Elvira SHISHENINA | Henri CALANDRA | Charles MOUSSA | Yuan YAO

Variational Quantum Eigensolver

Identification & validation of use-cases

Computing the ground state energy with VQE

A.Peruzzo et al. A variational eigenvalue solver on a quantum processor (2014). arXiv:1304.3061

TOTAL

VQE | electronic Schrödinger equation

Finding the ground state energy = solving an eigenvalue problem

$$\hat{H}|\Psi(\mathbf{R})\rangle = E(\mathbf{R})|\Psi(\mathbf{R})\rangle$$

intractable problem in general!

VQE | from fermions to qubits

I. Fermionic Hamiltonian

$$\hat{H}|\Psi(\mathbf{R})\rangle = E(\mathbf{R})|\Psi(\mathbf{R})\rangle$$

II. Second quantization

$$\hat{H} = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

III. Mapping from fermions to qubits – qubit Hamiltonian
(Jordan-Wigner or Bravyi-Kitaev transformation)

$$H_q = \sum_\alpha h_\alpha P_\alpha \,, \qquad P_\alpha = \sigma_1^{\alpha_1} \otimes \sigma_2^{\alpha_2} \otimes \ldots \sigma_N^{\alpha_N}$$

VQE | from fermions to qubits

OpenFermion

- open source library for compiling and analyzing quantum algorithms to simulate fermionic systems, including quantum chemistry.
- plugins available for electronic structure computation (Psi4, PySCF)

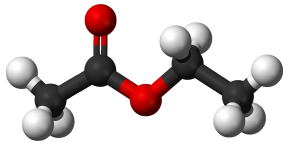
```
basis = 'sto-3g'
miltiplicity = 1
charge = 0


geometry = [('H',(0.,0.,0.)),('H',(0.,0.,bond_length))]
h2_molecule = MolecularData(geometry, basis, multiplicity, charge)
h2_molecule_psi4 = run_psi4(h2_molecule, run_mp2=True, run_ccsd=True, run_fci=True)
h2_qubit_Hamiltonian = jordan_wigner(get_fermion_operator(h2_molecule_psi4.get_molecule_hamiltonian()))

```

```
{(): 5.0607407984801229,
 ((0, 'X'), (1, 'X'), (2, 'Y'), (3, 'Y')): -0.039042564775674672,
 ((0, 'X'), (1, 'Y'), (2, 'Y'), (3, 'X')): 0.039042564775674672,
 ((0, 'Y'), (1, 'X'), (2, 'X'), (3, 'Y')): 0.039042564775674672,
 ((0, 'Y'), (1, 'Y'), (2, 'X'), (3, 'X')): -0.039042564775674672,
 ((0, 'Z'),): 0.30083789380435055,
 ((3, 'Z'),): -0.72647678971997243
 }
```


TOTAL

VQE | design

fermionic problem



qubit Hamiltonian

$$H_q = \sum_\alpha h_\alpha P_\alpha$$

optimize

prepare trial state QPU

$$|\Psi(\boldsymbol{\theta})\rangle$$

measure expectation value

$$h_\alpha \langle \Psi(\boldsymbol{\theta}) | P_\alpha | \Psi(\boldsymbol{\theta}) \rangle$$

calculate energy CPU

$$E_q(\boldsymbol{\theta}) = \langle \Psi(\boldsymbol{\theta}) | H_q | \Psi(\boldsymbol{\theta}) \rangle = \sum_\alpha h_\alpha \langle \Psi(\boldsymbol{\theta}) | P_\alpha | \Psi(\boldsymbol{\theta}) \rangle$$

