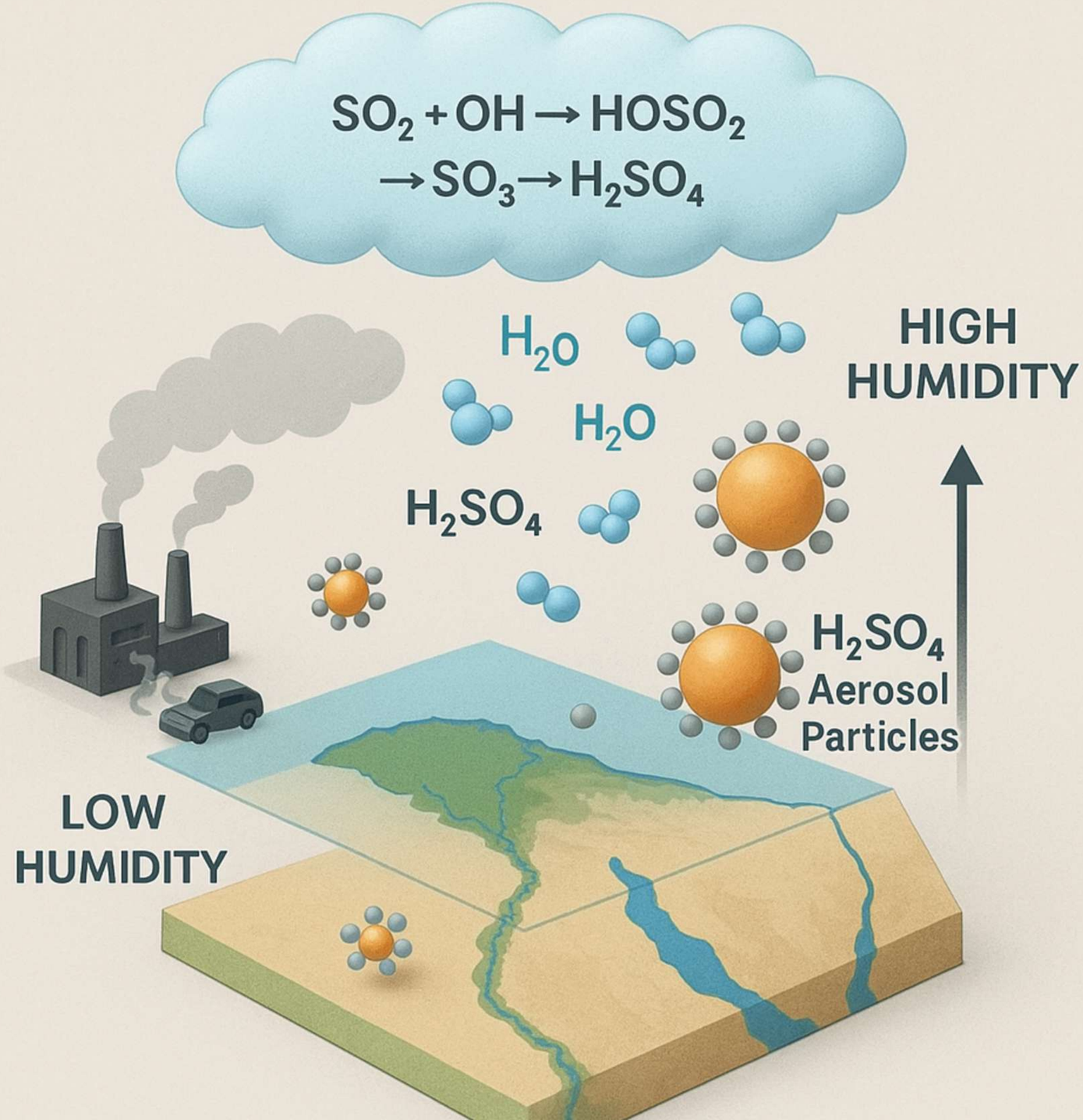
QUANTUM COMPUTING FOR ATMOSPHERIC CHEMISTRY - TEAM 12

Simulating Aerosol Formation in Humid Climates

Research Question

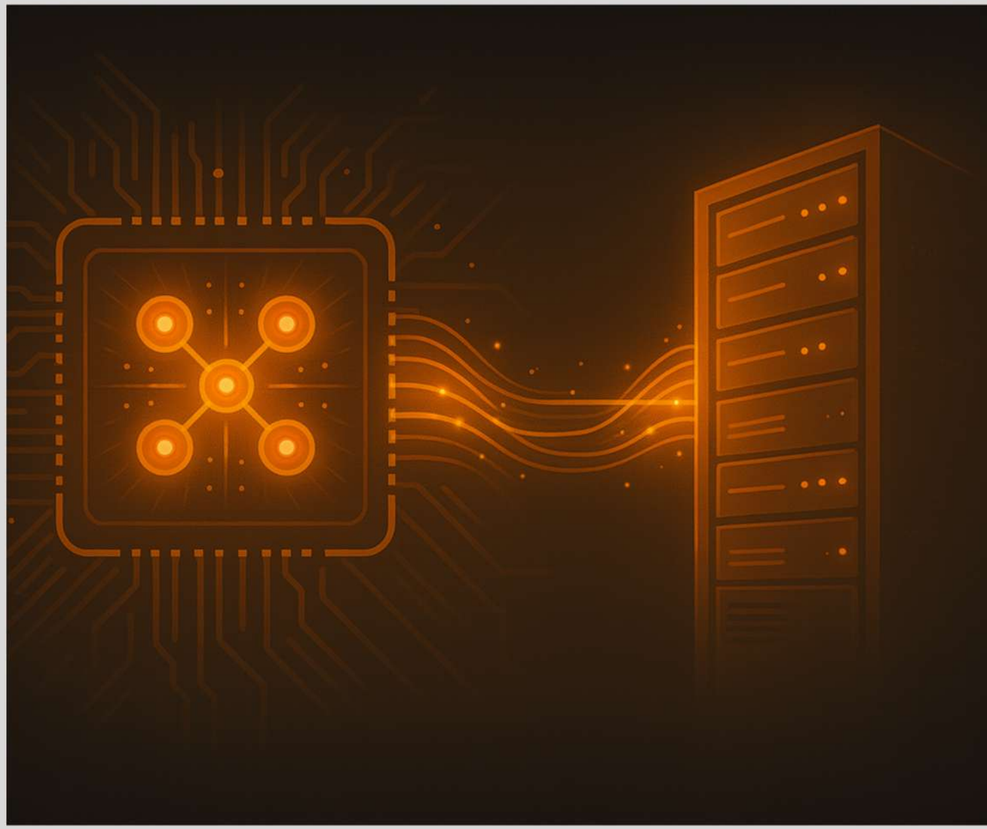
How aerosol formation in the Nile Delta can be affected by humidity?


$SO_2 + OH \rightarrow HOSO_2$
$\rightarrow SO_3 \rightarrow H_2SO_4$
H_2O
H_2O
H_2SO_4
HIGH HUMIDITY
H_2SO_4 Aerosol Particles
LOW HUMIDITY

Our Solution: A Hybrid Quantum-Classical Model

Quantum Part:

- Used VQE to compute ground-state energies of:
  - **H_2O, SO_3, H_2SO_4**
- Challenge with big molecule (SO_3, H_2SO_4) qubit reduction and term reduction:
  - **SO_3: Qubits: 46 → 6**
  - **H_2SO_4: Hamiltonian terms: 1.8M → 2628**
- Techniques:
  - Freezing the core electrons
  - Orbital reduction
  - 2-qubit tapering



