QUANTUM-ACCELERATED SUPERCOMPUTING FOR MATERIALS SCIENCE: HOW TO?

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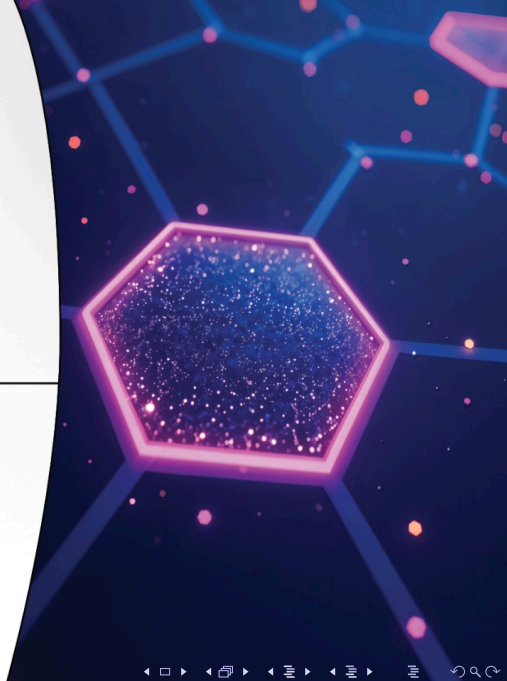

Quantum-Accelerated Supercomputing for Materials Science

Atomistic use case of HPC-QC algorithms integration Quantum Computing with HPC for

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Motivation and Goals

- **Challenge**: Materials simulations consume significant HPC resources using classical methods
- **Opportunity**: Quantum computing as a new accelerator in the HPC paradigm to run quantum methods
- **Example application**: Examine environmental friendly alternative corrosion inhibitors for aerospace and automotive industries
- **Goal**: Demonstrate quantum-HPC integration for important material science problem

The use case in a nutshell

Demonstration of quantum-accelerated corrosion inhibitor screening using hybrid HPC-quantum workflow

Quantum Computing in Materials Science

- Electronic structure calculations are perfect for quantum computers
- Current limitation: Small molecules only (few qubits available)
- Solution: Quantum embedding - treat critical regions with quantum accuracy

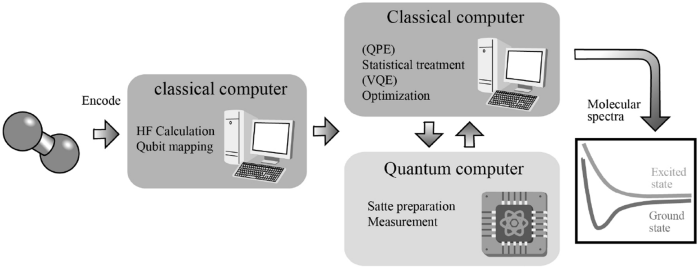


Figure: Typical quantum chemistry workflow [1]

Applying the above workflow beyond small molecules to larger molecules or periodic systems can be difficult at the moment due to large number of qubits needed

Materials Systems in Different Dimensions

Focus on materials science simulations like solid-state systems is picking up using quantum computing algorithms, those systems are often modeled as periodic systems and simulation cell can have hundreds of atoms and system can be 1D, 2D or 3D

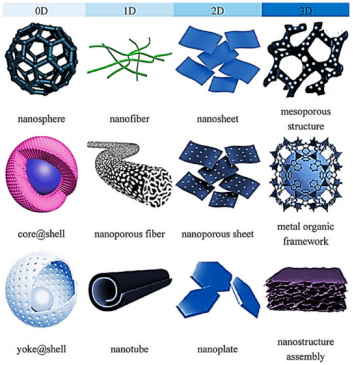


Figure: from [2]: Examples of materials systems in 1D, 2D and 3D

Computational materials science in a nutshell

- Modeling and computing materials properties is solving the electronic structure problem for the system of interest to predict a physical variable of interest
- Electronic structure of molecules and solids is the starting point in a computational materials science workflow
- Models and embedding help simplify complex quantum calculations

