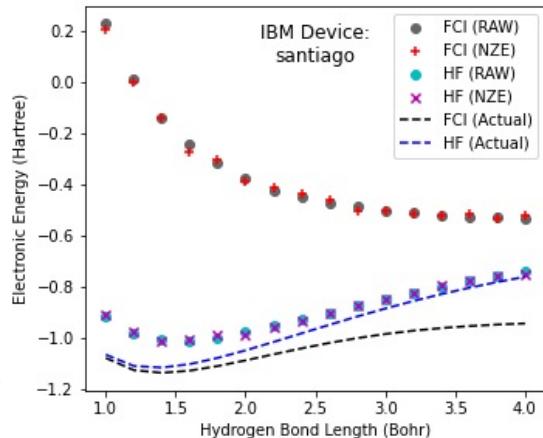
Potential Energy Surface for H₂ using various IBMQ Device Noise Models

Open Providers

Best performing

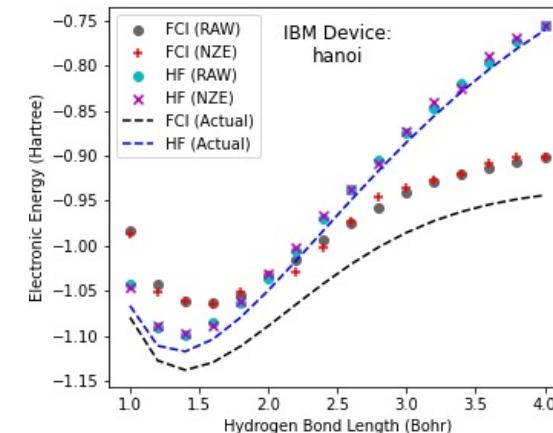


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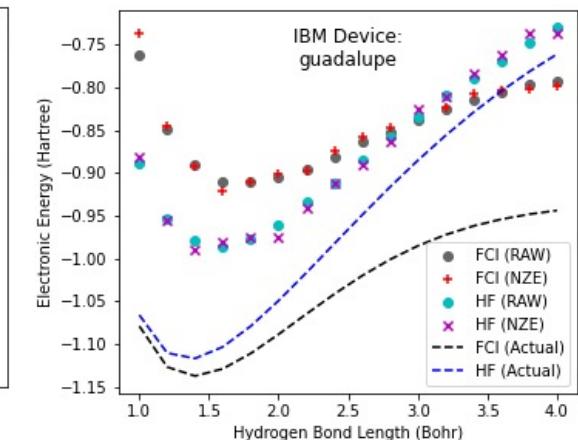


Exclusive Providers

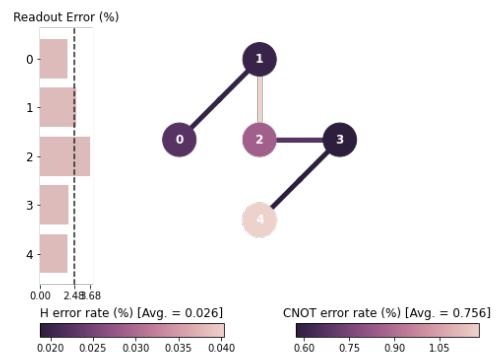
Best performing



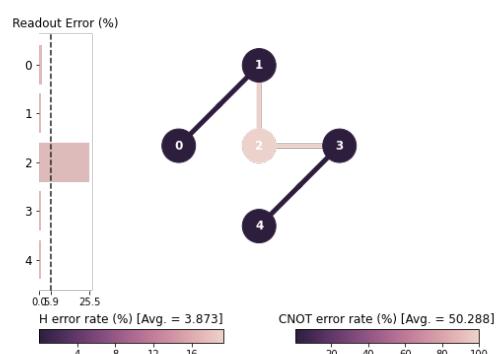
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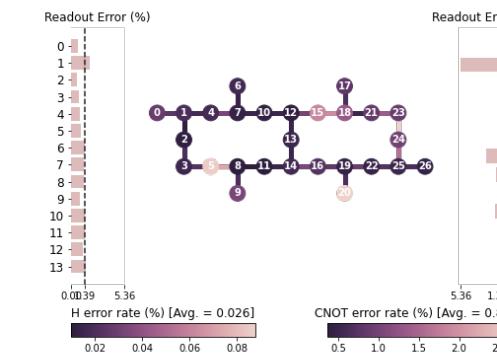
ibmq manila Error Map