Our Solution: A Hybrid Quantum-Classical Model

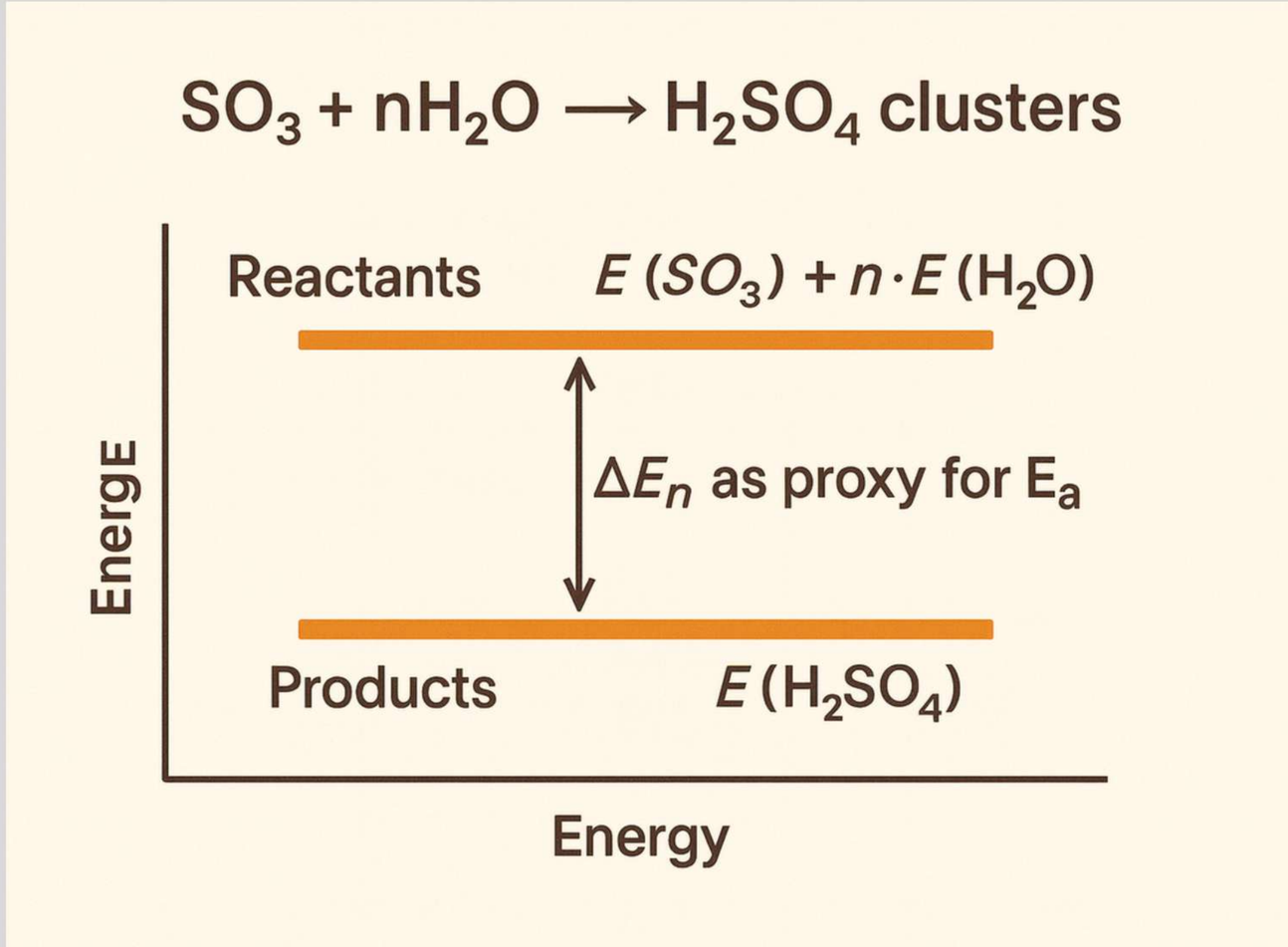
Energy Difference (ΔE):

- $\Delta E_n = E(H_2SO_4) - [E(SO_3) + n \cdot E(H_2O)]$
- Used ΔE as **activation energy proxy**

Estimate how humidity affects reaction speed Using Arrhenius equation:

