Quantux Climate Challenge Report

Please see https://github.com/buttercutter/quantum-climate-challenge-2023/

Team

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Task 1A

Problem

Calculate a combination of interaction molecules and calculate with a quantum algorithm the minimum of Potential Energy Surface.

Solution

Classical algorithm

Our team calculated energy levels with a classical computation in Quantistry solution for the combination molecules:

- Co 2+ CO2, Co 2+ H2O, Co 2+ N2
- Cu 2+ CO2, Cu 2+ H2O, Cu 2+ N2
- Fe 2+ CO2, Fe 2+ H2O, Fe 2+ N2
- Mn 2+ CO2, Mn 2+ H2O, Mn 2+ N2
- Ni 2+ CO2, Ni 2+ H2O, Ni 2+ N2

VQE Quantum algorithm

Our team calculated energy levels with a quantum computation with Qiskit and IBM Quantum for the energy combinations:

- Co 2+ CO2
- Fe 2+ CO2

We created a quantum algorithm UCCSD for the molecular problem.

Our most time consuming problem was to analyze how to reduce the problem size with a quantum computer approach. We researched the FreeCore and ActiveSpace transformers in Qiskit and raised two issues to ask for more detailed information on the usage.

The coordinate calculation was also a time consuming task.

Our approach was to use the Quantistry coordinates and use those in the quantum computation and then reduce the problem size with a transformer.

Born-Oppenheimer Potential Energy Surface (BOPES)
We implemented a Born-Oppenheimer potential energy surface for the calculations.

Quantum Phase Estimation

We created a Quantum Phase estimation to calculate the energy level with Pauli Trotterization evolution and a quantum simulation environment.

The simulation results can be seen under the notebook https://github.com/buttercutter/quantum-climate-challenge-2023/blob/main/notebooks/deloitte_2023_quantux.ipynb under topic Exact energy vs Quantum phase estimation in noiseless simulation.

Running the algorithm

Simulation

The runtime of the algorithm in a real quantum computer is high mostly because of the wait que in the real machine. We run the algorithm on a simulation environment with the following results.

The simulation results can be seen under the notebook https://github.com/buttercutter/quantum-climate-challenge-2023/blob/main/notebooks/deloitte_2023_quantux.ipynb under topic Exact energy vs VQE Noiseless simulation.

Real quantum computer

We have run the VQE on a Co 2+ CO2 interaction with a real quantum computer IBM Jakarta. The run is a reduced problem with the Freeze Core Transformer by removing orbitals 13 - 31.

The results can be seen under the notebook https://github.com/buttercutter/quantum-climate-challenge-2023/blob/main/notebooks/deloitte_2023_quantux.ipynb under topic Exact energy vs VQE Real quantum computer.

Quantistry
With Quantistry we created calculations for each combination of the interactions.

References
During the task we created issues for questions that came up during the task.

Qiskit https://github.com/Qiskit/qiskit-nature/issues/1087#issuecomment-1456015083

TensorCircuit
https://github.com/tencent-quantum-lab/tensorcircuit/issues/120#issuecomment-1447920148

Task 1B

Problem

Compare your solution to at least one classical solution, describing advantages and disadvantages of the approaches.

Solution

We used Gaussian16 as well as xtb software to perform DFT simulation. We will try TD-DFT as well as CASSCF https://gaussian.com/cas/ later.