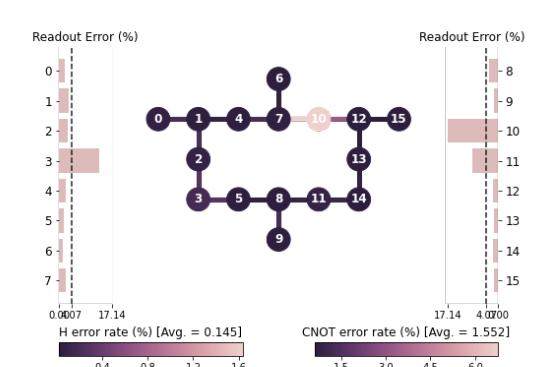
ibmq_santiago Error Map



ibm hanoi Error Map

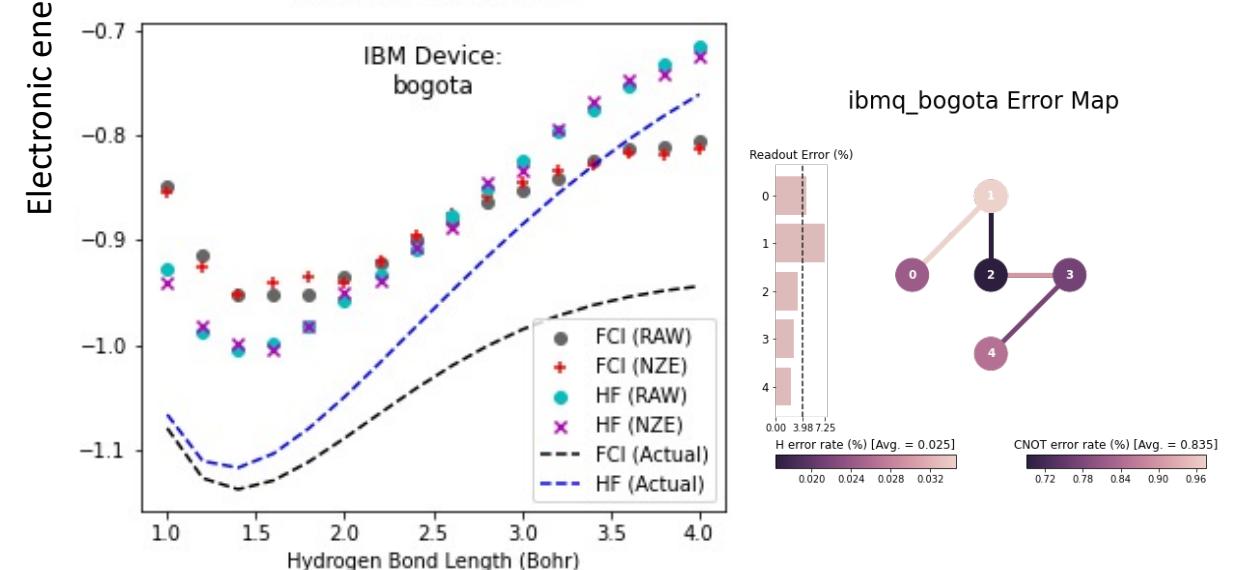