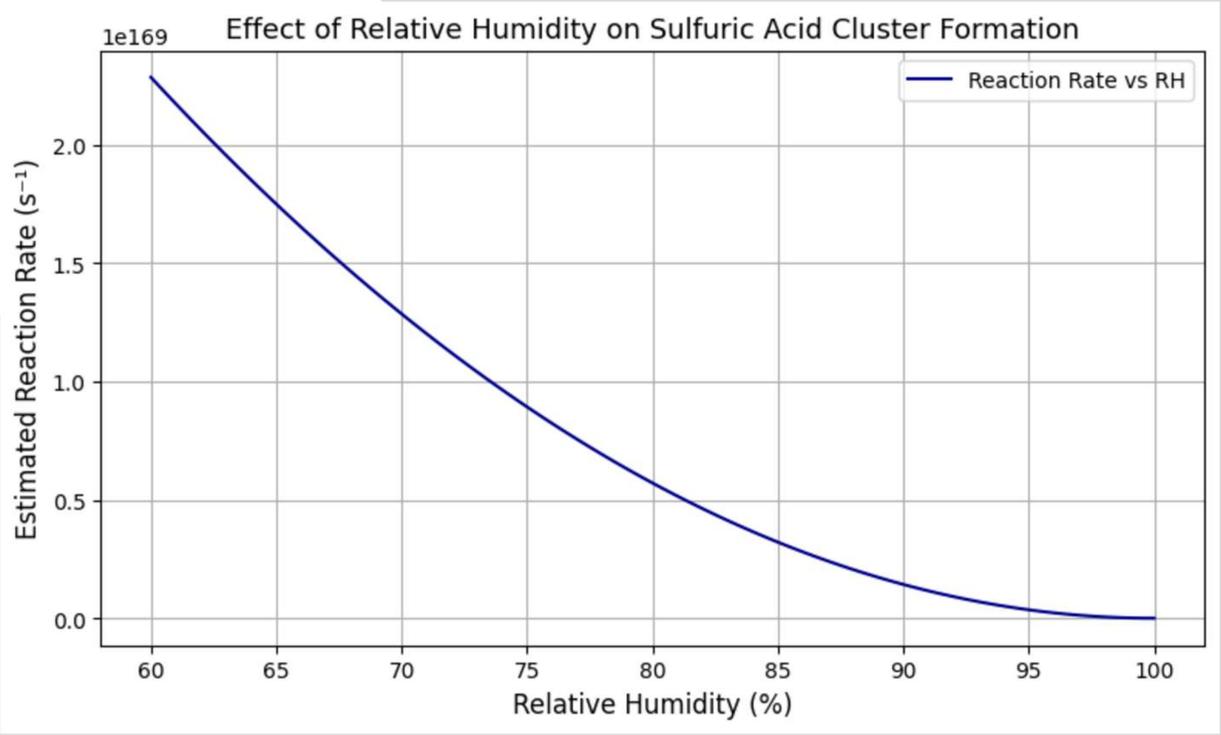
$k(T) = A \cdot e^{-Ea/RT}$

where: $Ea \approx \Delta E$



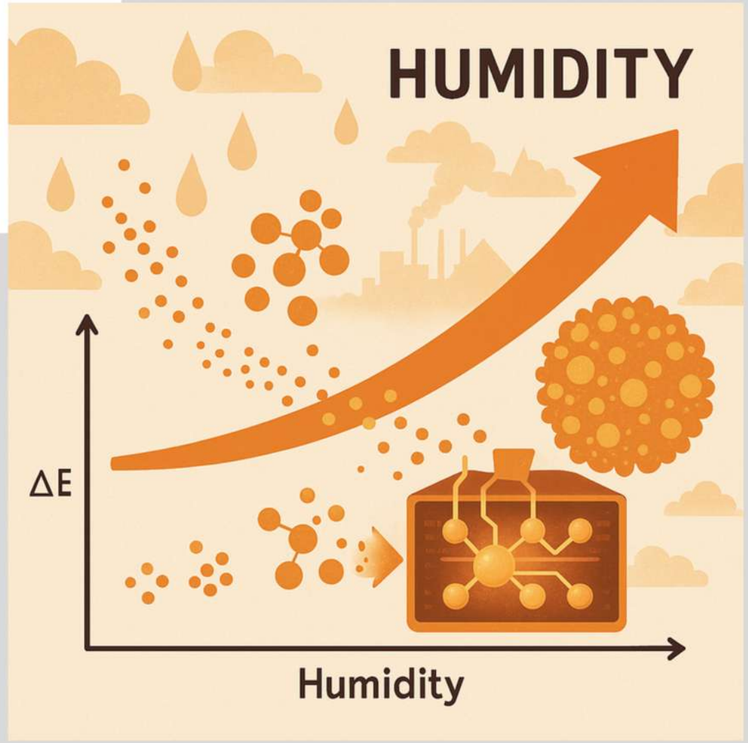
Methodology - Humidity-Dependent Reaction Rates

- **Relative Humidity (RH) Mapping:**
  - $x \in [0, 1]$ where $x = 0$ at 60% RH and $x = 1$ at 100% RH.
- **Quadratic Basis Weights:**
  - $w_1 = (1 - x)^2$
  - $w_2 = 2x(1 - x)$
  - $w_3 = x^2$



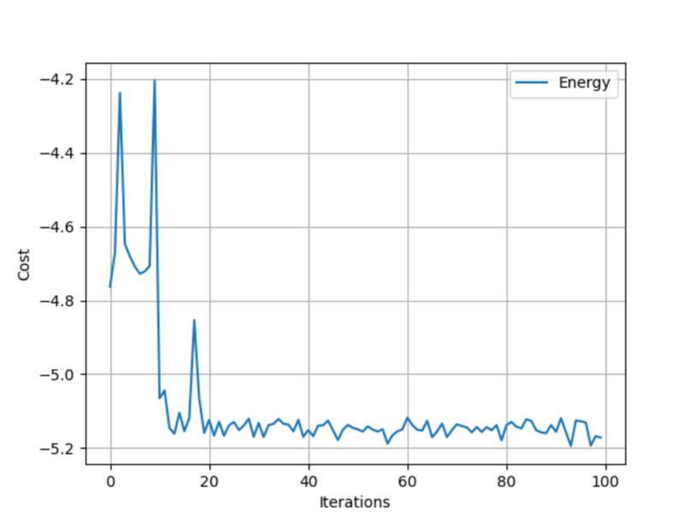
Methodology - Humidity-Dependent Reaction Rates