adjust parameters

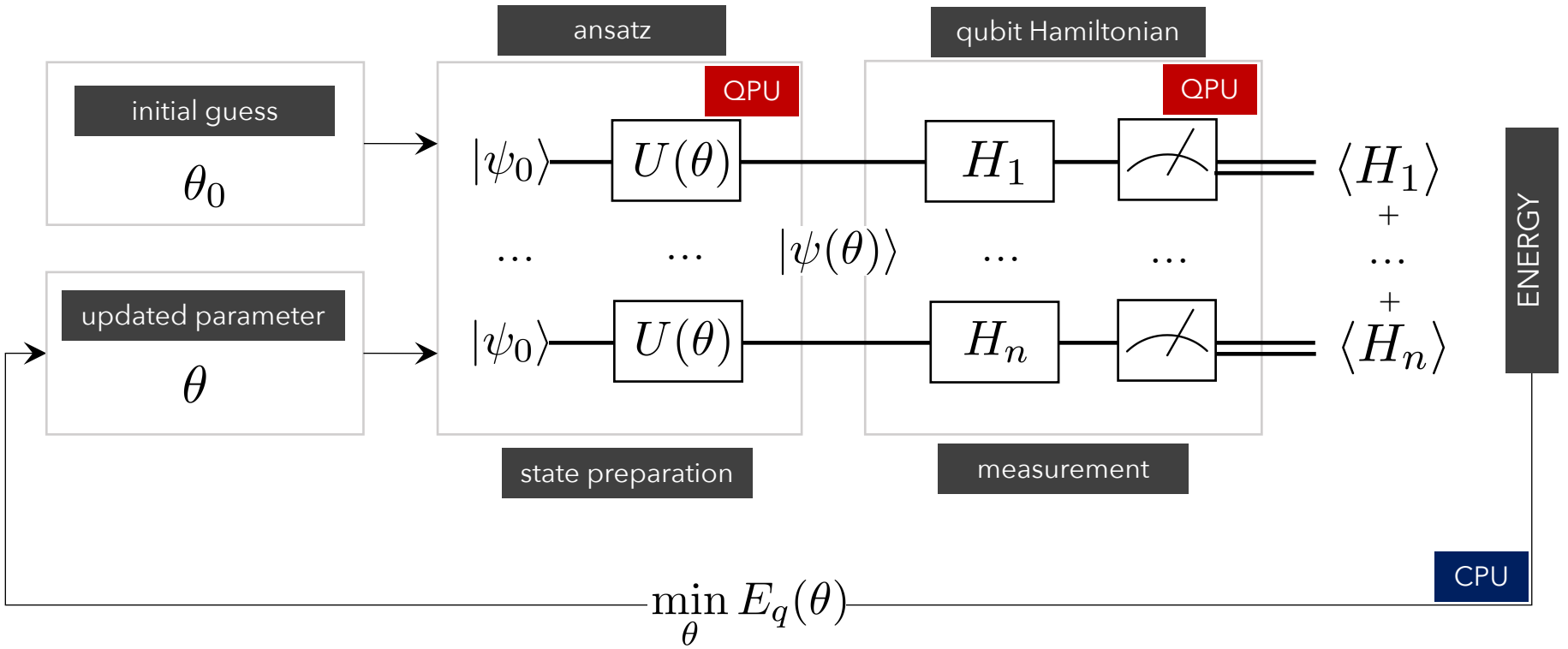
$$(\boldsymbol{\theta})$$

solution

$$E_q^{\min}$$

TOTAL

VQE | optimization loop



TOTAL

VQE | design

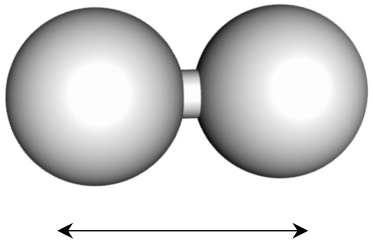
VQE library

```
from qat.linalg import get_qpu_server
from molecular_vqe.vqe import VQE
from molecular_vqe.ansatz import RYRZ
qpu = get_qpu_server

# define VQE parameters
number_qubit = 10
depth = 3
num_shots = 500
maxiter = 500
minimizer = 'COBYLA'

ansatz_ryrz = RYRZ(number_qubit, depth=depth)
vqe = VQE(number_qubit, qpu, openfermion_dict,
          ansatz_ryrz, minimizer=minimizer,
          num_shots=num_shots, maxiter=maxiter)

# run VQE
param_run = np.random.rand(ansatz_ryrz.get_num_parameters())
energy = vqe.run_minimize(init_params = param_run)


