2025

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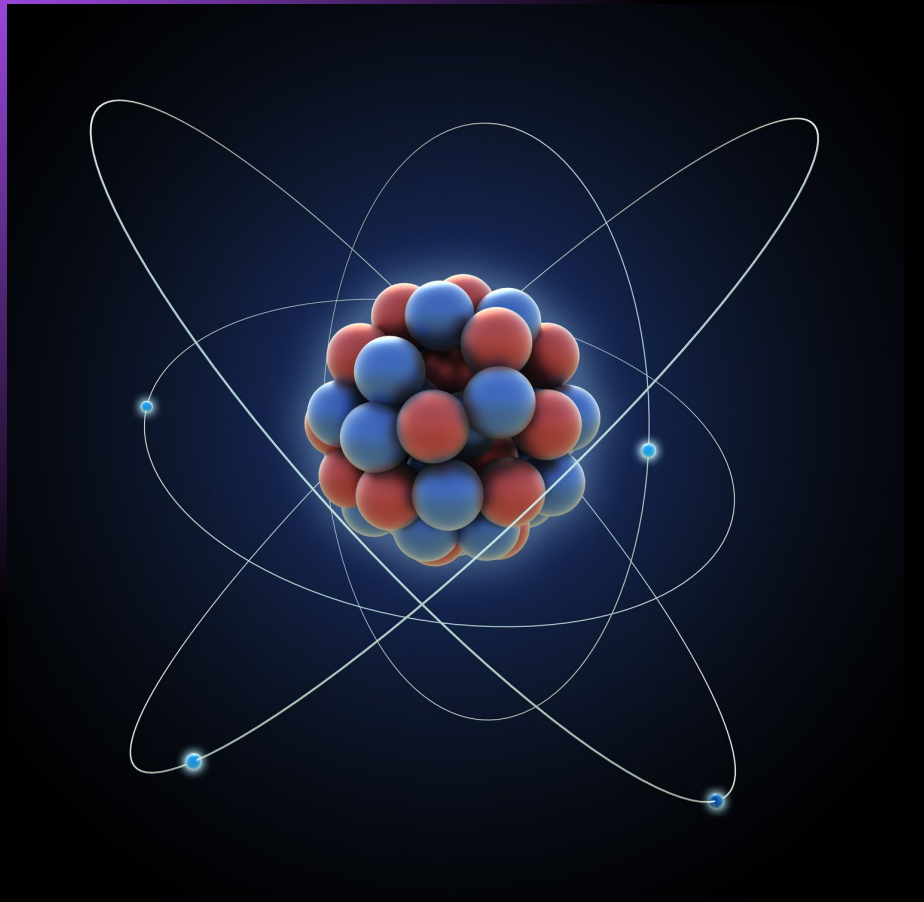
Basic Quantum Chemistry:

Simulating Hydrogen Molecules

Agenda

Why Chemistry?

- Describes the Universe
- Using Quantum, we can simulate and create new molecules much faster and safer
- Unique Approach to learning Quantum



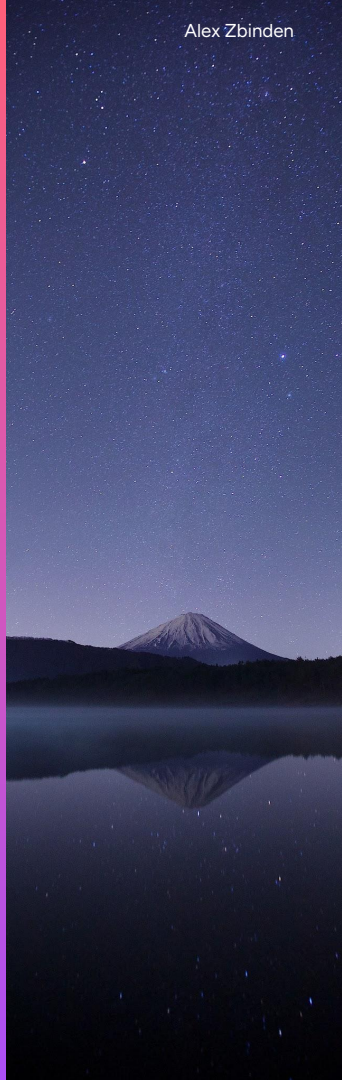
THE VISION:

Simulate Hydrogen Bonds, and Measure their Lengths and Energy Change over Time.

What does this Mean?!?

All Matter has Energy. At the Atomic Level, Energy is much harder to measure.