- **Effective Activation Energy:**
  - $\Delta E_{eff}(RH) = w_1 \cdot \Delta E_1 + w_2 \cdot \Delta E_2 + w_3 \cdot \Delta E_3$
  - *Where $\Delta E_1, \Delta E_2, \Delta E_3$ are activation energies at reference RH points.*
- **Humidity-Dependent Reaction Rate:**
  - $r(RH) \propto \exp\left(-\frac{\Delta E_{eff}}{kT}\right)$

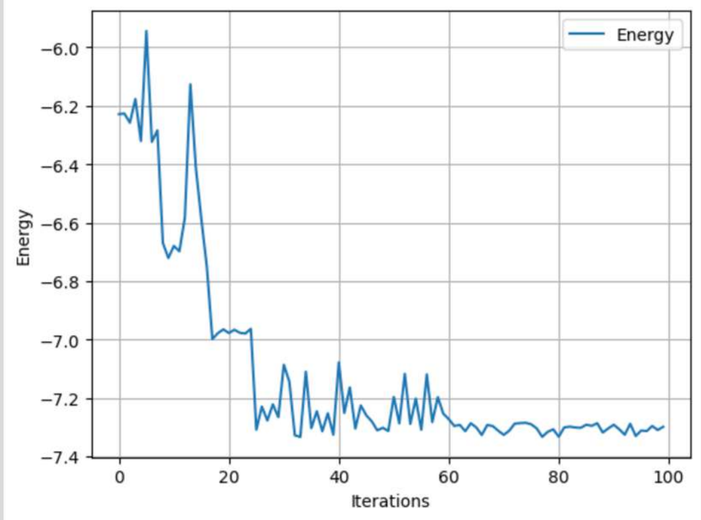


Results & Key Findings

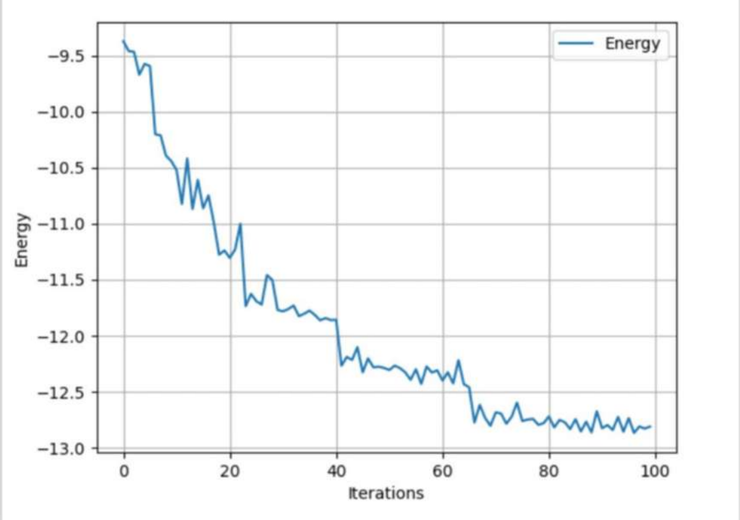
Noisy Simulation



Ground Energy: H_2O: -5.194307 Ha



SO_3: -7.333326 Ha



H_2SO_4: -12.867377 Ha

Reaction Energies: $\Delta E = E(H_2SO_4) - (E(SO3) + n \cdot E(H2O))$

cluster_1, cluster_2, cluster_3

(0.3397450000000063, 4.854562, 10.048868999999998)

Experiment setup:

