HAIQU

Molecules Ground State Energies during chemical reactions

Our Team

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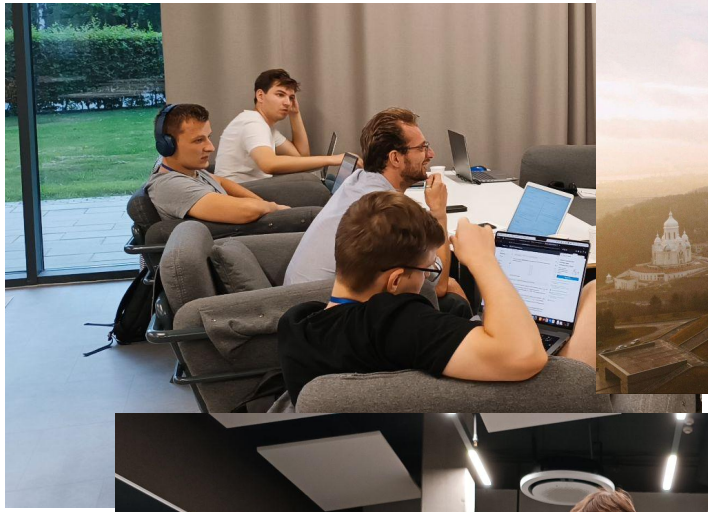
Yarema Sirskyy - *software engineer.*

Mariia Khlystiuk - *Ph.D. in physics.*

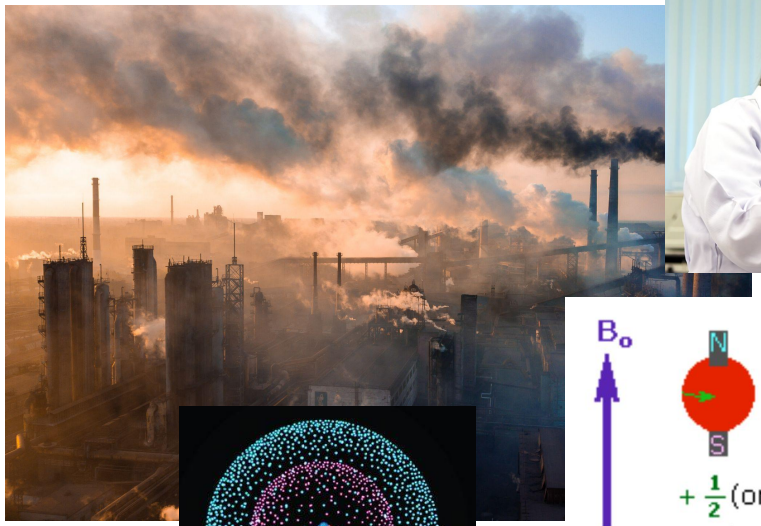


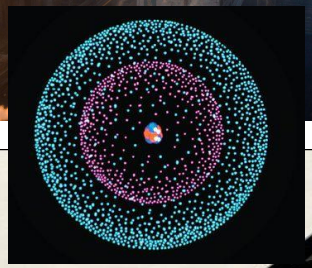
P.s. Many thanks to Maxence Grandadam!

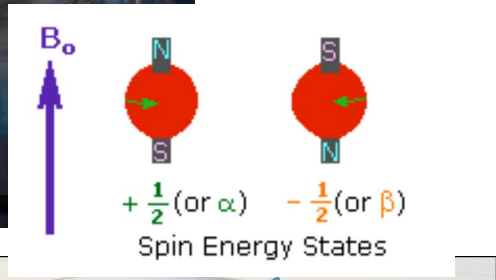
Motivation

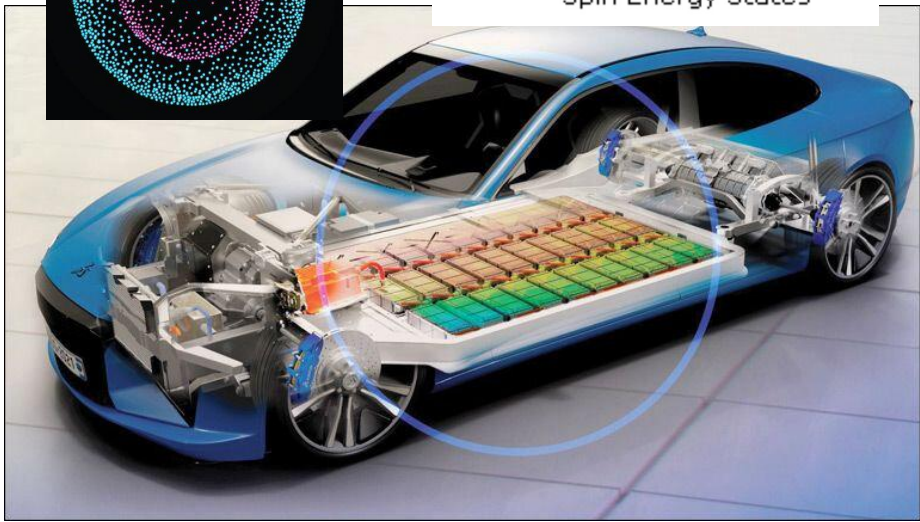
To Study a chemical reaction
LiH + H2O <-> LiOH + H2
by finding the ground state energy of molecules:

- Molecular dynamic simulations
- Medicine
- Quantum Chemistry Fundamental investigations
- Nuclear physics
- Material Engineering
- Hydrogen Storage
- Adsorption improvement





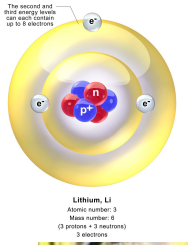




Our task specification

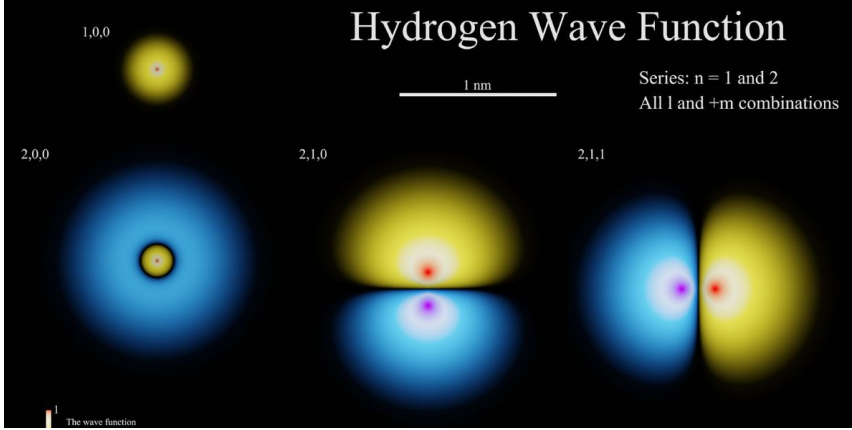
> For LiOH batteries production for electrical devices and vehicles;

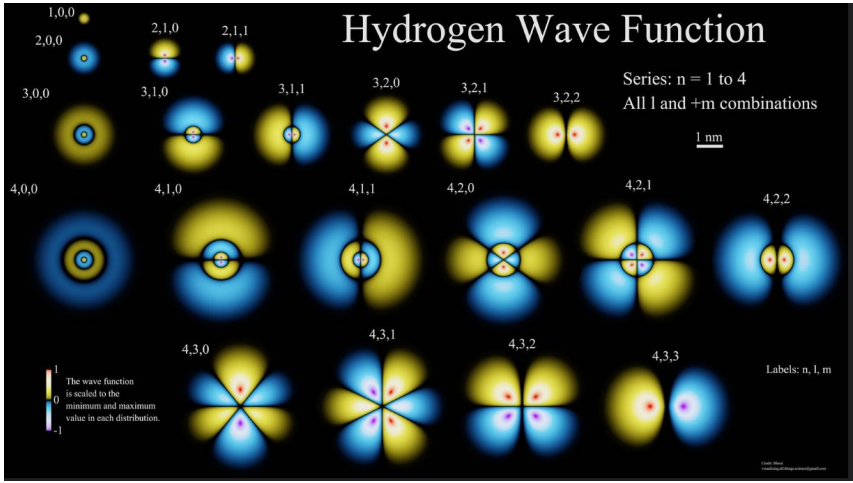
> BI - is to sell this instrument to experimental labs and educational institutions, cooperate with automobile and airplane companies (our top stakeholders) > update and add functionality, hire more people >>

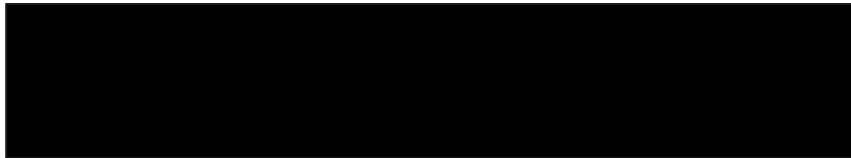


Deliverables

- ★ Which side is more stable? Does the geometry of the molecules change that? etc...