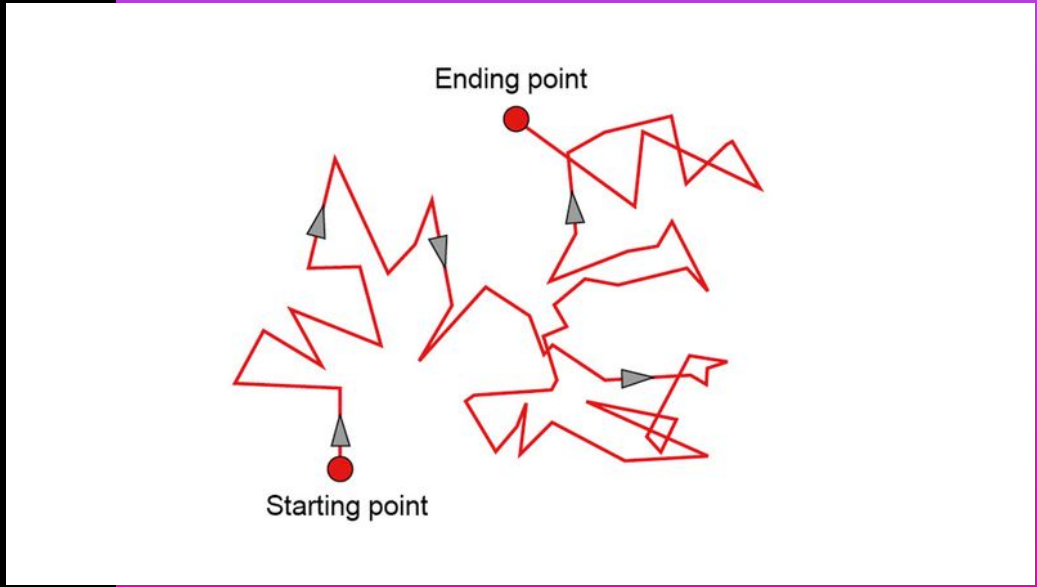
In essence, we want to take H_2, which is two hydrogen atoms bonded to each other, and observe how they 'interact' with each other, and the "space" around them.



The Plan

Step 1 - Run Brownian Motion (Random Walk) simulations on the bond lengths

Step 2 - Run Hamiltonian time evolution on energy levels of the bonds



```python
# ---------- Core pipeline functions ----------
def get_hamiltonian_for_h2(bond_length):
    symbols = ["H", "H"]
    coords = np.array([[0.0, 0.0, 0.0],
                       [0.0, 0.0, bond_length]])
    H, n_qubits = qchem.molecular_hamiltonian(symbols, coords)
    return H, n_qubits


def hamiltonian_matrix_and_energies(H):
    # sparse_hamiltonian returns a sparse matrix
    sparse_H = H.sparse_matrix()
    H_dense = sparse_H.toarray()
    eigvals, eigvecs = np.linalg.eigh(H_dense)
    # eigvals sorted ascending, ground state is eigvals[0]
    return H_dense, eigvals, eigvecs

def make_energy_qnode(H, n_qubits):
    dev = qml.device("default.qubit", wires=n_qubits)

    @qml.qnode(dev)
    def energy_for_state(statevector):
        qml.StatePrep(statevector, wires=range(n_qubits))
        return qml.expval(H)

    return energy_for_state

def make_time_evolution_qnode(H, n_qubits):
    dev = qml.device("default.qubit", wires=n_qubits)

    @qml.qnode(dev)
    def evolve(t):
        qml.BasisState(np.array([1] + [0]*(n_qubits-1)), wires=range(n_qubits))
        qml.ApproxTimeEvolution(H, t, 1)
        return qml.expval(H)

    return evolve
```

