

Quantum Climate Challenge 2023

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Deloitte's Quantum Climate Challenge 2023 - Direct Air Capture

Goal of the Challenge

Deloitte's Quantum Climate Challenge 2023 aims to investigate how quantum computers may help to improve materials used in direct air capture (DAC) of carbon dioxide (CO_2).

In particular, it will be evaluated how metal organic frameworks (MOFs) can be leveraged in DAC by calculating the potential energy surface of atmospheric gas molecules (CO_2 , H_2O , N_2) in the vicinity of the MOFs' preferential binding sites.

Further, a general concept to calculate the ideal CO_2 binding capacity per filter volume of MOFs on near term quantum computers will be developed. Based on the findings, it will be estimated what is needed for quantum hardware to solve this problem at scale and when this hardware might be available.

Due to the limitations of currently accessible quantum hardware, the goal of the challenge is twofold:

Task 1

An efficient way to evaluate the binding energy within a system of highly reduced complexity is to be found and evaluated on current quantum computing hardware. Here, the focus lies on developing or improving an algorithm that efficiently and accurately calculates the potential energy surface for chemical systems related to carbon dioxide capture using MOFs.

Task 2

A path towards solving more and more complex versions of the problem shall be devised. Here, the focus lies on developing a concept for quantum or hybrid methods that may assist the improvement of MOFs for DAC on further advanced quantum computers.

This document provides background information on the relevancy of direct air capture, on the role MOFs may play in DAC, and a brief introduction to quantum simulation.

Carbon Capture as a Necessity to Combat Climate Change

The increase in global temperature and alterations of weather pattern are an undeniable reality today. One driving factor of this human-made climate crisis is the increase of the amount of CO₂ in the earth's atmosphere. The CO₂ concentration in the earth's atmosphere has increased from a pre-industrial level of 280 parts per million to more than 410 parts per million today. In pre-human ages it would take between 5000 to 20000 years to see a similar increase in CO₂ levels than what humans have caused in the last 60 years.¹ This leads to a vast increase in near-surface temperature of earth since CO₂ absorbs sunlight that would otherwise be reflected into space, effectively acting as a temperature trap. This in turn has devastating effects on the whole earth system.

It is therefore of utmost importance to drastically reduce anthropogenic CO₂ emissions to slow down climate change. During the Paris Climate Conference (COP21) the member countries of the United Nations Framework Convention on Climate Change (UNFCCC) agreed to take all necessary actions to keep the projected increase of the mean global temperature well below 2°C in the year 2100 as compared to pre-industrial 1900. This amounts to a calculated remaining carbon budget for a 50% likelihood to limit global warming to 2°C of 1270 GtCO₂ from the beginning of 2022, equivalent to 32 years assuming 2021 carbon emission levels. To reach net-zero CO₂ emissions by 2050, anthropogenic CO₂ emissions need to be cut by about 1.4 GtCO₂ [Friedlingsstein2021]

Even if all measures were taken to achieve net zero emissions, current models predict, that humanity will overshoot this CO₂ budget. Hence, to achieve the 2°C goal, carbon dioxide removal (CDR) from the

atmosphere is necessary. The IPCC (Intergovernmental Panel on Climate Change) estimates the need for CO₂ removal per year at about 10 GtCO₂ by the year 2050 to still achieve the goals stated in the Paris agreement.²

Today, CDR is far from mainstream, but interest is spiking. For instance, Microsoft has committed to become carbon negative by 2030 investing \$1 Billion to get there^{3,4} the XPRIZE foundation together with Elon Musk has announced a \$100 Million prize to scale DAC beyond the GtCO₂ scale⁵ and European direct air capture company Climeworks has recently raised \$ 650 million in funding.⁶

As of today, several approaches to remove CO₂ from the atmosphere are pursued. Some of the most prominent ones are outlined here.

Afforestation

Since plants convert sunlight and CO₂ to biomass, planting trees where there were none before presents the most intuitive approach of capturing CO₂. While the simplicity of this approach has its merits, its impact is unfortunately limited. An average tree amounts for 0.025 tCO₂ captured each year. This is roughly equivalent to needing to plant 192 trees per person, or approximately 1.5 trillion trees in total, to account for today's emissions. The best estimate for the CO₂ reduction potential of afforestation in 2050 is 0.5-3.6 GtCO₂/year.⁷

Bioenergy with carbon capture and storage (BECCS)

Following the same rationale as afforestation, in this approach plants are used to capture CO₂ out of the atmosphere. The biomass is then collected and combusted while capturing the emissions from the combustion and supplying heat energy as

a resource. Here, the focus lies on rapidly growing plants and plants that efficiently turn CO₂ into biomass. One of the advantages of this approach is that BECCS generates a tradable resource that can generate profits that help pay for the costs of carbon capture. The best estimate for the CO₂ reduction potential of BECCS in 2050 is 0.5-5 GtCO₂/year.⁷

Enhanced Weathering

The reactions certain minerals undergo with water and air – also called weathering – is another natural process that captures CO₂ from the atmosphere. This process can be technologically enhanced, e.g., by increasing the air exposed surface of the mineral which can be achieved by finely grinding rocks and spreading the ground minerals on a surface. The best estimate for the CO₂ reduction potential of BECCS in 2050 is 2-4 GtCO₂/year.⁷

Ocean fertilization

The earth's oceans represent one of the largest CO₂ sinks, mainly due to the algae that grow there. Promoting their growth by fertilizing the earth's oceans shows a great potential to capture CO₂ due to the large area of the earth's oceans. However, it comes with several side effects, such as, e.g., alteration of local to regional food cycles by phytoplankton production. Estimates for the CO₂ reduction potential vary to a great extend – ranging from <0.01 GtCO₂/year up to 98 GtCO₂/year.⁷



Direct Air Capture

A technical solution that does not rely on natural processes to capture CO₂ from the atmosphere is called direct air capture (DAC). In DAC, an engineered CO₂ filter is placed behind a fan that draws in air. The filter material is designed to specifically bind CO₂ molecules, ideally without capturing other atmospheric gas molecules that would otherwise clog the filter. When the filter is saturated, it is heated in a closed compartment to release the captured CO₂ in a controlled manner. The released CO₂ is then captured and stored or transformed to high value-added chemical compounds or fuels. The regenerated filter is afterwards used again to capture CO₂ from the atmosphere. This whole process is illustrated in Figure 1.

Due to the enhanced movement of air and the potentially high amount of CO₂ that can be captured per area this technical solution is more area and time efficient than biomass-based solutions.⁸

Fans draw in air from the atmosphere through a filter that captures CO₂. The filter compartment is subsequently closed, and the captured CO₂ is released in a controlled fashion.

As of today, 15 direct air capture plants are in operation in the EU, US and Canada. In total, they capture around 9000 tCO₂/year. So far, most of these plants serve as demonstrators of the technology and industrial scale-up of the process still needs to be shown.

One of the most significant challenges for the technology is connected to its energy need. For one, CO₂ is very diluted in the earth's atmosphere. Hence, a large volume of air must be passed through the filter to capture a significant amount of CO₂. The operation of these fans as well as the heating cycle to regenerate the filters is very energy consuming. Due to the two-phase process of capturing and releasing CO₂, the ratio of capture time and release time is directly related to the capacity of the filter. Hence, filters with a large CO₂ adsorption capacity are highly sought after.

Leveraging the potential of quantum computers to improve the filters used in DAC of atmospheric CO₂ is at the center of this challenge.