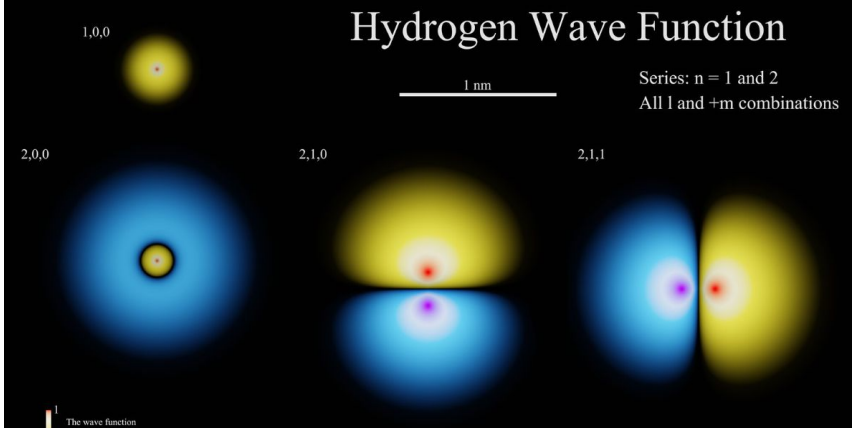


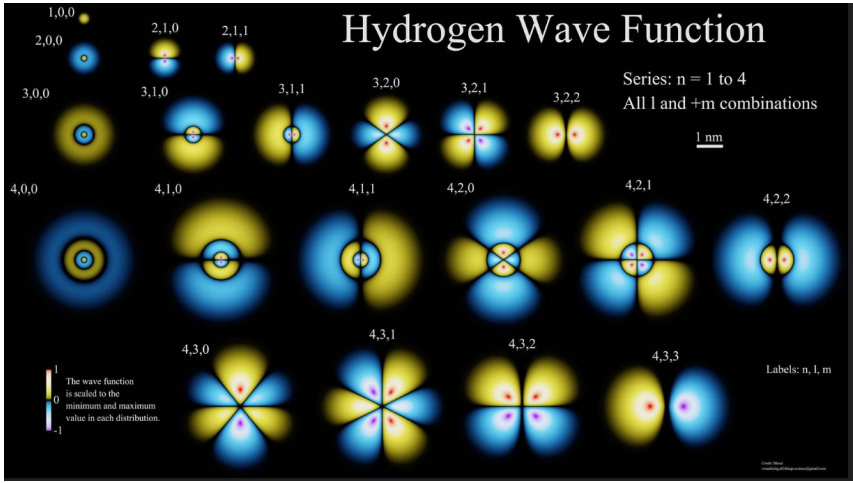




Deliverables

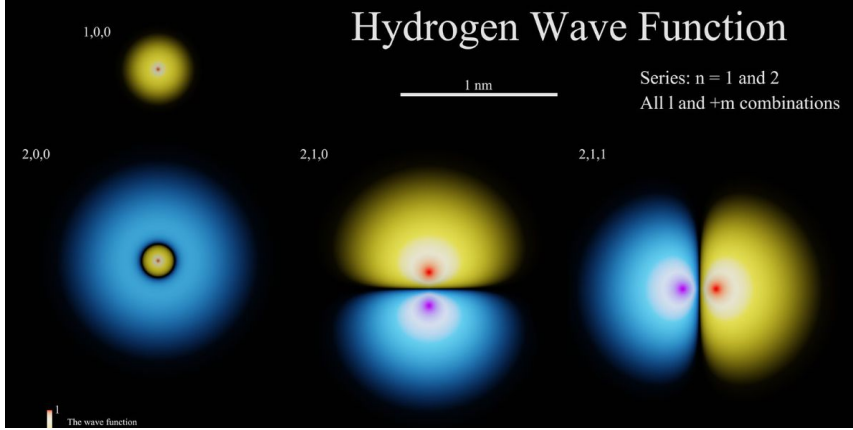
- ★ Which side is more stable? Does the geometry of the molecules change that? etc...
- ★ Look at the excited states, which are important for the optical properties of materials

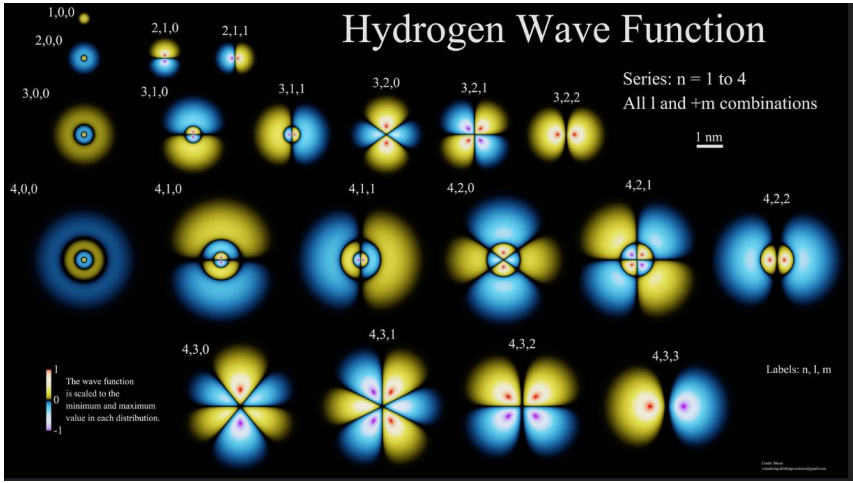




Deliverables

- ★ Which side is more stable? Does the geometry of the molecules change that? etc...
- ★ Look at the excited states, which are important for the optical properties of materials
- ★ Measure physical quantities such as magnetization, dipolar moment, etc...



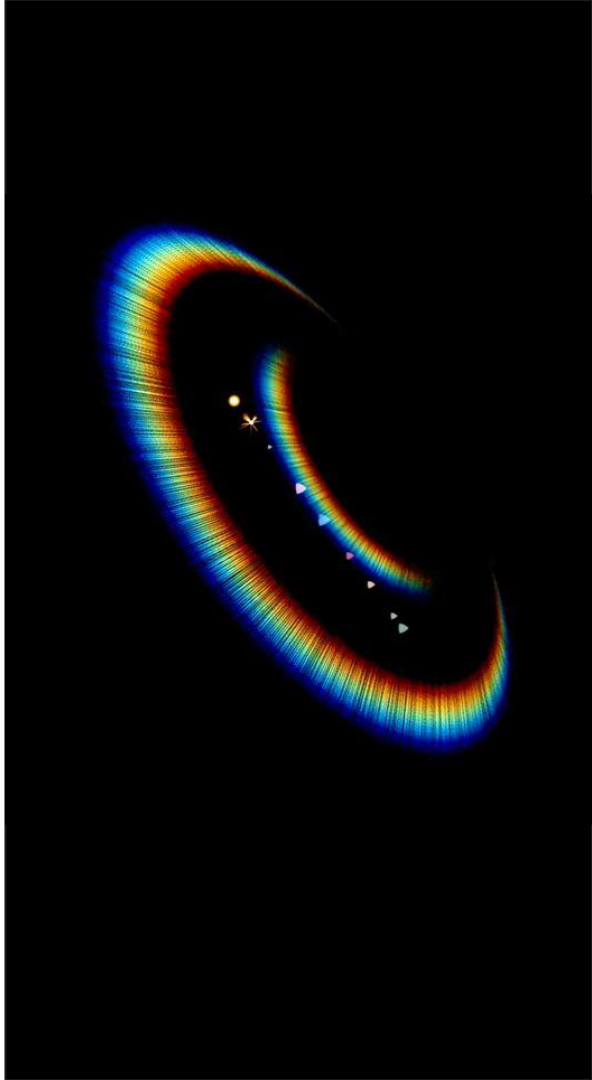


The uniqueness

- **LiH + H2O** and **LiOH + H2** are not as commonly studied as more basic molecules (like H2, LiH, H2O alone) in the context of VQE

- Detailed geometry of those molecules in the reaction process is yet to be fully described

- While VQE itself is widely researched, applying it to specific molecules like LiH and their interactions can yield novel results



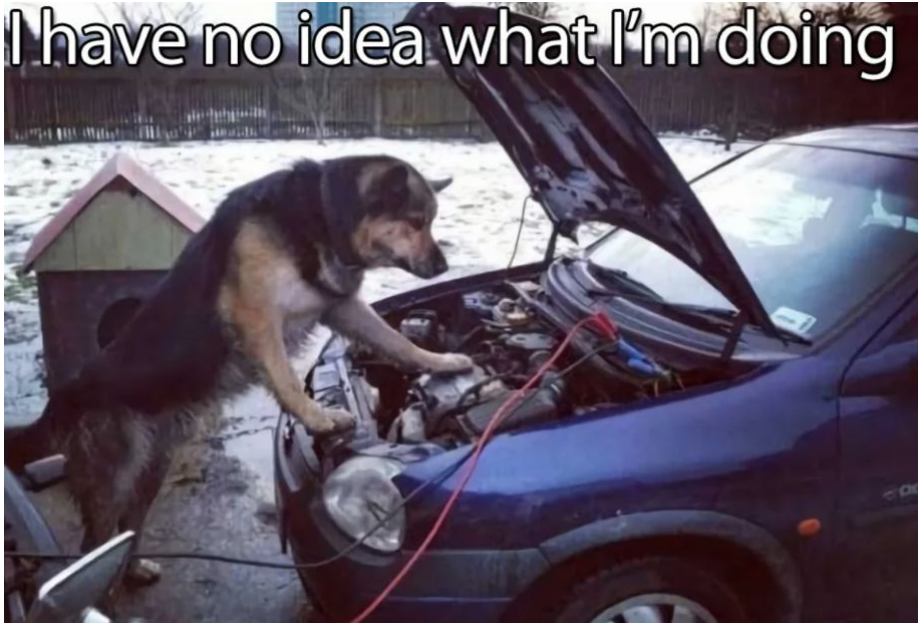
Why QA?

Variational Quantum Eigensolver (VQE) and Quantum Phase Estimation (QPE), are designed to find the ground state energy of molecules **more efficiently** than classical methods.

The Project

Plan for BI:

- Discovery phase (**many thanks to Maxence Grandadam!**)
- Data collection and encoding
- Model implementation (simulators)
- Error mitigation and correction
- Result analysis
- Project validation and testing
- Model (real QC device)
- Requirements and Design Mockups
- Web app development
- Deploy and maintenance



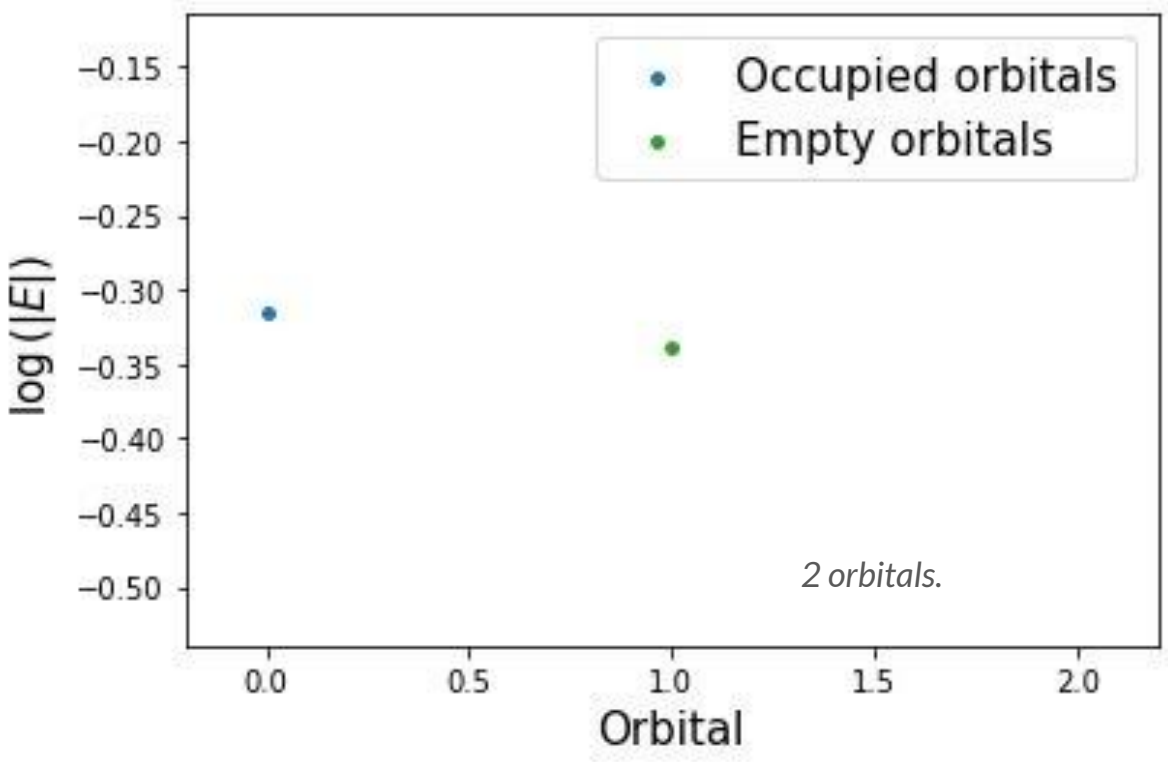
Result details

For each molecule:

- Orbitals visualization (obtained with help of PySCF & qiskit packages)
- Ground state Energies (**VQE** & **Exact Solver**)
  - *Optimizer*: Cobyla
  - *Mapper*: ParityMapper
  - *Ansatz*: UCCSD

- Exact Solver: NumPyMinimumEigensolver
- Error (difference between **Exact Solver** and **VQE** results)

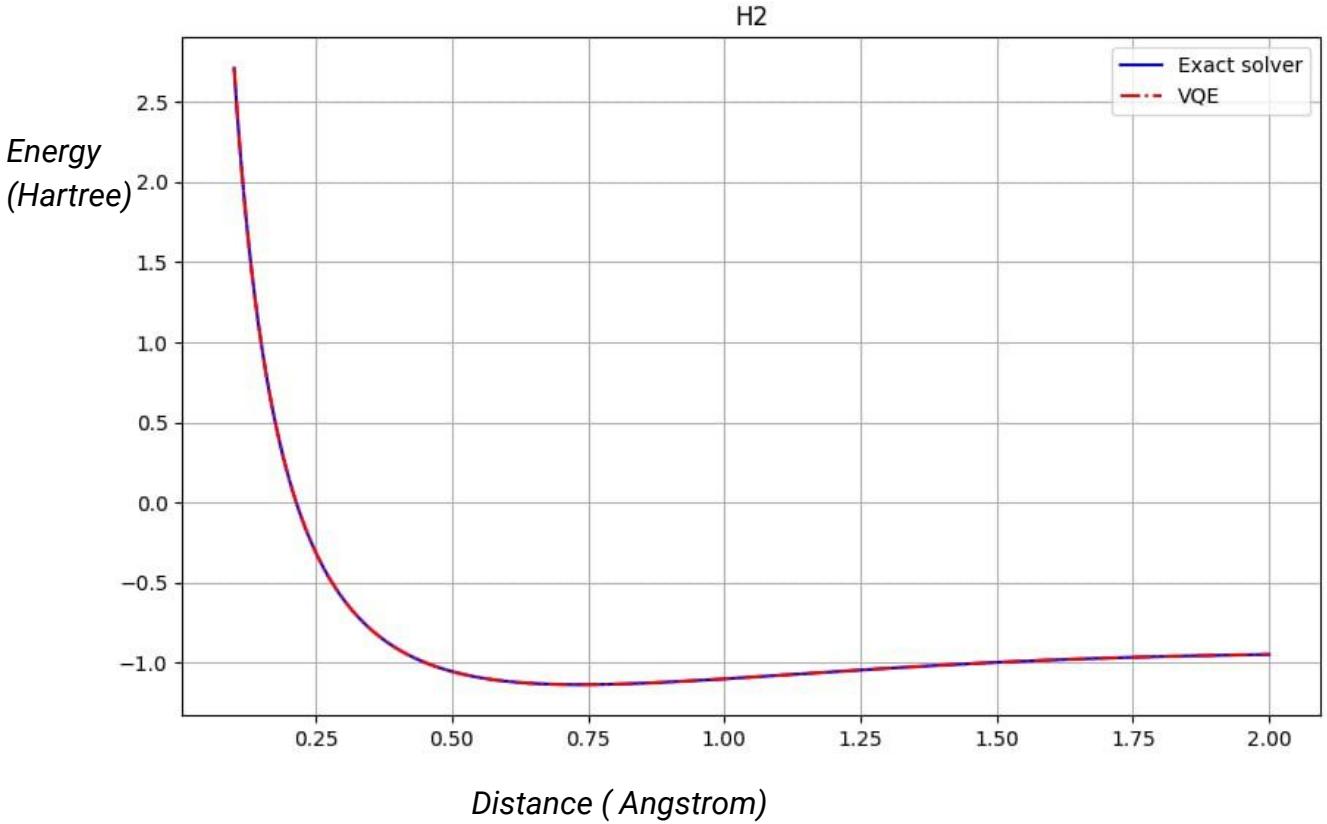
Orbitals (H_2)



2 orbitals.

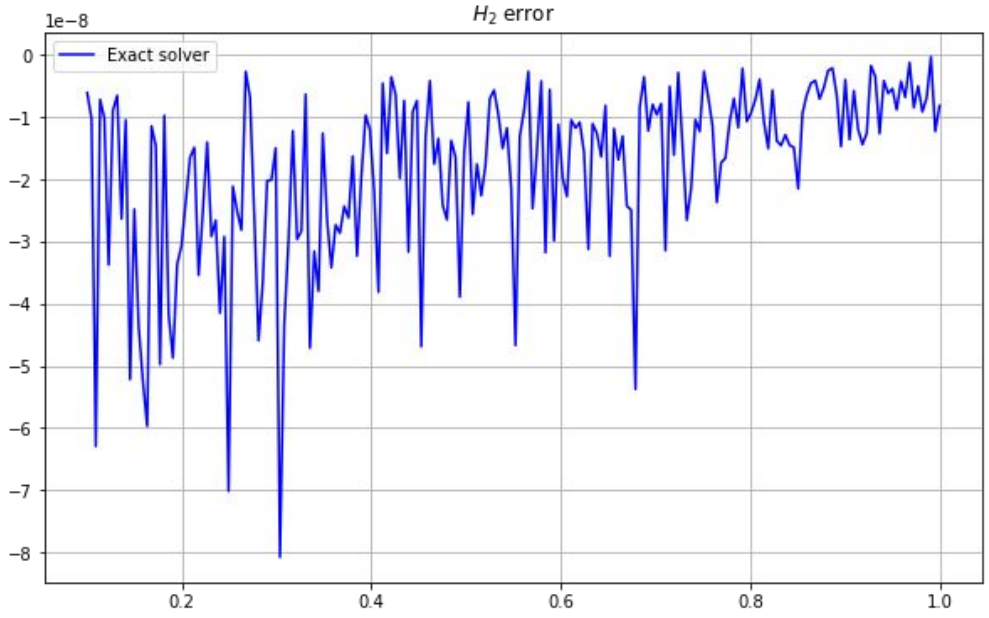
Ground State Energy (H_2)

VQE vs Exact Solver

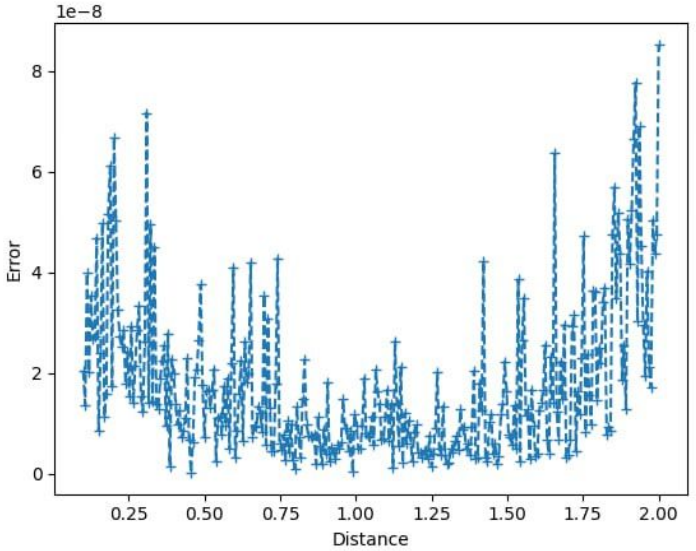


Error (H_2)

VQE vs Exact Solver

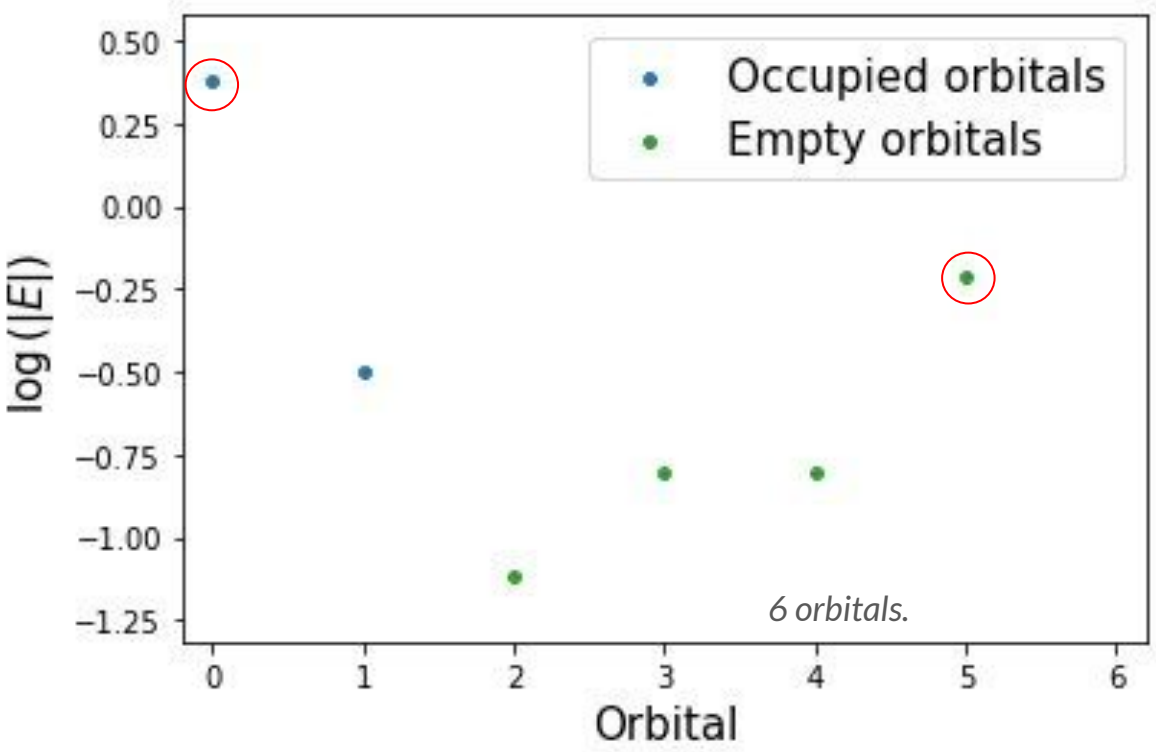


(np.linspace(0.1, 1, 200), COBYLA.maxiter=5000)