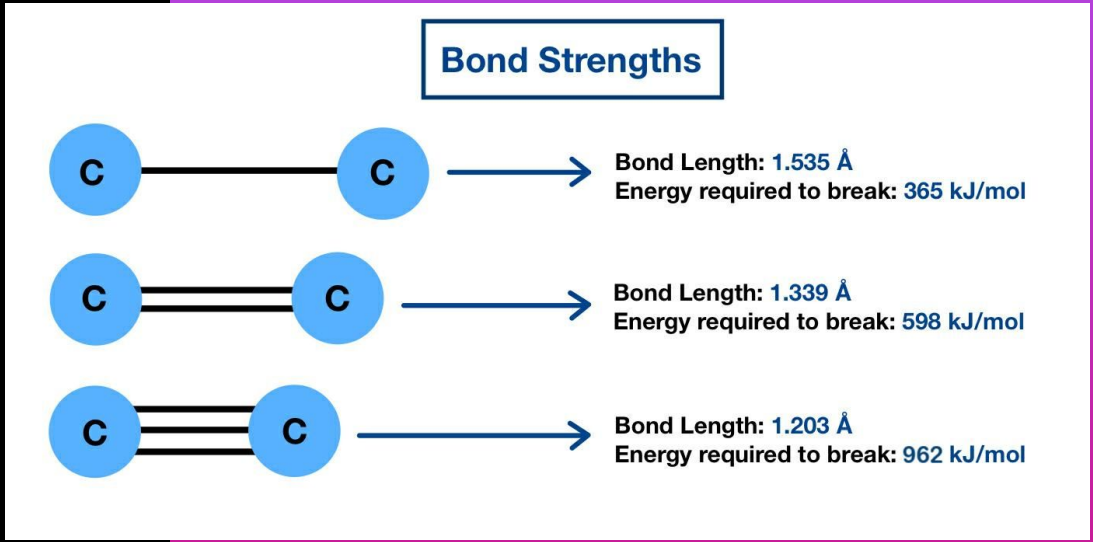
<- Two main functions I used when calculating the energy, they initialize the Hamiltonian matrix and return the matrices eigenvalues. These are called for each time step

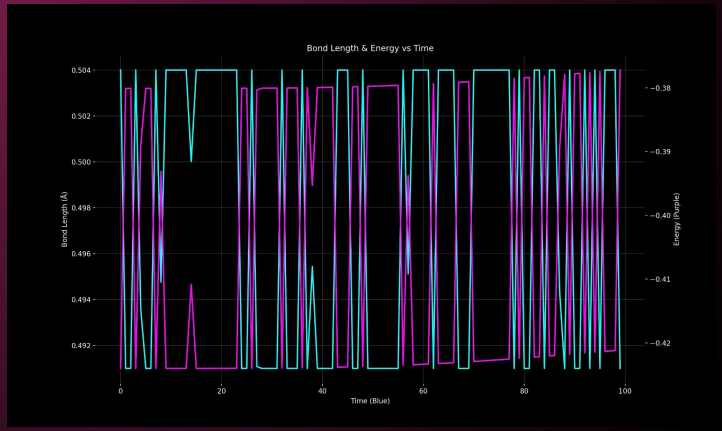
<- Two functions that initialize the energy and evolution model, these are only called once per bond

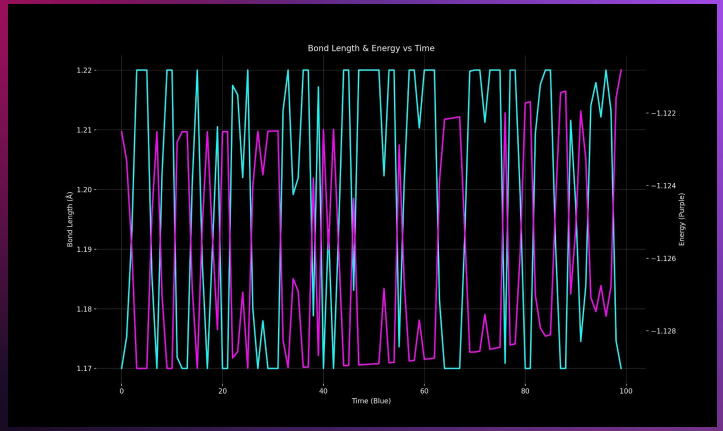
Expected Results

Here's what we would expect:

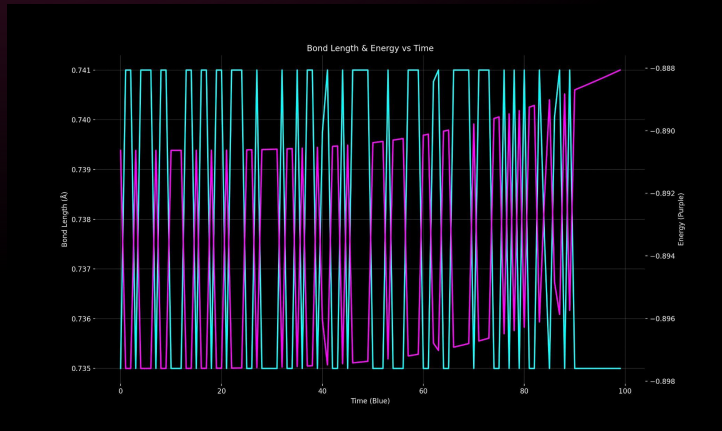
Bond lengths and energy levels are dependent on each other, with the results one should expect that with smaller bond lengths comes more energy, and with larger bond lengths comes less energy (weaker bonds).

