Efficient Ground State Energy Calculation of $LiCoO_2$ using Variational Quantum Eigensolver

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Group 9: Quantum Computer Aided Engineering (**Q-CAE**) Team

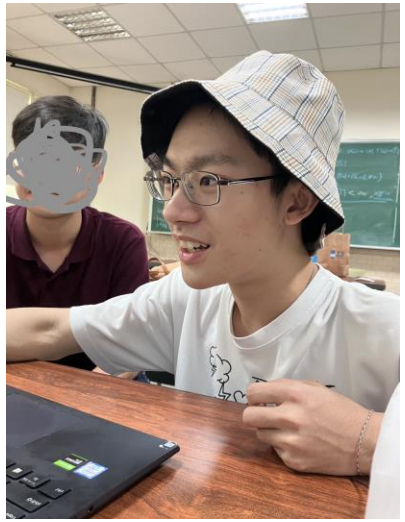
Yuto Terashima
Computational Mechanics

Conceptualization
Qubit Tapering

Yi-Kai Lee
Statistics

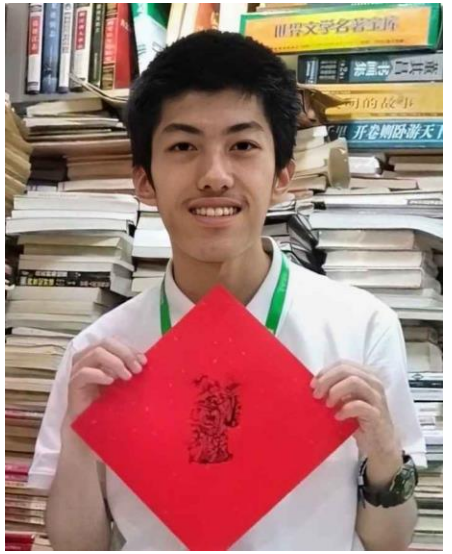
Visualization
Data Assimilation

Chun-Yu Lu
Computer Science



Visualization
Active Space Calculation

Zi-Yan Shi
Engineering Science



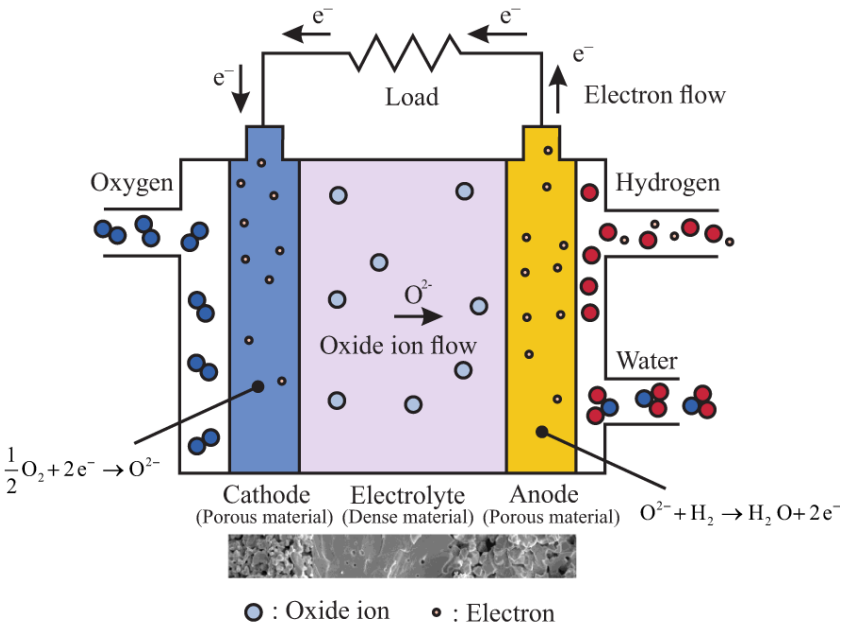
Programming
Verification & Validation

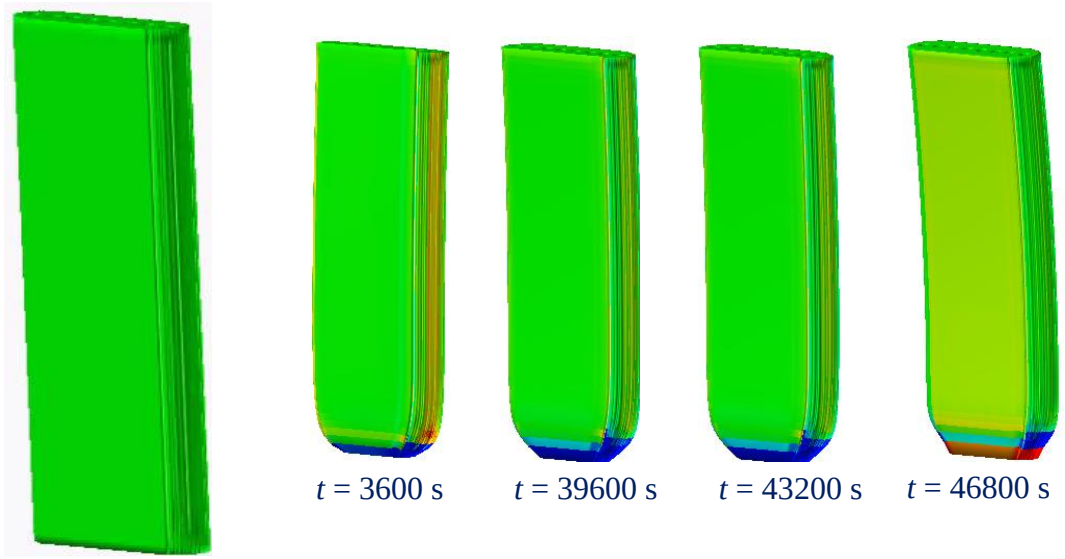
We are here to implement quantum computing technologies into engineering problems!