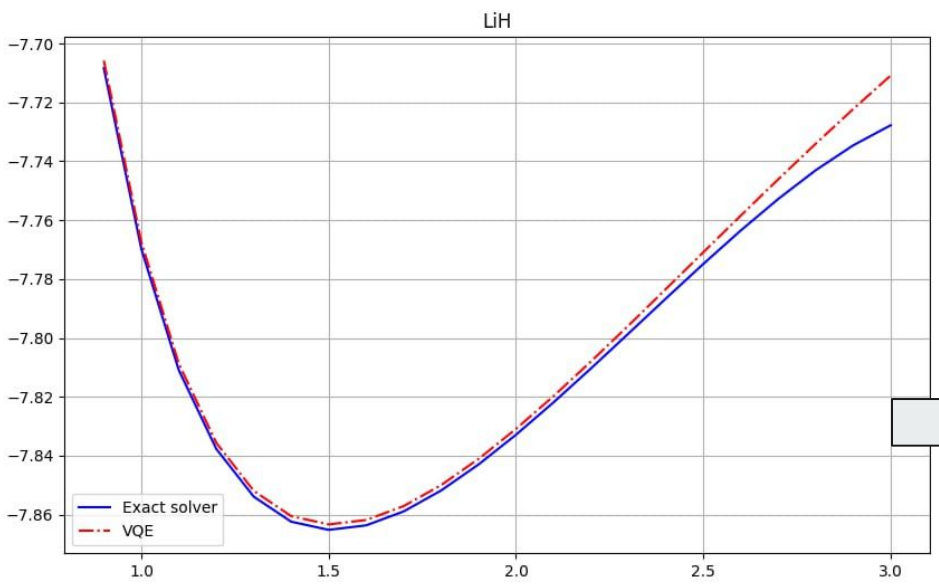


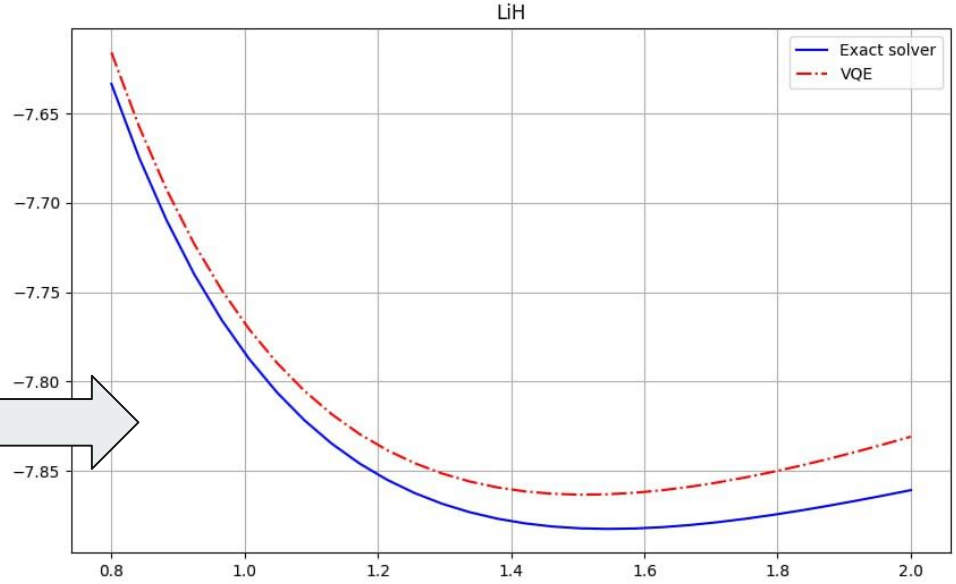
(np.linspace(0.1, 2, 300), COBYLA.maxiter=3000).

Orbitals (LiH)



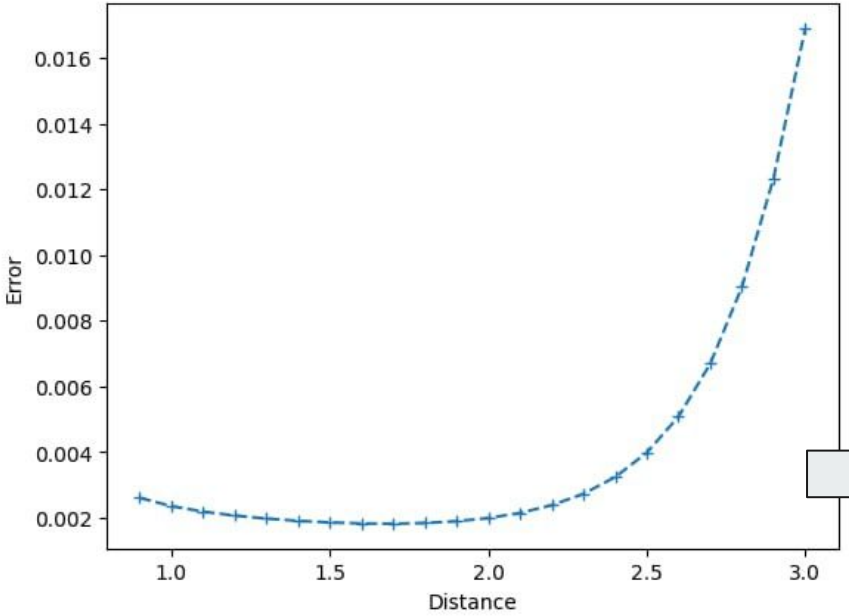
Ground State Energy (LiH)

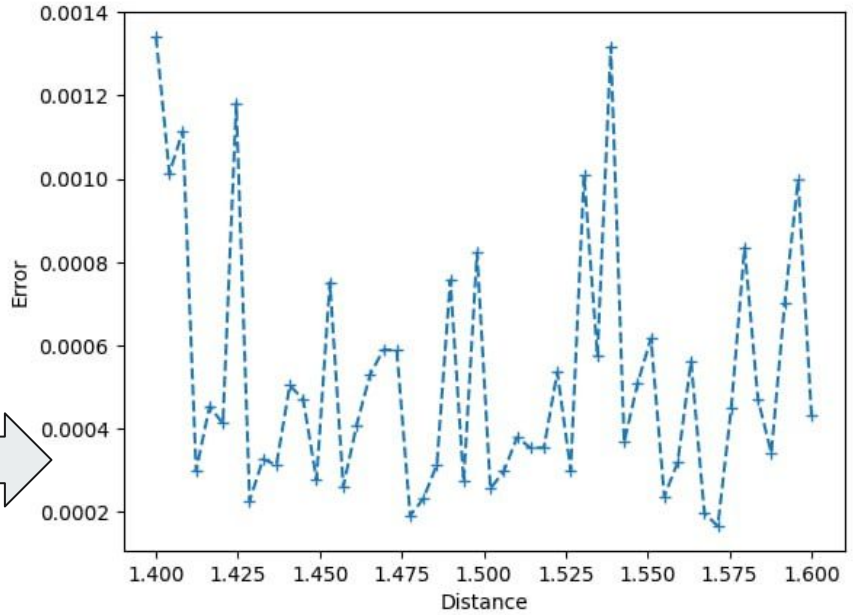




(np.linspace(0.8, 3, 30), COBYLA.maxiter=15)

Error (LiH)

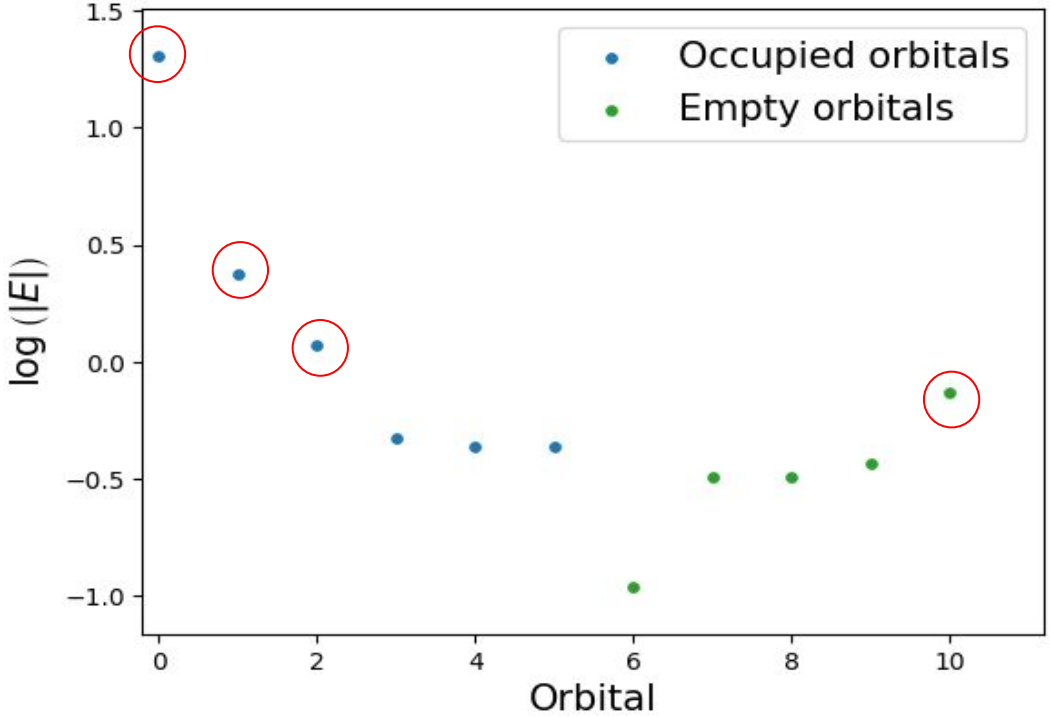




(np.linspace(0.8, 2, 30), COBYLA.maxiter=15)

linspace(1.4, 1.6, 50). COBYLA(maxiter=60, tol=0.0001)

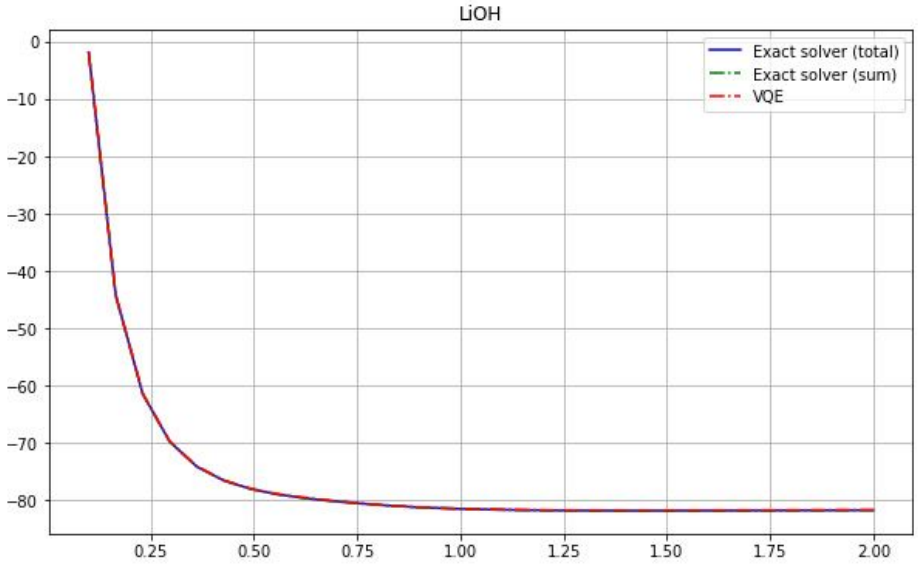
Orbitals (LiOH)