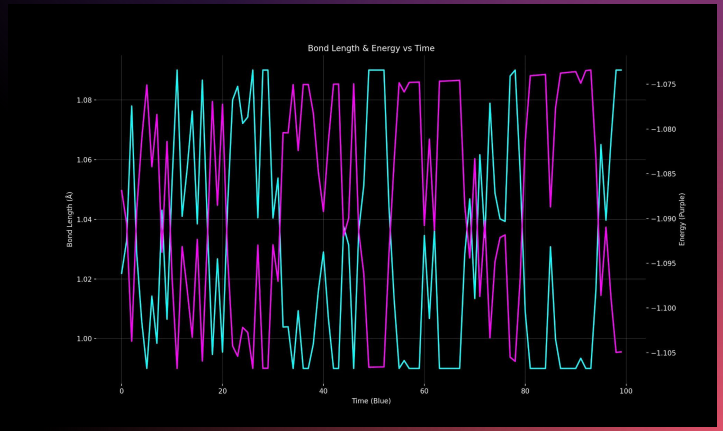



Bond Length & Energy vs Time
Bond Length (Å)
Energy (Purple)
Time (Blue)
0.504
0.502
0.500
0.498
0.496
0.494
0.492
−0.38
−0.39
−0.40
−0.41
−0.42
0
20
40
60
80
100


Bond Length & Energy vs Time
Bond Length (Å)
Energy (Purple)
Time (Blue)
1.22
1.21
1.20
1.19
1.18
1.17
−1.122
−1.124
−1.126
−1.128
0
20
40
60
80
100

RESULTS

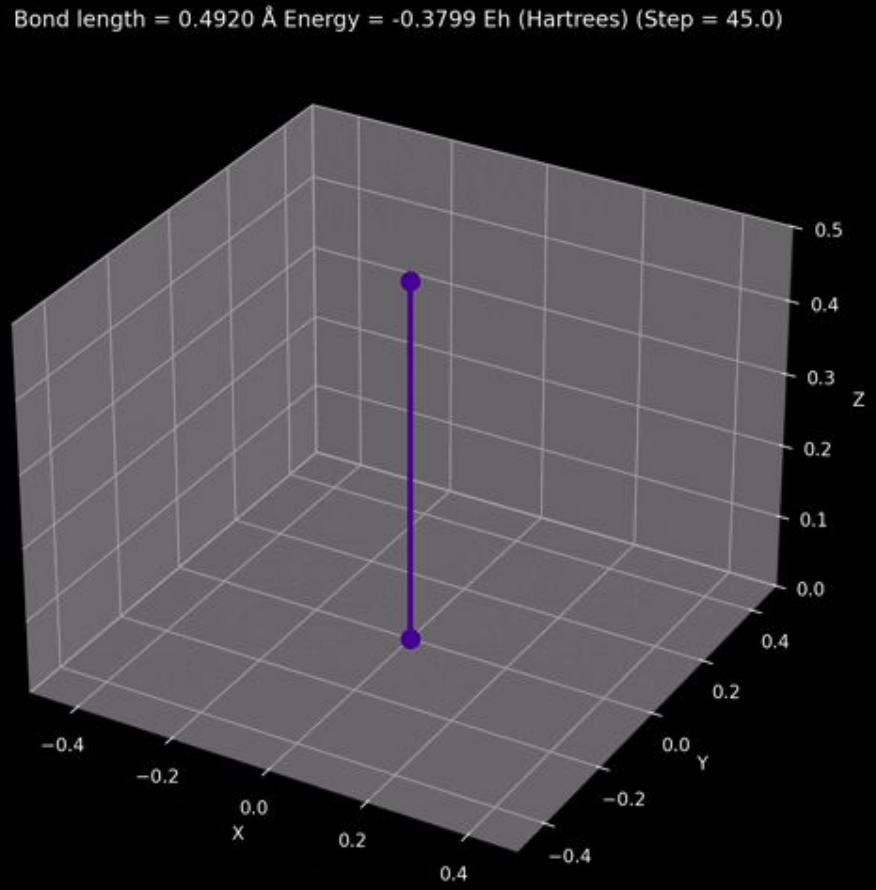

Bond Length & Energy vs Time
Bond Length (Å)
Energy (Purple)
Time (Blue)
0.741
0.740
0.739
0.738
0.737
0.736
0.735
−0.888
−0.890
−0.892
−0.894
−0.896
−0.898
0
20
40
60
80
100