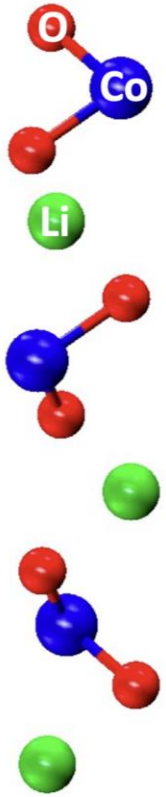
Difficulty in Safe Utilization of Novel Batteries

Multi-physics Simulations for the Prediction of Long-term Influence of Batteries

- ✓ Batteries are one of the closest materials in our modern life
- ✓ We are required to take control of it for safe utilization
- ✓ Batteries require multi-physics and multi-scale simulations for safe utilization







Source: [O'Hayre *et al.*, 2009; Yang *et al.*, 2013)

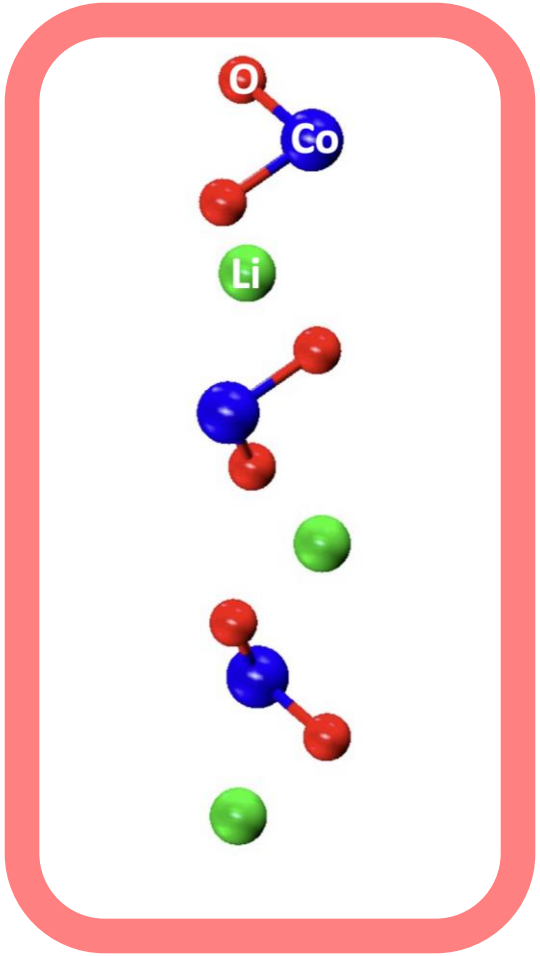
Voltage Calculation of Ion Batteries

Density Functional Theory (DFT) for Understanding Microscopic Properties of Batteries

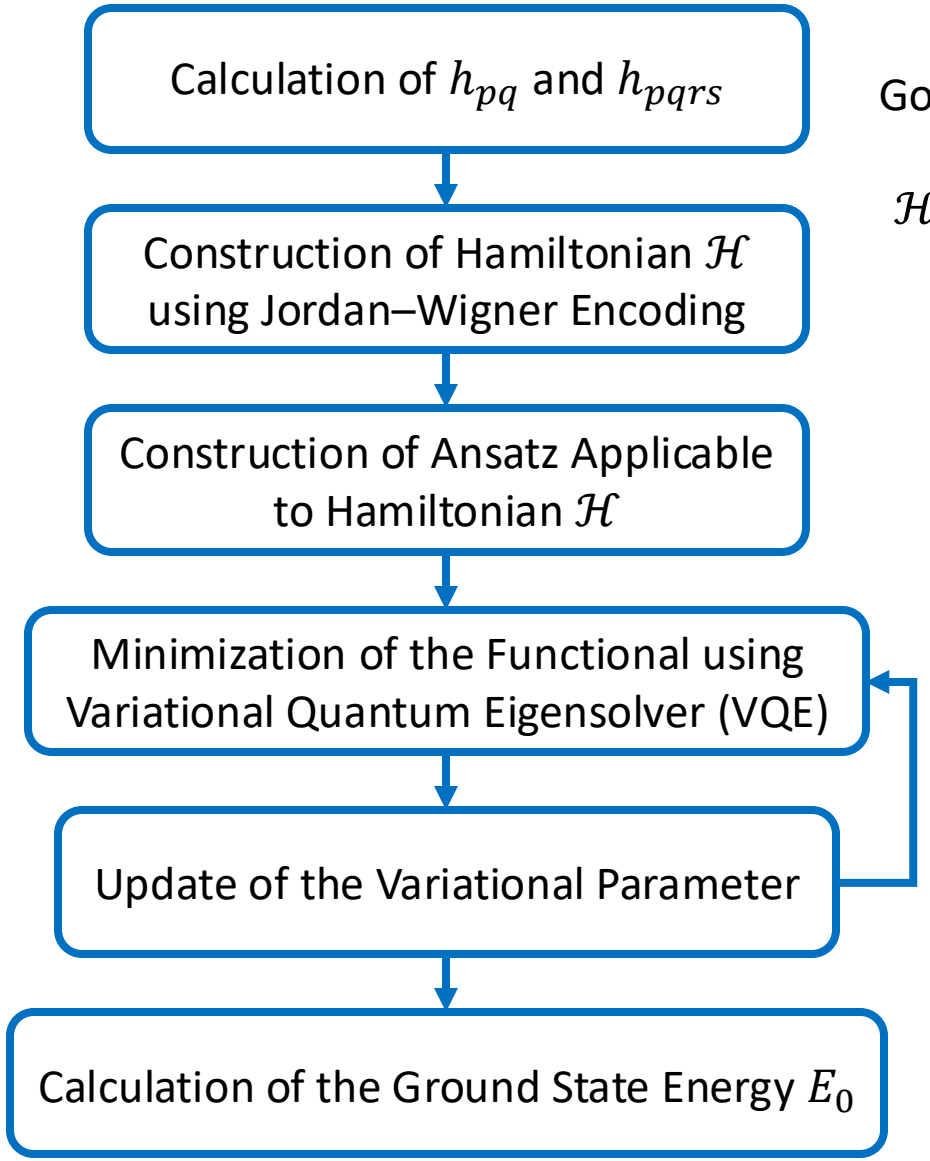
- ✓ One of the core technologies of batteries should consider the micro–mechanics
- ✓ DFT analyzes electron interactions based on quantum physics
- ✓ Molecular dynamics analyzes the atomic interactions within a finite temperature

$$V \approx -\frac{E(\mathrm{LiCoO_2}) - E(\mathrm{CoO_2}) - E(\mathrm{Li})}{e} \ [\mathrm{eV}]$$

Micro–physics can be incorporated in quantum physics!
→ In the scheme of quantum computer, too.