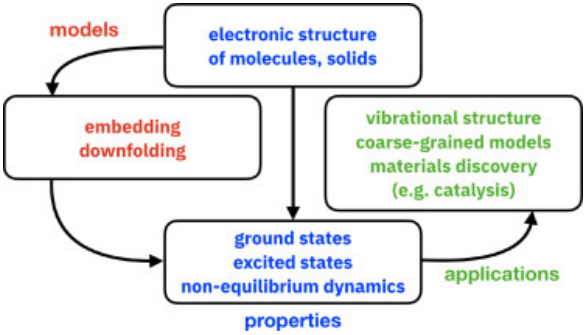
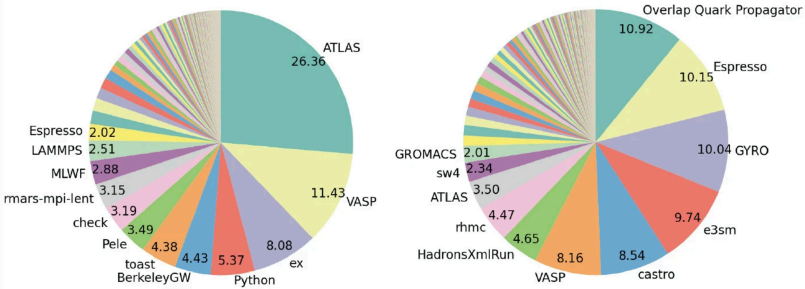


Figure: From [3]

Connection to HPC resources

From: Analyzing Resource Utilization in an HPC System: A Case Study of NERSC's Perlmutter



(a) CPU-only nodes. (b) GPU-accelerated nodes.

Decomposition of node-hours by applications. Infrequent applications are not labeled.

Figure: From [4]

Connection to HPC resources

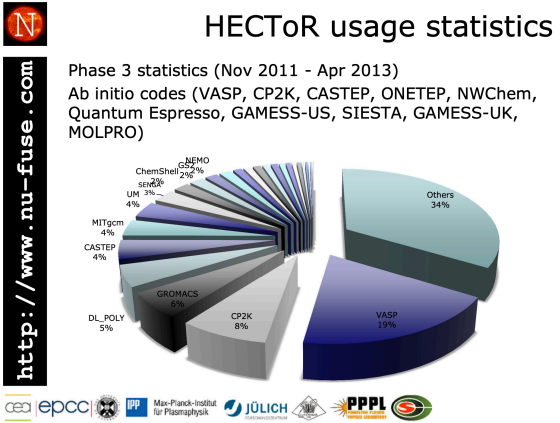


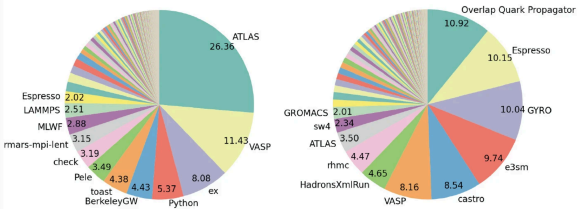
Figure: From [5]

Connection with current codes

Connection to HPC resources

Typically those systems require many cores and nodes and fill-up big portion of HPC time, for example through Density Functional Theory (DFT) calculations (by famous codes like VASP, Quantum ESPRESSO, ABINIT, etc.)

From: **Analyzing Resource Utilization in an HPC System: A Case Study of NERSC's Perlmutter**



(a) CPU-only nodes. (b) GPU-accelerated nodes.

Decomposition of node-hours by applications. Infrequent applications are not labeled.

