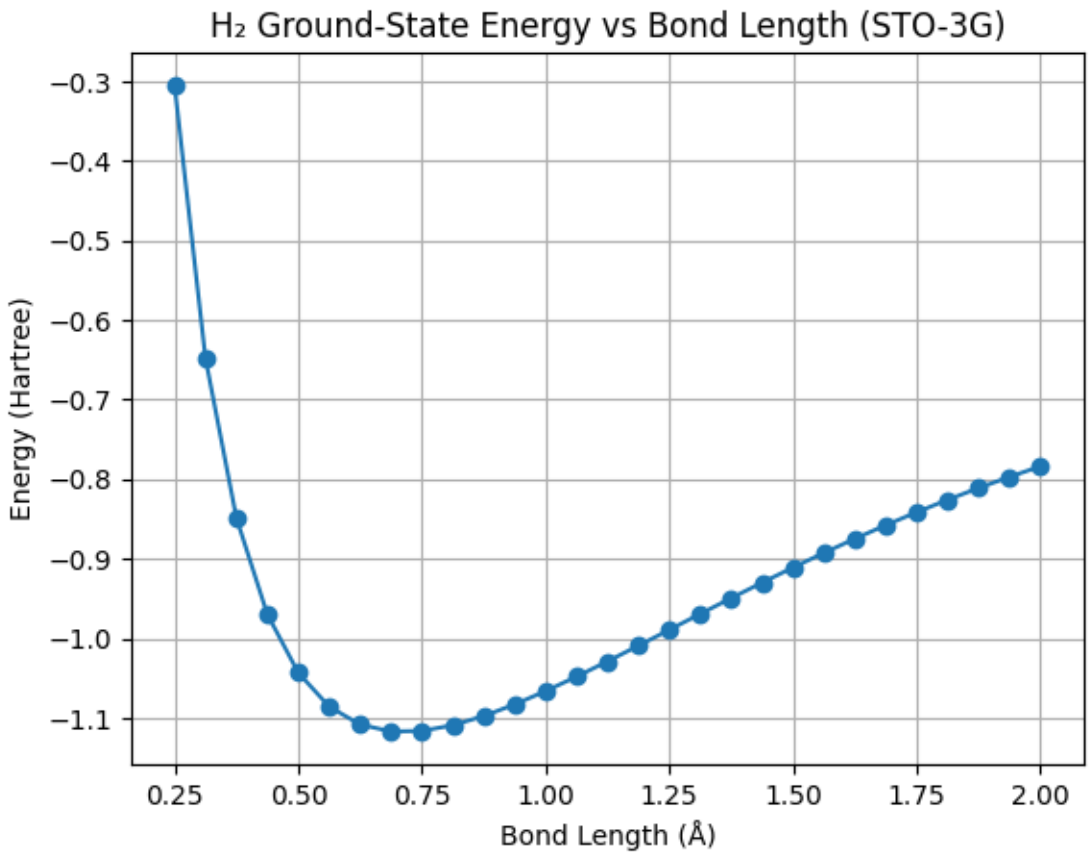
Hydrogen_Molecule_BondLength

January 12, 2026

[ ]:
```python
import numpy as np
import pandas as pd

from qiskit_nature.second_q.drivers import PySCFDriver
from qiskit_nature.units import DistanceUnit

# Bond lengths in Angstrom
bond_lengths = np.linspace(0.25, 2.0, 29)

energies = []

for r in bond_lengths:
    # Define H2 geometry
    geometry = f"H 0 0 0; H 0 0 {r}"

    # PySCF driver
    driver = PySCFDriver(
        atom=geometry,
        basis="sto3g",
        spin=0,
        charge=0,
        unit=DistanceUnit.ANGSTROM,
    )

    # Run electronic structure calculation
    problem = driver.run()

    # Ground-state energy (electronic + nuclear repulsion)
    energy = problem.reference_energy

    energies.append(energy)

# Create table
df = pd.DataFrame({
    "Bond Length (Å)": bond_lengths,
    "Energy (Hartree)": energies
})
```

```
print(df)
import matplotlib.pyplot as plt

plt.plot(bond_lengths, energies, marker='o')
plt.xlabel("Bond Length (Å)")
plt.ylabel("Energy (Hartree)")
plt.title("Classical: H  Ground-State Energy vs Bond Length (STO-3G)")
plt.grid(True)
plt.show()
```

