Introducing qc2: A Modular Open-Source Software for Quantum Chemistry with Quantum Computers

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Conf24 Quantum Computing

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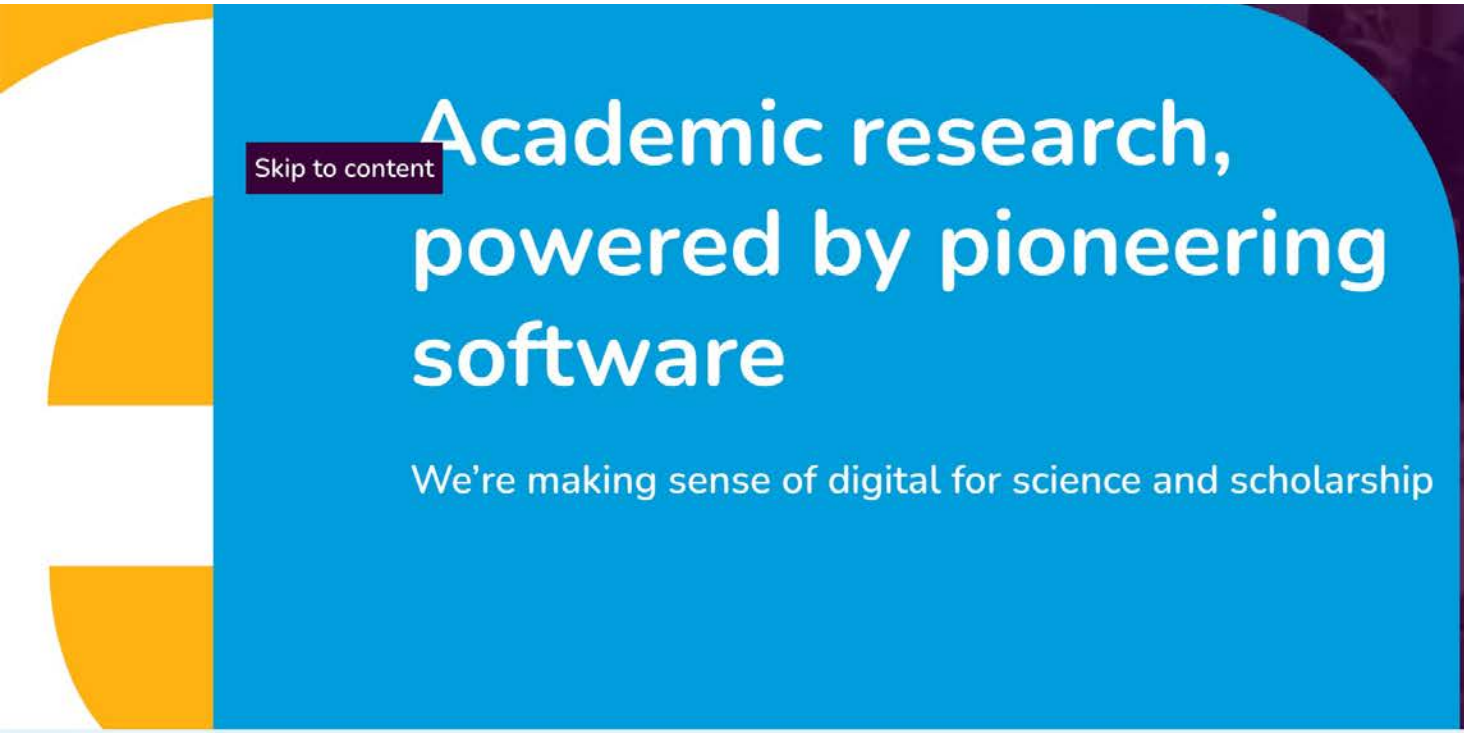

Strategy 2021-2025

VISION

a robust research community, in which all investigators in all domains are able to exploit advanced digital technologies to answer curiosity-driven questions, keeping the Netherlands at the forefront of cutting-edge international research.

MISSION

empowering researchers across all disciplines through innovative research software.

AMBITION 1 collaboratively designing software for research

= Research projects with research partners

AMBITION 2 building digital expertise

= Workshops, Fellowship Programme, Tech blogs, NL-RSE etc.

STRATEGIC PRIORITIES

- ✔ institutional alignment
- ✔ software sustainability

- open calls for eScience domain research
- collaborations in advanced eScience technologies
- workshops & training
- community building & networking