Computational Method: VQE–DFT



Governing Equation (Second Quantization)

$$\mathcal{H} = \sum_{p,q}^{M} h_{pq} c_p^\dagger c_q + \sum_{p,q,r,s}^{M} h_{pqrs} c_p^\dagger c_q^\dagger c_r c_s$$

Problem of VQE–DFT is that we cannot execute large systems, e.g., ion batteries ($LiCoO_2$)
In the case of $LiCoO_2$:

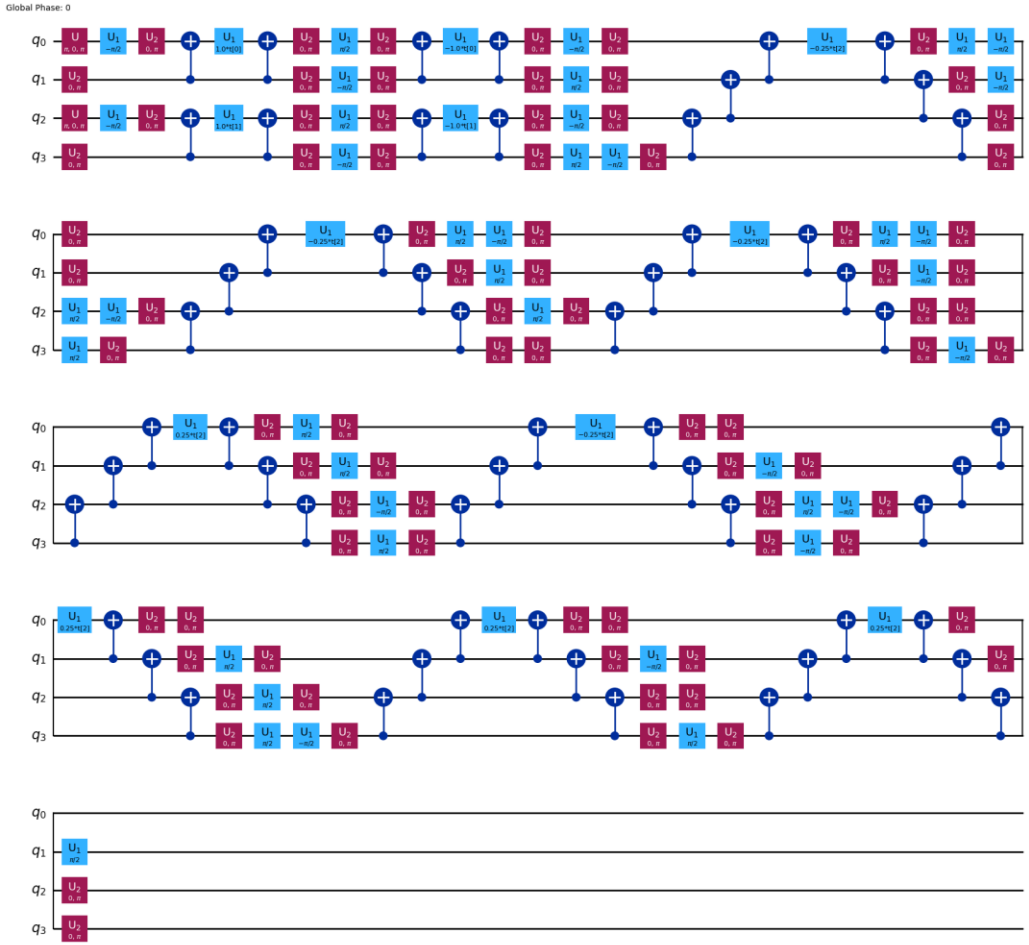
2^{76} states (76 qubits) are required!

We reduced the calculation costs in two points:

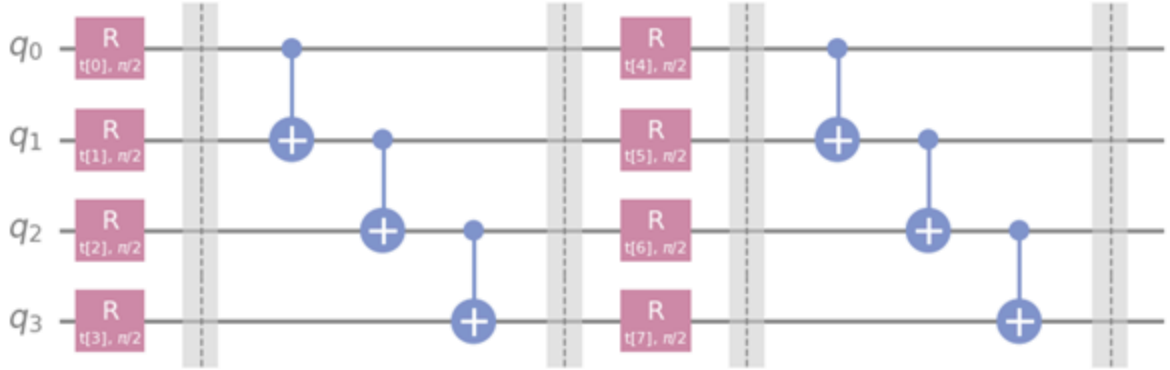
1. Physical Aspects of **the Gates and Qubits**
2. Mathematical **Tapering of the Hamiltonian**

Gate Reduction: Selection of the Ansatz for VQE

Unitary Coupled Cluster (UCC) Ansatz



Hardware Efficient Ansatz (HEA)