	Bond Length (Å)	Energy (Hartree)
0	0.2500	-0.305001
1	0.3125	-0.648096
2	0.3750	-0.848599
3	0.4375	-0.969726
4	0.5000	-1.042996
5	0.5625	-1.085710
6	0.6250	-1.108150
7	0.6875	-1.116848
8	0.7500	-1.116151
9	0.8125	-1.109016
10	0.8750	-1.097454
11	0.9375	-1.082838
12	1.0000	-1.066109
13	1.0625	-1.047931
14	1.1250	-1.028797
15	1.1875	-1.009089
16	1.2500	-0.989114
17	1.3125	-0.969121
18	1.3750	-0.949314
19	1.4375	-0.929855
20	1.5000	-0.910874
21	1.5625	-0.892468
22	1.6250	-0.874712
23	1.6875	-0.857660
24	1.7500	-0.841349
25	1.8125	-0.825800
26	1.8750	-0.811026
27	1.9375	-0.797026
28	2.0000	-0.783793



[11]:
```
import numpy as np
import pandas as pd

from qiskit_algorithms import VQE
from qiskit_algorithms.optimizers import SLSQP
from qiskit.primitives import Estimator

from qiskit_nature.second_q.drivers import PySCFDriver
from qiskit_nature.second_q.mappers import JordanWignerMapper
from qiskit_nature.second_q.circuit.library import UCCSD, HartreeFock
from qiskit_nature.second_q.algorithms import GroundStateEigensolver
from qiskit_nature.units import DistanceUnit

bond_lengths = np.linspace(0.25, 2.00, 29)
vqe_energies = []

for R in bond_lengths:
    # --- Driver ---
    driver = PySCFDriver(
```

```
        atom=f"H 0 0 0; H 0 0 {R}",
        basis="sto3g",
        unit=DistanceUnit.ANGSTROM,
        charge=0,
        spin=0
    )

    problem = driver.run()

    # --- Mapper ---
    mapper = JordanWignerMapper()

    # --- Ansatz ---
    num_particles = problem.num_particles
    num_spatial_orbitals = problem.num_spatial_orbitals

    hf_state = HartreeFock(
        num_spatial_orbitals,
        num_particles,
        mapper
    )

    ansatz = UCCSD(
    num_spatial_orbitals=num_spatial_orbitals,
    num_particles=num_particles,
    initial_state=hf_state
    )
    ansatz.qubit_mapper = mapper


    # --- VQE ---
    optimizer = SLSQP(maxiter=1000)
    estimator = Estimator()

    vqe = VQE(
        estimator=estimator,
        ansatz=ansatz,
        optimizer=optimizer,
        initial_point=np.zeros(ansatz.num_parameters)
    )

    solver = GroundStateEigensolver(mapper, vqe)
    result = solver.solve(problem)

    vqe_energies.append(result.total_energies[0].real)

df = pd.DataFrame({
```

```
    "Bond Length (Å)": bond_lengths,
    "VQE (UCCSD) Energy (Ha)": vqe_energies
})

print(df)

import matplotlib.pyplot as plt

plt.plot(bond_lengths, vqe_energies, marker='o')
plt.xlabel("Bond Length (Å)")
plt.ylabel("Energy (Hartree)")
plt.title("VQE: H  Ground-State Energy vs Bond Length (STO-3G)")
plt.grid(True)
plt.show()
```

```
/tmp/ipykernel_33134/1446953903.py:52: DeprecationWarning: The class
``qiskit.primitives.estimator.Estimator`` is deprecated as of qiskit 1.2. It
will be removed no earlier than 3 months after the release date. All
implementations of the `BaseEstimatorV1` interface have been deprecated in favor
of their V2 counterparts. The V2 alternative for the `Estimator` class is
`StatevectorEstimator`.
  estimator = Estimator()
```

	Bond Length (Å)	VQE (UCCSD) Energy (Ha)
0	0.2500	-0.312270
1	0.3125	-0.656269
2	0.3750	-0.857883
3	0.4375	-0.980336
4	0.5000	-1.055160
5	0.5625	-1.099669
6	0.6250	-1.124161
7	0.6875	-1.135188
8	0.7500	-1.137117
9	0.8125	-1.132929
10	0.8750	-1.124672
11	0.9375	-1.113751
12	1.0000	-1.101150
13	1.0625	-1.087577
14	1.1250	-1.073563
15	1.1875	-1.059522
16	1.2500	-1.045783
17	1.3125	-1.032606
18	1.3750	-1.020189
19	1.4375	-1.008673
20	1.5000	-0.998149
21	1.5625	-0.988663
22	1.6250	-0.980220
23	1.6875	-0.972794

24	1.7500	-0.966335
25	1.8125	-0.960773
26	1.8750	-0.956027
27	1.9375	-0.952013
28	2.0000	-0.948641