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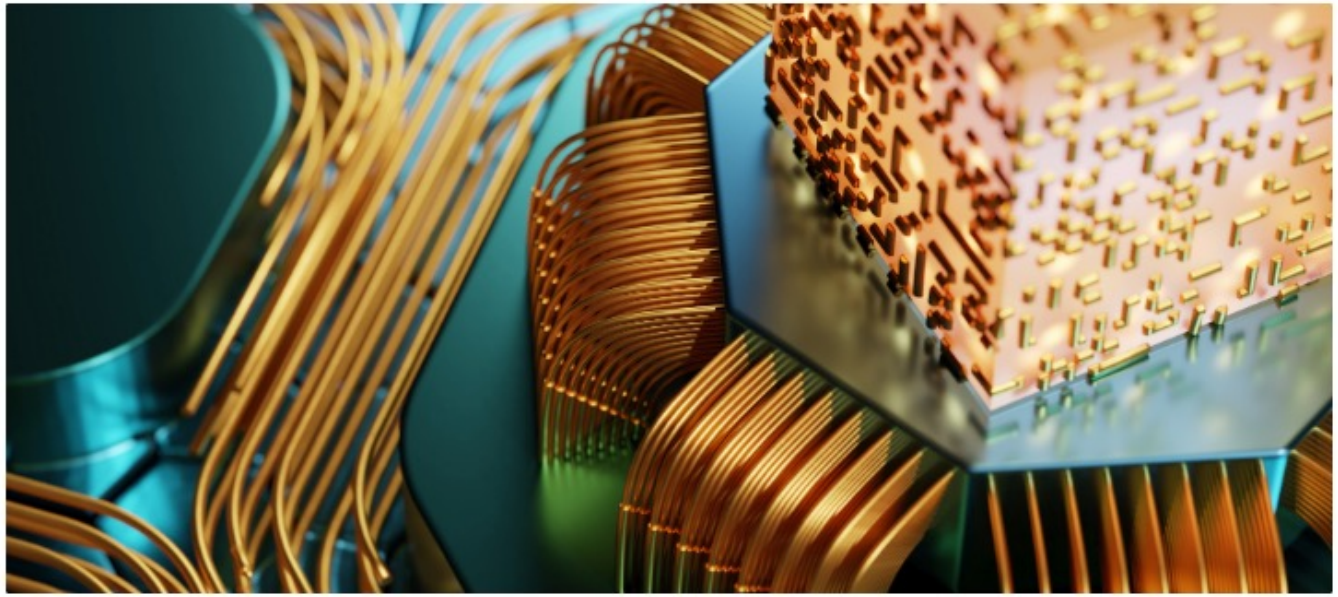
QCforQC

Bridging Quantum Chemistry and Quantum Computing



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Quantum chemistry might be one of the main application area for near term quantum computing. The evaluation of multi-electron integrals by traditional quantum chemistry codes, such as pyscf, ADF, NWCHEM, are usually used to map the physical electrons of the simulated system to the qubits of a quantum circuits. The use of dedicated quantum circuits can then significantly accelerate the calculation of the system's properties. In this project we are aiming at developing dedicated software to facilitate the interoperability between classical computational chemistry codes and quantum architecture without any programming overhead for the developers or users.

Status

Jan 2023 — Dec 2024

In progress

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SURF

Project links

Project repo

Research domains

PE: Physical Sciences And Engineering

Keywords

Quantum Chemistry

Quantum Computing

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https://research-software-directory.org/projects/qcforqc