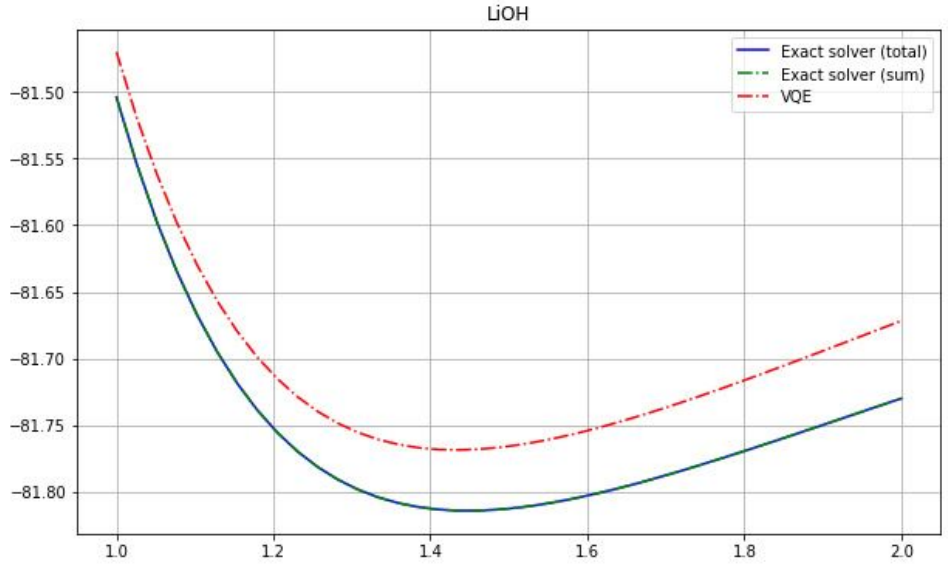
*11 orbitals —> 7 orbitals. Orbitals [**0**, **1**, 2, 10] are frozen*

Ground State Energy (LiOH)

VQE vs Exact Solver

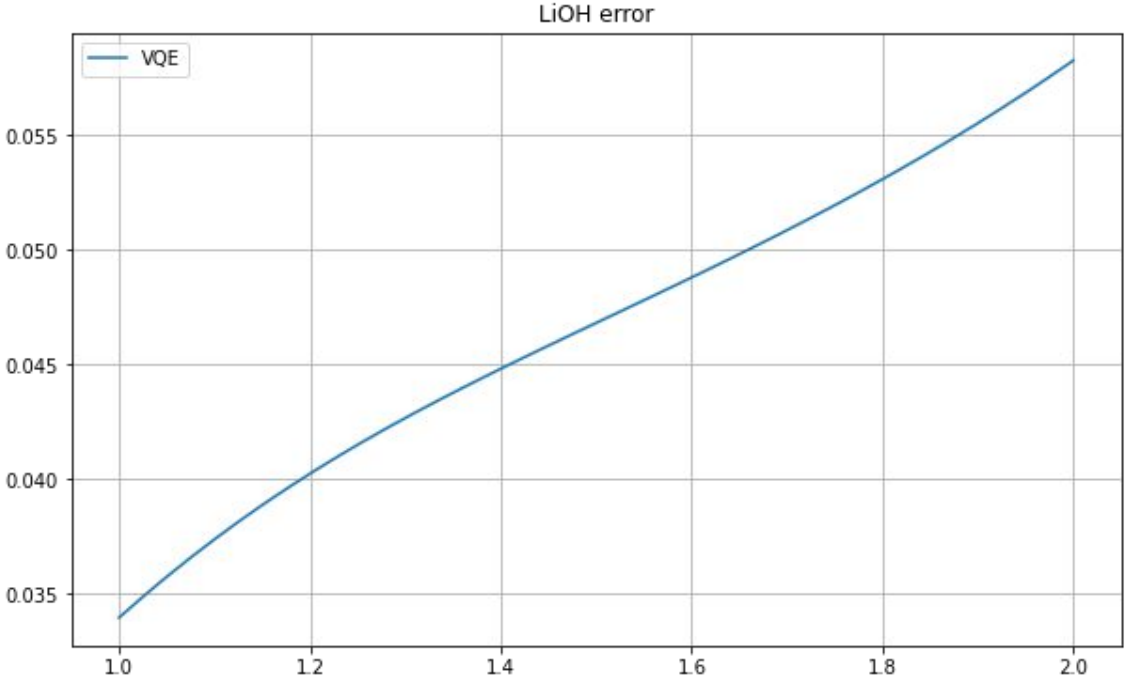


np.linspace(0.1, 2, 30), COBYLA.maxiter=10.



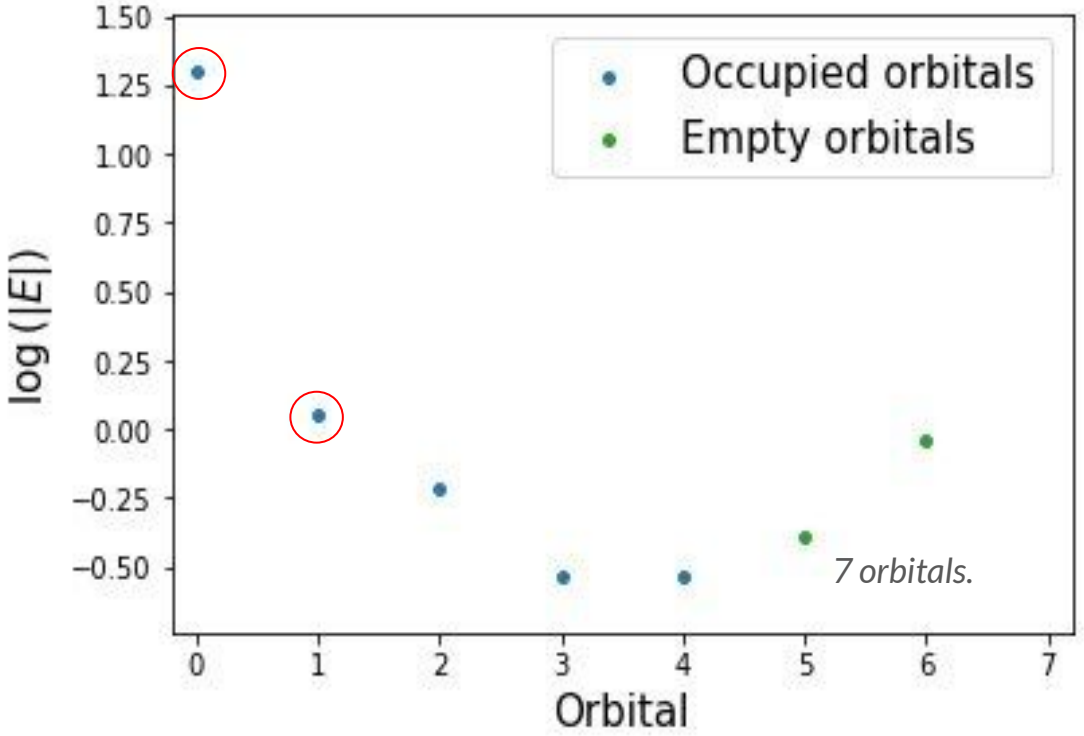
np.linspace(1, 2, 40)

Error (LiOH)



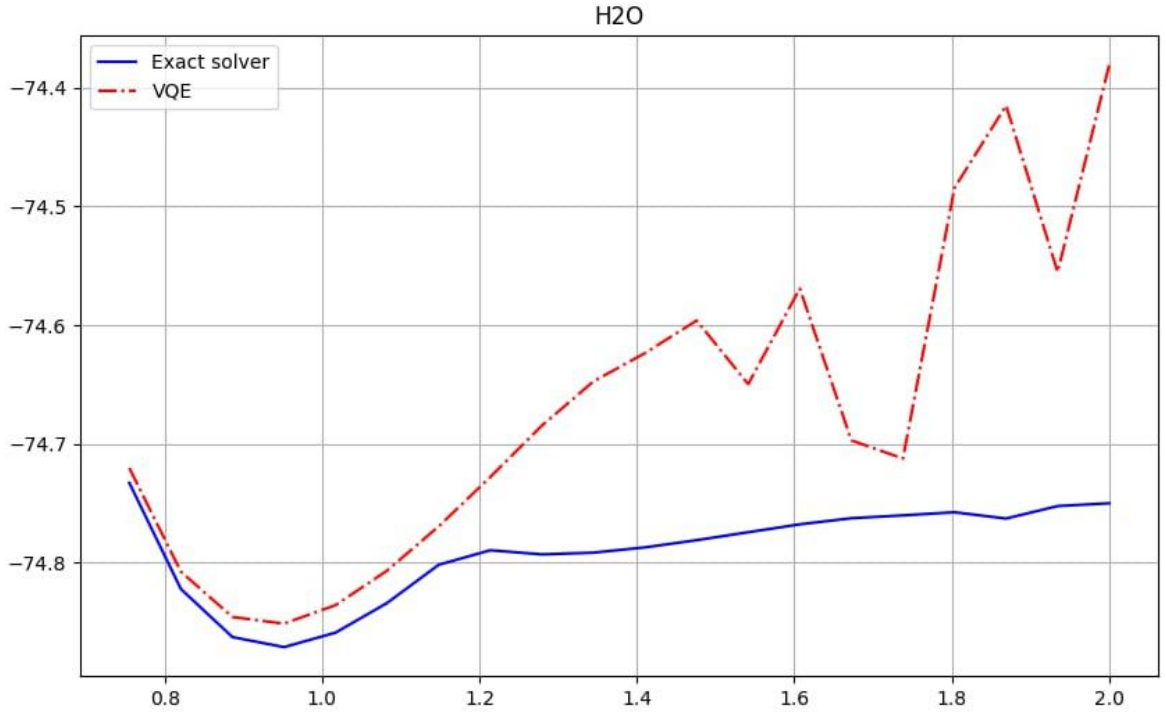
lioh_dist_domain = np.linspace(1.6, 1.7, 25) COBYLA(maxiter=70, tol=0.0001)

Orbitals (H_2O)