UCC is originated from the coupled cluster theory

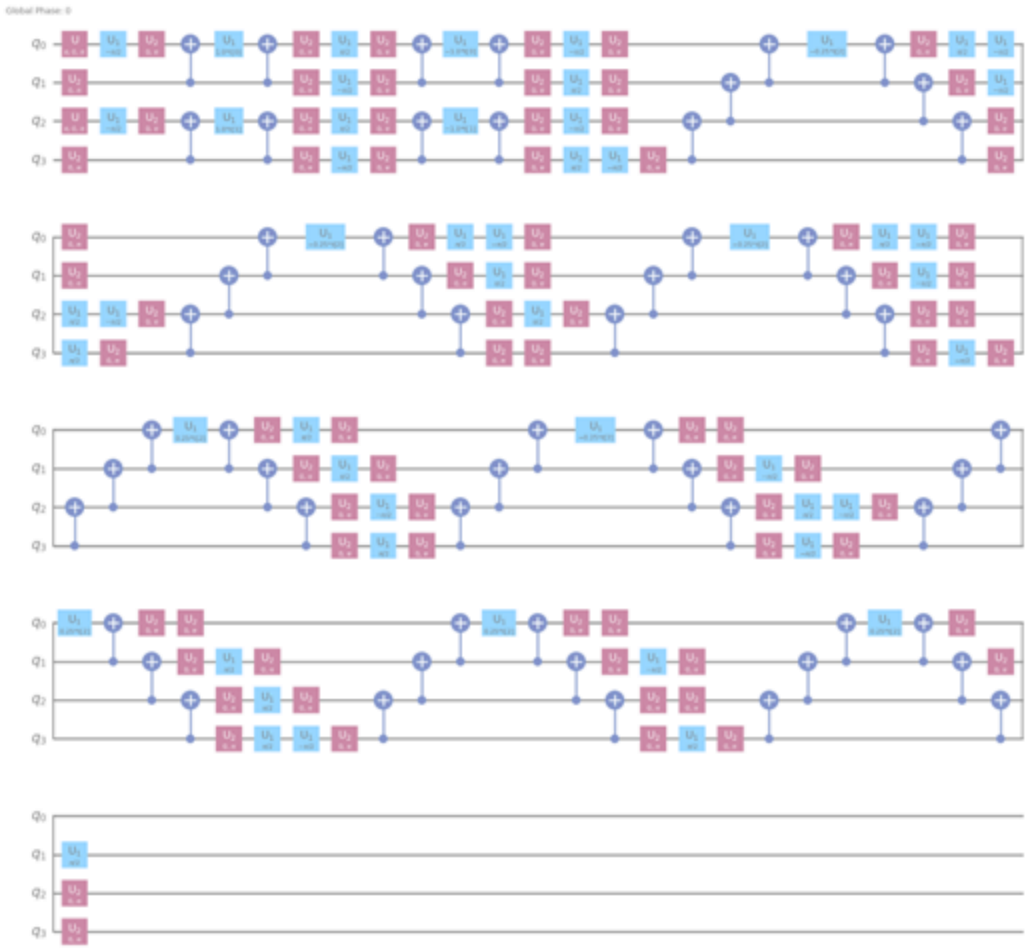
\+ Accurate VQE–DFT calculation can be achieved

− Deep Gate might not be suitable to NISQ

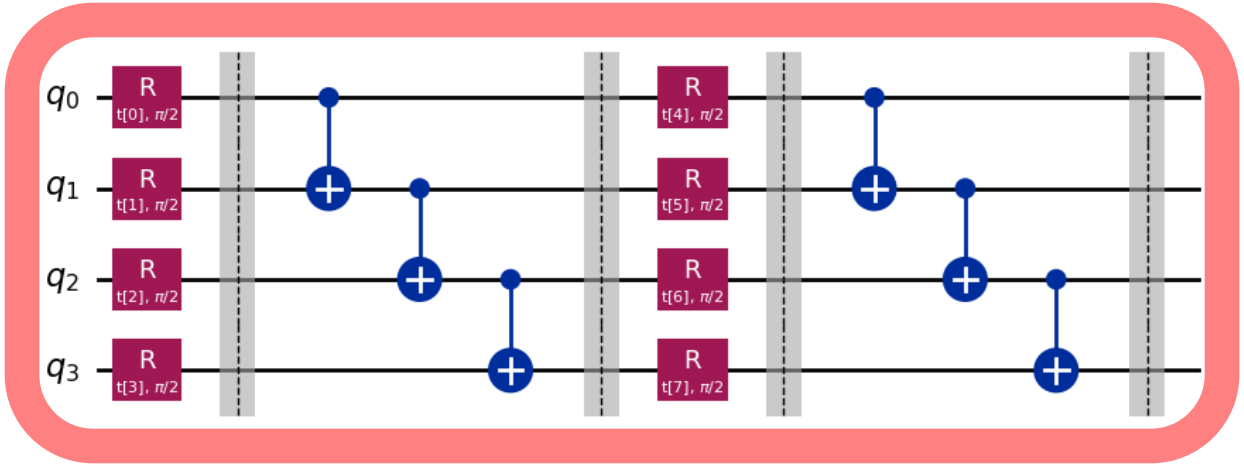
Ansatz with shallow gates should be considered

Gate Reduction: Selection of the Ansatz for VQE

Unitary Coupled Cluster (UCC) Ansatz



Hardware Efficient Ansatz (HEA)



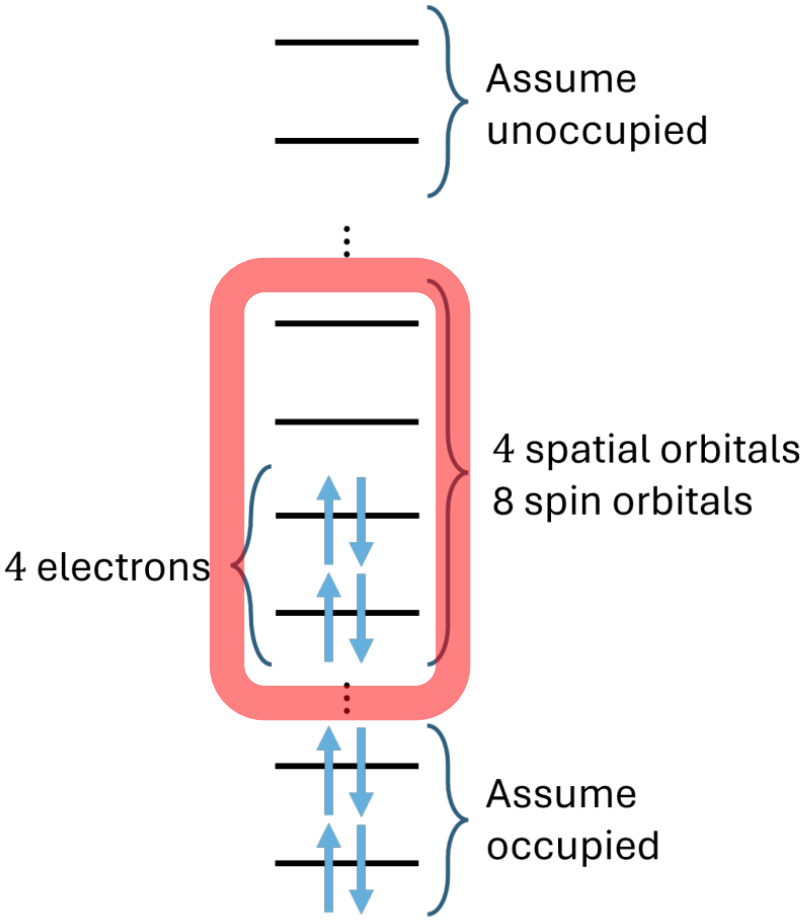
HEA is general ansatz developed for NISQ