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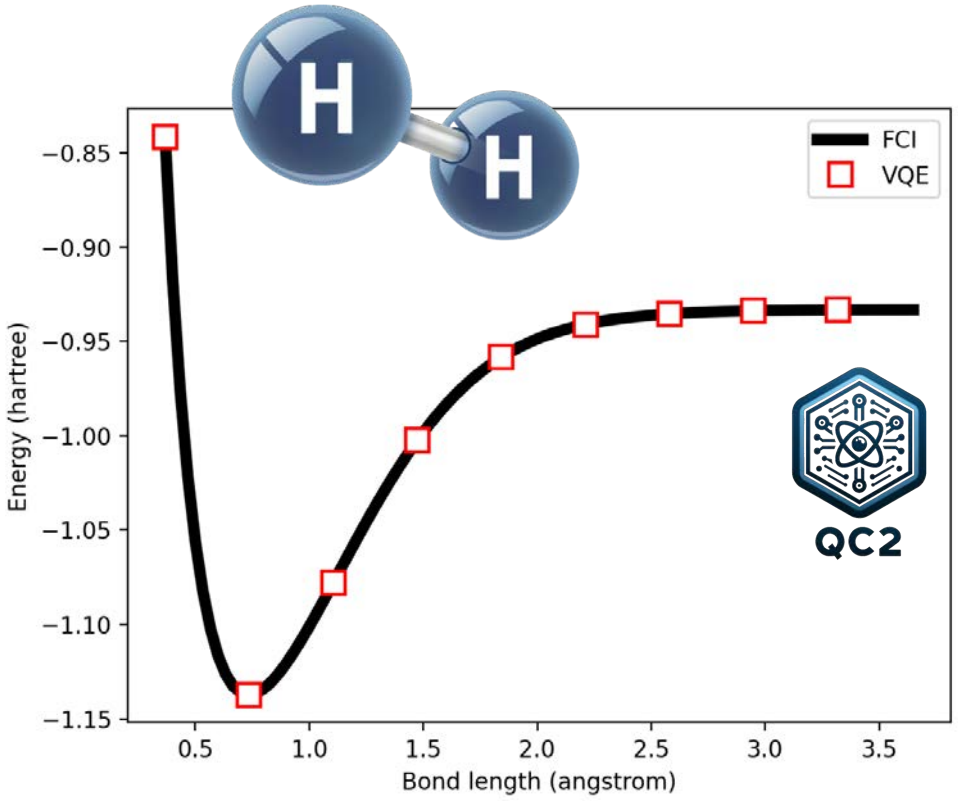
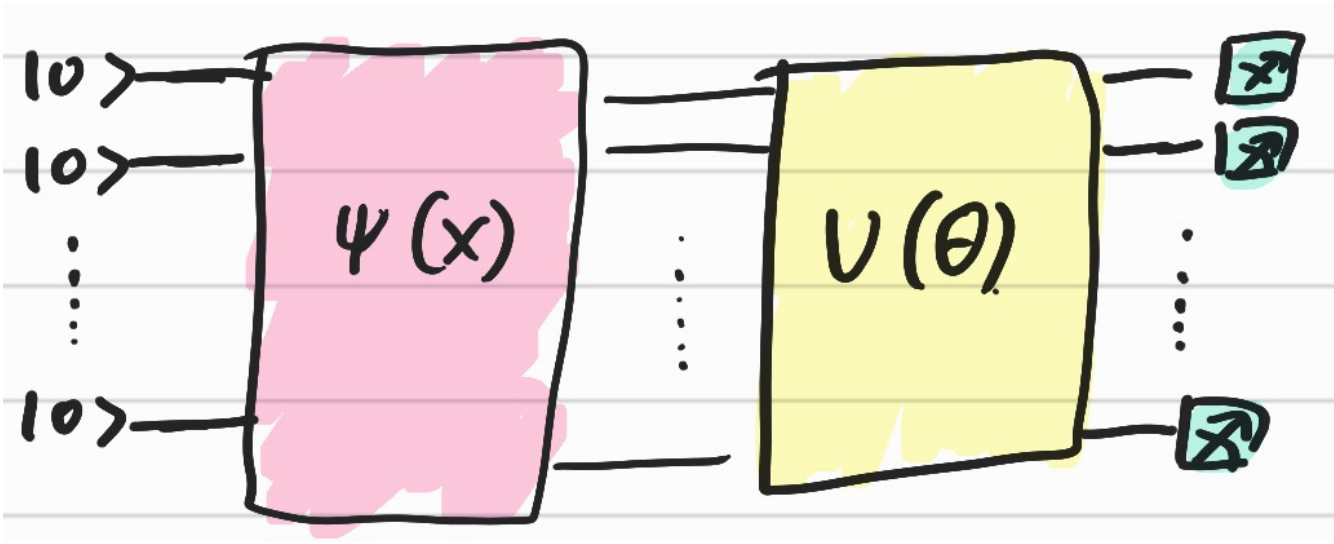
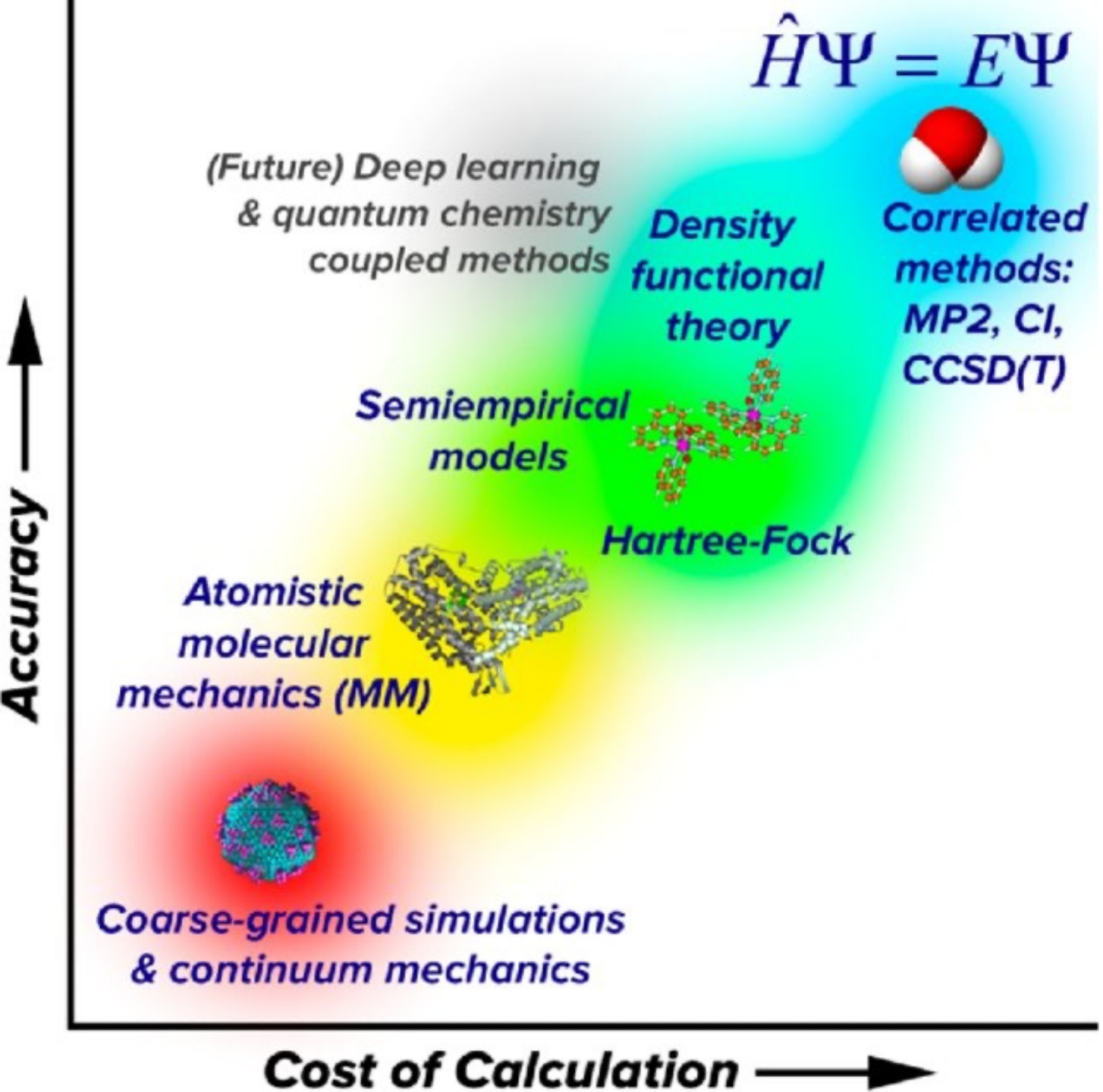
Objectives