```


TOTAL

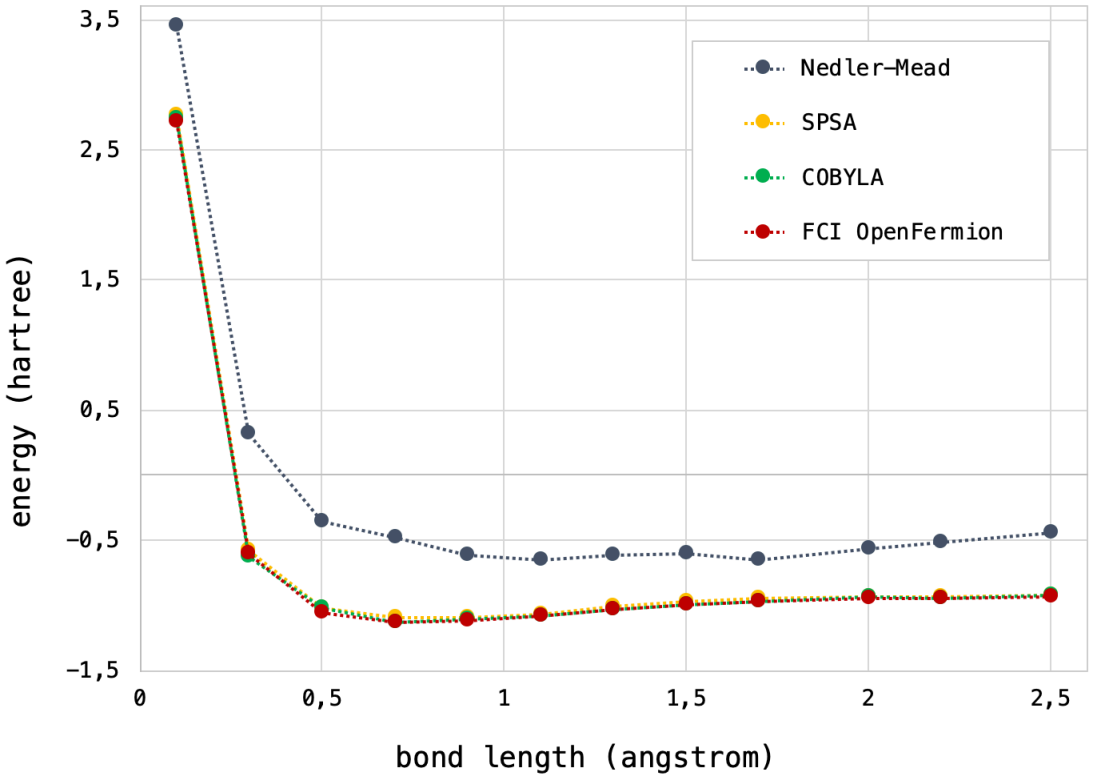
VQE | benchmarking

H_2



bond_length

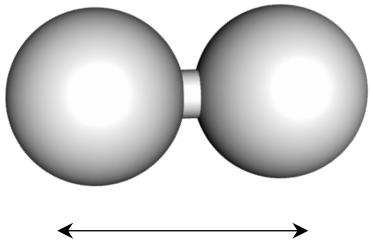
```
charge = 0
multiplicity = 1
basis = 'sto-3g'
number_qubit = 4   # bravyi-kitaev
```