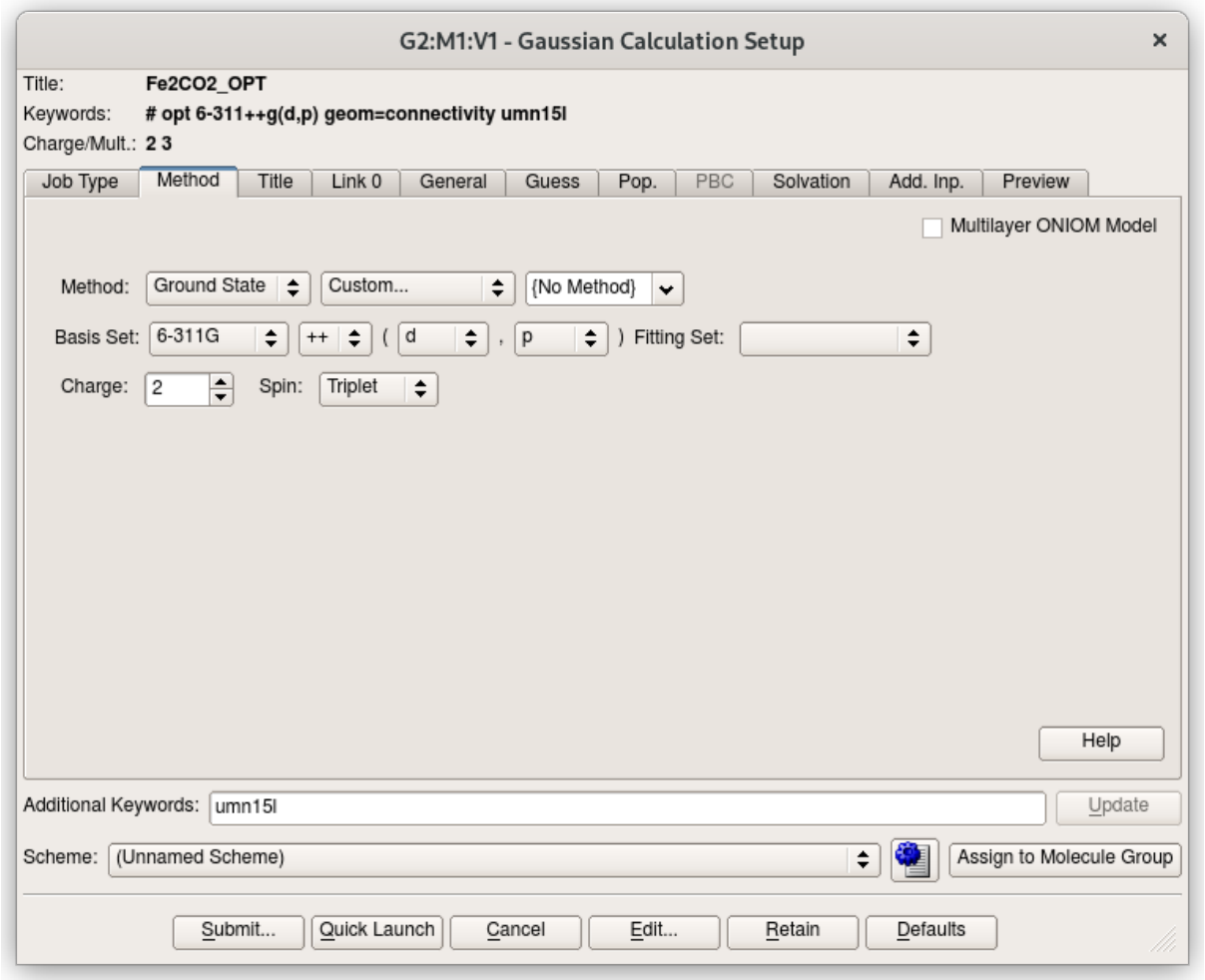
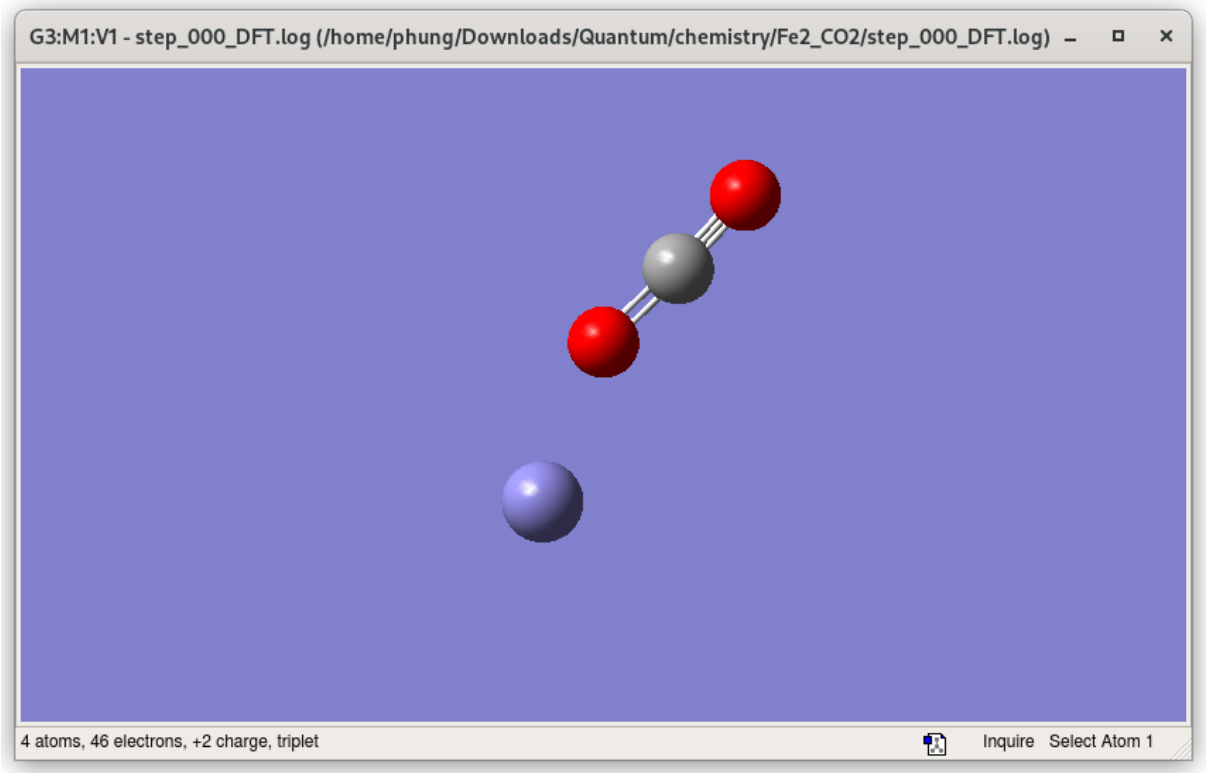