\+ Shallow gate contributes to the stable calculation

△ Consideration of the accuracy is required

We utilize HEA for VQE-DFT calculation

Qubit Reduction: Active Cite Calculation



Active Chemical Interaction

- ✓ DFT incorporates all of the electron interactions
- ✓ However, there are inactive cites, which can be cutoff
- ✓ We observed such active and inactive cites in the qubit interactions

```
------------------------------------------------------------------------------
Active space selection finished
------------------------------------------------------------------------------

-> Selected an active space of 14 electrons in 12 orbitals.
ActiveSpace: 14 electrons in 12 orbitals
  active MO indices: [16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27]
```

We made a code for automatic selection of the active cite .

Tapering of Hamiltonian: Qubit Tapering with Z_2 Symmetry

Qubit Tapering against the Hamiltonian Operator in VQE

- ✓ Molecular simulation can be simply described in Z Gate (Qubits can be described in 0 or 1)
- ✓ Hamiltonian operator $\mathcal{H}$ can be decomposed using Z_2 symmetry
  - ✓ We can cutoff the symmetric states from the calculation which stabilize in the same quantum state

For example, simulation results for H_2O:

```
# 2979: -74.696555: 3.1416
# 2980: -74.696555: 3.1416
# 2981: -74.696555: 3.1416
# 2982: -74.696555: 3.1416
# 2983: -74.696555: 3.1416
# 2984: -74.696555: 3.1416
# 2985: -74.696555: 3.1416
# 2986: -74.696555: 3.1416
# 2987: -74.696555: 3.1416
Energy: -74.69655465020367
```

```
# 1144: -74.144545: 3.5069
# 1145: -74.144545: 3.5069
# 1146: -74.144545: 3.5069
# 1147: -74.144545: 3.5069
# 1148: -74.144545: 3.5069
# 1149: -74.144545: 3.5069
# 1150: -74.144545: 3.5069
# 1151: -74.144545: 3.5069
# 1152: -74.144545: 3.5069
# 1153: -74.144545: 3.5069
# 1154: -74.144545: 3.5069
# 1155: -74.144545: 3.5069
Energy: -74.1445451756479
```

Tapering of Hamiltonian: Qubit Tapering with Z_2 Symmetry

Qubit Tapering against the Hamiltonian Operator in VQE

- ✓ Molecular simulation can be simply described in Z Gate (Qubits can be described in 0 or 1)
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For example, other small molecule results :

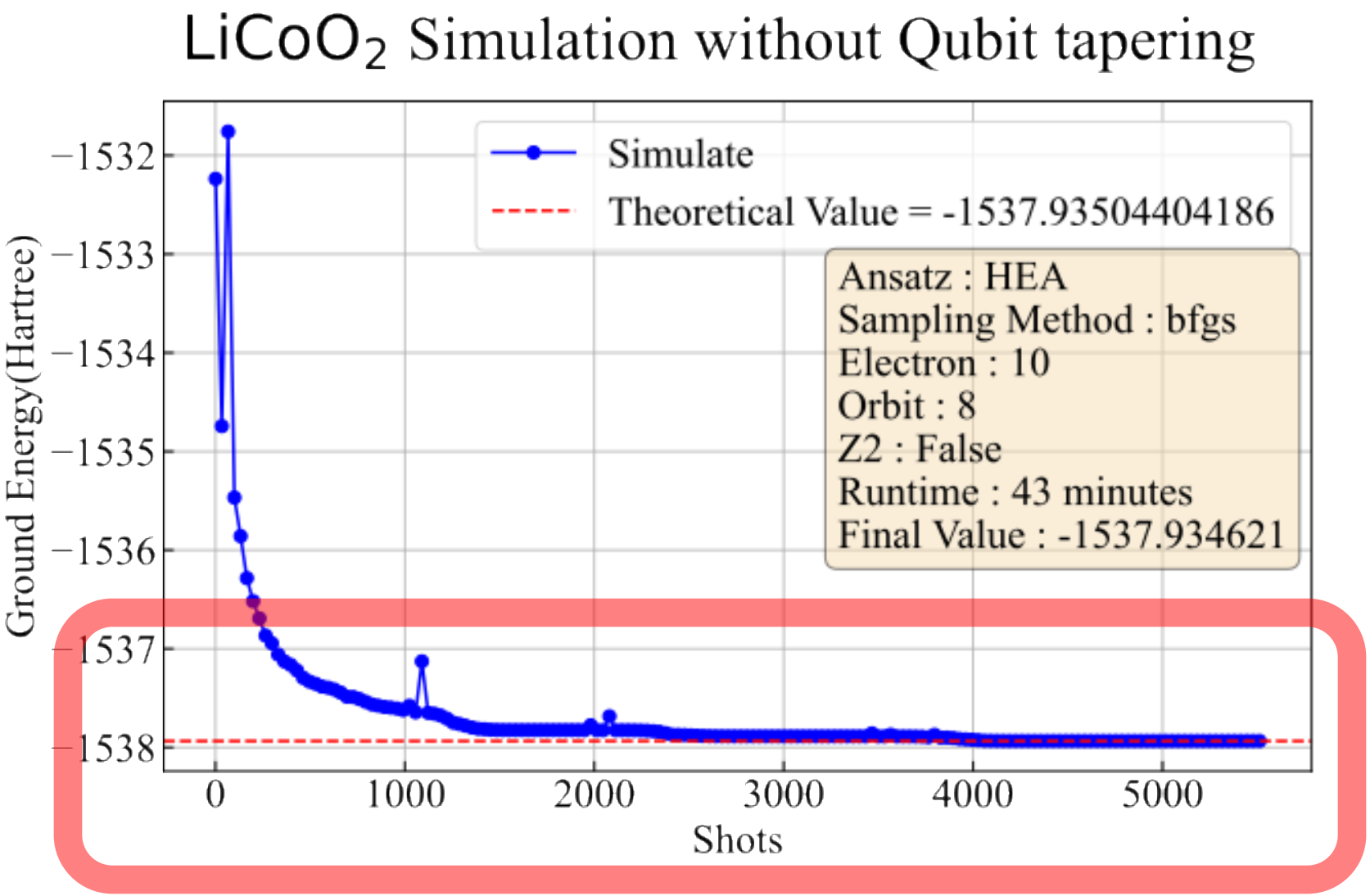
```
H2O hea vqe before tapering
theoretical SCF energy = -74.8801743517023
iteration : 8323
nOrb : 7
nElec: 10
hamiltonian SparsePauliOp numbers : 1086
approximated energy : -74.88017435152771
runtime : 40 minutes


H2O hea vqe after tapering without picking active space
theoretical SCF energy = -74.8801743517023
iteration : 8323
nOrb : 7
nElec: 10
number of tapered operations : 16
SparsePauliOp numbers of each hamiltonian : 1035
approximated energy : -73.73967919953907
runtime : 22 seconds
```