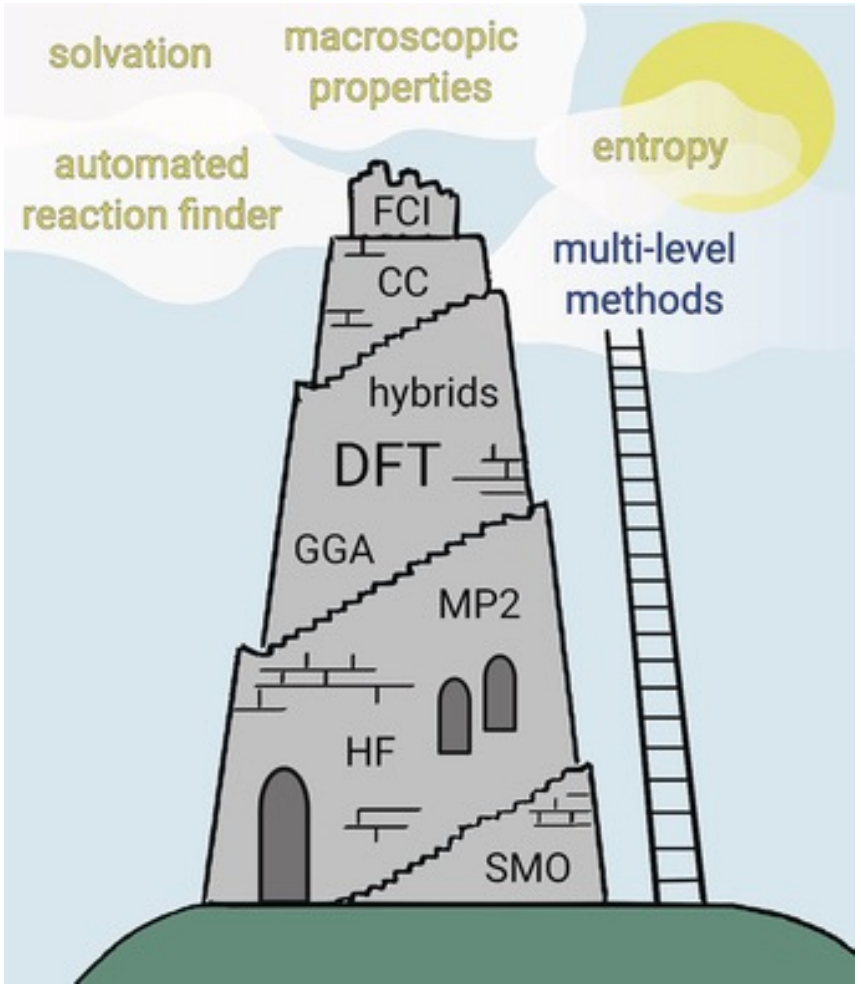
"Develop a dedicated software (qc2) to facilitate the interoperability between traditional computational chemistry codes and quantum architecture."





Quantum Chemistry in various contexts and scales





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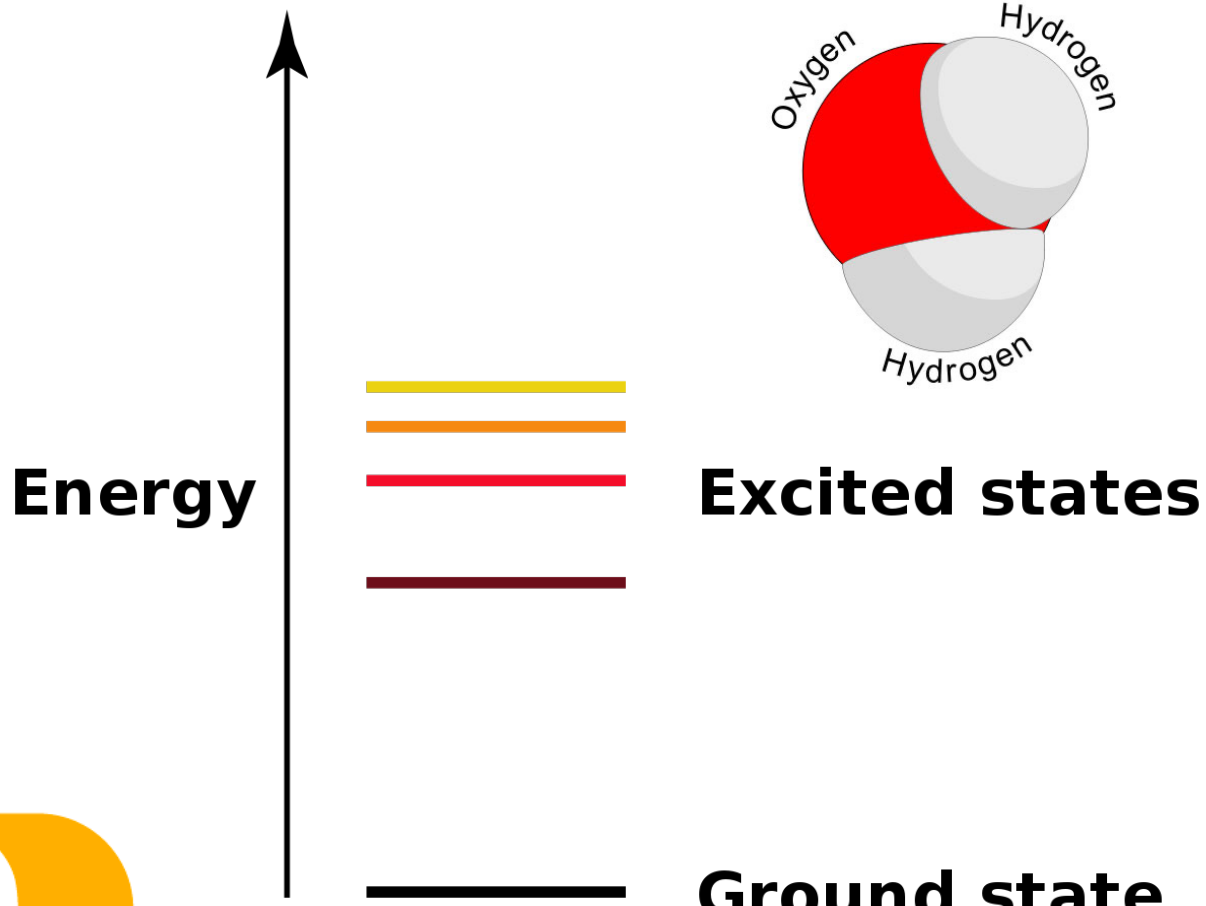
Molecules and quantum mechanics