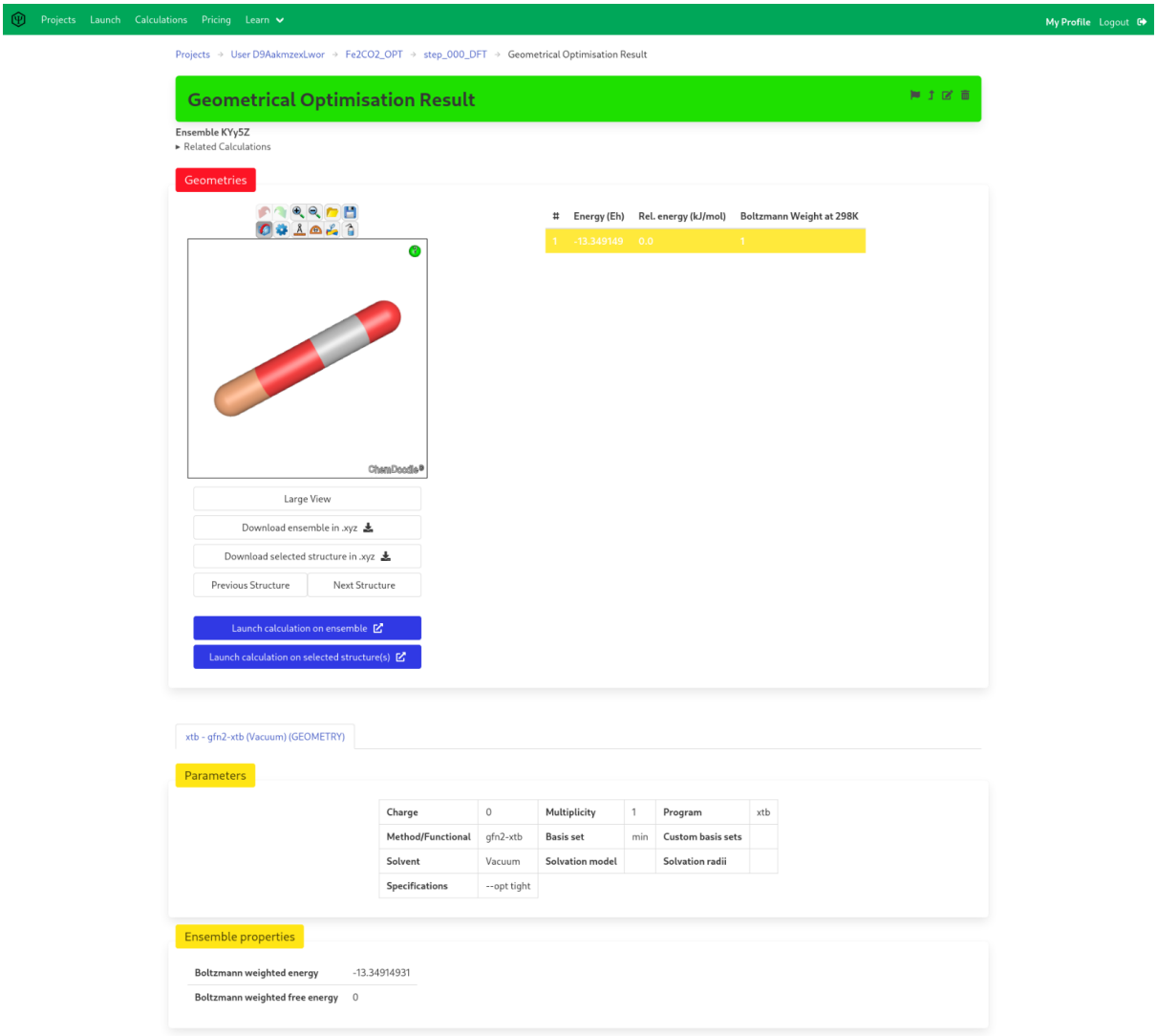
Fig: Gaussian16 setup for DFT simulation

We use the MN15L functional, we tried CAM-B3LYP functional before. But as advised by Igors Mihailovs , CAM-B3LYP functional is not suited for transition metal like Fe.