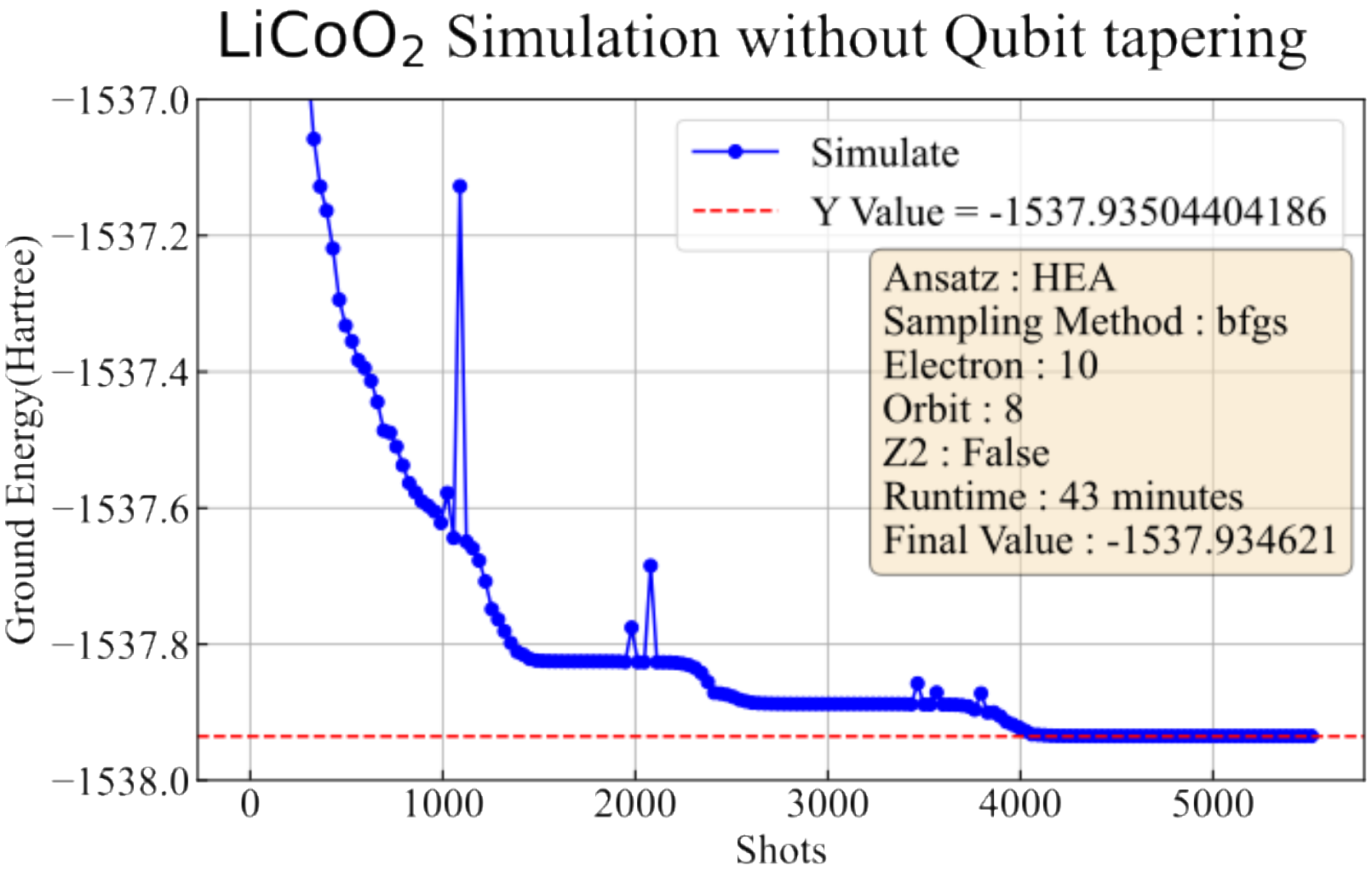
```
C2H4 hea vqe before tapering
theoretical SCF energy = -77.0720875637473
nOrb : 14
nElec: 16
hamiltonian SparsePauliOp numbers : 8919
runtime : too complex and too long to run


C2H4 hea after tapering without picking active space
theoretical SCF energy = -77.0720875637474
iteration : 8323
nOrb : 14
nElec: 16
number of tapered operations : 32
SparsePauliOp numbers of each hamiltonian : 8914
approximated energy : -73.285786075257
```