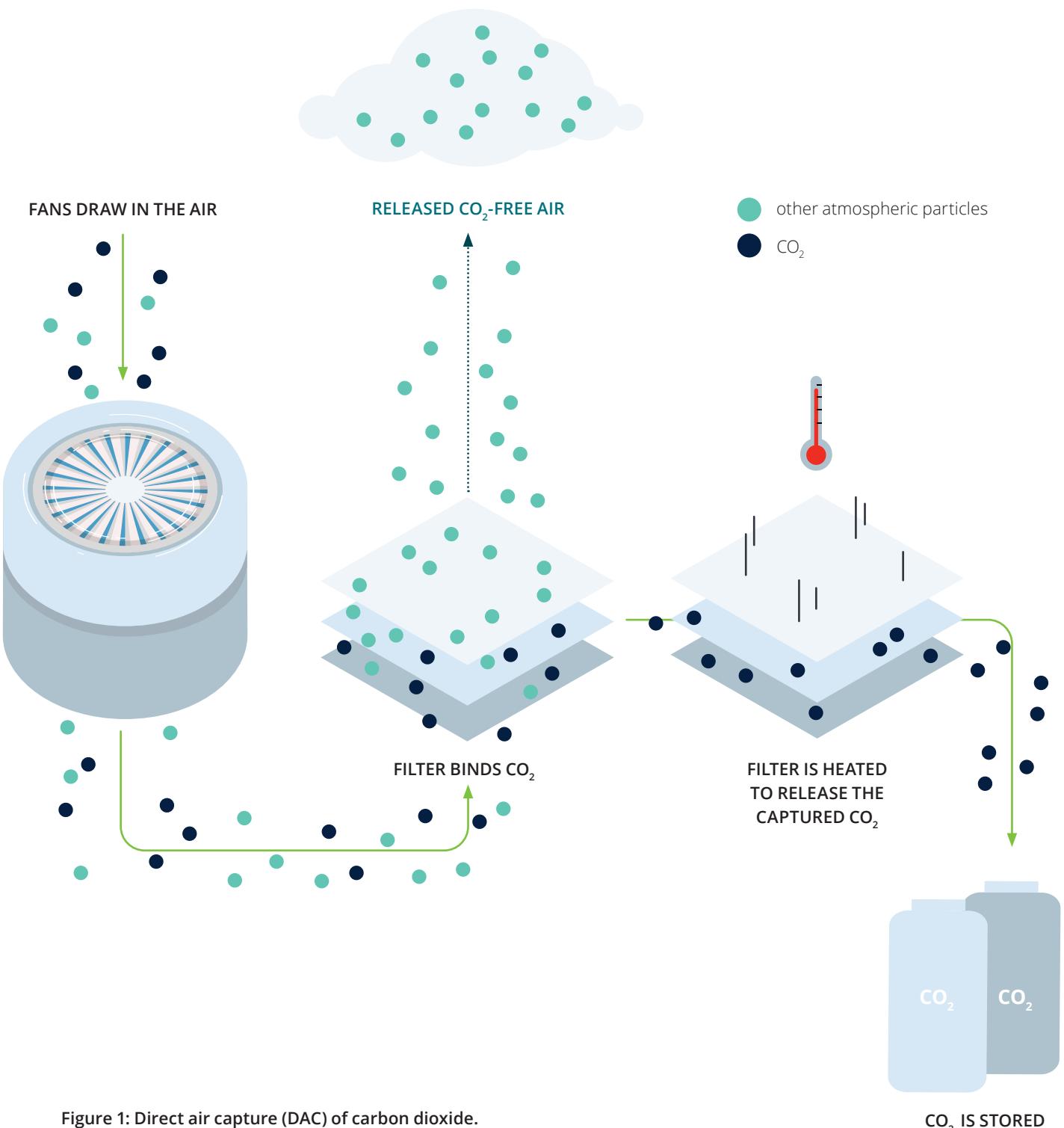


Figure 1: Direct air capture (DAC) of carbon dioxide.

CO₂ IS STORED

Metal-Organic Frameworks as CO₂ Filters

Several materials and technologies for the adsorption of CO₂ have been developed over the years, they involve the use of metal oxides, zeolites, activated carbons, fluorinated solvents, molecular sieves, and metal-organic frameworks (MOFs).

MOFs are often crystalline compounds that are constituted of metal ions or metal ion clusters coordinated to organic ligands, forming three-dimensional, porous structures.

Their typically high surface area, tunable pore size and low heat capacity have put MOFs in the spotlight for carbon capture applications. Their structures have to be specifically designed to ensure high CO₂ uptake capacity and selectivity towards CO₂, high stability in production and regeneration at reasonable energy cost. To be considered a competitive filter material, MOFs need to demonstrate a CO₂ adsorption

capacity of 3.0 mmol/g or higher. First pilot-scale demonstrators of MOF-based DAC already show great potential, with regeneration energy consumptions as low as 1.6 kWh / kgCO₂ and at an estimated operational cost below US\$ 350 per tCO₂.⁹

To accelerate material development, electronic and structural information obtained via computational chemistry are crucial.^{10, 11, 12}

Among the known MOFs, so called MOF-74 type analogs are of particular interest, since they present open metal sites (OMSs), that can act as CO₂ adsorption sites, within hexagonal channels aligned along one axis. Within those MOFs, one mechanism of CO₂ capture is the formation of M-OCO complexes (where M is the metal, O oxygen and C carbon). Figure 2 shows such complex formation within one unit cell of the MOF-74 analogue Mg/DOBDC.¹³

MOF-74s are constituted of divalent

metallic cations and the organic ligand 1,5-dihydroxybenzene-1,4-dicarboxylate (DOBDC). A wide diversity of combinations of divalent metallic cations and organic ligands with both larger sizes and added functional groups leads to many possible MOF-74 analogues with similar expected properties. Figure 3 shows their general chemical structure, including some exemplary linker molecules. MOF-74 type analogues differ in the metal ion used as CO₂ binding site as well as in the organic linker molecule that determines the relative locations of these binding sites. Both are likely to greatly influence the MOFs CO₂ adsorption capacity. For instance, length of the organic linker affects the pore size of the MOF and thereby potentially influences the carbon dioxide uptake and the required energy to regenerate the filter. It might also affect the water uptake and thereby the specificity of the filter to bind CO₂ over H₂O.