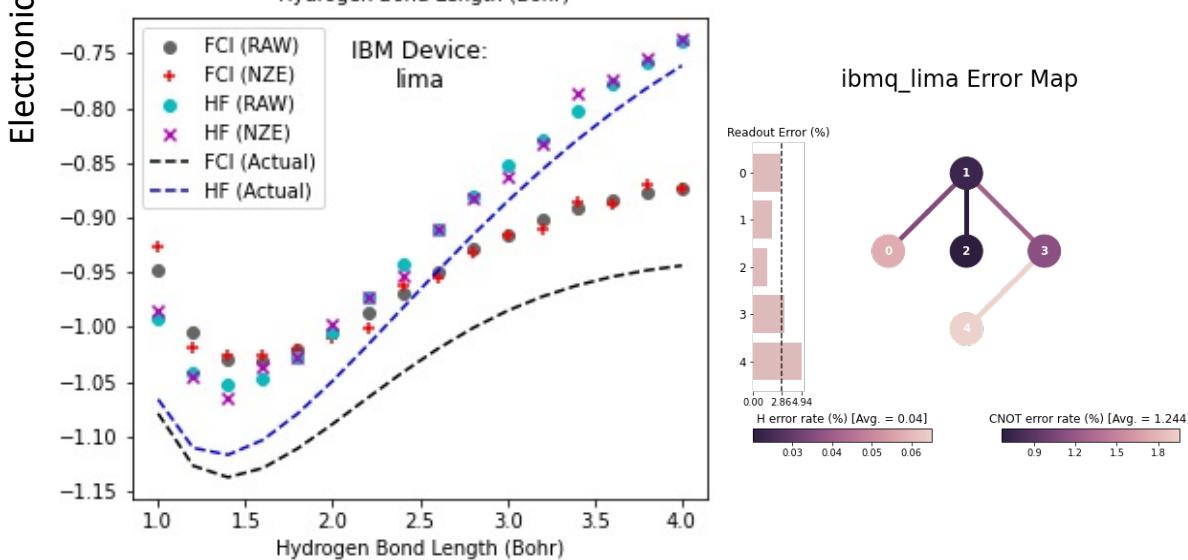
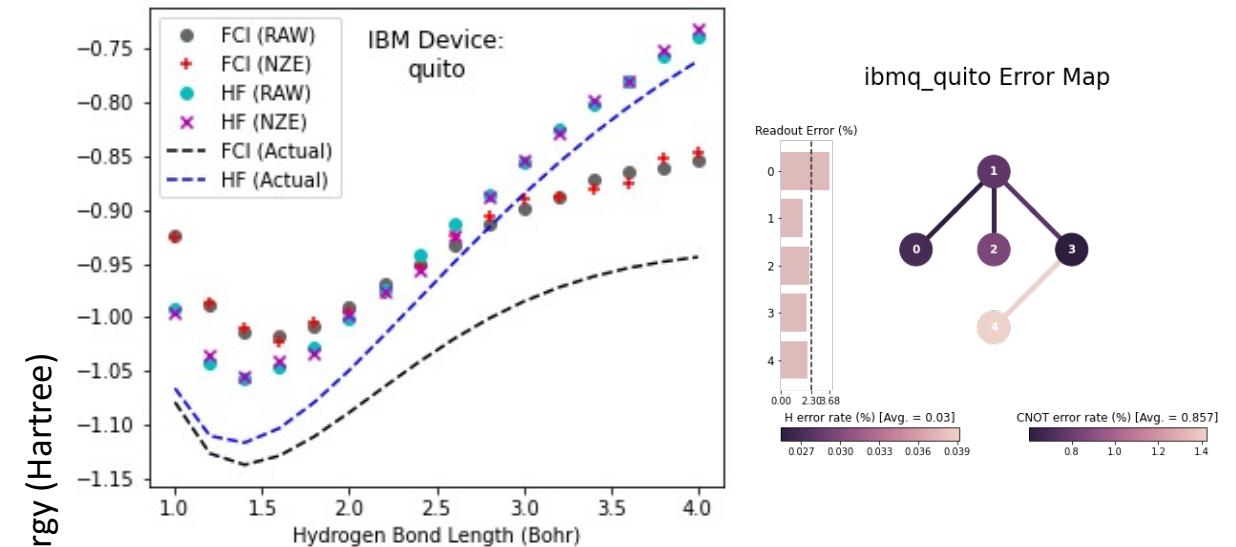
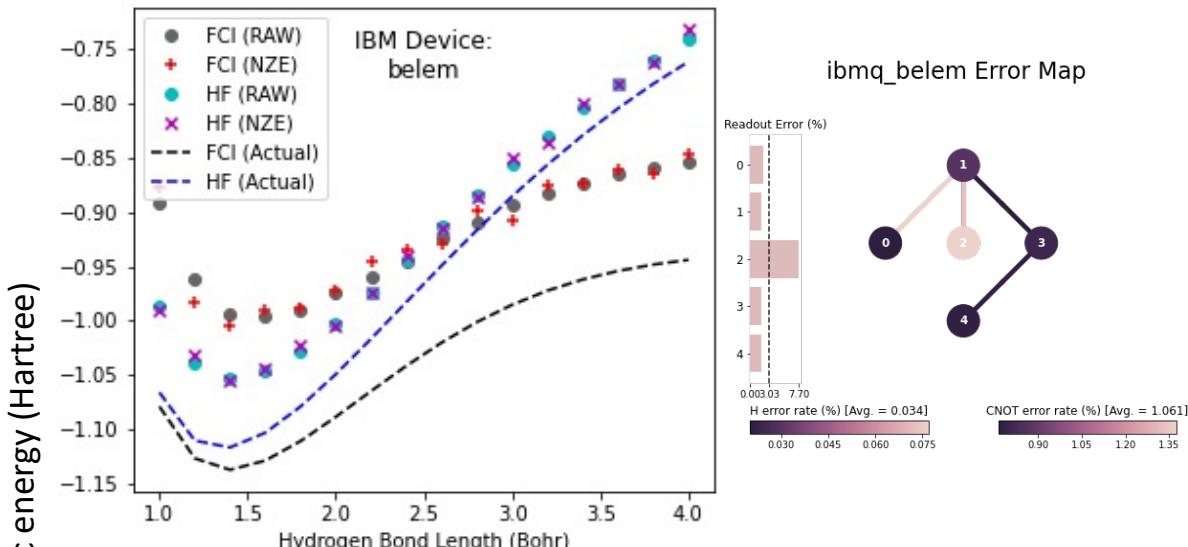