TOTAL

VQE | benchmarking

H_2



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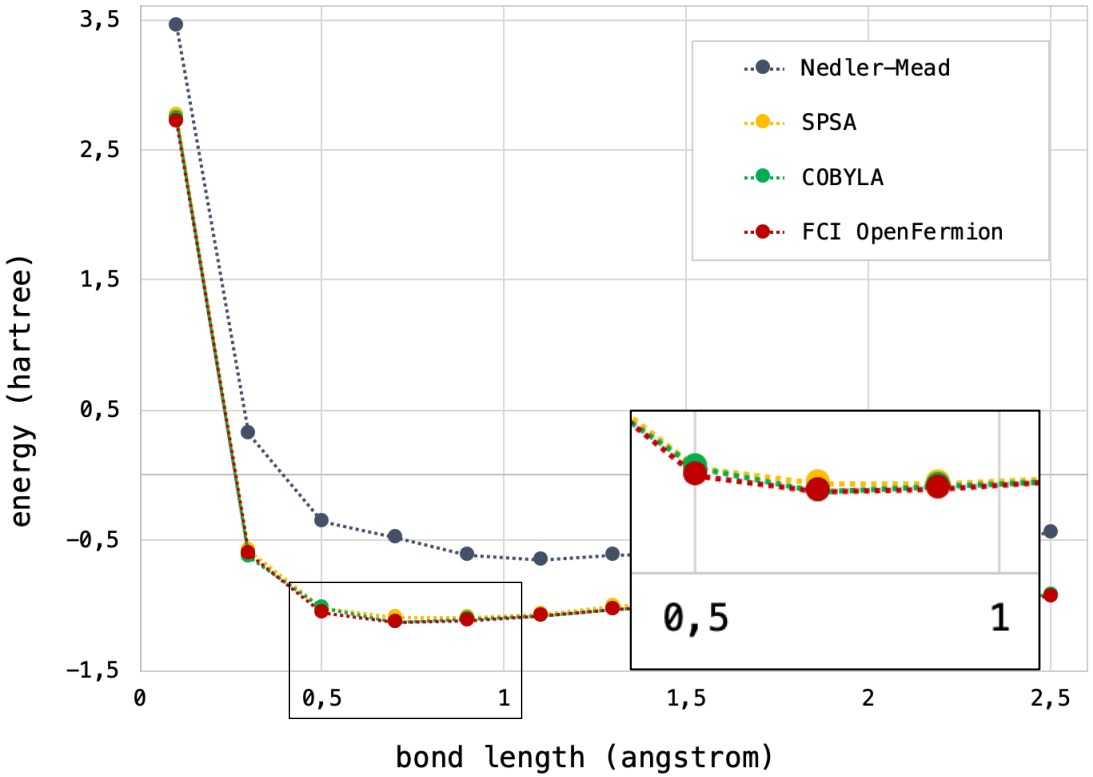
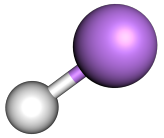
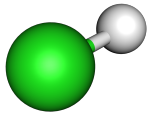
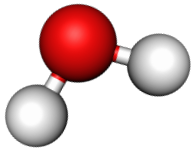
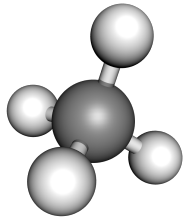
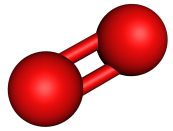
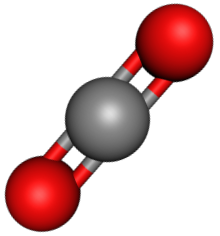
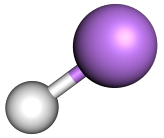
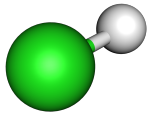
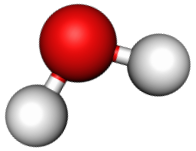
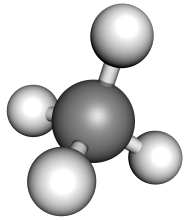
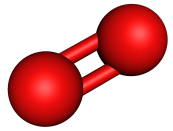
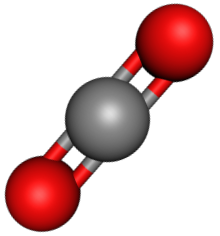


VQE | benchmarking

ground state energies						
	LiH	BeH	H_2O	CH_4	O_2	CO_2
VQE Total	-7.75927010033	-14.4365668914	-72.9137048216	-38.9700162812	-144.2795640017	-179.930380621
VQE Atos	-7.79160864682	-14.6002137511	-73.1510280024	-39.1240178446	-144.1520719862	-180.918374772
FCI OpenFermion	-7.86613635619	-14.9569336087	-74.9908117277	-39.8060539918	-147.7434954566	-185.231532228

TOTAL

VQE | benchmarking

ground state energies						
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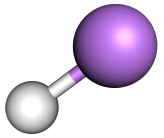
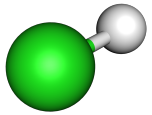
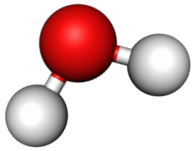
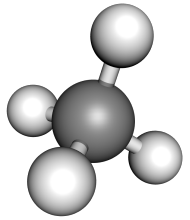
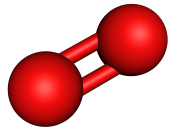
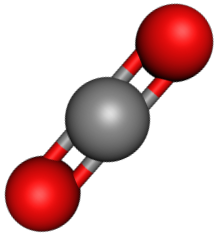
1 - 3 % error