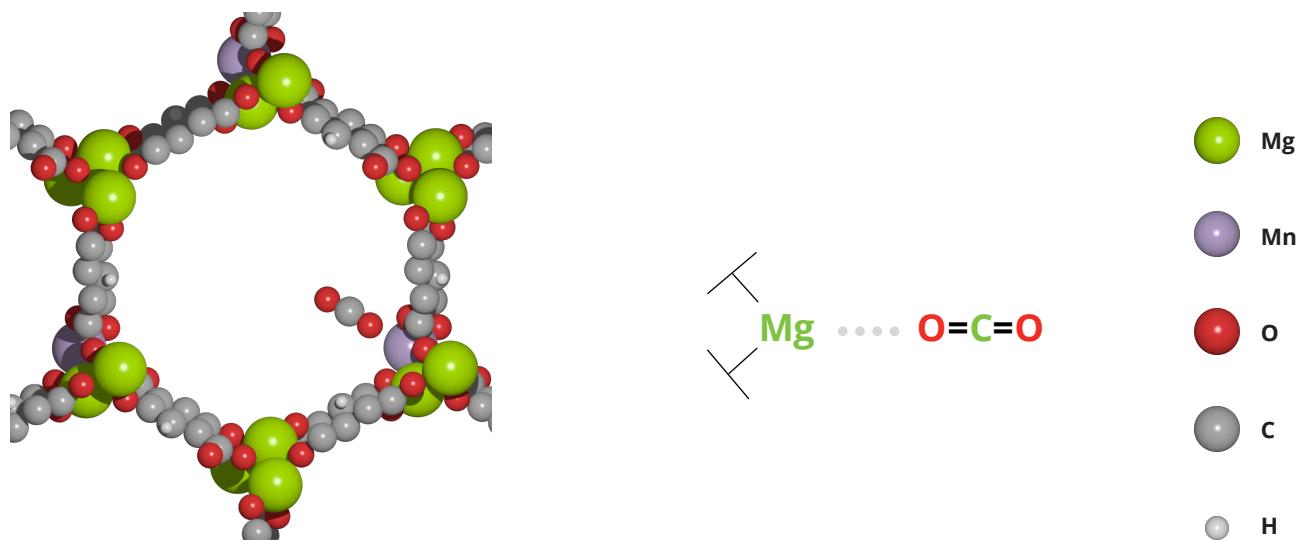


Figure 2: MOF-74 analogs for CO₂ capture: Left: 1D structure of the hexagonal unit cell. Right: Proposed CO₂ absorption mechanism of Mn-MOF-74 (adapted from [30], [31]).

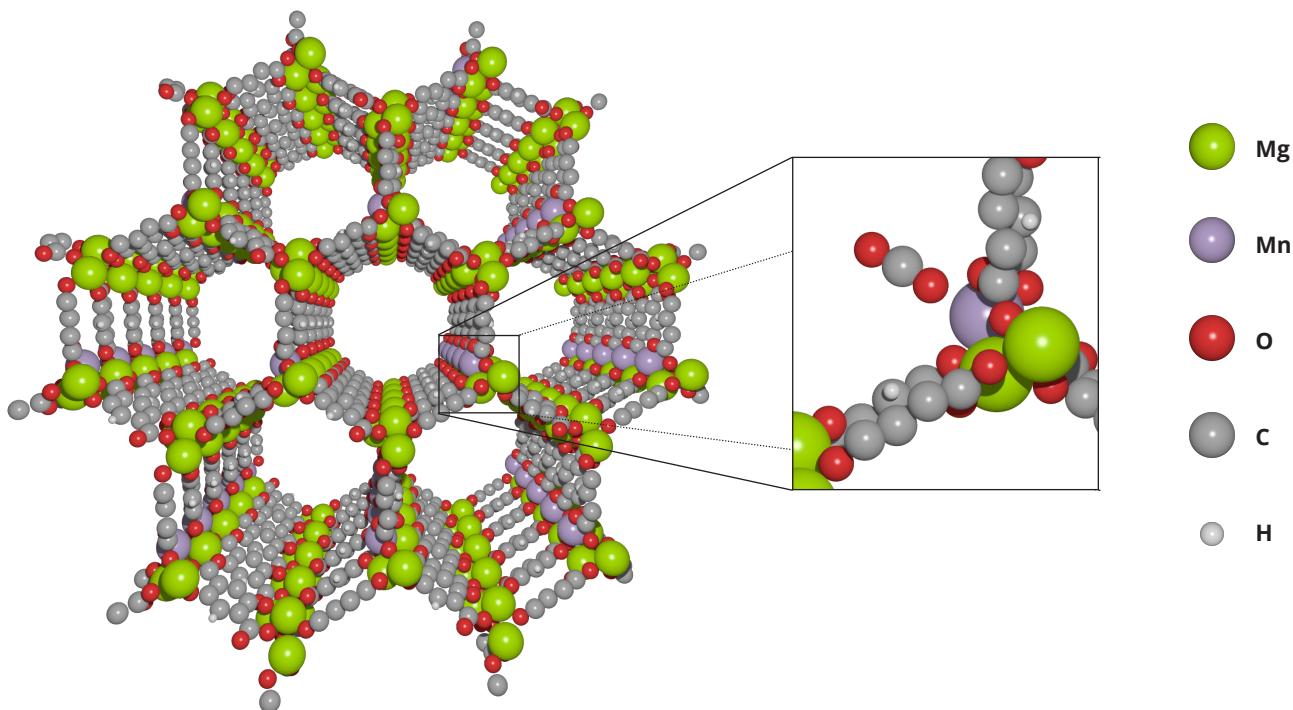


Figure 3: 3D structure of a group of MOF-74 unit cells repeated in two directions. The figure exemplifies the hexagonal channels aligned along the c-axis as well as their hexagonal dense packing. C-stacked unit-cells and integration of metal ion clusters in multiple unit cells are among the added complexities when considering a larger crystal as compared to one unit cell (adapted from [30], [31]).

To explore the feasibility of accelerating carbon capture MOF development using quantum computing in this challenge the potential energy surfaces in MOF-74 type analogs is calculated.

Task 1 of the challenge is to efficiently calculate the potential energy surface of a system of MOF constituents and atmospheric gas molecules, exploring which calculations are already possible on today's quantum computers and

comparing them to classical quantum chemistry calculations. Some proposed simplifications of the chemical problem to make it more tangible are given in the Chapter Task Description.

Task 2 focuses on developing a scheme to calculate the carbon dioxide uptake and evaluating the potentially accelerated development of MOFs for DAC when using more advanced quantum computers in the future.

Quantum Chemistry on Quantum Computers

The calculation of the ground state energy of a Hamiltonian is a ubiquitous challenge in classical quantum chemistry.

The wave function ψ is a complex-valued probability amplitude that all possible results of measurements made on a quantum-mechanical system, e.g., a charge carrier, can be derived from.

For instance, the probability density $\rho = |\psi|^2$ relates to the probability to find an electron at a given location in space. The energy levels of a molecule can be calculated as eigenvalues of the molecular Hamiltonian \hat{H} in the time-independent Schrödinger equation:

$$\hat{H}\psi(\vec{r}_1, \dots, \vec{r}_N) = E\psi(\vec{r}_1, \dots, \vec{r}_N)$$

where \vec{r}_i are the location vectors to all electrons and E is the energy of the system. The molecular Hamiltonian is constituted of operators describing the kinetic energy, the potential energy, and the electron-electron interaction energy. Since the electron-electron interaction energy includes the interaction between all electrons, this term grows exponentially with the number of electrons in a system. Calculating the eigenvalue of this many-body problem is hence an exponentially growing computational challenge.

Methods to calculate the accurate solutions to the Schrödinger equation, such as the full configuration integration (FCI) method exist but have expectedly shown to scale exponentially with the number of atoms.¹⁴ In classical quantum chemistry, this scaling challenge is addressed using approximation schemes. After decades of research multiple methods balancing the trade-off between accuracy and compute

time have been proposed and routinely used to calculate molecular properties. Methods employed today include approximations of FCI based on coupled clusters (CC), such as the coupled cluster single and double excitations (CCSD), as well as mean-field methods such as Hartree-Fock (HF) and Density Functional Theory (DFT). A general-purpose, well-scaling and highly accurate electronic structure calculation method applicable to arbitrary molecules is, however, still lacking.¹ In 1982, Richard Feynman theorized that simulating quantum systems would be most efficiently done using another, more controllable quantum system.¹⁶ In a lecture he proposed the development of a quantum computer for quantum chemistry and is famously quoted:

Nature isn't classical, dammit,
and if you want to make a
simulation of nature, you'd
better make it quantum
mechanical, and by golly, it's a
wonderful problem, because it
doesn't look so easy.