Figure: HPC usage at NERSC [4]

- DFT codes dominate HPC usage
- VASP alone: 20% of resources
- Materials science: Major HPC consumer
- Hybrid quantum-classical workflows could unlock new computational capabilities

Quantum-Centric Supercomputing

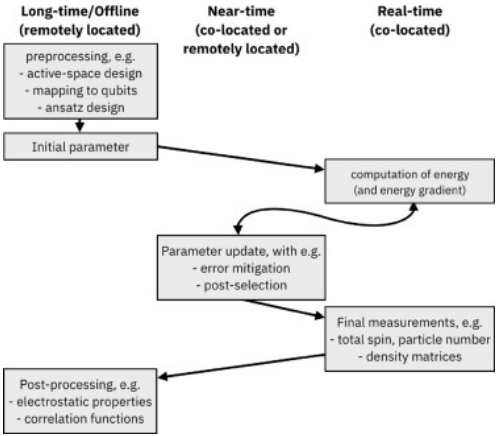


Figure: Integration of classical HPC and quantum resources [3]

- QPUs as specialised accelerators
- Hybrid workflows leverage strengths of both paradigms
- This example shows the VQE steps of the calculation connected by arrows describing the flow of operations that require "long-time/near-time/real-time" interaction between HPC and quantum computers

Material science codes that utilise HPC resources could have the potential to combine the best of both worlds, revealing the higher accuracy of quantum methods and the efficiency of classical methods in accelerated material science

Corrosion Inhibition: a practical usecase application on Quantum Computing for Materials

- **Problem**: Cars and Aeroplanes body corrosion costs billions annually
- **Traditional solution**: Use chromium-based corrosion inhibitors (toxic)
- **Eco-friendly alternative**: organic inhibitors (such as: triazole derivatives)
- **Challenge**: Predicting the effectiveness of those alternatives requires expensive calculations
- **Solution**: examining the adhesion power of those alternative inhibitor molecules on top of metal alloys surfaces that form the body of a car or aeroplane. The calculations could employ a workflow that benefit from accurate quantum calculations to correct for energies computed by classical calculations

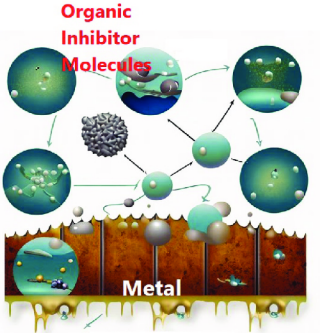


Figure: Inhibition mechanisms [6]

Quantum Embedding: bridging quantum simulations to material science workflows

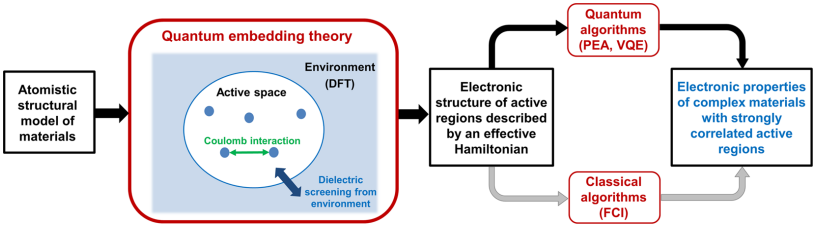


Figure: General strategy for quantum simulations of materials using quantum embedding [7]

- Use the classical resources to do the calculations as usual and focus the quantum part on the important interactions that can benefit from the quantum algorithms and feed the results back to the classical side
- simulations utilises active space approximation to reduce the resources required to model the system's electronic structure on a quantum workflow

Quantum Embedding Method for the Simulation of Systems on Quantum Computers I

$$E_{\text{SCF-in-DFT}}[\gamma^A_{\text{emb}};\gamma^A,\gamma^B] = E_{\text{SCF}}[\gamma^A_{\text{emb}}] + E_{\text{DFT}}[\gamma^A+\gamma^B] - E_{\text{DFT}}[\gamma^A] + \text{tr}[(\gamma^A_{\text{emb}}-\gamma^A)\nu_{\text{emb}}[\gamma^A,] + \alpha\text{tr}[\gamma^A_{\text{emb}}\mathbf{P}^B] \quad (1)$$

This relies on the projection-based wave function-in-DFT (WF-in-DFT) embedding method, where the total KS density matrix, γ, of the molecular system obtained from KS-DFT is partitioned into an active and environment subsystem, γ_A and γ_B

E_{SCF} is the energy of the embedded subsystem A at SCF level

$\mathbf{P}^B = S\gamma^B S$ is a projector for orbital orthogonality α is a scaling parameter, ν_{emb} includes all two-electron interactions