Schrödinger Equation

$$\hat{H}\,\Psi = E\,\Psi$$

Hamiltonian Operator (Energy operator)

Energy eigenvalue

Can only be solved exactly for one-electron systems, *e.g.* H atom!

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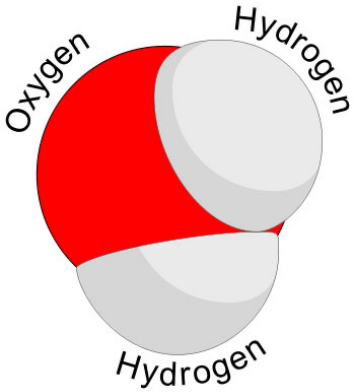
Approximate solutions to the SE



Variational Principle

$$|\psi\rangle \approx \alpha|\varphi_0\rangle + \beta|\varphi_1\rangle + \gamma|\varphi_2\rangle + \delta|\varphi_3\rangle + \ldots \qquad \langle\psi|H|\psi\rangle \geq E_{exact}$$

$$\mathbf{U}^{-1}\begin{pmatrix} \langle\varphi_0|H|\varphi_0\rangle & \cdots & \langle\varphi_0|H|\varphi_n\rangle \\ \vdots & \ddots & \vdots \\ \langle\varphi_n|H|\varphi_0\rangle & \cdots & \langle\varphi_n|H|\varphi_n\rangle \end{pmatrix}\mathbf{U} = \begin{pmatrix} E_0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & E_n \end{pmatrix}$$

FCI ~ $\mathcal{O}(2^{\text{nelec/orbitals}})$

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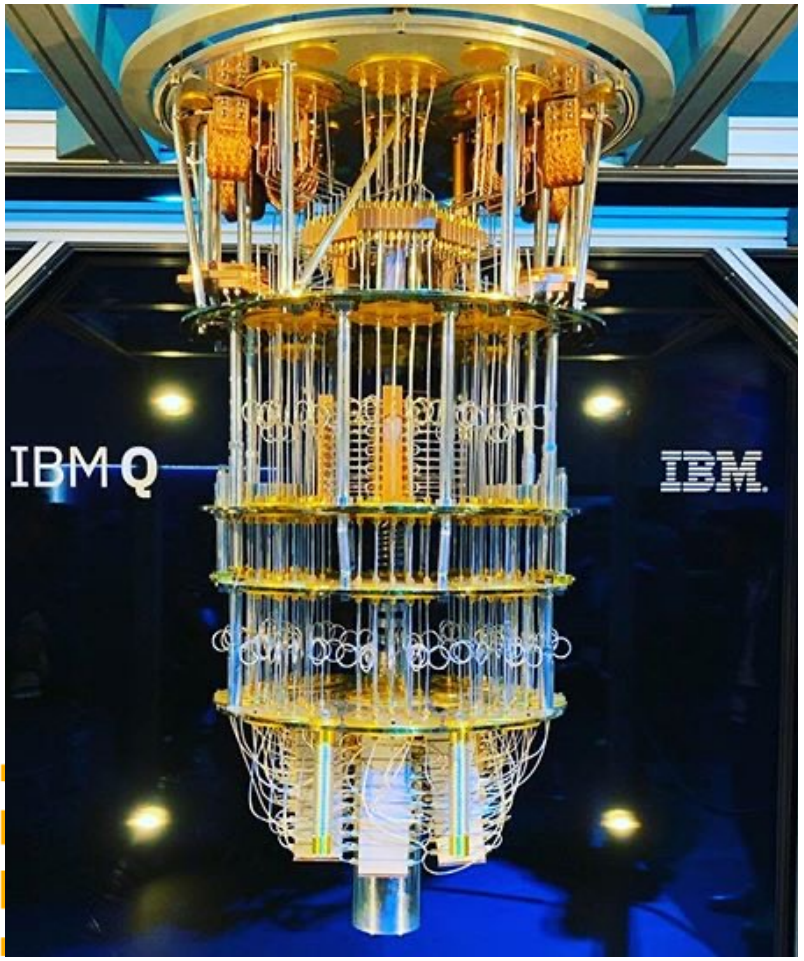
Quantum computation & chemistry



CHEMICAL REVIEWS

Review

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Quantum Chemistry in the Age of Quantum Computing

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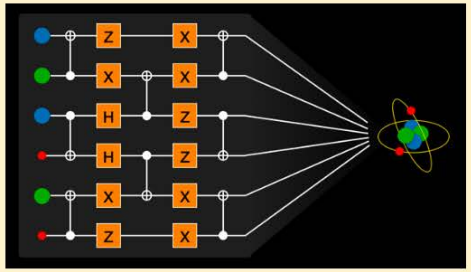
ABSTRACT: Practical challenges in simulating quantum systems on classical computers have been widely recognized in the quantum physics and quantum chemistry communities over the past century. Although many approximation methods have been introduced, the complexity of quantum mechanics remains hard to appease. The advent of quantum computation brings new pathways to navigate this challenging and complex landscape. By manipulating quantum states of matter and taking advantage of their unique features such as superposition and entanglement, quantum computers promise to efficiently deliver accurate results for many important problems in quantum chemistry, such as the electronic structure of molecules. In the past two decades, significant advances have been made in developing algorithms and physical hardware for quantum computing, heralding a revolution in simulation of quantum systems. This Review provides an overview of the algorithms and results that are relevant for quantum chemistry. The intended audience is both quantum chemists who seek to learn more about quantum computing and quantum computing researchers who would like to explore applications in quantum chemistry.