Then, we use the 6-311G basis set with ++ diffuse function. Fe2+ has a charge of 2 and it is a triplet as suggested by David Shobe . Since Fe2+ is of ferromagnetic characteristics, we actually added spin polarization settings.

```
~/D/Q/c/Fe2_CO2  grep -Einw "done|energy" step_000_DFT.log
175:       nuclear repulsion energy       178.7145642873 Hartrees.
227: Requested convergence on             energy=1.00D-06.
228: No special actions if energy rises.
232: SCF Done:  E(UMN15L) =  -1451.21329131     A.U. after   26 cycles
480: Predicted change in Energy=-6.953832D-03
523:       nuclear repulsion energy       173.2118596216 Hartrees.
577: Requested convergence on             energy=1.00D-06.
578: No special actions if energy rises.
579: SCF Done:  E(UMN15L) =  -1451.22296734     A.U. after   25 cycles
645: Predicted change in Energy=-4.900162D-03
688:       nuclear repulsion energy       167.5806983807 Hartrees.
742: Requested convergence on             energy=1.00D-06.
743: No special actions if energy rises.
744: SCF Done:  E(UMN15L) =  -1451.22817065     A.U. after   37 cycles
810: Predicted change in Energy=-1.327823D-03
853:       nuclear repulsion energy       165.5184004510 Hartrees.
907: Requested convergence on             energy=1.00D-06.
908: No special actions if energy rises.
909: SCF Done:  E(UMN15L) =  -1451.22870120     A.U. after   28 cycles
973: Predicted change in Energy=-5.201493D-04
1016:       nuclear repulsion energy       165.4000486045 Hartrees.
1070: Requested convergence on             energy=1.00D-06.
1071: No special actions if energy rises.
1072: SCF Done:  E(UMN15L) =  -1451.22926030     A.U. after   24 cycles
1137: Predicted change in Energy=-4.840015D-05
1180:       nuclear repulsion energy       165.5658216202 Hartrees.
1234: Requested convergence on             energy=1.00D-06.
1235: No special actions if energy rises.
1236: SCF Done:  E(UMN15L) =  -1451.22933856     A.U. after   26 cycles
1301: Predicted change in Energy=-4.496397D-05
1344:       nuclear repulsion energy       166.0448348018 Hartrees.
1389: Requested convergence on             energy=1.00D-06.
1390: No special actions if energy rises.
1391: SCF Done:  E(UMN15L) =  -1451.22939438     A.U. after   20 cycles
1457: Predicted change in Energy=-2.098594D-05
1500:       nuclear repulsion energy       166.4524077319 Hartrees.
1545: Requested convergence on             energy=1.00D-06.
1546: No special actions if energy rises.
1547: SCF Done:  E(UMN15L) =  -1451.22941697     A.U. after   19 cycles
1614: Predicted change in Energy=-1.680180D-06
1657:       nuclear repulsion energy       166.5626011393 Hartrees.
1702: Requested convergence on             energy=1.00D-06.
1703: No special actions if energy rises.
1706: SCF Done:  E(UMN15L) =  -1451.22941894     A.U. after   18 cycles
1772: Predicted change in Energy=-1.206624D-07
1815:       nuclear repulsion energy       166.5578247398 Hartrees.
1860: Requested convergence on             energy=1.00D-06.
1861: No special actions if energy rises.
1862: SCF Done:  E(UMN15L) =  -1451.22941908     A.U. after   21 cycles
1930: Predicted change in Energy=-5.167161D-10
~/D/Q/c/Fe2_CO2
```

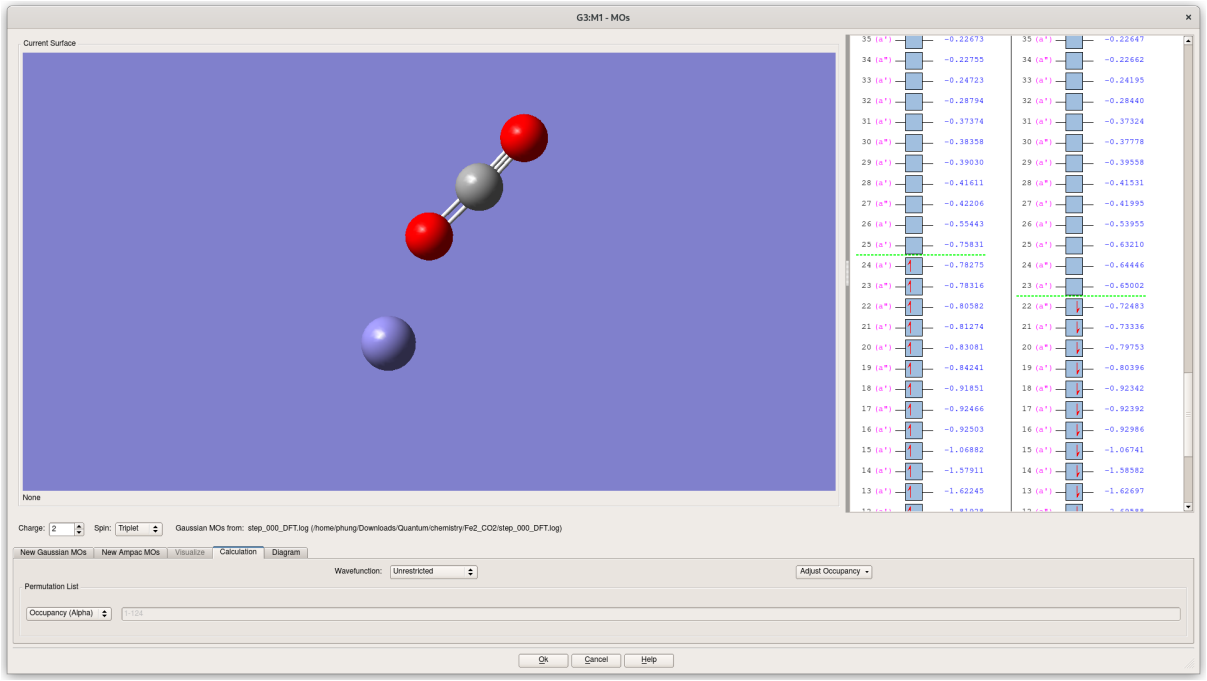

G3:M1:V1 - step_000_DFT.log (/home/phung/Downloads/Quantum/chemistry/Fe2_CO2/step_000_DFT.log)
4 atoms, 46 electrons, +2 charge, triplet
Inquire
Select Atom 1