– Richard Feynman¹⁷

Building a true quantum simulator has indeed turned out to be a dauntingly challenging task.

Now, more than 4 decades later, tremendous progress in isolating, manipulating, and detecting single quantum systems has moved Feynman's dream within reach. Today, quantum simulation – the simulation of quantum chemical properties using quantum computers – is widely believed to be one of the first applications where quantum computers will demonstrate a quantum advantage over classical computers. The Quantum Phase Estimation Algorithm (QPEA) was the first algorithm proposed to solve electronic structure problems leveraging the power of quantum computers. It can be used to compute

a precise eigenvalue of a Hamiltonian from a given approximated value. While QPEA can be used to calculate energy levels at very high levels of precision, it does so using quantum circuits of depths that are far beyond reach for near-term noisy-intermediate scale quantum (NISQ) hardware. [19]

Therefore, another algorithm is widely recognized as the 'flagship' of quantum simulation today: the Variational Quantum Eigensolver (VQE). It has emerged as a quantum-classical algorithm promising to solve the eigenvalue problem in polynomial time, while being feasible on NISQ hardware. The latter is due to the comparatively shallow circuits required for computation. Further, variational algorithms have shown to be resilient to noise in quantum hardware to some extent. This makes VQE one of the most promising near-term applications of quantum computing.

The following paragraphs give a broad overview over the VQE algorithm. This introduction is geared towards those, who are new to quantum simulation. It aims to provide a comprehensive starting point rather than an exhaustive review of VQE. Of course, VQE is just one way to tackle the challenge of electronic structure calculations via quantum computers. The tasks of the Deloitte's Quantum Climate Challenge 2023 can thus also be solved using other methods.

The VQE algorithm assumes the calculation of the ground state energy to be an optimization problem. The molecular Hamiltonian and a parameterized quantum circuit preparing the quantum state of the molecule serve as inputs,

whereas the expectation value of the Hamiltonian serves as the cost function to be minimized.

Finding the ground state of a given Hamiltonian is therefore equivalent with optimizing the circuit. In VQE, the optimization is carried out by a classical optimizer, while the cost function is evaluated by a quantum computer.



Richard Feynman¹⁸

The general steps to calculate the ground state energy using VQE are:

01: Construct the molecular Hamiltonian

First, the system the ground state should be calculated for has to be defined. For molecules, this starts by defining the specific geometry, i.e., the locations of all atoms in the molecule. Constructing the molecular Hamiltonian then involves finding specific operators and their weights between so called basis functions describing the physical problem. These basis functions represent individual single-particle degrees of freedom and span the solution space for the total energy associated with a wave function. For electronic structure calculations, these can for example be molecular orbitals from a prior mean-field calculation, plane-wave functions, or local atomic functions.

In quantum simulation frameworks this step can, e.g., include importing the geometry and picking a basis set as well as potentially choosing a classical chemistry framework to supply the prior computation of the orbitals.

02: Encode the Fermionic operators to Pauli operators

In step 1, fermionic asymmetry with respect to permutation of any two particles is often ensured by expressing the Hamiltonian in terms of fermionic operators. Since qubit registers on quantum computers can only measure observables expressed in a Pauli basis, a basis transformation of the fermionic operators to spin operators is required. This step is also referred to as encoding. It enables the measurement of

the expectation value of the previously constructed Hamiltonian on a quantum computer. The resulting qubit Hamiltonian can then be reduced further using tapering off methods based on symmetries.^{20, 21, 22} It can further be optimized to be hardware-efficient on a specific quantum computer.

Encodings that are commonly used and implemented in most quantum simulation frameworks include the Jordan-Wigner mapping and the Bravyi-Kitaev mapping.

03: Decide on a measurement strategy

For the execution on a real quantum computer, the expectation values of the operators have to be extracted from the trial wave function. Generally, to achieve a precision of $\epsilon, O(1/\epsilon)$ repetitions, or shots, are required. There are several techniques today, that reduce the number of required repetitions, to speed up the overall computation as much as possible. One such method uses an efficient weighting of the number of measurements across the operators.^{23, 24, 25}

04: Prepare a parameterized ansatz and prepare the initial state

To find the ground state of the molecular Hamiltonian, a trial wave function is prepared. The structure of the parametrized quantum circuit preparing the trial wave function is referred to as ansatz. Successful optimization of the ansatz parameters results in the trial states becoming a model for the ground state wave function of the chemical problem. A variety of ansatzes are generally possible. The choice of ansatz that fits the problem at hand is a key aspect of VQE.

The ideal ansatz spans a large class of states in the Hilbert space, has a low number of parameters that are linearly independent and do not show vanishing gradients, and has a low depth while still appropriately approximating the ground state wave function.

In quantum simulation frameworks, standard parameterized ansatzes, such as the unitary coupled clusters single and double excitation (UCCSD) are readily available to be constructed automatically.^{26, 27}

05: Optimize the parameters to get the ground state

Each parameter set results in a corresponding expectation value of the Hamiltonian. To move from the initial trial state to the ground state, the parameters of the chosen ansatz need to be updated iteratively until convergence. The optimizer chosen for this task has a critical effect on the speed of the overall computation since it directly impacts the number of measurements required per parameter set as well as the number of iterations required to reach convergence. It also affects the ability to reach convergence at all.^{28, 29}