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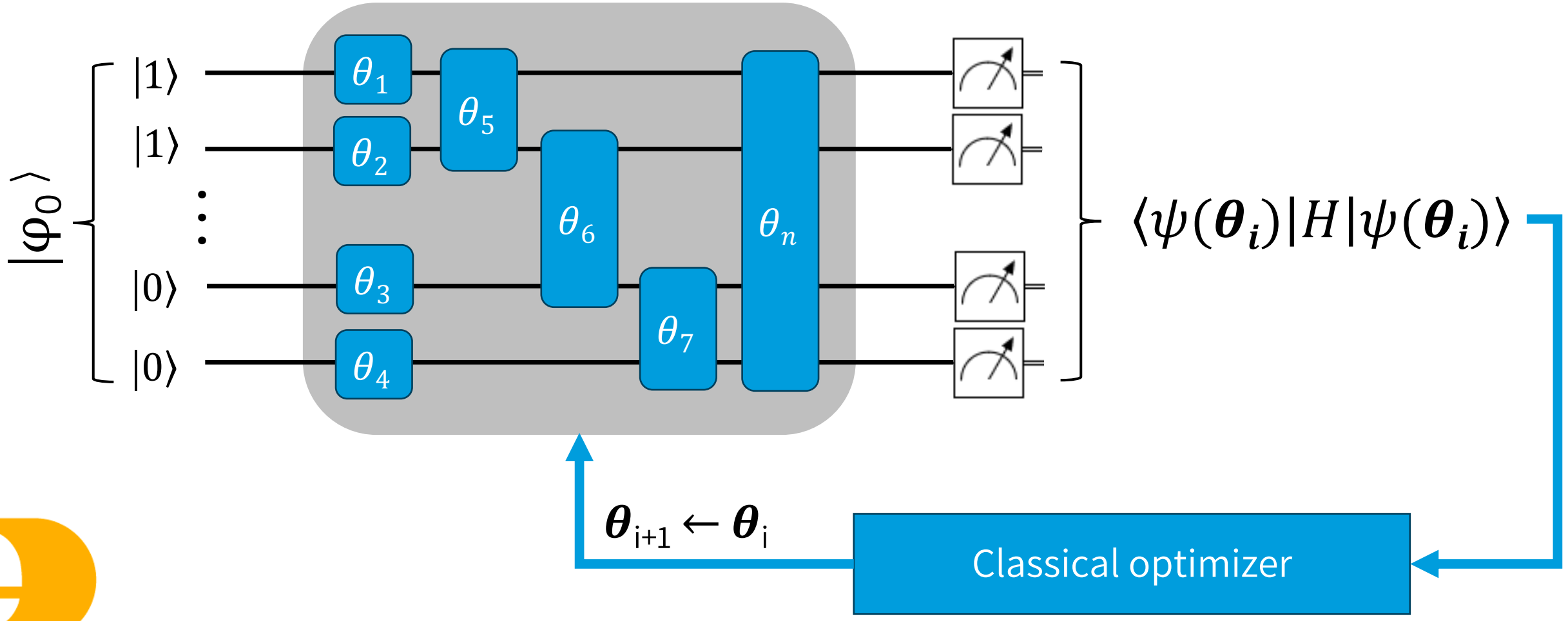
Variational Quantum Eigensolver