ibmq guadalupe Error Map



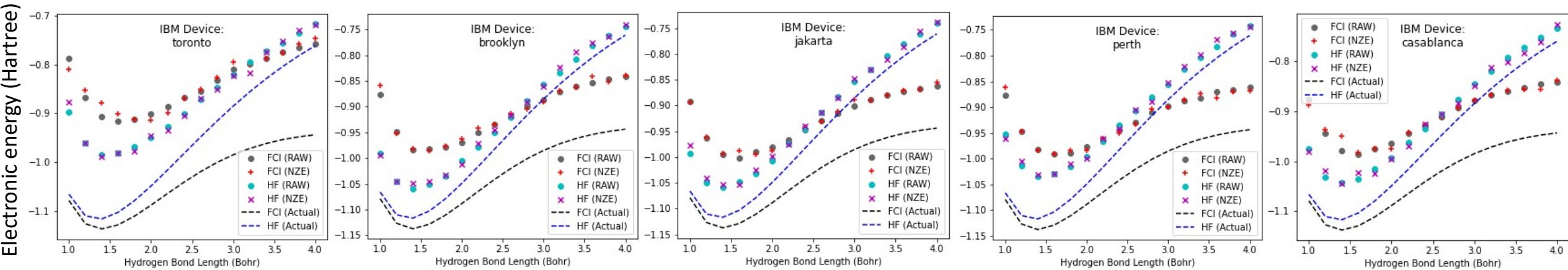
Potential Energy Surface for H₂ using various IBMQ Device Noise Models