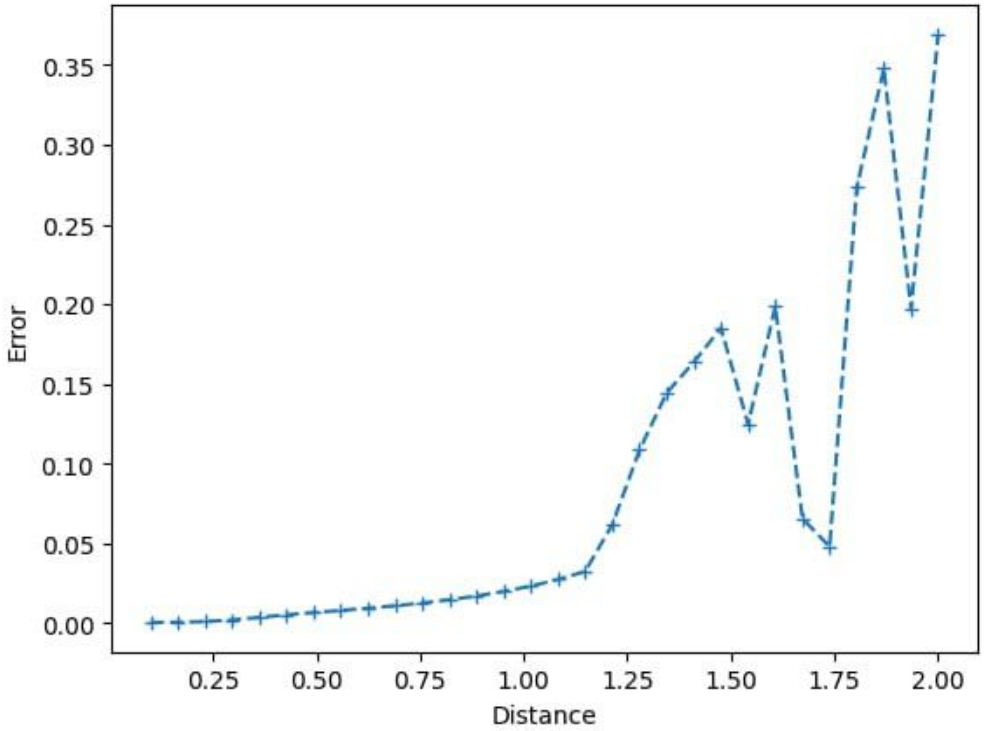
Ground State Energy (H_2O, distance)

VQE vs Exact Solver



linspace(0.1, 2, 30) COBYLA(maxiter=15, tol=0.0001)

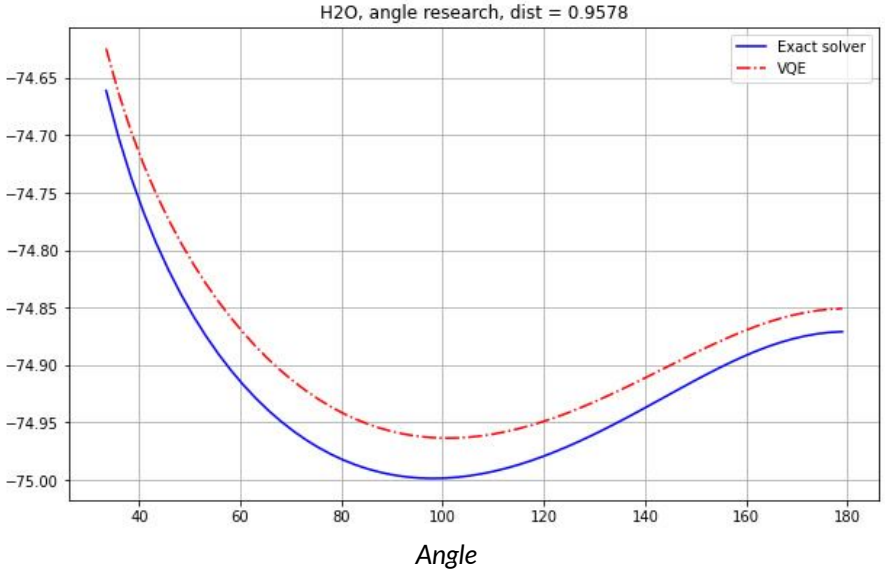
Error (H_2O, distance)

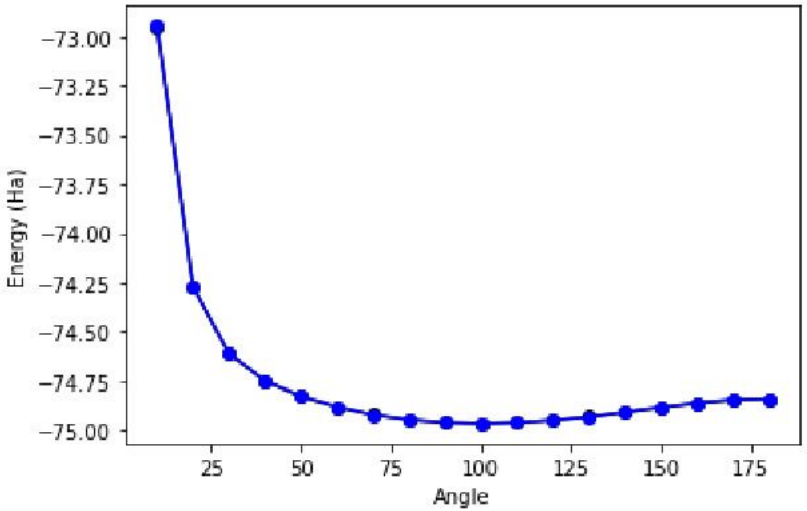


linspace(0.1, 2, 30) COBYLA(maxiter=15, tol=0.0001)

Ground State Energy (H_2O, angle)

VQE vs Exact Solver

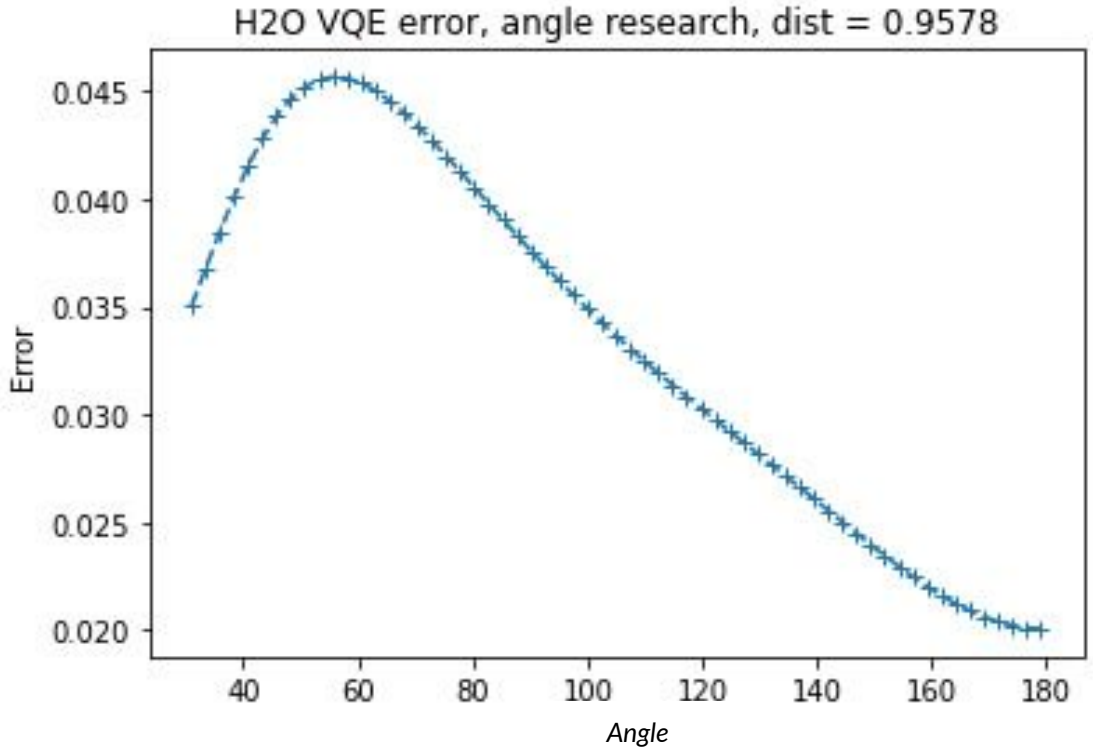




From: https://arxiv.org/pdf/2109.00401

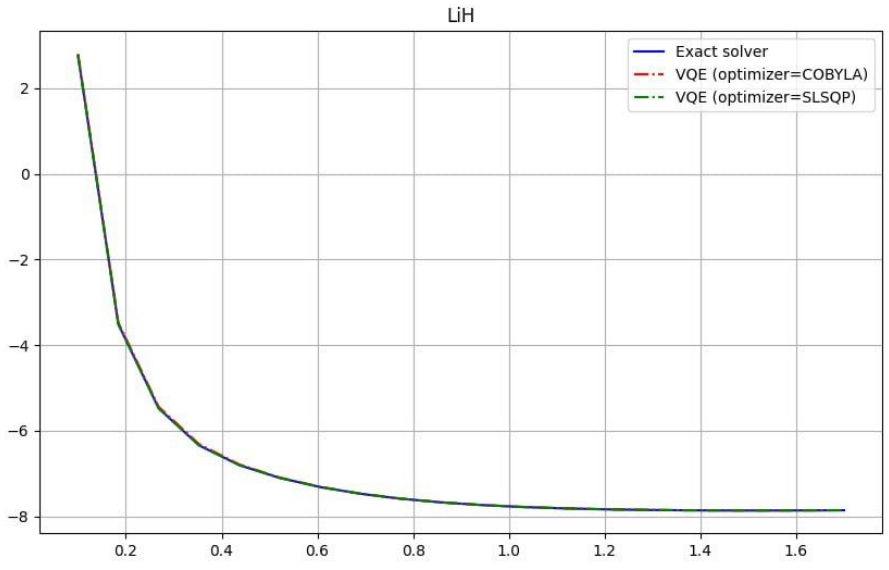
np.linspace(31, 179, 61) COBYLA(maxiter=60, tol=0.0001)

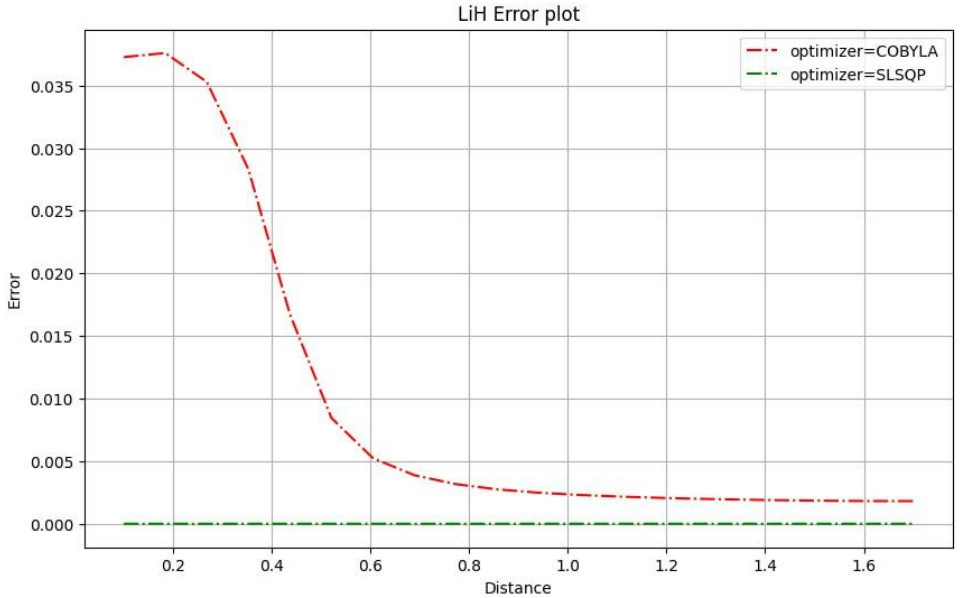
Error (H_2O, angle)



np.linspace(31, 179, 61) COBYLA(maxiter=60, tol=0.0001)