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VQE/qc2 data needs

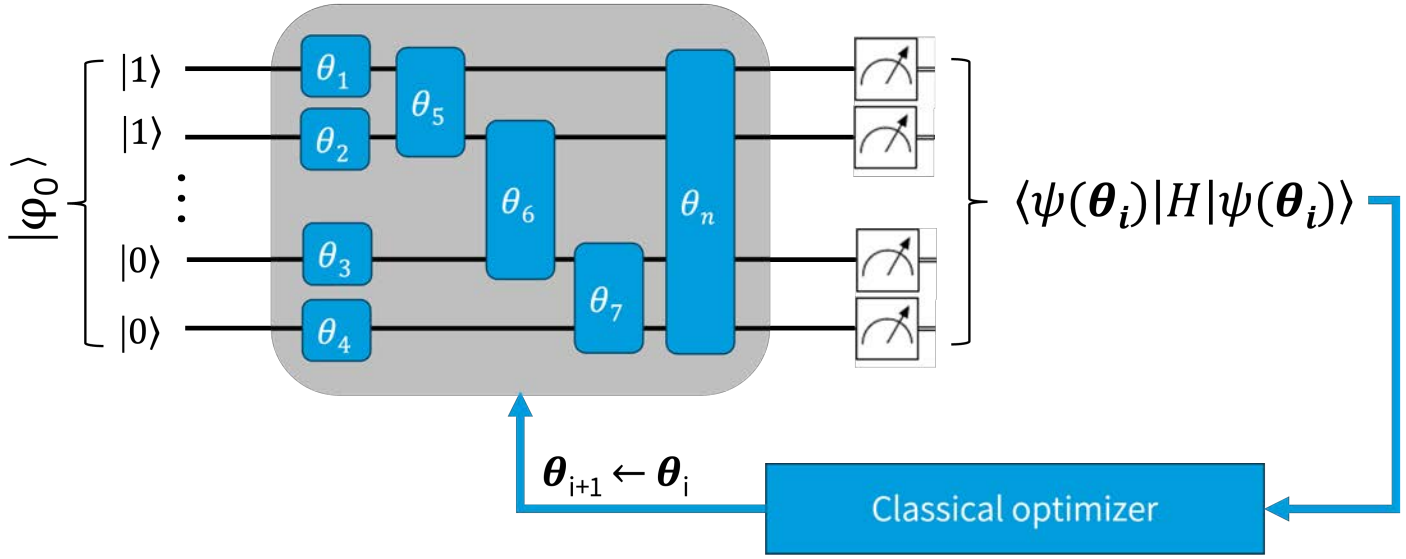
traditional quantum chemistry codes

- Reference state $|\psi_0\rangle$
- Variational form U($\boldsymbol{\theta}$)
- Initial parameters $\boldsymbol{\theta}$
- Qubit Hamiltonian H
- Classical optimizer

Hartree-Fock wave function

$$|\psi\rangle \approx \alpha|\varphi_0\rangle + \beta|\varphi_1\rangle + \gamma|\varphi_2\rangle + \delta|\varphi_3\rangle + \ldots.$$

One- & two-electron integrals + MO coefficients



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qc2 core design principles

- **Leveraging Existing Tools:** Interoperable with existing open-source qchem tools and adheres to standard data schemas
- **Seamless Integration with Popular Quantum Computing SDKs:** Designed to work effortlessly with Qiskit and Pennylane, ensuring a smooth experience for developers.
- **Modularity:** Highly modular, featuring a built-in algorithms package that simplifies extensions and enhancements.
- **User-Friendly Design:** Has an intuitive interface, enabling users to focus on their research and applications with minimal technical details.

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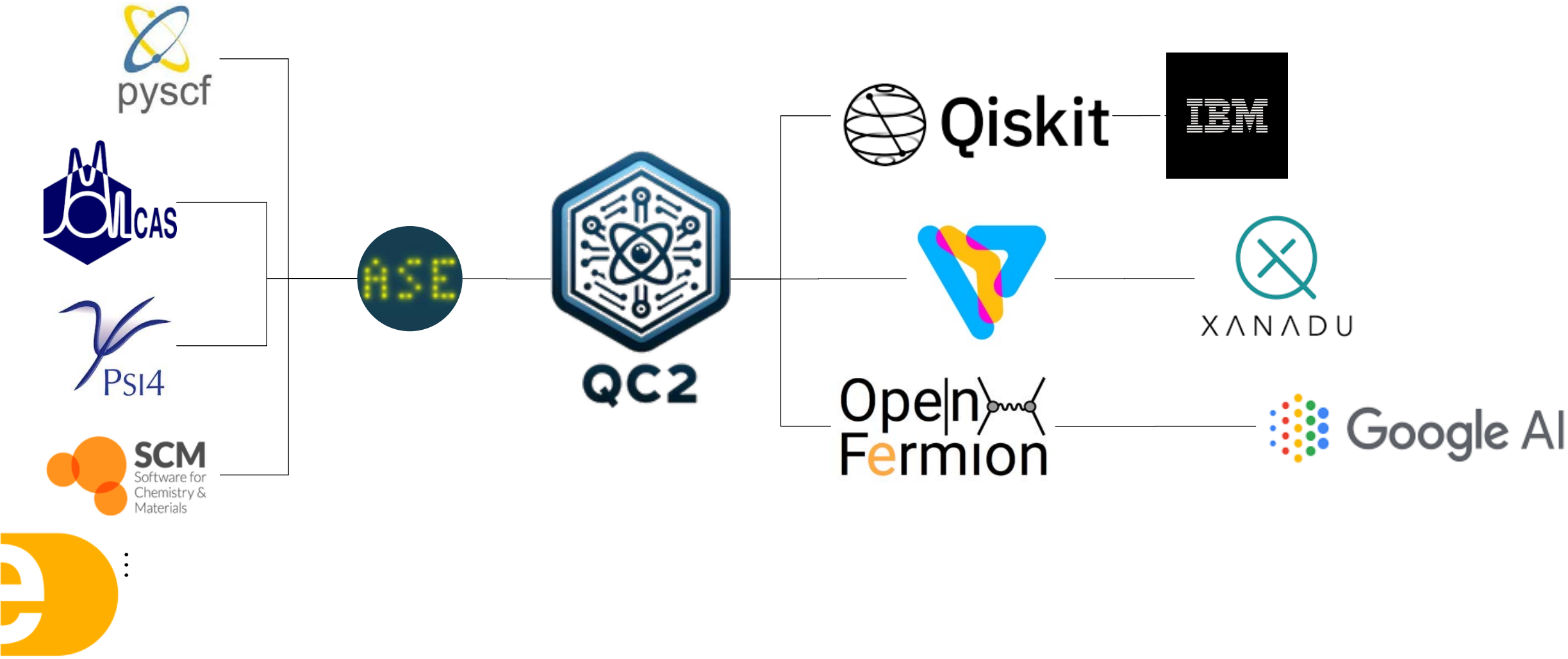
qc2: reusability and interoperability