Bond Length & Energy vs Time
Bond Length (Å)
Energy (Purple)
Time (Blue)
1.08
1.06
1.04
1.02
1.00
−1.075
−1.080
−1.085
−1.090
−1.095
−1.100
−1.105
0
20
40
60
80
100

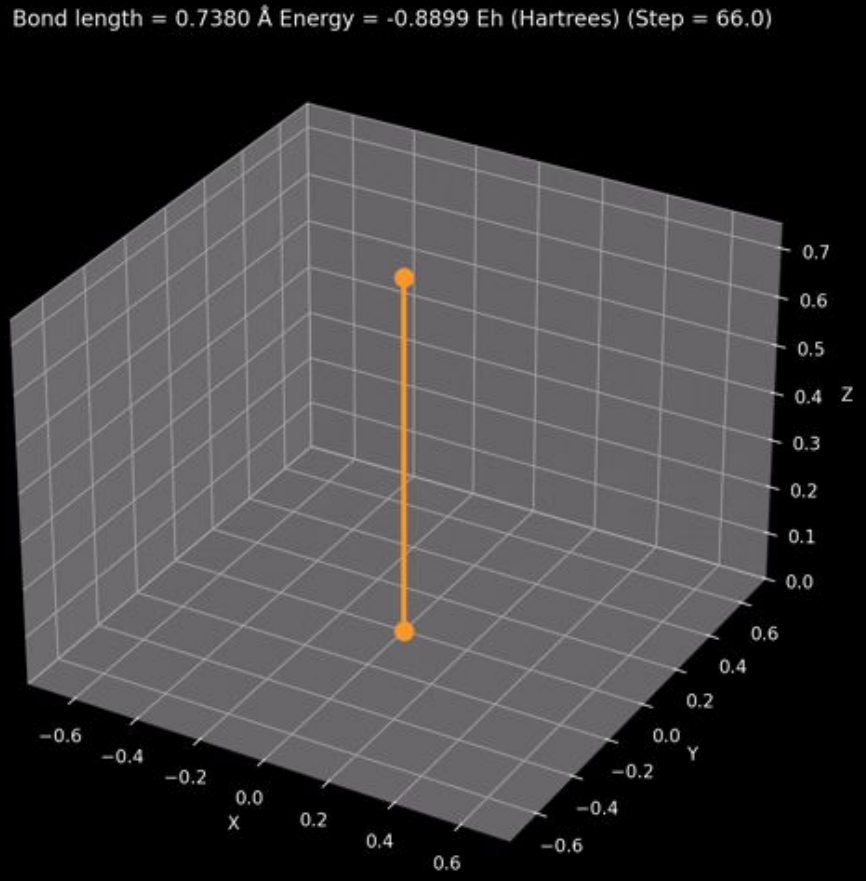
RESULTS


Bond Length & Energy vs Time
Bond Length (Å)
0.741
0.740
0.739
0.738
0.737
0.736
0.735
Energy (Purple)
−0.888
−0.890
−0.892
−0.894
−0.896
−0.898
0
20
40
60
80
100
Time (Blue)