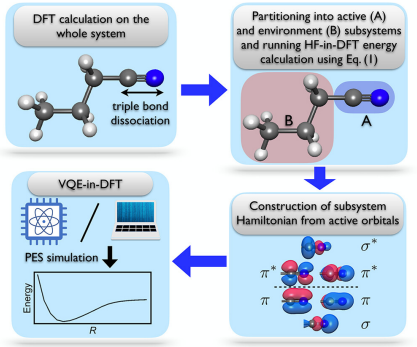


Figure: Quantum embedding in action [8]

Quantum Embedding Method for the Simulation of Systems on Quantum Computers II

ADAPT-VQE: Adaptive Derivative-Assembled Pseudo-Trotter VQE (ADAPT-VQE) is a solver technique that builds an ansatz iteratively from a predefined operator pool, which can efficiently converge to predict the ground state energy [9]

Then different pool of ansatz offered by UCCSD can be chosen then initial Hartree-Fock state can be formed then build the Hamiltonian

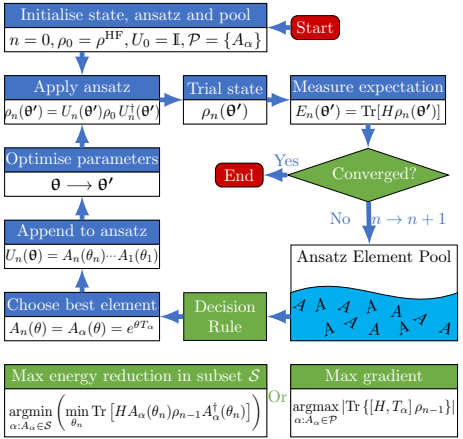


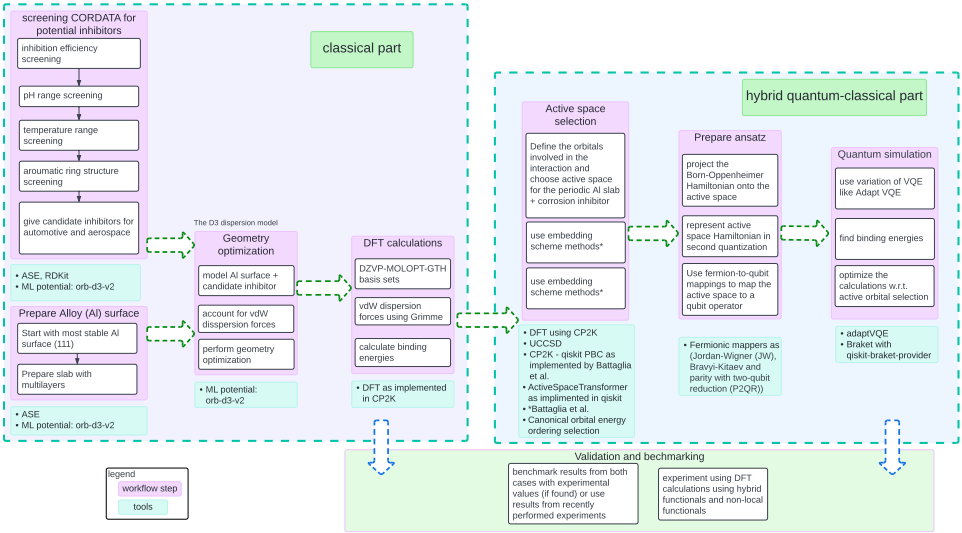
Figure: ADAPT-VQE procedure [10]

How to perform the quantum-centric supercomputing approach to simulation corrosion inhibition

- Build the DFT simulation workflow
- Identify the part of important interactions to study with the quantum algorithm (e.g. surface-adsorbate interactions where we choose orbitals around the Fermi level)
- Build Hybrid quantum-classical computational framework where calculations from DFT (implemented in CP2K) can talk to quantum algorithm calculation (adaptVQE implemented in Qiskit)