Results for the $LiCoO_2$ Ion Battery

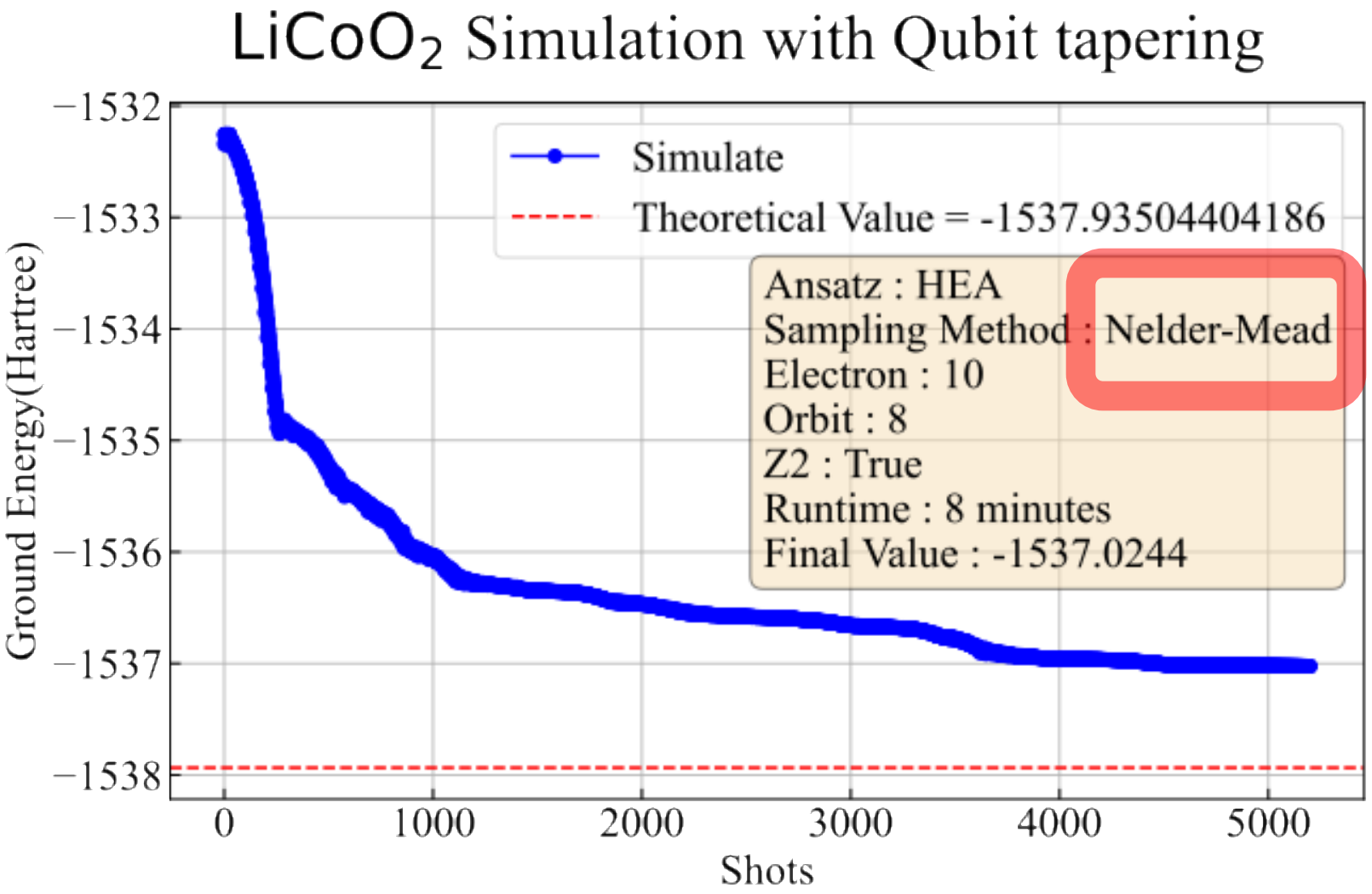


Results for the $LiCoO_2$ Ion Battery



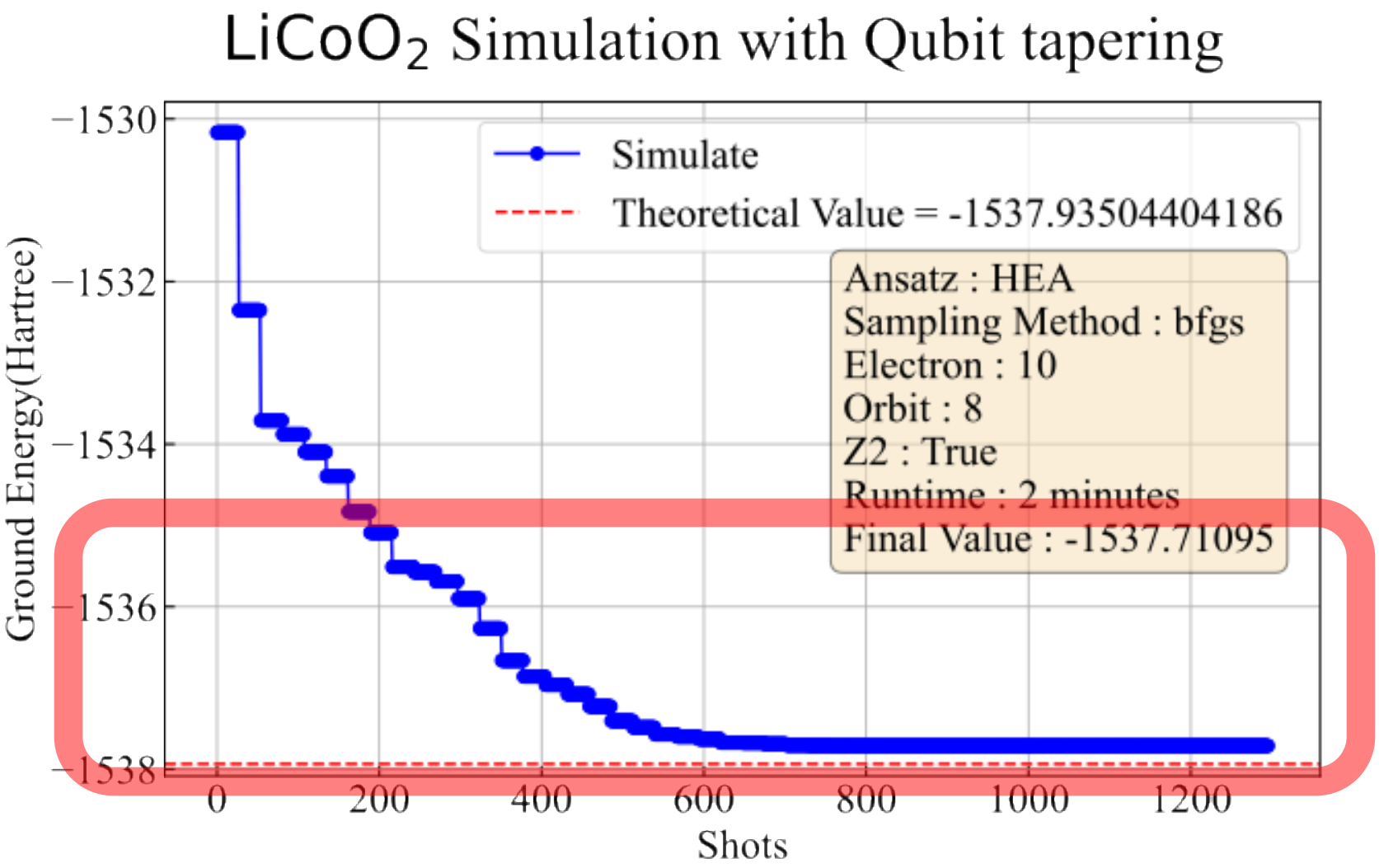
We automatically selected the active cite, and the results show nice convergence.