CalcUS

VERSION BETA 487DF7D

We actually used DFT simulation results to generate the molecular orbitals in order to deduce the active orbitals around the HOMO-LUMO bandgap. This is to be used for FreezeCore and ActiveSpaceTransformer during VQE computation to reduce the computation to a smaller problem.



VQE is a heuristic algorithm, and it actually depends on some of the outputs from classical algorithms to determine its computation starting point as well as computation complexity reduction.

References

https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Physical_Chemistry_(LibreTexts)/11%3A_Computational_Quantum_Chemistry/11.04%3A_Orbital_Polarization_Terms_in_Basis_Sets#:~:text=as%20(d%2C%20p).-,Diffuse%20Functions,-Another%20common%20addition

http://www.ccl.net/cgi-bin/ccl/message-new?2023+03+01+002
http://www.ccl.net/cgi-bin/ccl/message-new?2023+02+25+003

https://calcus.cloud/

https://www.basissetexchange.org/

https://joaquinbarroso.com/2017/06/20/dealing-with-spin-contamination/
https://docs.google.com/document/d/1ozLsxpzqxg1ZMz1YxFELq5vPqnhYEP9NtZCimbvuur0/edit

Task 2A

Problem

Conceptualize a quantum or hybrid solution to scale the calculation from one binding site to at least one 2D unit cell of the given MOF-family AND from one gas molecule to a larger amount of substance of the gas molecule.

Solution

From the pictures, it shows a slice of MOF layer is showing hexagonal structure -
Each vertex is Mg, so the total would be a layer of 24 Mg ions.

So per layer would be 24x binding energy needed.