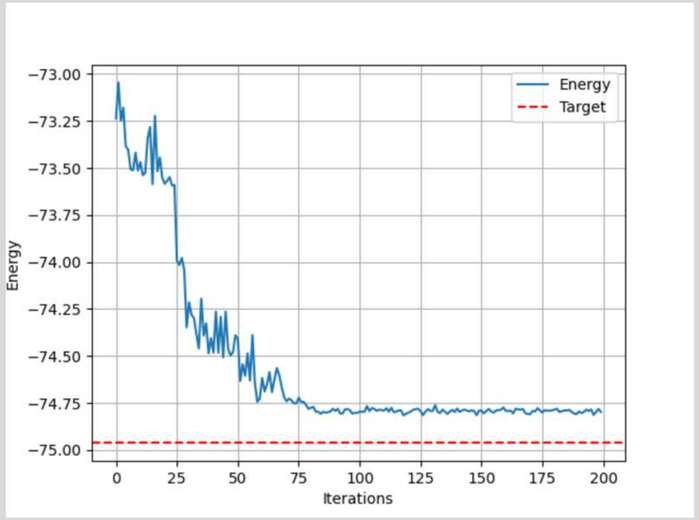
Framework: Qiskit

Simulator: FakeBrisbane

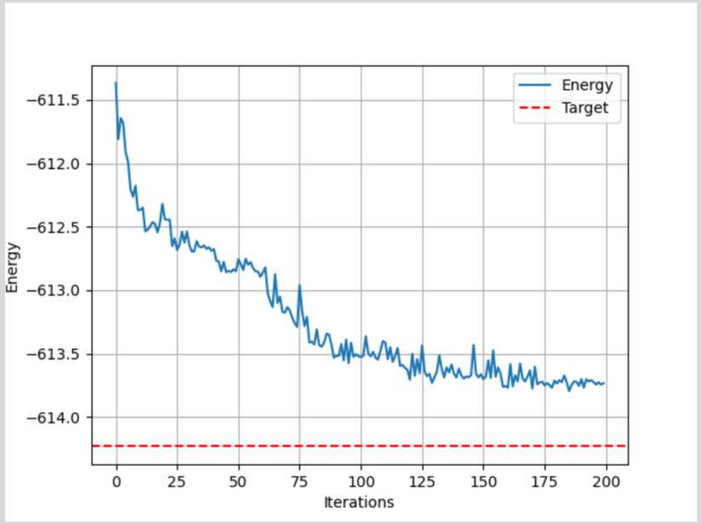
Quantum Algorithm: VQE

Results & Key Findings

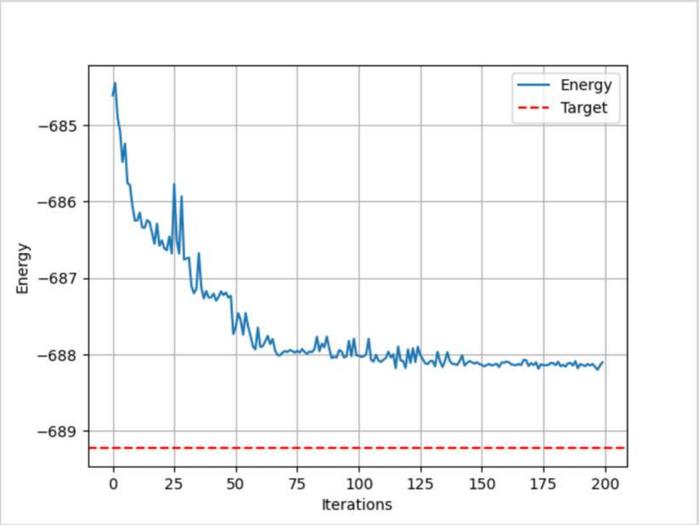
Ideal Simulation



Ground Energy: H_2O: -74.816034 Ha



SO_3: -613.795499 Ha



H_2SO_4: -688.199187 Ha

Reaction Energies: $\Delta E = E(H_2SO_4) - (E(SO3) + n \cdot E(H2O))$

ΔE1: 0.412346 Ha, ΔE2: 75.228380 Ha, ΔE3: 150.044414 Ha

Experiment setup:

Framework: Qiskit

Simulator: AerSimulator

Quantum Algorithm: VQE

Impact & Mapping to Aerosol Nucleation

- **Higher RH → more clustering → faster sulfate formation**
- **Can map rate increase to nucleation probability**
  - Useful for climate models and air pollution forecasting
- **Quantum advantage:**
  - Enables accurate energy estimates for complex hydrogen-bonded systems
  - Scalable to other reactions (e.g. nitric acid, ammonia)

Conclusion

- Built a full quantum-classical pipeline
- Simulated $SO_3 + nH_2O \rightarrow H_2SO_4$ for n = 1–3
- Predicted RH-dependent rates and mapped to nucleation insights
- First step toward quantum-enabled climate chemistry modeling

Thanks