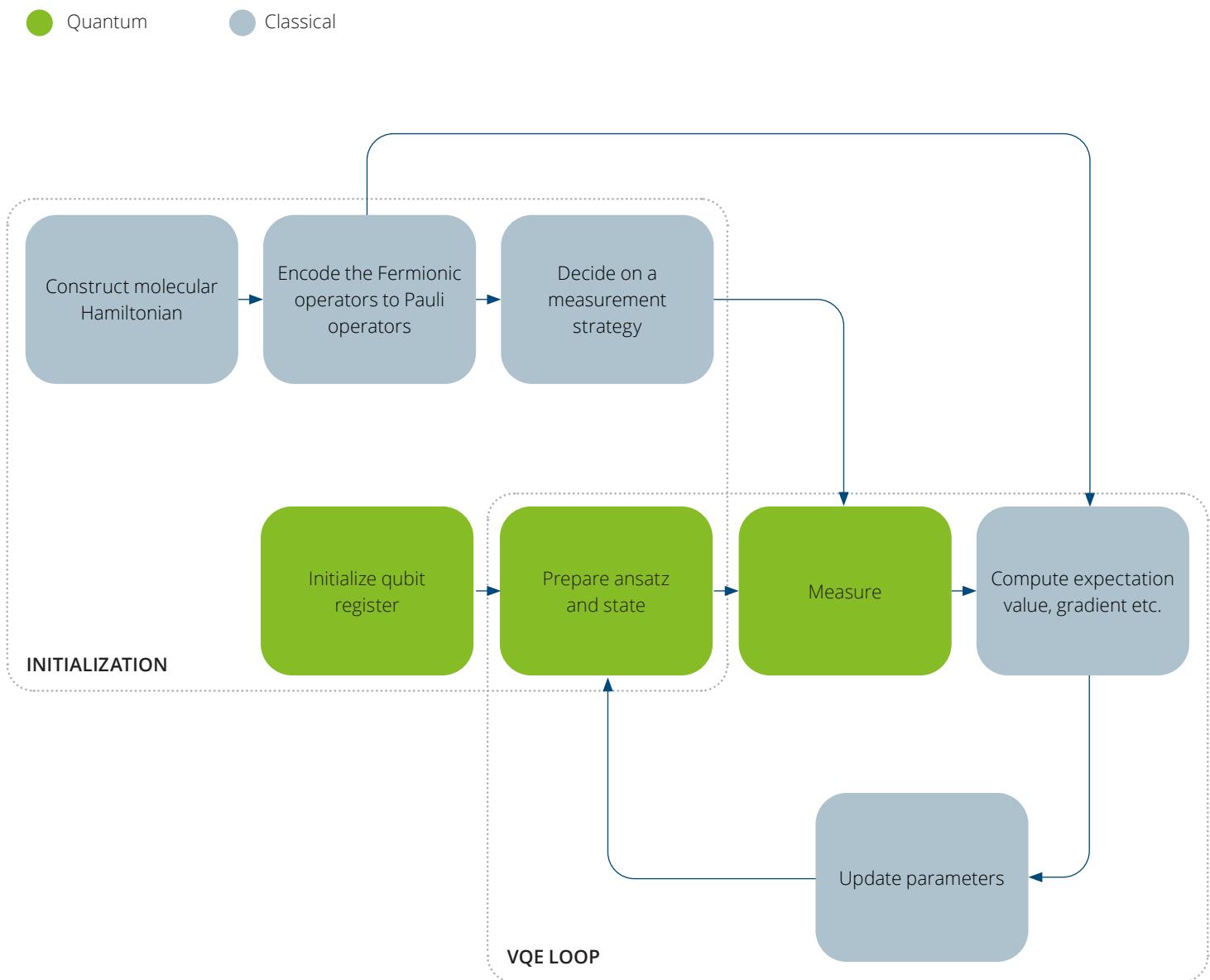


Figure 4: Schematic of the Variational Quantum Eigensolver (VQE), including its classical (grey) and quantum (green) components. The VQE loop is repeated until a convergence criterion is fulfilled or a fixed budget of quantum executions is used up.

The Potential Energy Surface

The potential energy surface (PES) describes the energy of a collection of atoms in terms of the position of the atoms. The surface can be defined as a function of one or more coordinates, e.g., positions, bond angles etc.

To sample the PES, all coordinates are sampled, and the ground state energy is determined using VQE at all combinations of sampled values. Then, the data can be interpolated and the configuration at which the total energy of the system is minimal can be determined. This is the most stable configuration of the system. A system of two atoms presents the simplest case for PES calculations, since the distance between the atoms is the only geometric coordinate of interest. Calculating the PES for H₂ is therefore often used as Hello world example in quantum simulation. (Note that the PES in 2D is sometimes referred to as *potential energy curve* or *energy profile*)

Introductions on how to perform this Hello world example in some of the most used, freely available chemistry frameworks can be found here:

[**Qiskit-Nature**](#)

by IBM
based on Qiskit

[**OpenFermion**](#)

by Google
based on Cirq

[**Q#Chem**](#)

by Microsoft
based on Q#

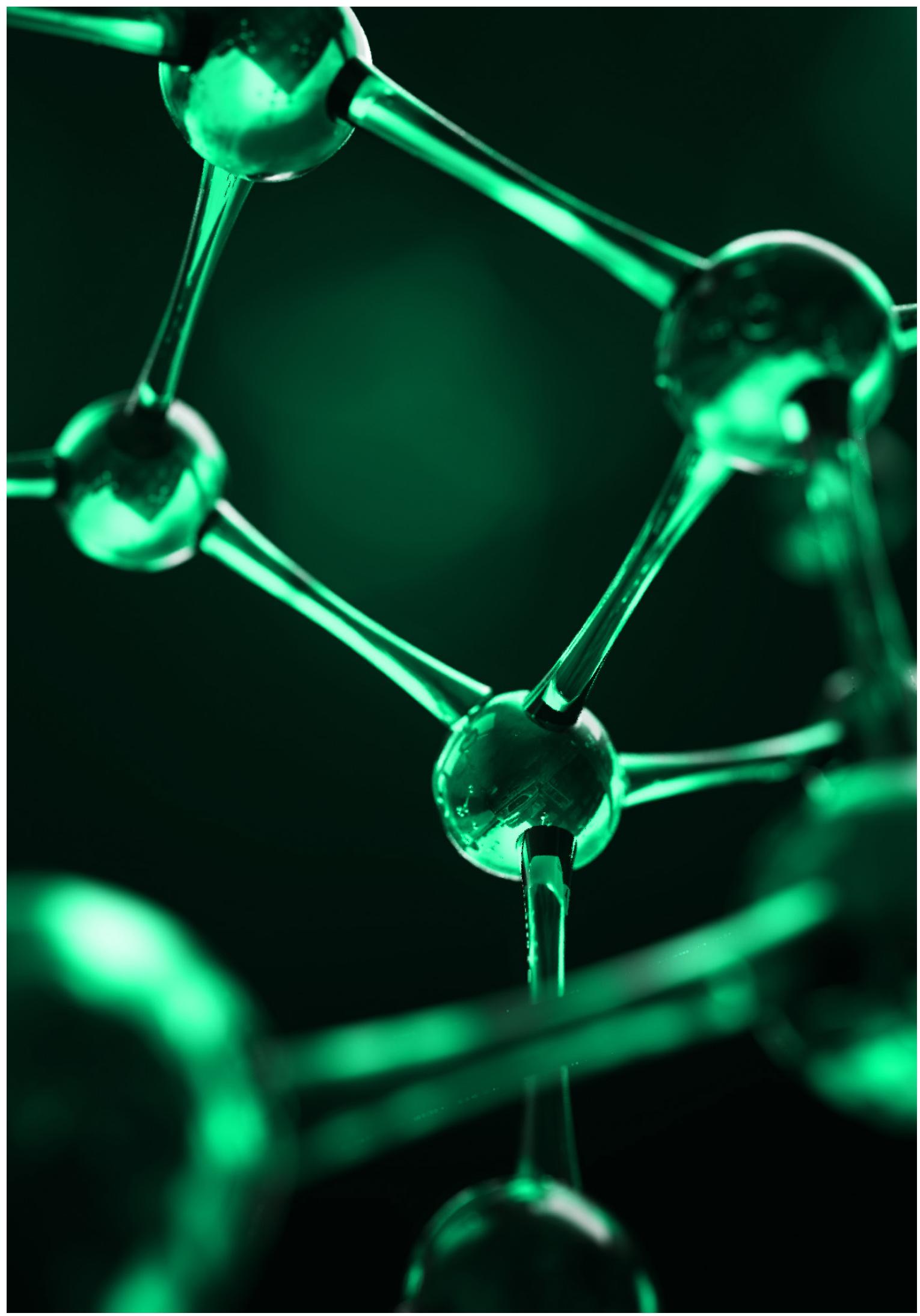
[**Qchem**](#)

by Xanadu
based on PennyLane

[**Braket**](#)

by Amazon
built with PennyLane-qchem

For a more detailed description of VQE, including some best-practices, the reader is referred to [Tilly et al.](#)²⁸



Tasks

Quantum chemical calculations can be performed using hybrid classical-quantum computation in a myriad of ways. For instance, there are multiple potential reduction schemes to reduce the chemical problem to a size that is feasible to compute on today's quantum computers. Further, hybrid algorithms offer multiple potential levers for optimization. For instance, the choice of a basis set, a molecular Hamiltonian to quantum Hamiltonian mapper, a circuit reduction scheme, an ansatz, and a classical optimizer are all levers to improve the performance of a Variational Quantum Eigensolver (VQE).