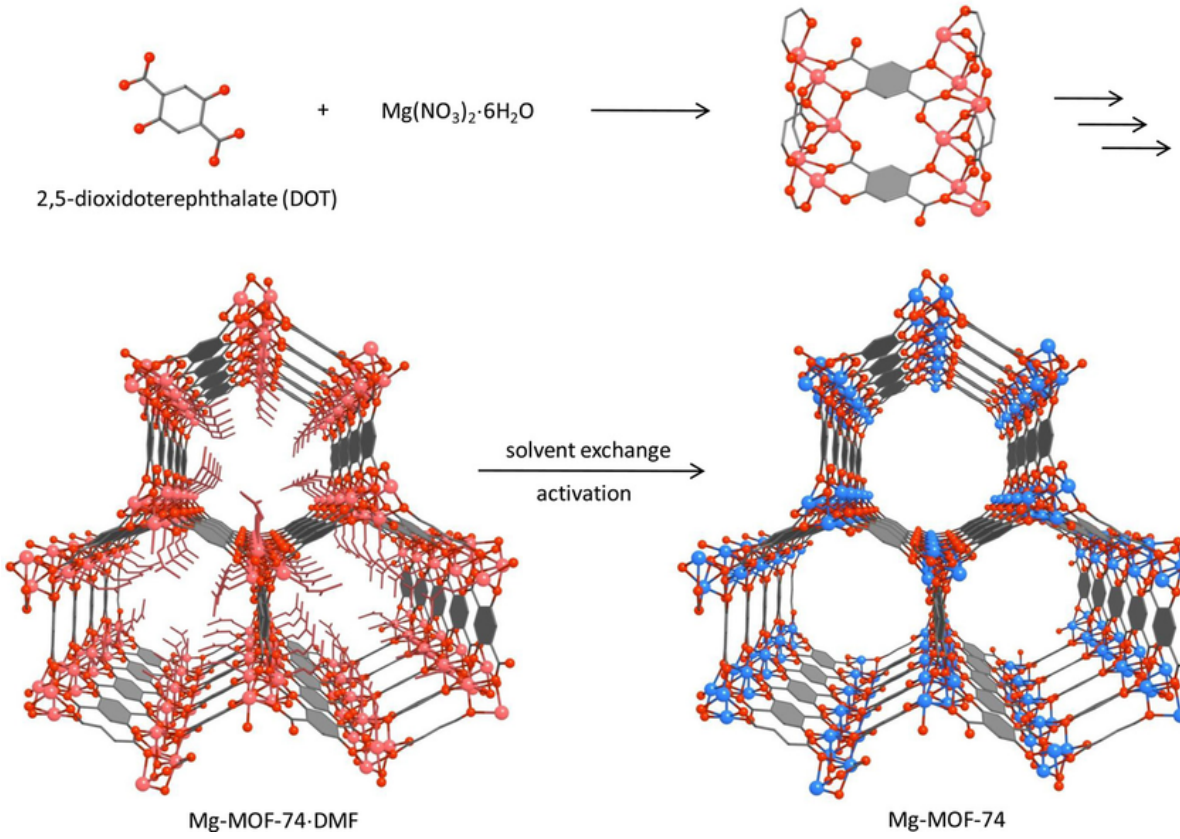
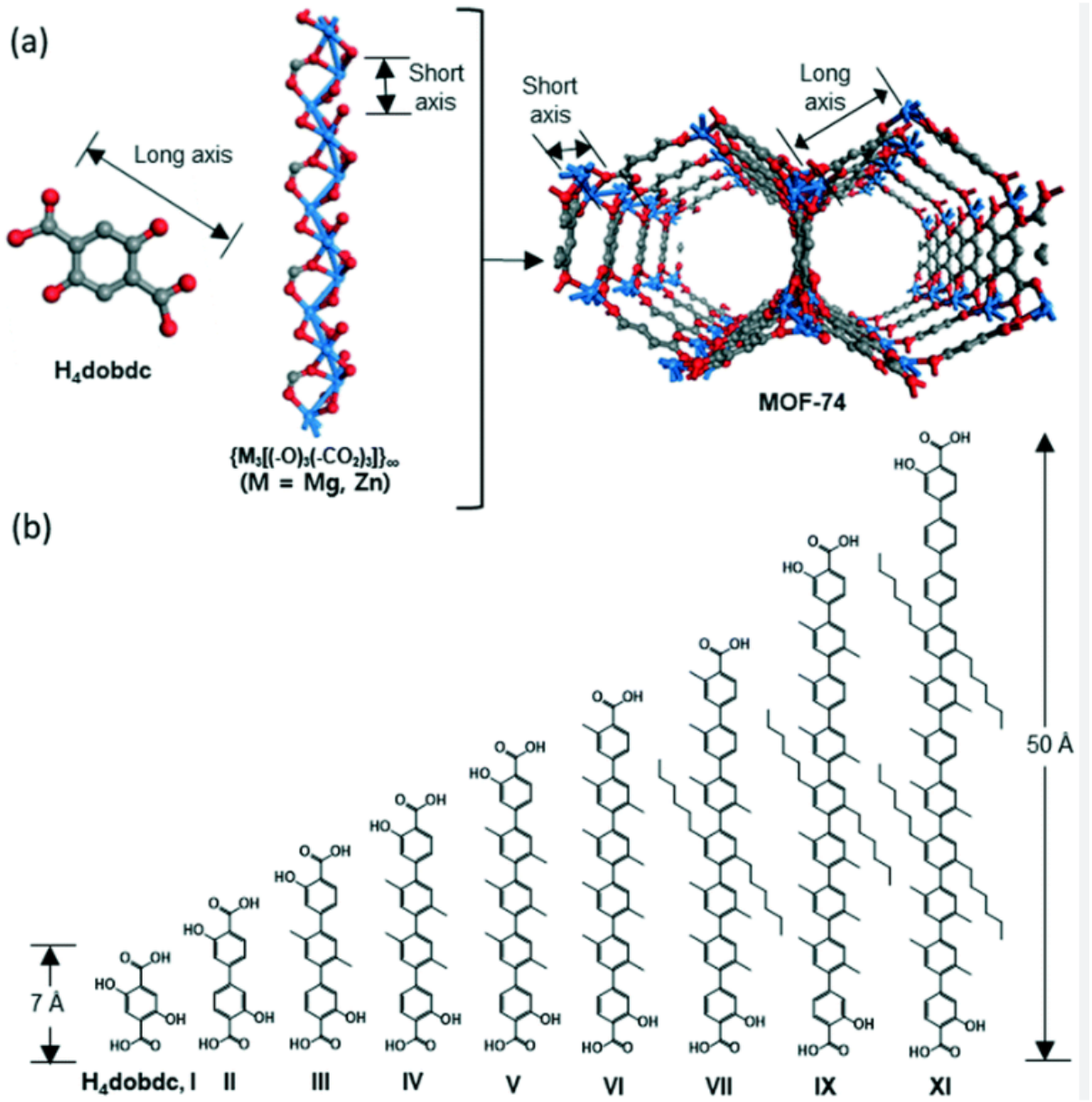


Image MOF



MOF-74-type frameworks: tunable pore environment and functionality through metal and ligand modification - CrystEngComm (RSC Publishing)...