Results for the $LiCoO_2$ Ion Battery

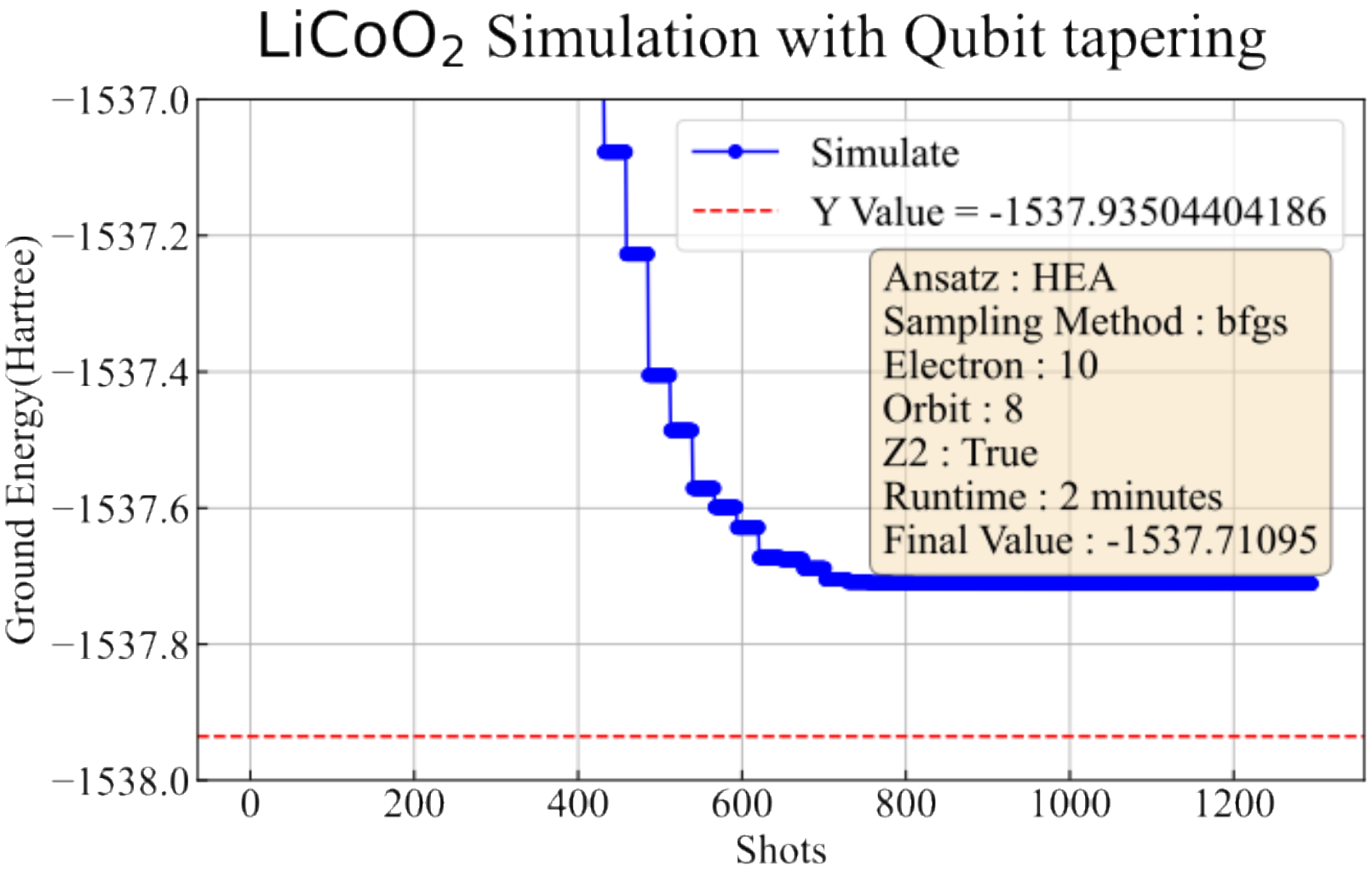


We utilized the Nelder–Mead sampling, and there were some differences in the result. The qubit tapering has accelerated the simulation.

Results for the $LiCoO_2$ Ion Battery



Results for the $LiCoO_2$ Ion Battery



We utilized the bfgs sampling with a nice convergence. The number of the shots decreased in **2 minutes.**

Conclusion & Future Perspective

We reduced the calculation costs in two points:

1. Physical Aspects of **the Gates and Qubits**
2. Mathematical **Tapering of the Hamiltonian**

Through this activity, we were able to calculate a computationally expensive simulation of ion batteries by reducing its calculation costs in **2 minutes**

We understand that

- quantum computing is interesting in both physics and mathematical aspects
- quantum algorithm itself can be passed down to

Future extension can be the VQE–DFT–MD simulation[1] for observing dynamical influences.

[1] H. Kashihara, Y. Suzuki, and K. Yasuoka. "A Study on Quantum Car-Parrinello Molecular Dynamics with Classical Shadows for Resource Efficient Molecular Simulation." *arXiv preprint arXiv:2406.18797* (2024).

We are open for new connections!

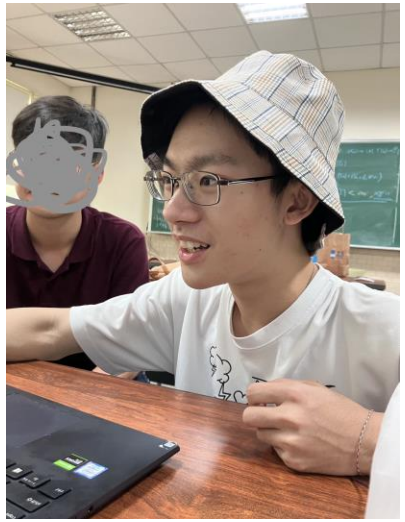
Yuto Terashima
Computational Mechanics

LinkedIn Account

Yi-Kai Lee
Statistics

LinkedIn Account

Chun-Yu Lu
Computer Science



Zi-Yan Shi
Engineering Science