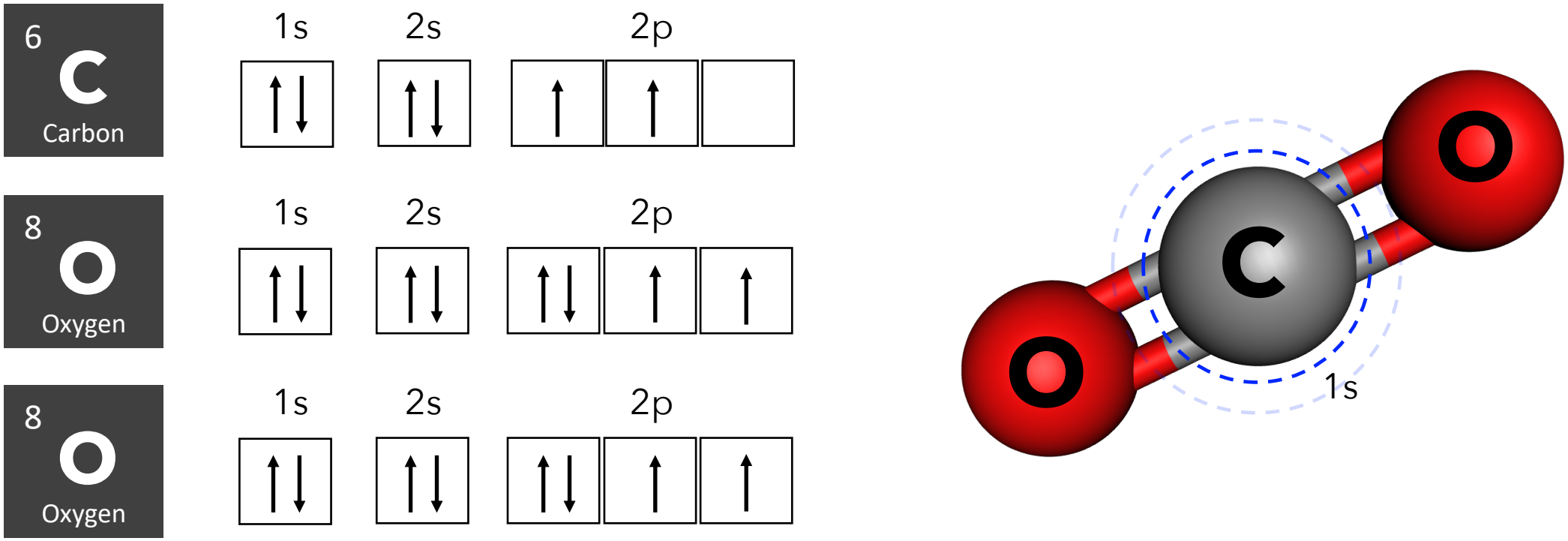
TOTAL

VQE | benchmarking

configuration						
	LiH	BeH	H_2O	CH_4	O_2	CO_2
num_orbitals	6	6	7	9	10	15
num_qubit	12	12	14	18	20	30