To reduce the complexity of the challenge to a level that is manageable in the given time frame, we provide some **guideposts**. These are meant as starting points, while encouraging independent exploration. Further, a non-exhausting list of ideas to increase the complexity of the problem and/or solution are given for each guidepost.

It is highly encouraged to analyze the problem as a whole and deviate from these guideposts to further improve performance of the calculations as well as to improve the fit of the calculated solution to the physical problem. Please clearly indicate where you chose to deviate from these guideposts and justify your choice. It is sufficient to solve the challenge using the guideposts. However, the more complex problem the solutions addresses the higher the chances to achieve a good ranking.



Task Summary

To successfully complete this challenge please complete the following tasks:

Task 1A

Create a quantum algorithm, a quantum hybrid or quantum inspired solution, that calculates the minimum of the potential energy surface of combinations gas molecules (CO_2 , H_2O , N_2) and ions (Mg^{2+} , Ni^{2+} , Fe^{2+} , Co^{2+} , Zn^{2+} , Mn^{2+} , Cu^{2+}). Pick at least one type of ion and calculate the PES for at least CO_2 and one more gas molecule. Run your algorithm on a quantum computer or simulator and supply some information on the resource requirements of your solution (e.g., total number of shots, compute time etc.)

Task 1B

Compare your solution to at least one classical solution, describing advantages and disadvantages of the approaches. Evaluate the performance differences of your solution versus the classical approach.

Task 2A

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. The goal is to calculate the amount of substance of CO_2 that can be captured per unit cell. Briefly discuss the limitations of your solution.

Task 2B

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. Requirements can be, e.g., the number of logical qubits needed, coherence times, external inputs like molecular geometries etc.

Task 3

Compile a report (as .pdf file) that includes a short problem statement and outline how you solved it. 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 (either in a repository or as file).

Details on how to access the simulators and quantum computers (on IBM Quantum and AWS Braket) as well as the Quantistry platform (to calculate the classical reference solution), as well as optimized geometries of the gas molecules can be found on the Confidential tab on the challenge webpage. It is only visible for registered participants.

Tasks 1,2 and 3 will be evaluated independently and each awarded 1-3 points.

The best solution for Task 1 and the best solution for Task 2 directly qualify for the pitch event. The remaining solutions will be ranked by average grade of all tasks (all weighted equally). The remaining spots for the pitch event will be awarded to the best overall solutions that are not already qualified.

Guideposts are given as an orientation to guide you towards one solution of a strongly reduced problem. It is sufficient to solve the challenge using all of them. Increasing the complexity of the problem your solution addresses will result in a better chance of winning the challenge.

Task Details and Guideposts

Predicting the carbon dioxide uptake of a MOF based on its chemical structure is a highly complex task. For a full picture a multi-scale simulation would be necessary, including Quantum Chemistry, Molecular Dynamics as well as fluid dynamics. In this challenge, the focus lies on Quantum Chemistry. Effects that can only be modelled using Molecular Dynamics or fluid dynamics are therefore disregarded. To further reduce the complexity of the problem for both tasks, assume that the molecular geometries stay fixed after the initial calculation. Specifically, they do not have to be optimized for each parameter sample.

Guideposts 1-1

Consider only the active binding site of

the MOF (the metal ion) and disregard the organic linker for your calculations.

Potential to increase the complexity:

- Include parts of the organic linker BOD..., or a whole unit cell of the material. You might need to come up with a suitable partitioning scheme and/or perform some of the calculations classically.
- Consider other potentially carbon dioxide capturing moieties, e.g., amine groups ($R-NH_2$, where R: rest, N: nitrogen, H: hydrogen) and calculate the PES for them as well.

Guideposts 1-2

Consider only one gas molecule in a fixed orientation and calculate the PES only versus the distance of metal ion and gas molecule.

For all molecules where all atoms lie on one axis (CO_2 , N_2), the molecule's main axis and the distance axis coincide. For H_2O , the line defined by the two H atoms is aligned with the distance axis. This is illustrated in Figure 5.

Potential to increase the complexity:

- Explore more geometric degrees of freedom (rotation/translation of the gas molecule around/along one axis or more). Each degree of freedom may be sampled at a different frequency.
- Consider more than one gas molecule of the same species and determine the PES dependent on their relative locations.
- Consider more than one type of gas molecule at the same time and determine the PES to determine which molecule is preferentially bound.

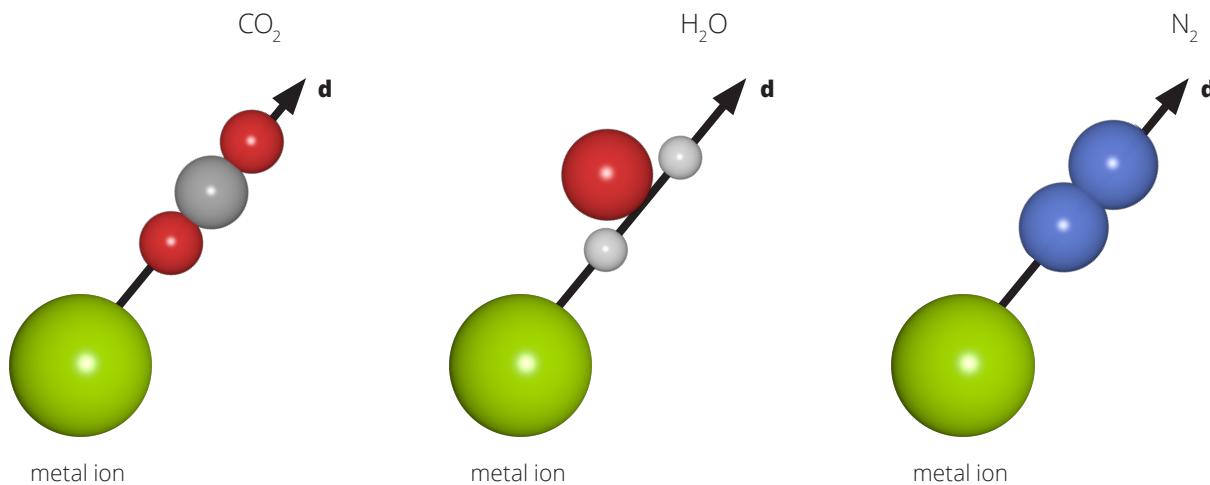


Figure 5: Definition of the distance axis for PES calculations. For N_2 and CO_2 the distance axis d and the molecular main axis are aligned, for H_2O the line defined by the two H atoms is aligned with the distance axis [31].

Guideposts 1-3

Use a Variational Quantum Eigensolver (VQE) to solve the problem. Start with a STO-3G basis set, use Jordan-Wigner mapping, a UCCSD ansatz and for the classical optimization part, use a Simultaneous Perturbation Stochastic Approximation (SPSA) optimizer. Freeze all inner electrons.