Visit

Image MOF

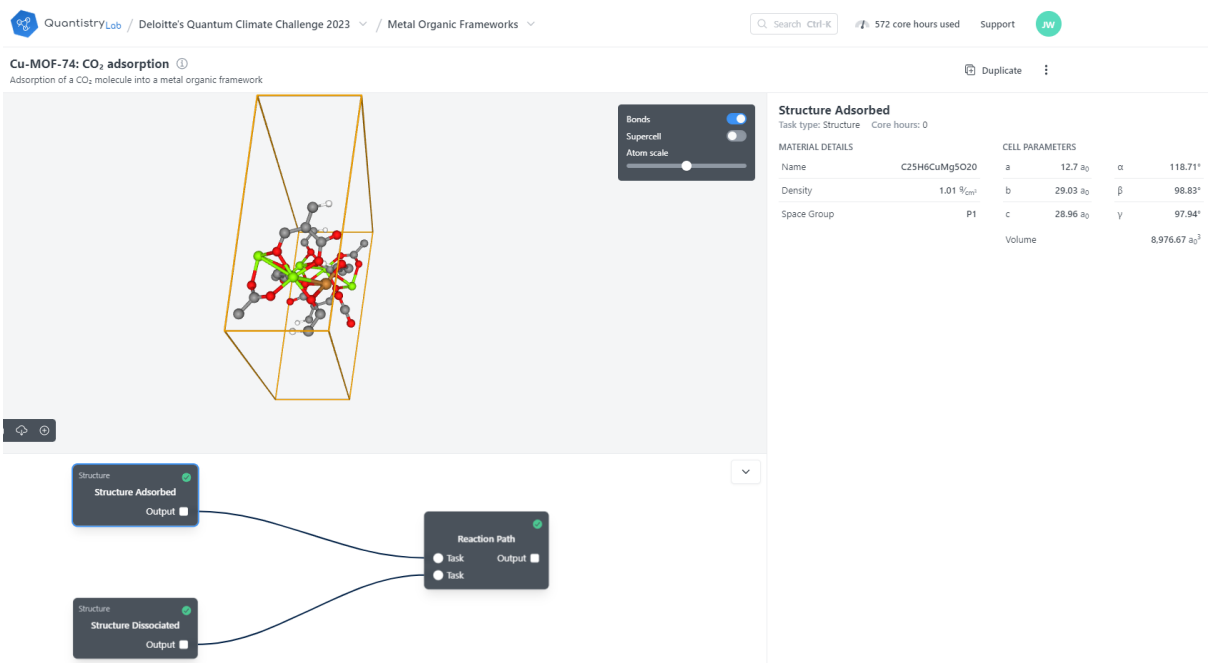


Image Quantistry Metal Organic Framework.

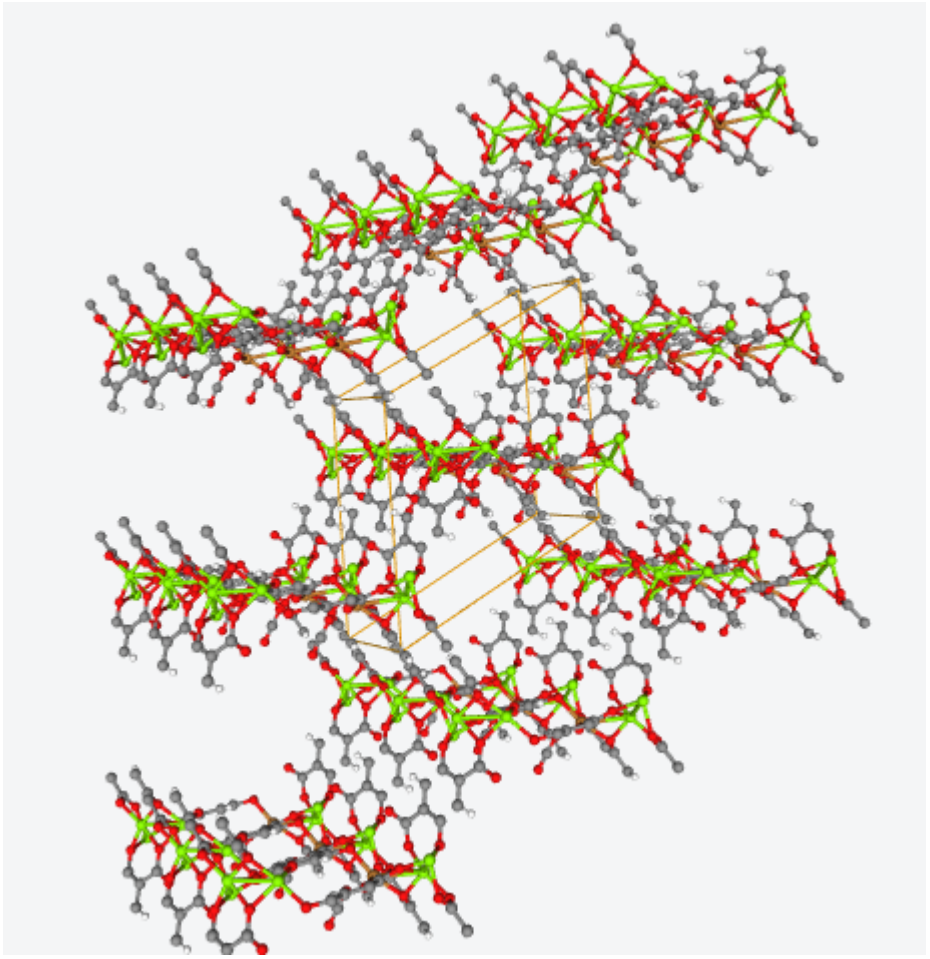
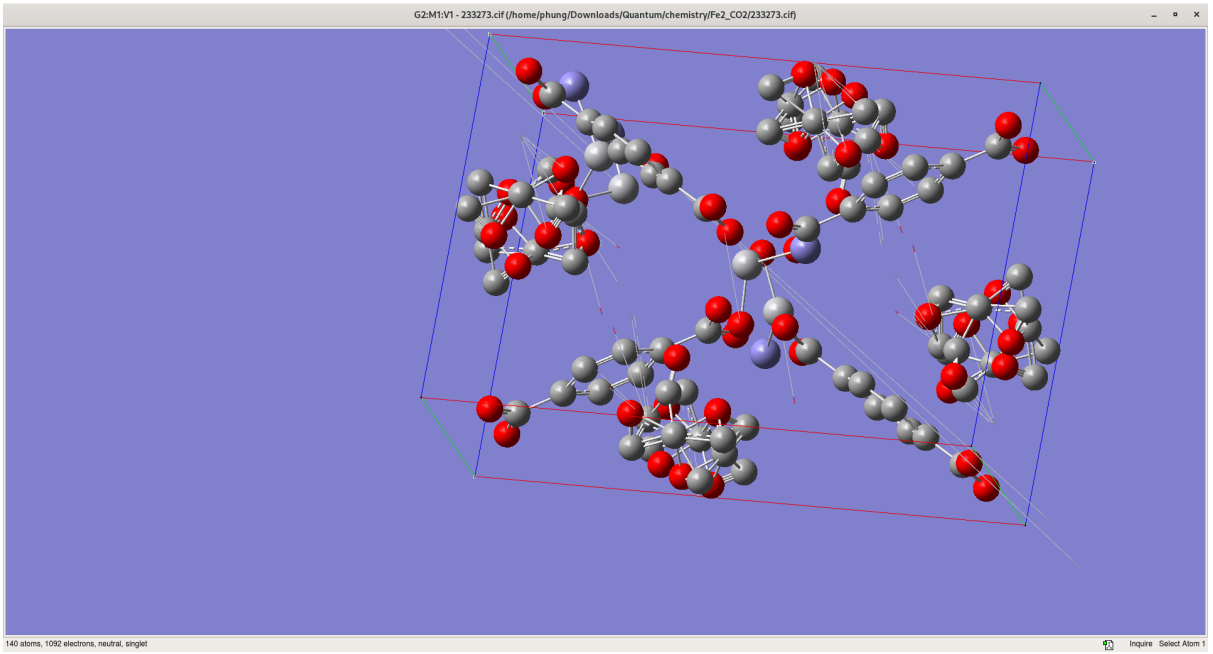