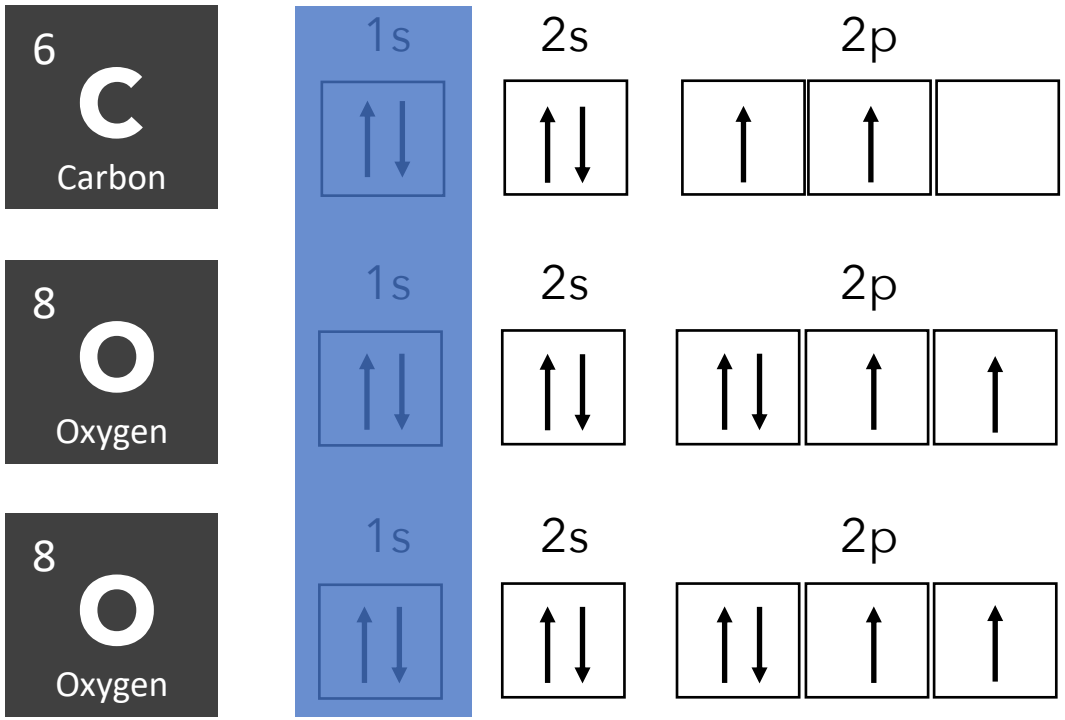
TOTAL

VQE | freezing orbitals

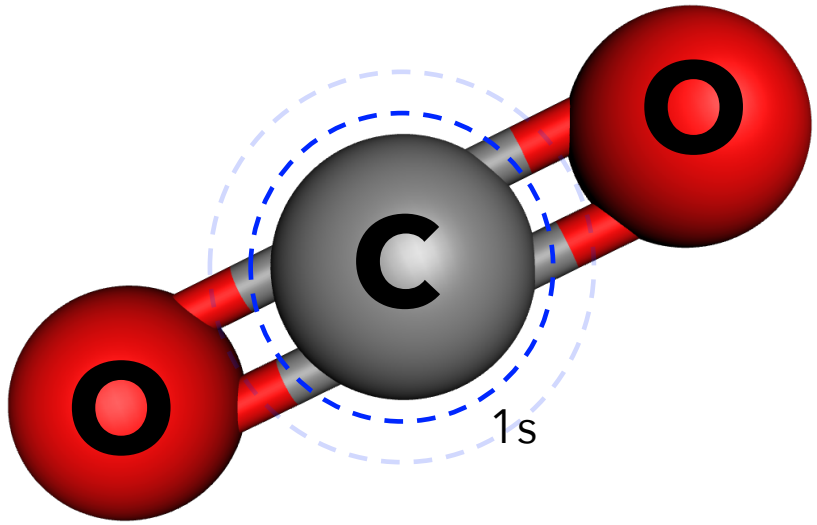


TOTAL

VQE | freezing orbitals



reduced from 30 to 24 qubits



TOTAL

VQE | freezing orbitals

excess renewable energy

CO_2
-179.9303

+H_2
-1.1719

HCO_2H
-186.2908

+H_2
-1.1719

-H_2O
-72.9137

H_2CO
-112.4542

+H_2
-1.1719

H_3COH
-113.5732

+H_2
-1.1719

-H_2O
-72.9137

CH_4
-38.9700

chemical value chain

energy content

carbon dioxide	acids, esters	aldehydes	alcohols, amines	hydro-carbons

Klankermayer J, Leitner W. 2016

TOTAL

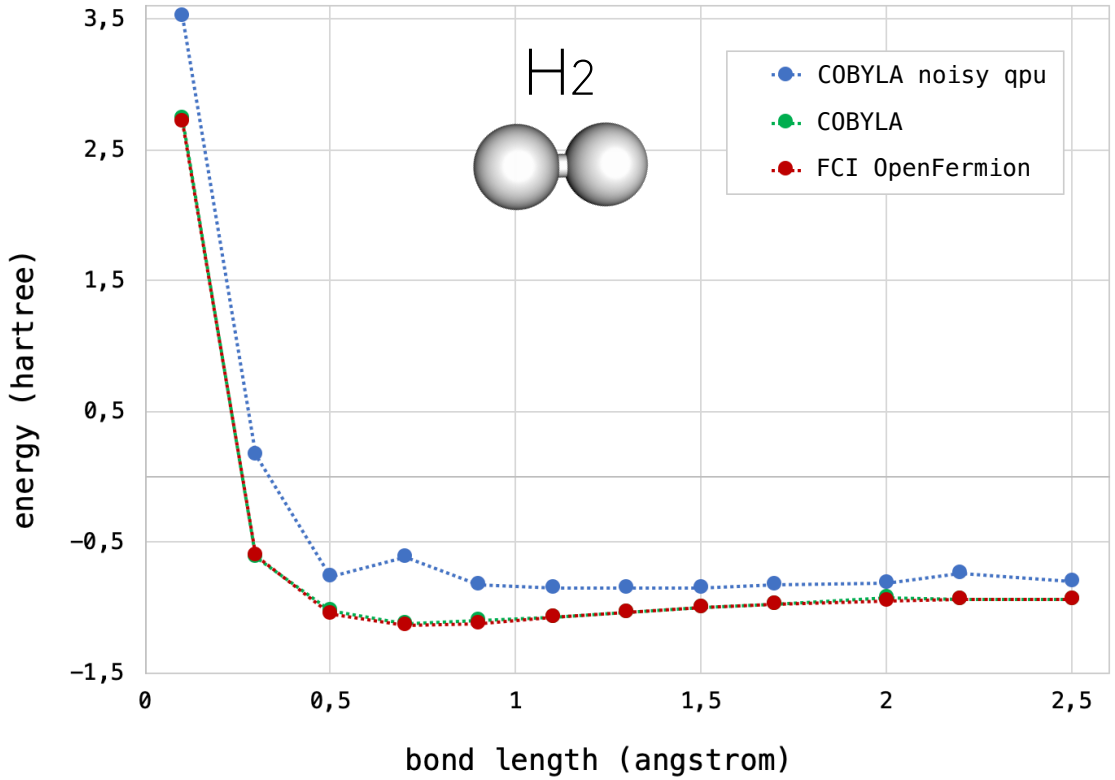
VQE | noisy QPU

1. Hardware model

```
gate_durations = {  "Z": 60, "H": 60, "X": 60, "Y": 60,
                    "RY": lambda angle: 60, "RX": lambda angle: 60,