Potential to increase the complexity:

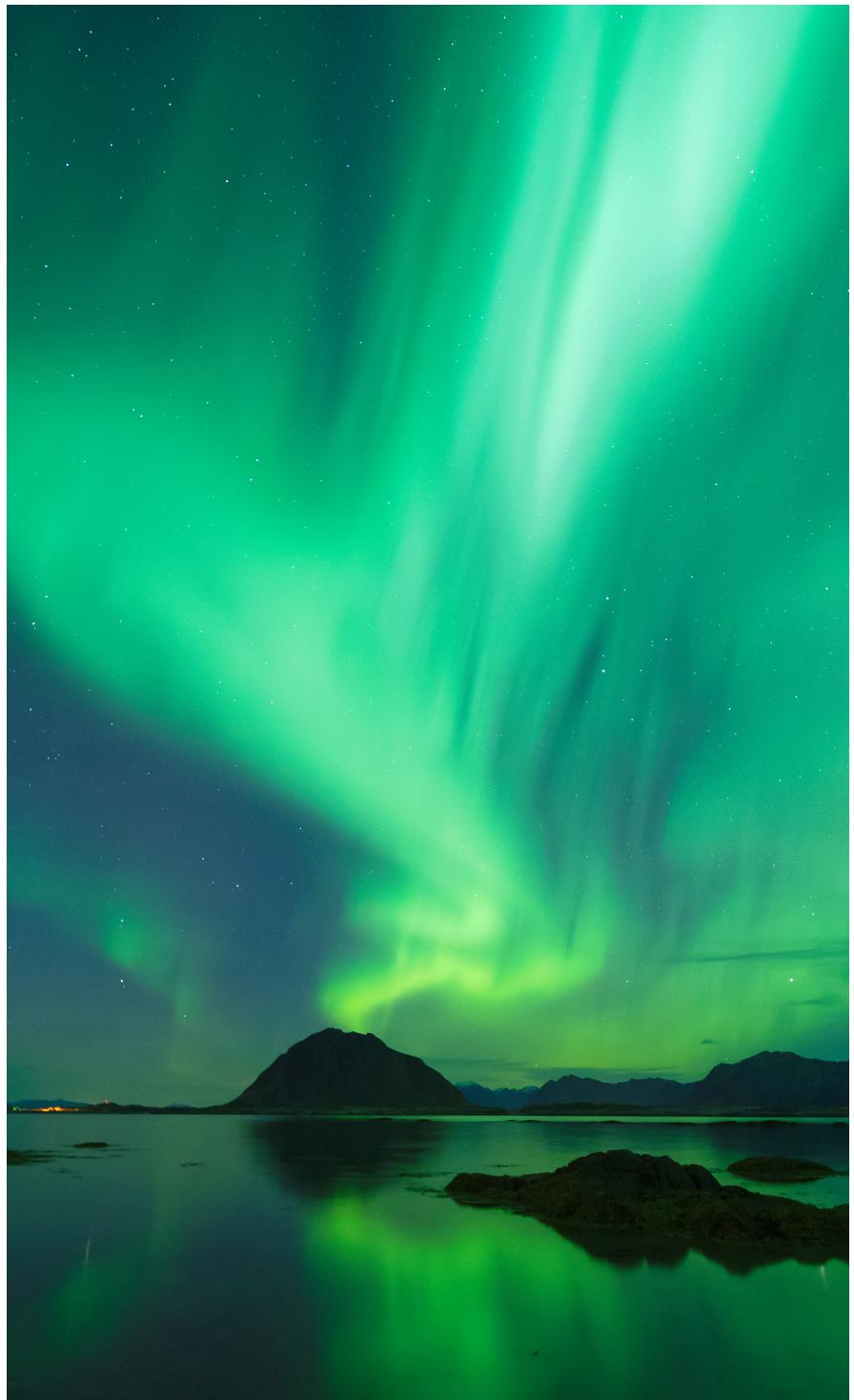
- Use a different basis set or basis set free method
- Explore different fermionic operator to spin operator mappings
- Taper the Pauli Hamiltonian to reduce the complexity of the circuit
- Choose different ansatzes or optimize the ansatz with respect to circuit complexity
- Optimize the circuit for specific hardware
- Choose the best optimizer for the problem at hand
- Pick your own measurement strategy to reduce the number of shots required
- Use a non-VQE approach to solve the problem

Guideposts for 2

Potential to increase complexity: All complexities proposed above also apply to Task 2.

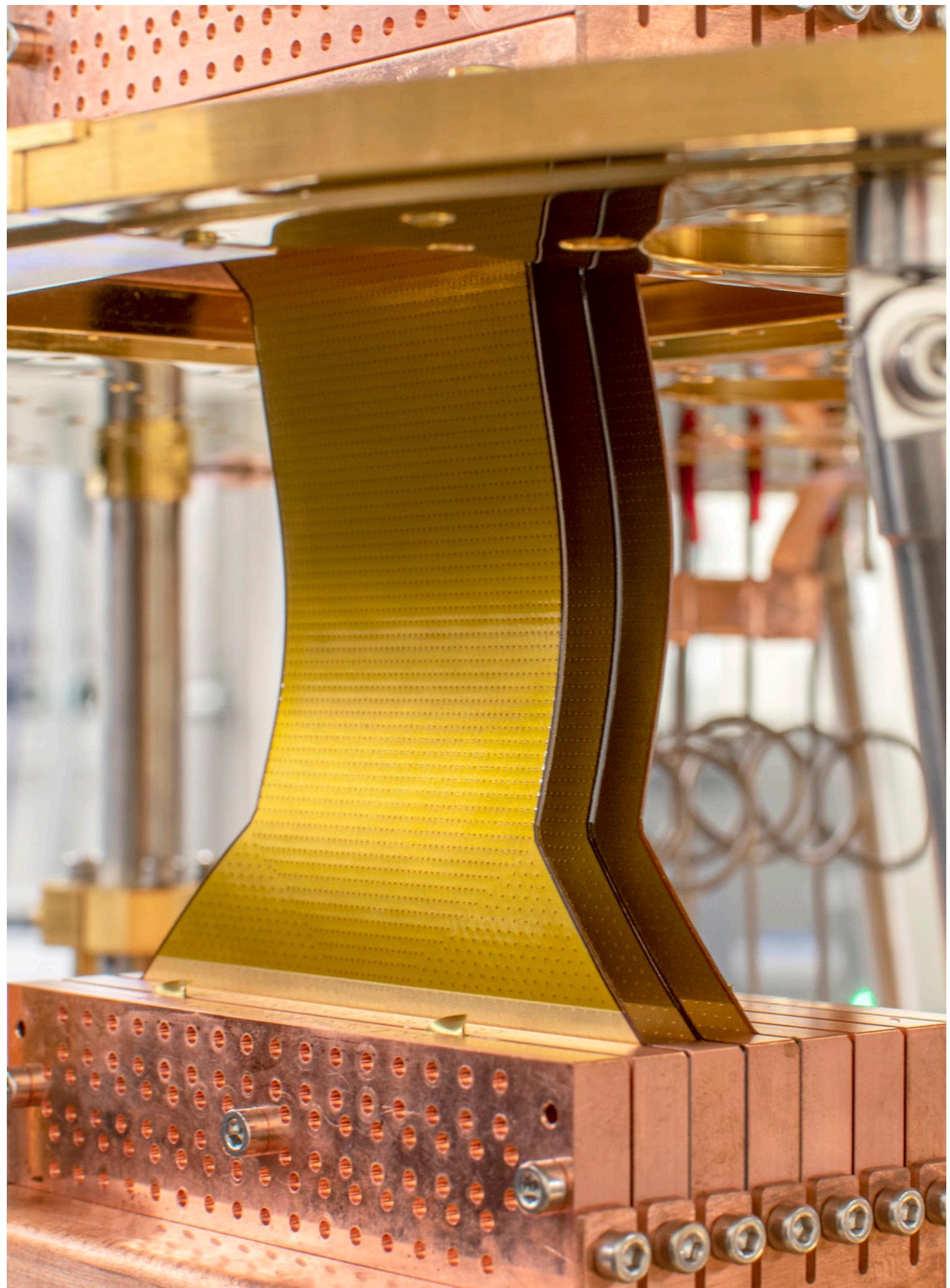
Additional complexity:

- Devise a scheme that automatically proposes a MOF that maximizes carbon adsorption under DAC relevant boundary conditions.