Ground State Energy and Error (LiH)

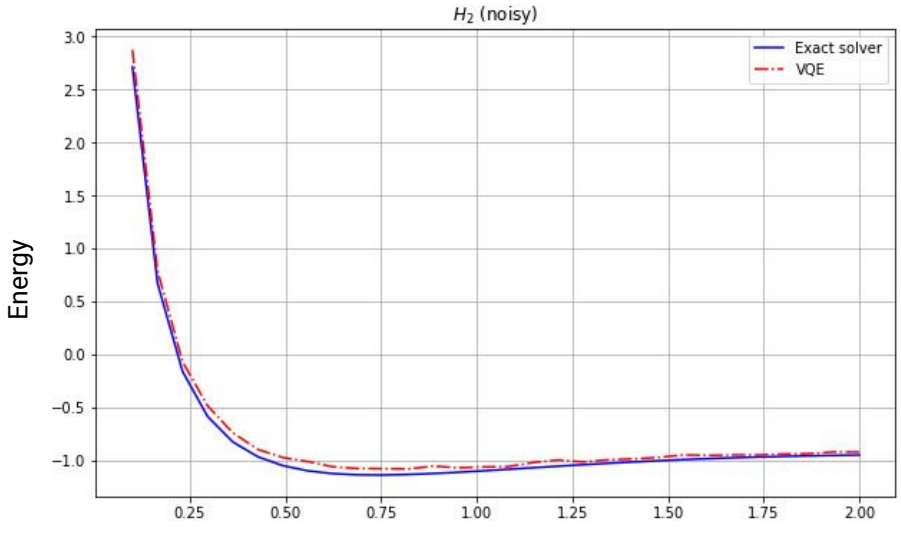


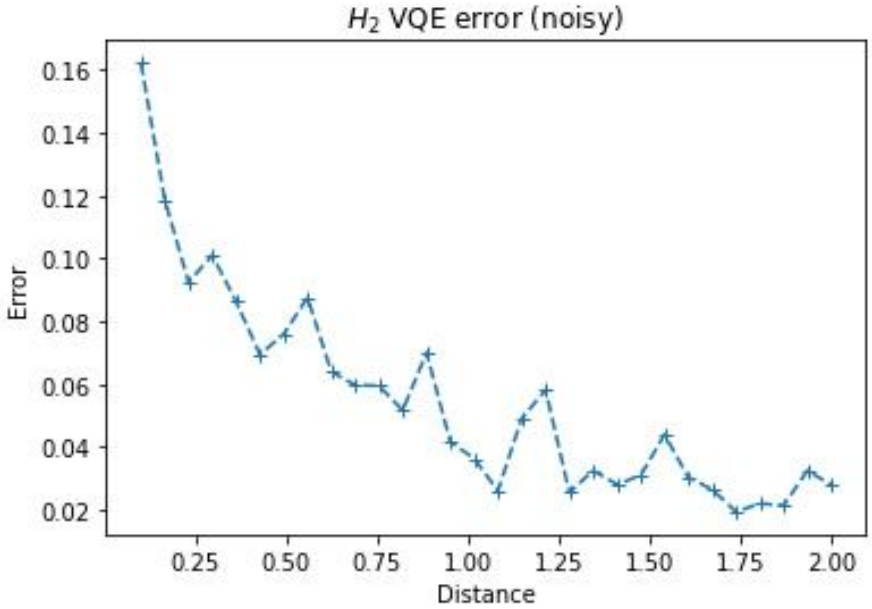


COBYLA = 1 min 15 sec
SLSQP = 2 min 47 sec

maxiter=10, tol=0.0001 linspace(0.1, 1.7, 20)

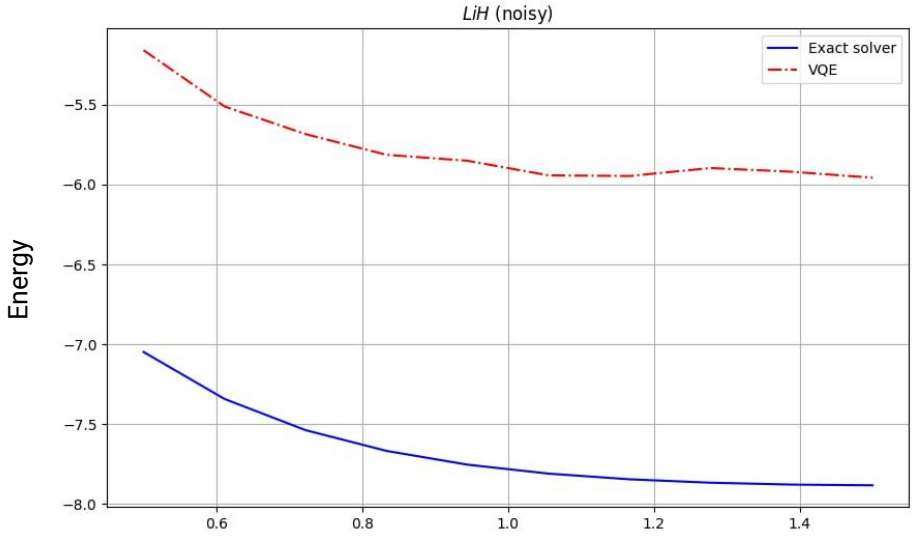
Noisy simulations (H_2)

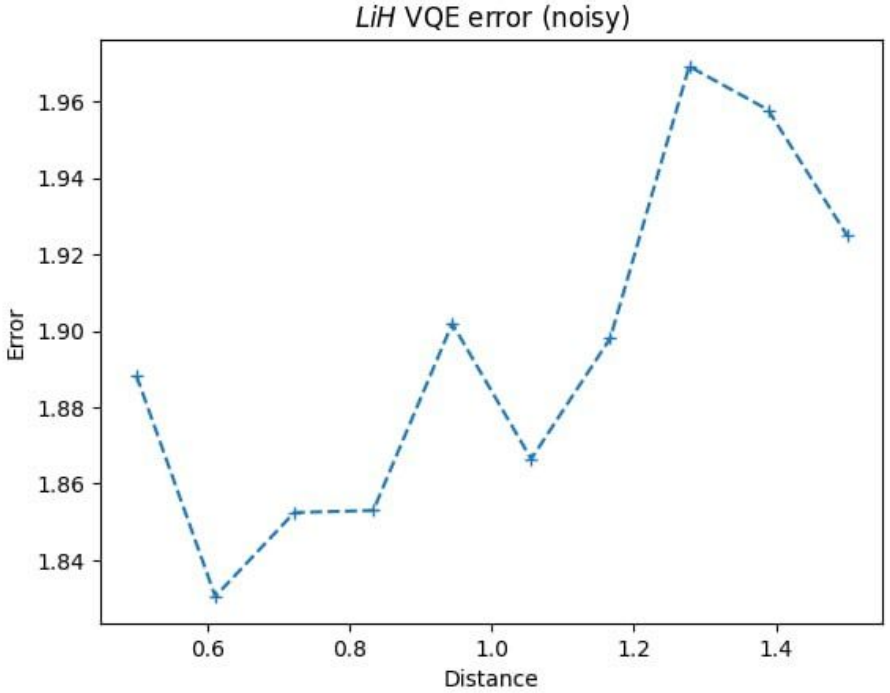




np.linspace(0.1, 2, 30), COBYLA(maxiter=15, tol=0.0001),
num of qubits = 2

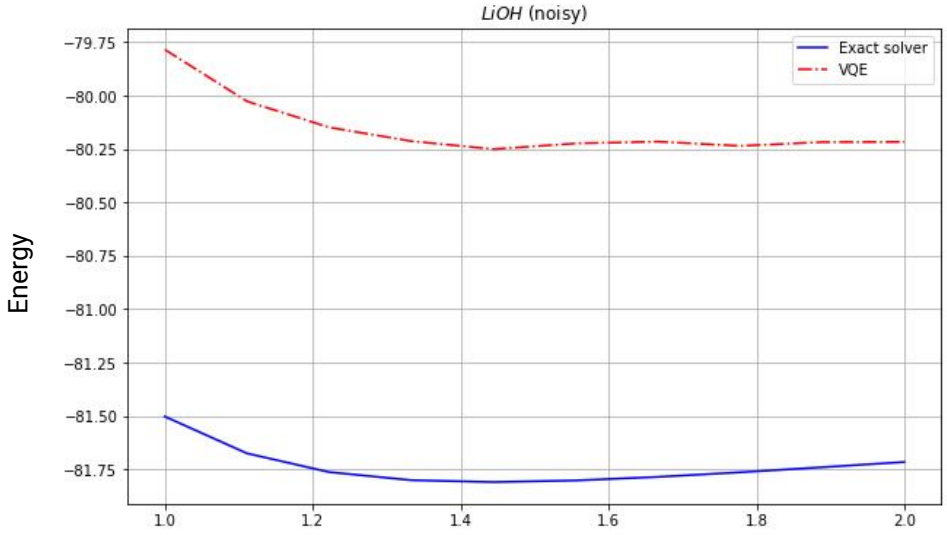
Noisy simulations (LiH)