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Ex. 1: VQE calculation on water

```python
# Import ASE-related modules
from ase.build import molecule

# Import qc2 modules
from qc2.data import qc2Data
from qc2.ase import PySCF
from qc2.algorithms.pennylane import VQE
from qc2.algorithms.utils import ActiveSpace

# Instantiate qc2Data class
qc2data = qc2Data(
    molecule=molecule("H2O"),
    filename="h2o.hdf5"
)

# Specify and run the quantum chemistry qc2-ASE calculator
qc2data.molecule.calc = PySCF(
    method="scf.RHF",
    basis="sto-3g",
)
qc2data.run()

# Instantiate VQE class
qc2data.algorithm = VQE(
    active_space=ActiveSpace(
        num_active_electrons=(2, 2),
        num_active_spatial_orbitals=4
    ),
)

# Run VQE algorithm
qc2data.algorithm.run()
```

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Ex. 2: oo-VQE calculation on water

```python
# Import ASE-related modules
from ase.build import molecule

# Import qc2 modules
from qc2.data import qc2Data
from qc2.ase import PySCF
from qc2.algorithms.qiskit import oo_VQE
from qc2.algorithms.utils import ActiveSpace

# Instantiate qc2Data class
qc2data = qc2Data(
    molecule=molecule("H2O"),
    filename="h2o.hdf5"
)

# Specify and run the quantum chemistry qc2-ASE calculator.
# If you already have "h2o.hdf5" from a previous run,
# you can skip this step.
qc2data.molecule.calc = PySCF(
    method="scf.RHF",
    basis="sto-3g",
)
qc2data.run()

# Instantiate oo_VQE class
qc2data.algorithm = oo_VQE(
    active_space=ActiveSpace(
        num_active_electrons=(2, 2),
        num_active_spatial_orbitals=4
    ),
)

# Run oo-VQE algorithm
qc2data.algorithm.run()
```

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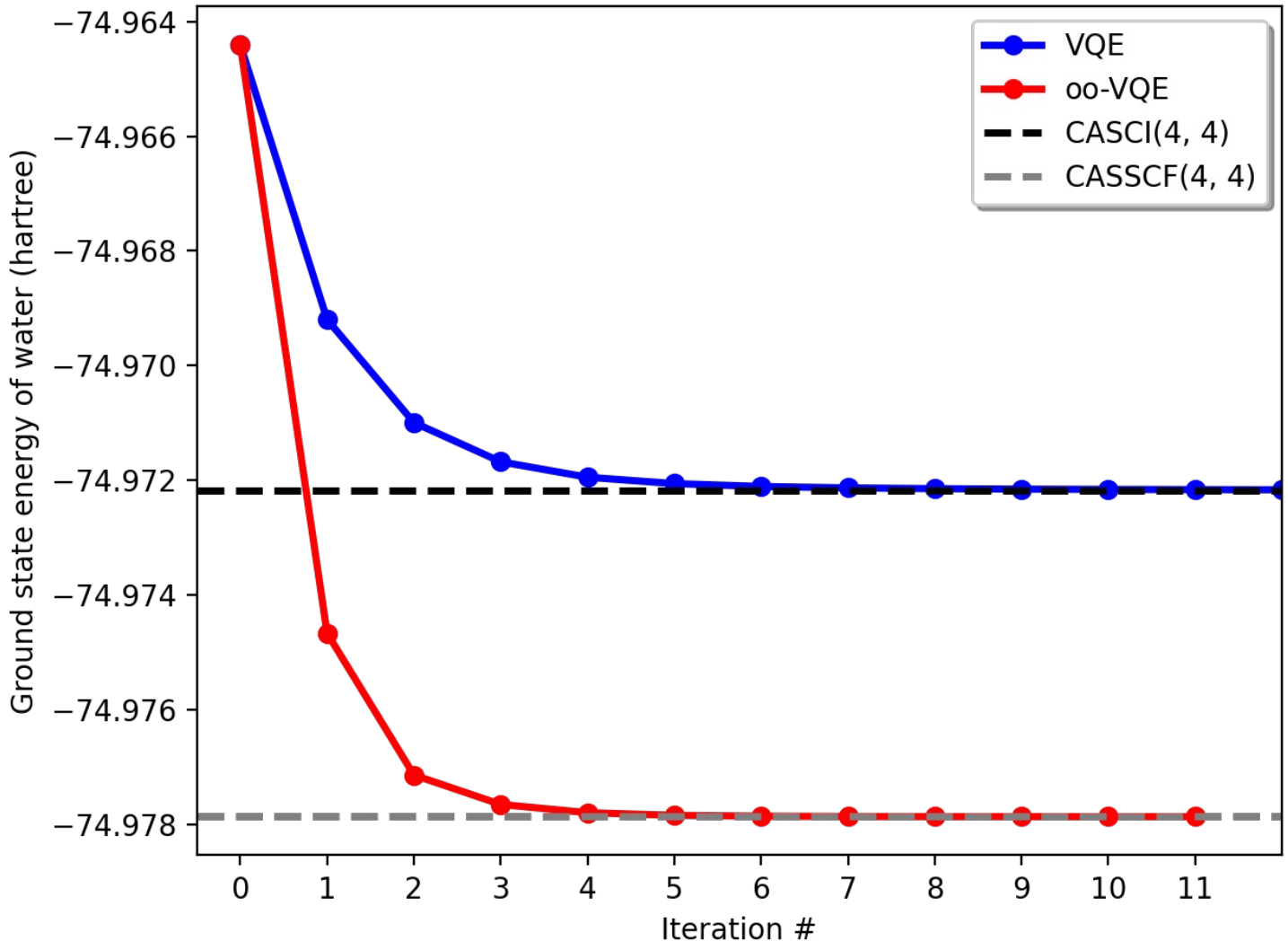
Energy convergence of ground-state water



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Final remarks

qc2 is an ever-growing open-source project, constantly enriched by new algorithms and features.

We warmly welcome your contributions!

https://github.com/qc2nl/qc2

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Thank you!

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