Image Quantistry Metal Organic Framework.

Cu-MOF-74 for N2 absorption has another formula: C24H6CuMg5N2O18

Cu-MOF-74 for H2O absorption: C24H8CuMg5O19

We also tried MIL-53 which is based of Fe2+ , but given the molecular compound complexity, Gaussian16 computation quickly runs into out-of-memory issues. In light of this, we feel that it might be more feasible to use a different wavefunction or incremental FCI methodology.



References

https://www.ccdc.cam.ac.uk/structures/Search?Compound=MIL-53&DatabaseToSearch=Published

https://www.linkedin.com/posts/feiphung_chemistry-computationalchemistry-compchem-activity-7027200867992821760-8Ret

Task 2B

Problem

Discuss the requirements for your solution to 2A to be implemented in real quantum computers and give an estimate for the time horizon at which it may become feasible.

Solution

We have implemented the pipeline on calculating the binding energy using BOPES (refer to Github on the full BOPES pipeline), which includes our call to IBM's real quantum computer providers, matching the suitable no. of qubits as per initial circuit and no. of element conditions, using that we triggered the options on transpiler optimization level as well as noise resilience levels via the AerEstimator primitive circuits before calling the VQE algorithms.

The CO2 solution's implementation on a real quantum computer requires approximately 60 qubits. If the number of qubits needed per 1g of CO2 would be log4(1.3 x 10^22) / log4 ~ 60 qubits then.

The larger MOF solutions implementation calculation we do not yet have.

One proposed solution to the computation problem is to use photonic computation that is using classical logic computation but in a photonic chip computing unit. The proposed computation unit would increase the computation speed. We are working with the design of these upcoming quantum chips.

Task 3

Problem

Give an overview of your research and the resources used during the challenge, provide *.csv or* .xls files for all data resulting from the calculations in your report and supply your comprehensively commented code

Solution

Final quantum computing notebook with Variational Quantum Eigensolver approach.
https://github.com/buttercutter/quantum-climate-challenge-2023/blob/main/notebooks/deloitte_2023_quantux.ipynb

Quantistry reference calculations for combination molecules in csv and coordinate data.
https://github.com/buttercutter/quantum-climate-challenge-2023/tree/main/notebooks/quantistry

Quantux solution presentation
https://github.com/buttercutter/quantum-climate-challenge-2023/blob/main/deloitte_2023_quantux_presentation.pptx