Other Open Providers

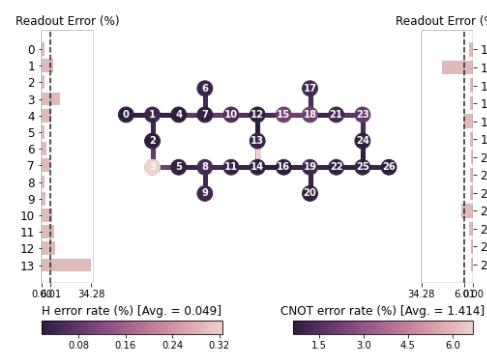


Potential Energy Surface for H₂ using various IBMQ Device Noise Models

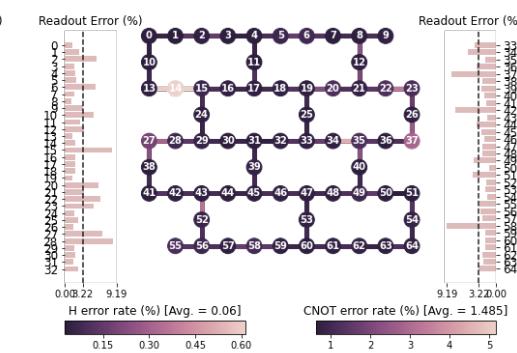
Other Exclusive Providers



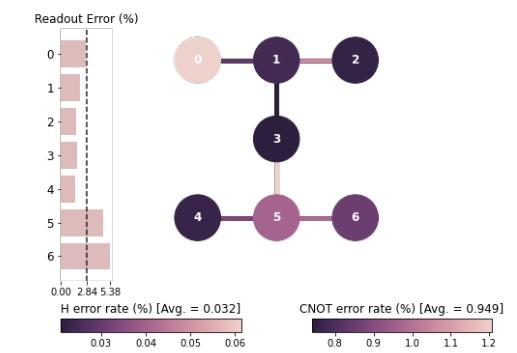
ibmq_toronto Error Map



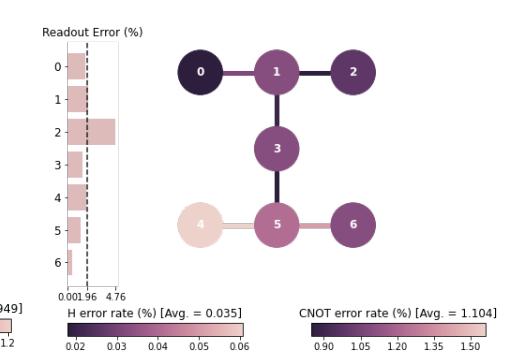
ibmq_brooklyn Error Map



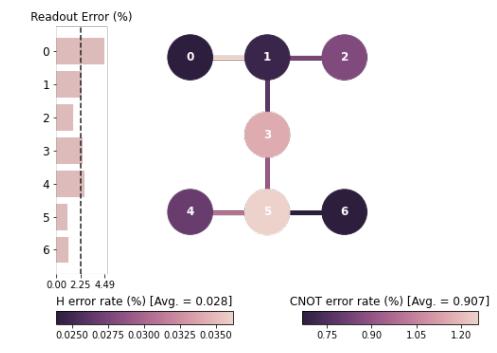
ibmq_jakarta Error Map



ibm_perth Error Map

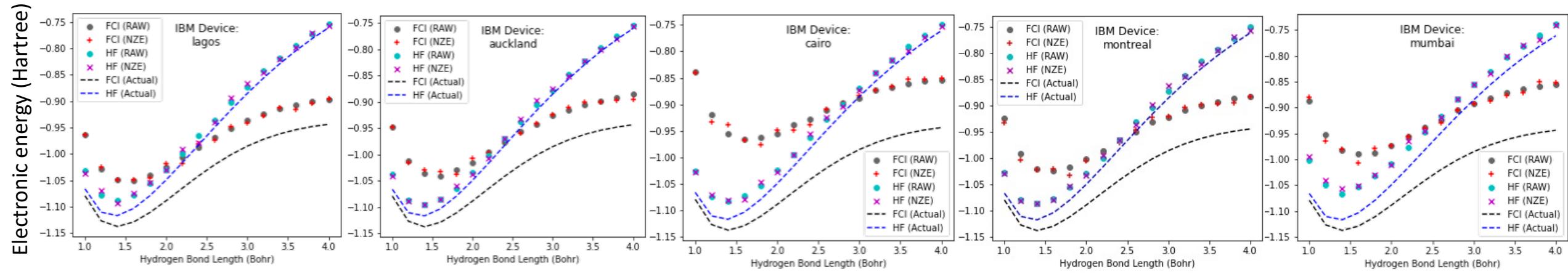


ibmq_casablanca Error Map