References

- ¹ "nationalacademies.org," 2022. [Online]. Available: <https://www.nationalacademies.org/based-on-science/climate-change-humans-are-causing-global-warming>.
- ² P. e. a. Friedlingstein, "Global Carbon Budget 2021," *Earth System Science Data*, vol. 14, pp. 1917–2005, 2022.
- ³ "Microsoft will be carbon negative by 2030," Microsoft Blog, [Online]. Available: <https://www.microsoft.com/en-us/corporate-responsibility/sustainability/climate-innovation-fund?activetab=pivot1:primaryr6>. [Accessed 17 October 2022].
- ⁴ "Microsoft Climate Innovation Fund," Microsoft, [Online]. Available: Climate Innovation Fund | Microsoft CSR]. [Accessed October 2022].
- ⁵ "\$100M Prize for Carbon Removal," XPRIZE Foundation, [Online]. Available: \$100M Prize For Carbon Removal | XPRIZE Foundation. [Accessed October 2022].
- ⁶ "CO2-Startup Climeworks sammelt halbe Milliarde Euro ein," Business Insider, [Online]. Available: <https://www.businessinsider.de/gruenderszene/perspektive/das-co2-star-tup-zweier-deutscher-bekommt-halbe-milliarde-euro/>. [Accessed October 2022].
- ⁷ S. e. a. Fuss, "Negative emssions --- Part 2: Costs, potentials and side effects," *Environmental Research Letters*, vol. 12, no. 064002, 2018.
- ⁸ K. Z. H.-J. G. P. Lackner, "Carbon Dioxide Extraction from Air: Is It An Option?," in 24th Annual Technical Conference on Coal Utilization and Fuel Systems, Clearwater, FL(US), 1999.
- ⁹ M. B. M. F. C. , T. N. W. H. H. T. Sadiq, "A Pilot-Scale Demonstration of Mobile Direct Air Capture Using Metal-Organic Frameworks," *Advanced Sustainable Systems*, vol. 4, no. 12, p. 2000101, 2020.
- ¹⁰ C. G. & L. S. Piscopo, "Strategies to enhance carbon dioxide capture in metal-organic frameworks..," *ChemPlusChem*, no. 85, pp. 538-547, 2020.
- ¹¹ H. & H. M. R. Li, "Low-energy CO₂ release from Metal-Organic Frameworks triggered by external stimuli," *Accounts*, vol. 50, p. 778–786, 2017.
- ¹² O. L. J. F. R. & W. C. Shekhar, "MOF thin films: existing and future applications..," *Chem. Soc. Rev.*, vol. 40, p. 1081–1106, 2011.
- ¹³ Y. Liu, J. Hu, X. Ma, J. Liu and Y. Lin, "Mechanism of CO₂ adsorption on Mg/DOBDC with eleveated CO₂ loading," *Fuel*, vol. 181, pp. 340-346, 2016.
- ¹⁴ T. Helgaker, P. Jorgensen and J. Olsen, *Molecular Electronic-Structure Theory*, John Wiley & Sons, 2014.
- ¹⁵ Y. e. a. Coah, "Quantum Chemistry in the Age of Quantum Computing," *Chemical Reviews*, vol. 119, pp. 10856-10915, 2019.
- ¹⁶ R. P. Feynman, "Simulating physics with computers..," *International Journal of Theoretival Physics*, vol. 21, no. 6-7, pp. 467-488, 1982.
- ¹⁷ A. Trabesinger, "Quantum simulation," *Nature Physics*, vol. 8, p. 263, 2012.
- ¹⁸ Copyright Tamiko Thiel 1984 (https://commons.wikimedia.org/wiki/File:Richard-Feynman-PaineMansionWoods1984_copyrightTamikoThiel_bw.jpg), „Richard-Feynman-PaineMansionWoods1984 copyrightTamikoThiel bw“, <https://creativecommons.org/licenses/by-sa/3.0/legalcode>
- ¹⁹ M. W. N. S. K. W. D. T. M. Reiher, "Elucidating reaction mechanisms on quantum computers..," *Proceedings of the National Academy of Sciences*, vol. 114, no. 29, p. 7555–7560, 2017.
- ²⁰ S. G. J. M. A. T. K. Bravyi, "Tapering off qubits to simulate fermionic Hamiltonians," 2017. [Online]. Available: <https://arxiv.org/abs/1701.08213v1>.
- ²¹ K. C. R. R. J. M. A. P. M. W. J. Setia, "Reducing qubit requirements for quantum simulations using molecular point group symmetries..," *Journal of Chemical Theory and Computation*, vol. 16, no. 10, p. 6091–6097, 2020.
- ²² W. T. A. L. P. Kirby, "Contextual subspace variational quantum eigensolver," *Quantum*, vol. 5, p. 456, 2021.
- ²³ D. H. M. T. M. Wecker, " Progress towards practical quantum variational algorithms..," *Physical Review A*, vol. 4, no. 92, p. 042303, 2015.
- ²⁴ N. B. R. M. J. Rubin, "Application of fermionic marginal constraints to hybrid quantum algorithms," *New Journal of Physics*, vol. 5, no. 20, p. 053020, 2018.
- ²⁵ A. C. L. S. R. C. P. Arrasmith, "Operator sampling for shot-frugal optimization in variational algorithms," 2020. [Online]. Available: [arXiv:2004.06252](https://arxiv.org/abs/2004.06252).
- ²⁶ Z. S. K. C. M. C. P. Holmes, "Connecting ansatz expressibility to gradient magnitudes and barren plateaus..," 2021. [Online]. Available: <https://arxiv.org/abs/2101.02138v1>.
- ²⁷ K. Y. N. Nakaji, "Expressibility of the alternating layered ansatz for quantum computation," *Quantum*, vol. 434, p. 5, 2021.
- ²⁸ J. e. a. Tilly, "The Variational Quantum Eigensolver: a review of methods and best practices," *Physics Reports*, vol. 986, pp. 1-128, 2022.
- ²⁹ K. F. K. T. S. Nakanishi, "Sequential minimal optimization for quantum-classical hybrid algorithms..," *Physical Review Research*, vol. 2, no. 4, 2020.
- ³⁰ A.S. Rosen, J.M. Notesteina and R.Q. Snurra, "Comparing GGA, GGA+U, and meta-GGA functionals for redox-dependent binding at open metal sites in metal-organic frameworks", *J. Chem. Phys.*, 152, 224101,2020.
- ³¹ Chemical visualizations (Figures 2, 3 & 5) provided by Quantistry.



IBM's new high-density control signal delivery with flex wiring to provide a 70% increase in wire density. Credit: Connie Zhou for IBM

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