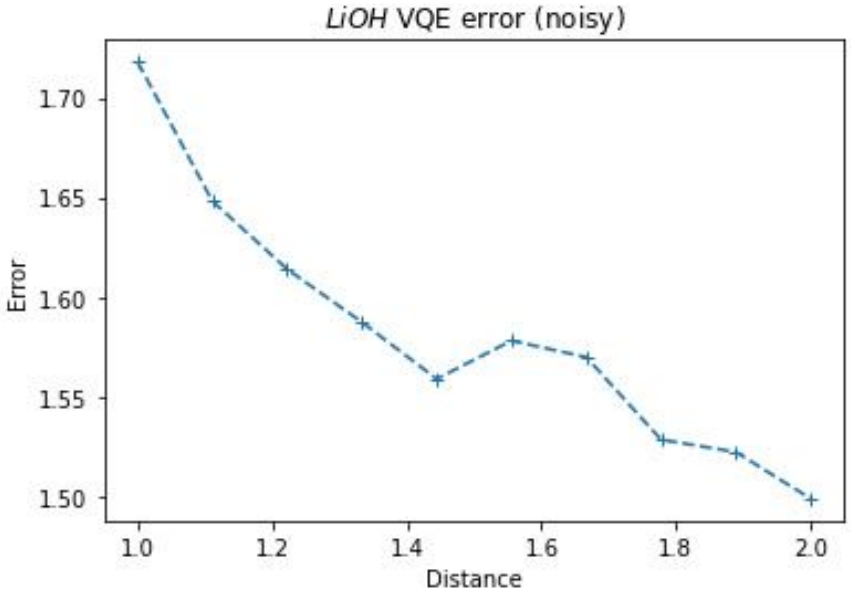




linspace(0.5, 1.5, 10), COBYLA(maxiter=10, tol=0.0001), num of qubits = 8

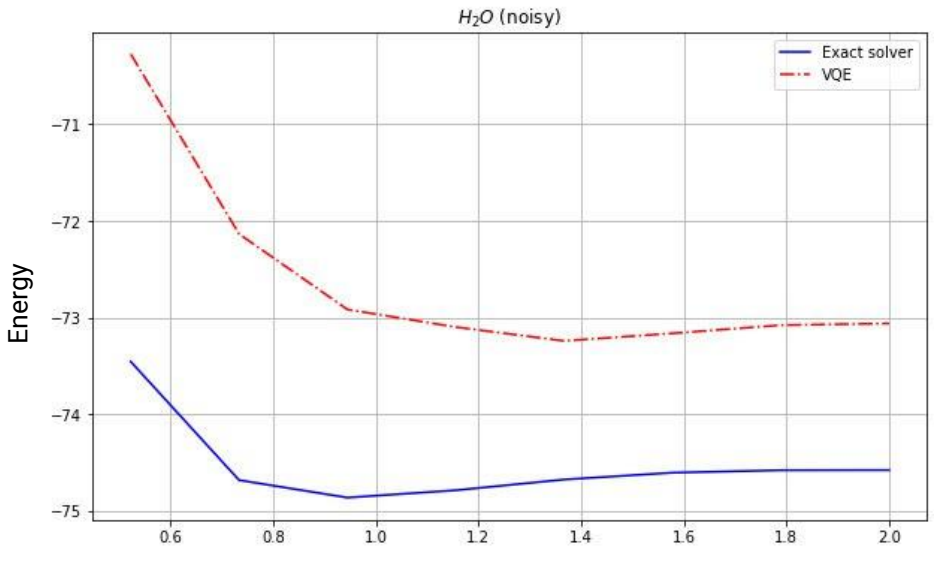
Noisy simulations (LiOH)

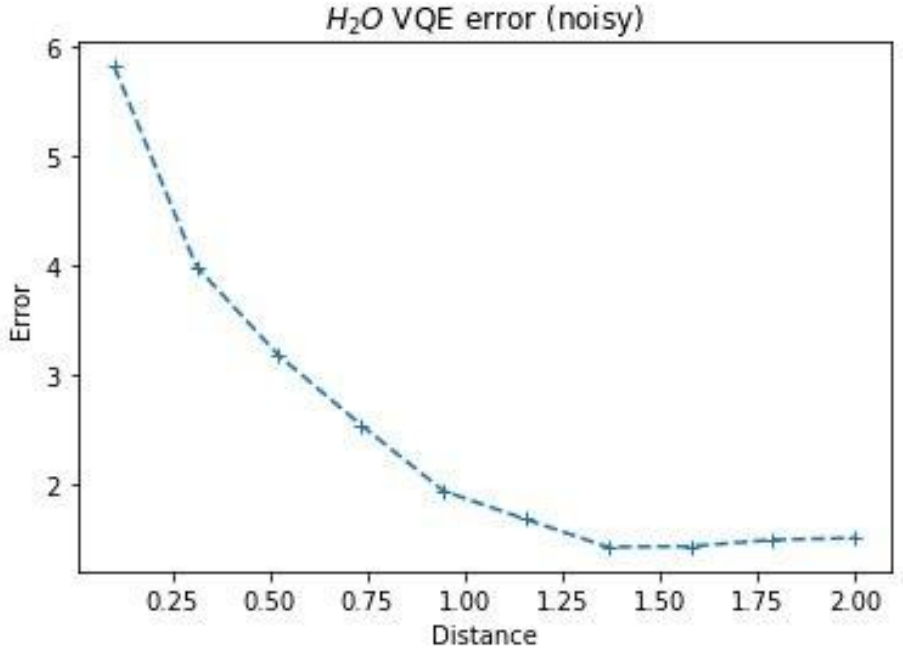




linspace(1, 2, 10), COBYLA(maxiter=10, tol=0.0001),
num of qubits = 8

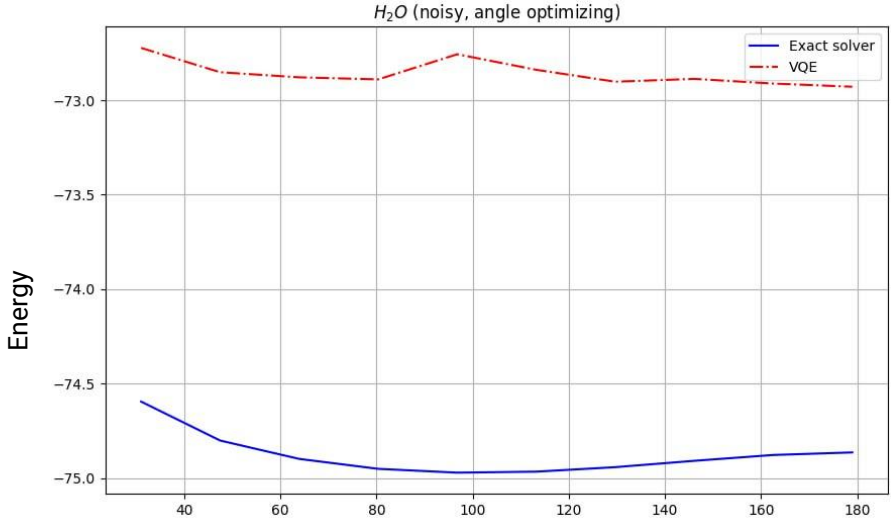
Noisy simulations (H_2O)

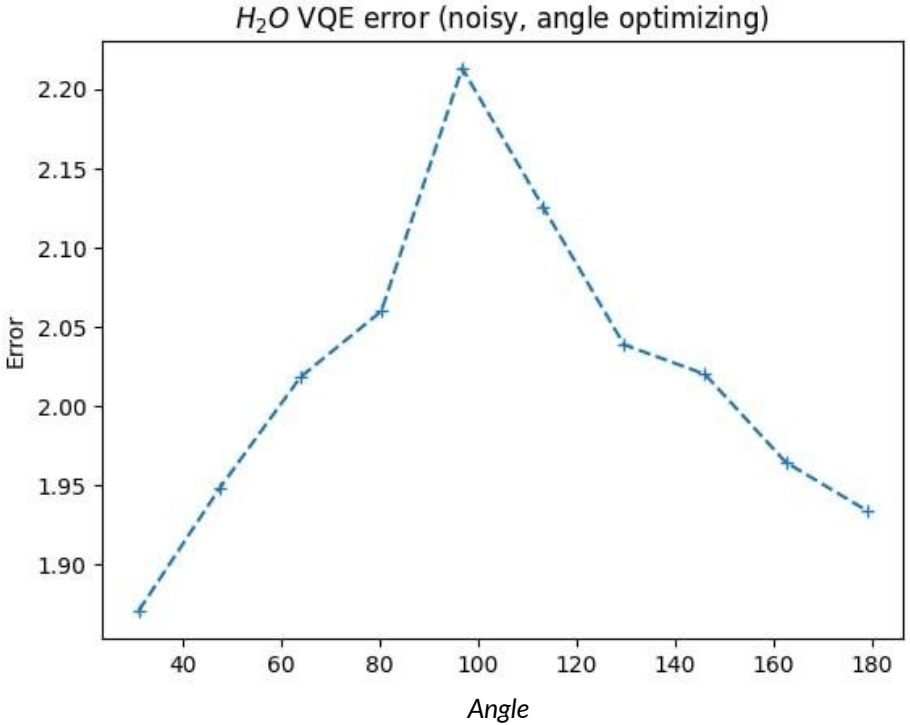




np.linspace(0.1, 2, 10) COBYLA(maxiter=15, tol=0.0001)
orbitals_to_fix=[**0**, 1, 6], num of qubits = 6

Noisy simulations (H_2O, angle)





np.linspace(31, 179, 10) COBYLA(maxiter=15, tol=0.0001)
orbitals_to_fix=[**0**, 1, 6], num of qubits = 6

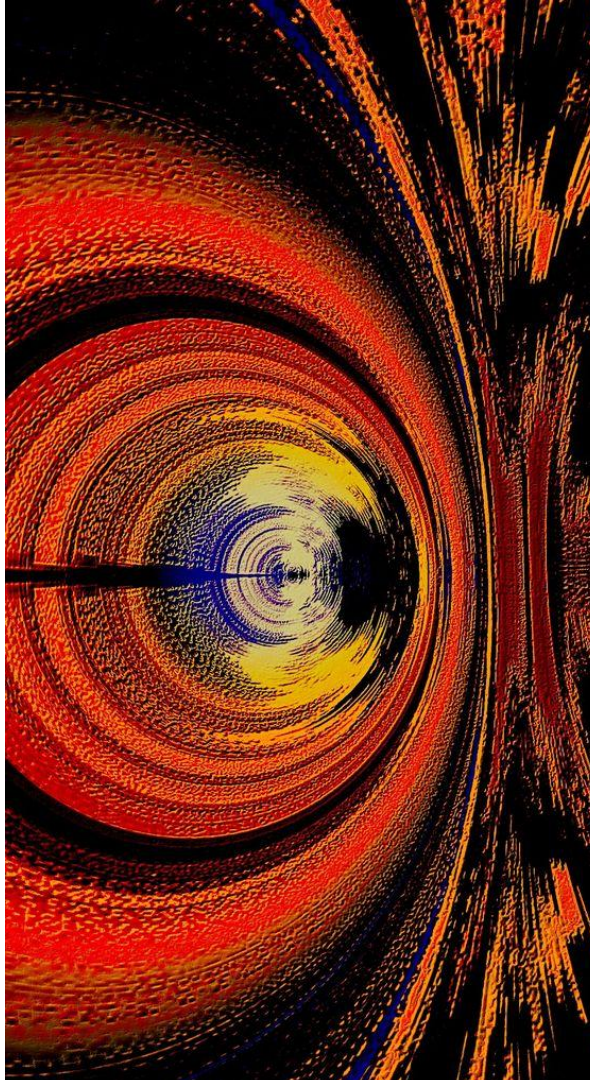
Summary: Energy equation ($LiH + H_2O \Rightarrow LiOH + H_2$)

- **Exact Solver** energies:
  a. **LiH**: -7.86384169490822
  b. **H_2O**: -74.99707745452083
  c. **LiOH**: -81.80516685184013
  d. **H_2**: -1.1371170673457303
- **VQE**:
  a. **LiH**: -7.863795155155253
  b. **H_2O**: -74.96316193784605
  c. **LiOH**: -81.75676315654546
  d. **H_2**: -1.1371170561574413

- Left part:
  a. **Exact**: -82.86091914942905
  b. **VQE**: -82.82695709300131
- Right part:
  a. **Exact**: -82.94228391918585
  b. **VQE**: -82.8938802127029
- Delta (Right - Left):
  a. **Exact**: -0.08136476975680296
  b. **VQE**: -0.06692311970158471

Results and conclusions

- Out of the box coding tools
- Low Error rates, especially at extr. points
- Calculated energies so we show that they are not equal on both sides
- Struggle with intermediate states (dynamics)
- Successive POC and base for future investigations



Our GitHub:

https://github.com/QMLcobyla/chemistry