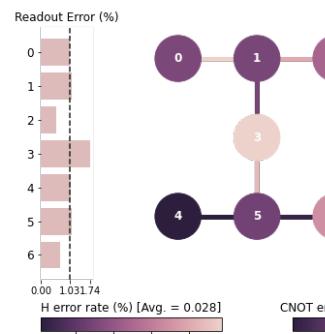


Potential Energy Surface for H₂ using various IBMQ Device Noise Models

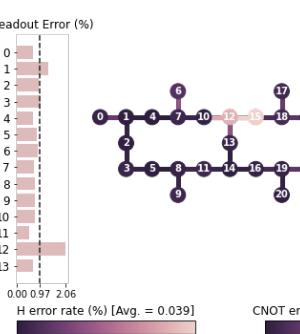
Other Exclusive Providers



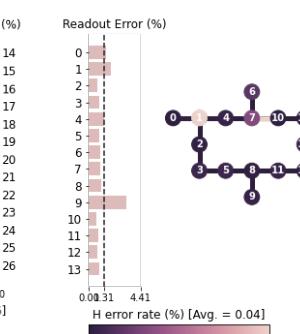
ibm_lagos Error Map



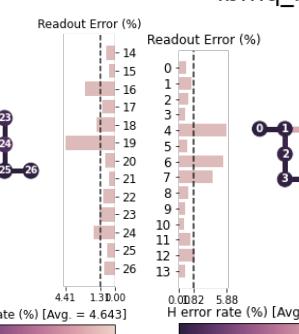
ibm_auckland Error Map



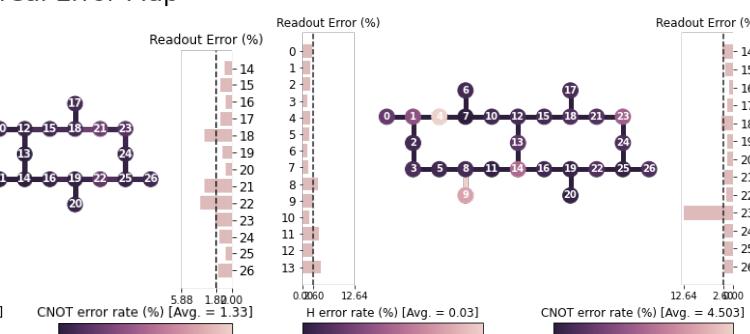
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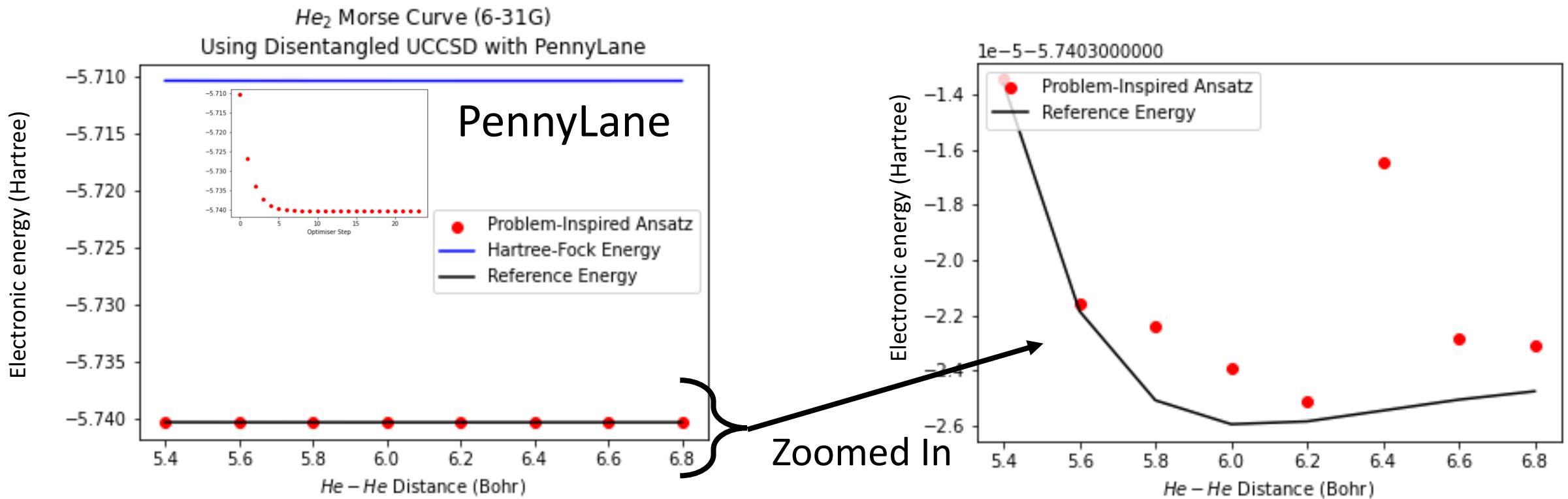
ibmq_montreal Error Map