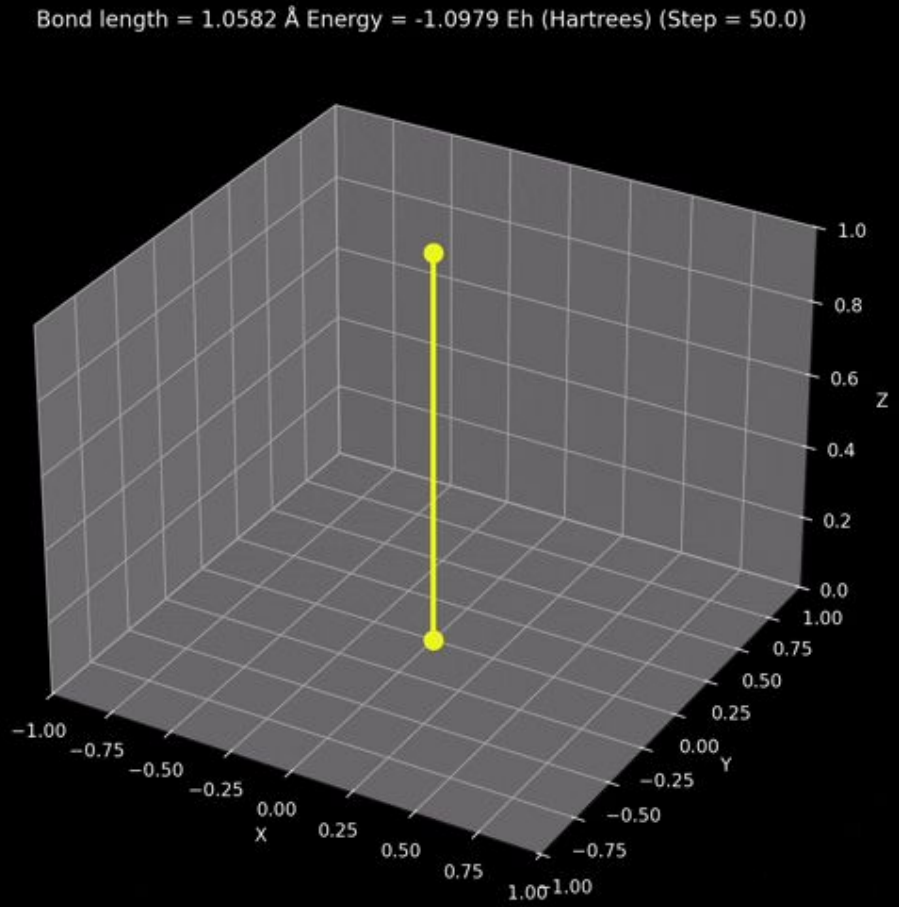
Bond 1 - Smallest length, therefore closest energy to 0 Eh. The color change represents the energy change over time to some degree, although very miniscule.



Bond 2 - Larger length, so a bit more negative. Also a drastic color change since the energy is lower



Bond 3 - Even larger length, so a bit more negative. Color change is minimal since the bond is not too much longer than bond 2, so the energy levels are similar to some degree.



Bond 4 was nearly the same as bond 3.

Results - Analysis

Bond Lengths

- → The lengths were extremely random
- → The brownian motion created by our quantum simulation revealed this randomization
- → Visuals and the plots showed this as well

Energy Levels

- → The energy levels rose in general over time
- → They correlated inversely to the bond lengths
- → Visualization was not as effective animation wise, as the energy changes were minimal

Lengths vs Energy

- → Energy went down as bond length increased
- → Bond length did not see a general increase or decrease, while energy went up on average over time

Comparison to real Results

- → Energy should decrease as the bond lengths increase (i.e. weaker bond since it is longer)
- → Energy in this instance is expected to increase over time since we are simulating in a vacuum
- → When simulating with real physics, energy is not conserved in a system so this increase will not always occur in practice

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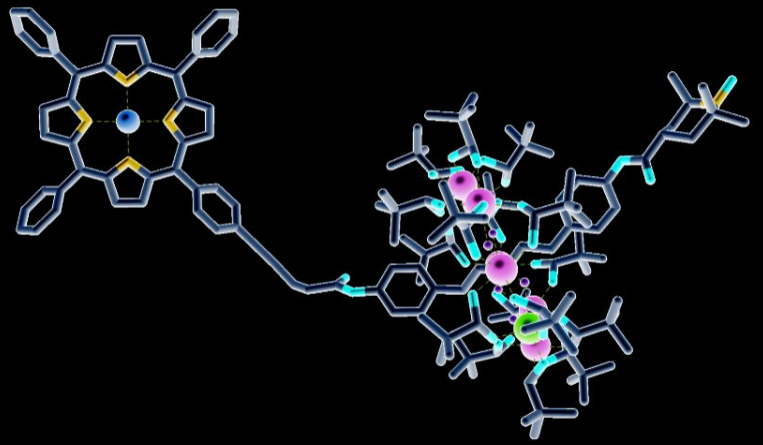
Possible Ideas for Extending the Project

Future Ideas -

- Creating a real Quantum Variational Eigensolver (VQE), the project here uses a built in Pennylane function that works for small Molecules like our H_2
- Allow simulation of more complex molecules
- Simulate more parameters like reaction energies and activation energy for a given molecule



THANK YOU

Any questions?

Sources:

https://pennylane.ai/topics/hamiltonian-simulation

https://pennylane.ai/blog/2021/04/qhack-qml-challenge-walkthrough-variational-quantum-eigensolver/

https://www.ibm.com/quantum/case-studies/modeling-realistic-chemistry