                    "RZ": lambda angle: 60, "CNOT": 150
                 }
amp_damping = ParametricAmplitudeDamping(T_1 = 1000)
pure_dephasing = ParametricPureDephasing(T_phi = 2000)
hw_model = HardwareModel(DefaultGatesSpecification(gate_durations),
                         idle_noise = [amp_damping, pure_dephasing]
                         )
```

2. Simulation method

```
noisy_qpu = get_noisy_qpu_server(hardware_model=hw_model,
                                 sim_method="deterministic"
                                 )
```

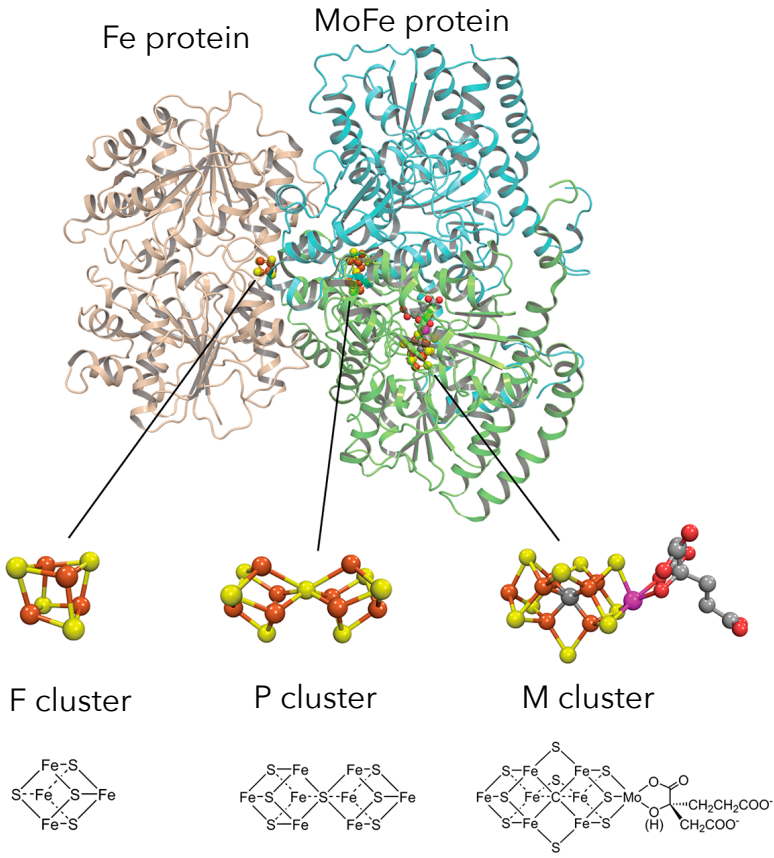


TOTAL

VQE | further steps

- Investigating the scalability of VQE
- Benchmarking against Imaginary Time Evolution (ITE)
- Extending VQE in order to estimate the rest of excited states
- Exploring more complex use-cases