ibmq_mumbai Error Map

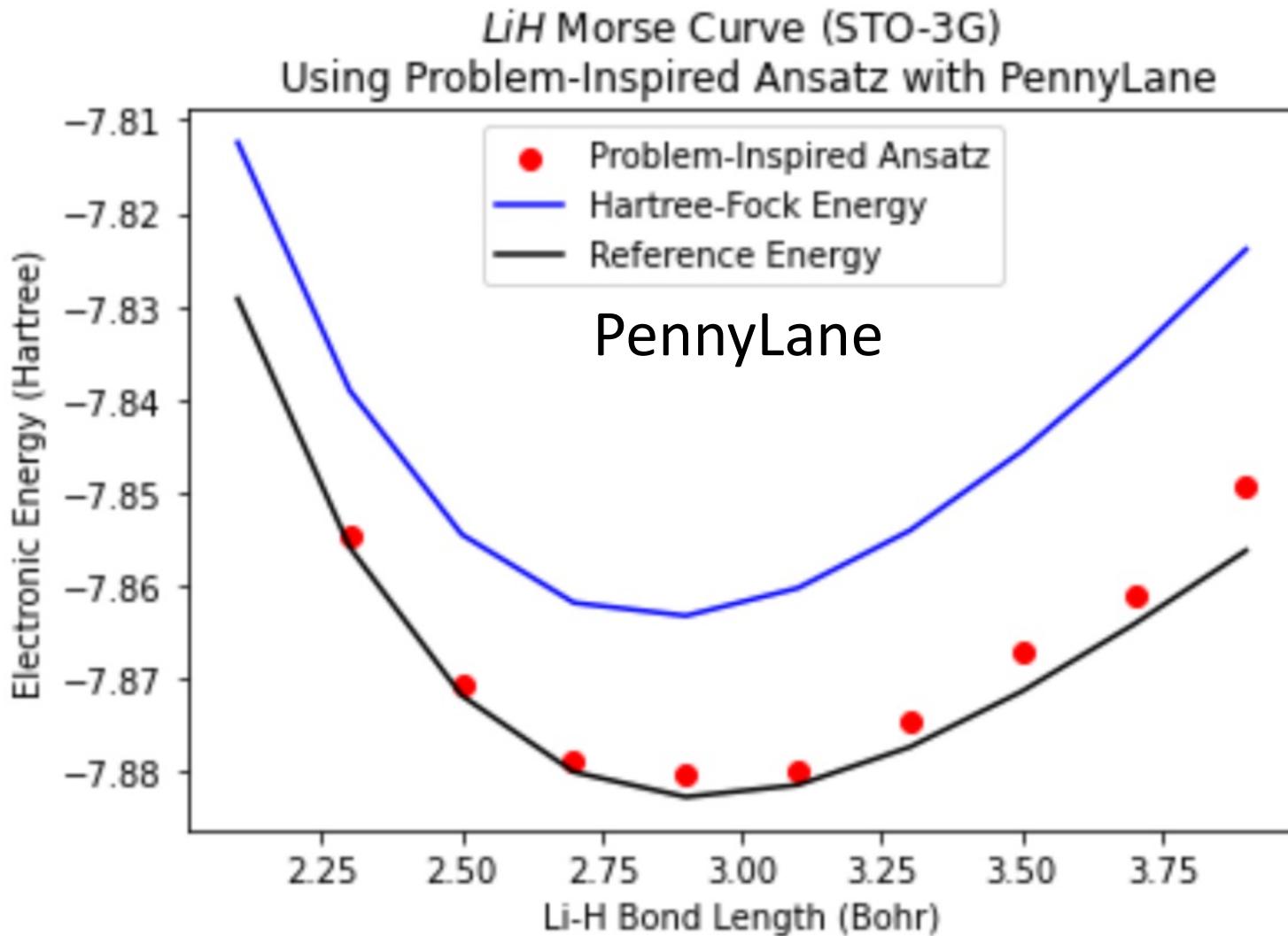


Potential Energy Surface for He_2 using Exact Quantum simulator

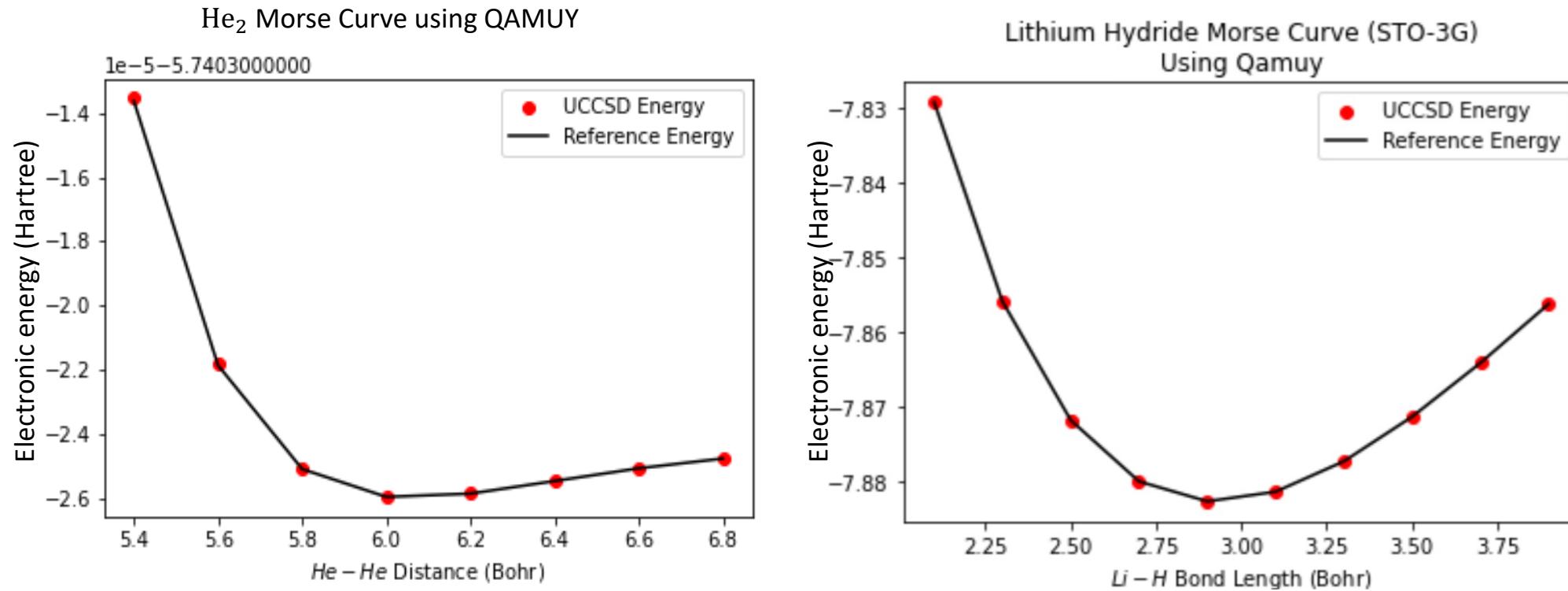


- Optimizers provided by PennyLane were unsuccessful in converging to the reference energy in a limited number of steps (30 Iterations Max)

Potential Energy Surface for LiH using Exact Quantum simulator



(BONUS) Potential Energy Surface for He_2 and LiH with QAMUY using their UCCSD Ansatz



PES curves for Helium Dimer and Lithium Hydride obtained using the optimizers provided with QAMUY compared with their reference values