Afterwards



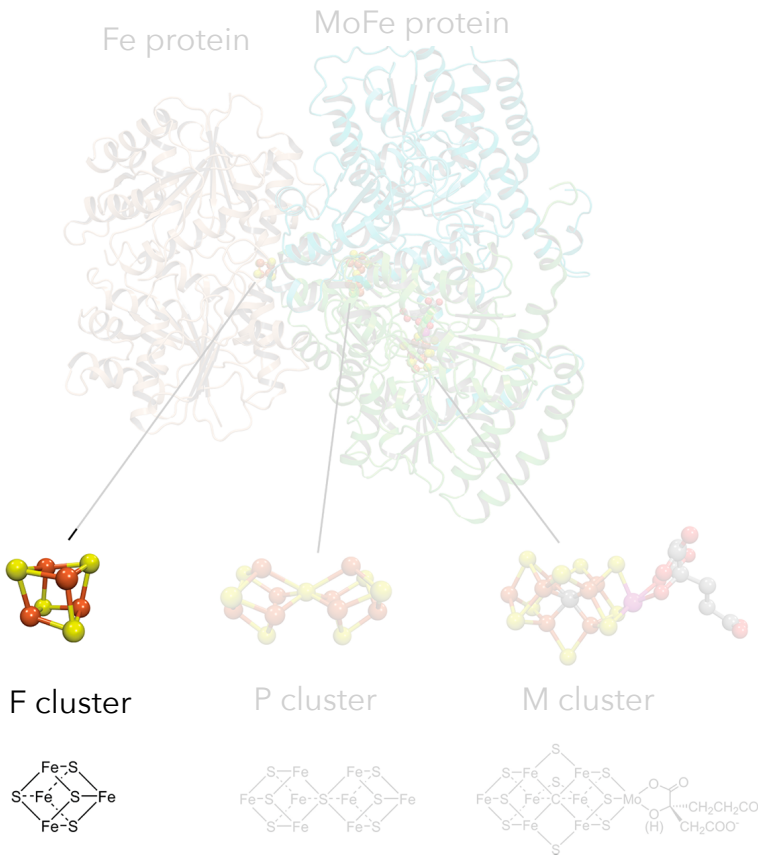
Molybdenum nitrogenase

—— Iron sulfide clusters (Fe_S_) of different sizes

B.Hoffman et al. Mechanism of nitrogen fixation by nitrogenase (2014). dx.doi.org/10.1021/cr400641x

Afterwards

Simulating F cluster is at the limit of classical computers! *(IBM Research, 2018)*



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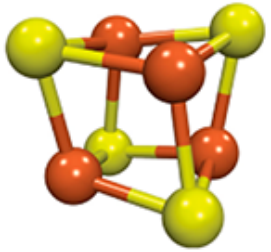
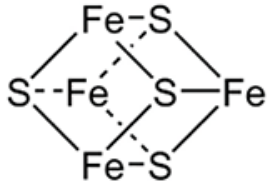


F cluster



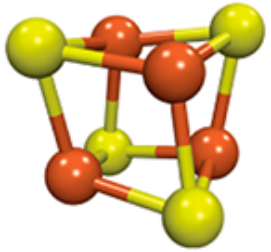
4Fe - 4S

4 x 26 + 4 x 16 = 168 electrons

~ 10^50 permutations

TOTAL

Afterwards



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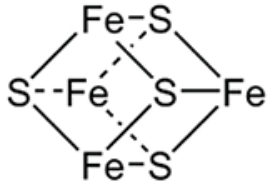

4Fe - 4S

4 x 26 + 4 x 16 = 168 electrons

~ 10^50 permutations

~ 192 qubits

(3-5 years)

TOTAL

Thank You!