Paper: open here Code: GitHub repository [11] Materials Cloud Archive 2024.211 (2024) raw data to reproduce the workflow
Demo video on YouTube: video demo

Computational Workflow Overview



System Setup and Inhibitor Selection

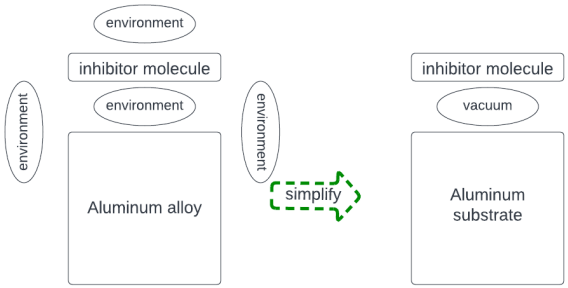
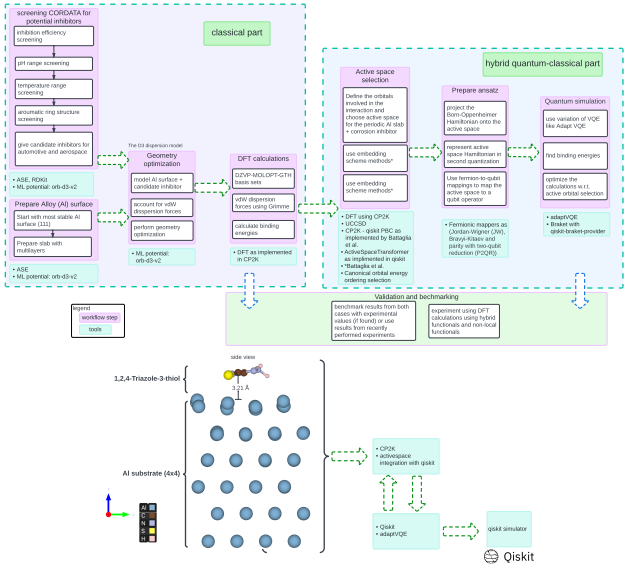


Figure: Model simplification approach: we simplify our system to make the calculations easy to compute and focus on the two parts which are the DFT and the adaptVQE calculations

- Al(111) surface (4×4 supercell)
- Two inhibitors studied:
  - 1,2,4-Triazole
  - 1,2,4-Triazole-3-thiol
- Binding energy as effectiveness metric
- Active space: 2 electrons in 5 orbitals

Case Study: Workflow with Example System



From: [12]

CP2K-Qiskit Integration

- Socket-based communication
- FCIDUMP format for integrals
- Self-consistent embedding loop
- ADAPT-VQE algorithm for quantum part

most important article here!

This figure is from [13]

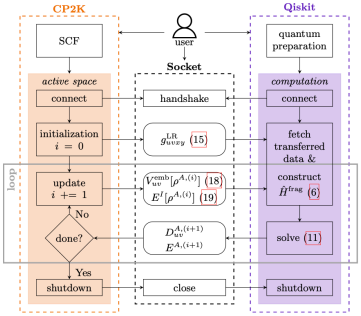


FIG. 2. Workflow diagram depicting the interaction of CP2K and Qiskit Nature. The user configures the two classical processes and the socket for the IPC. Each process then follows the computational steps (rectangular boxes) outlined inside of their respective frames. The data that gets computed and transferred is indicated by the rounded boxes. Numbers in parentheses refer to the respective equations in this manuscript. The self-consistent embedding requires a loop which is highlighted by the gray box. This loop is terminated based on the decision (diamond shape) taken by the CP2K process.

Computational Parameters

Component	Details
Classical (DFT)	
Software	CP2K with PBE functional
Basis Set	DZVP-MOLOPT-GTH
Dispersion	Grimme D3 correction
ML Potential	orb-d3-v2 for geometry optimisation
Quantum	
Algorithm	ADAPT-VQE
Active Space	2e, 5o (10 spin-orbitals)
Mapping	Parity with 2-qubit reduction
Optimiser	SPSA (1000 iterations)
HPC Resources	
CPU	AMD EPYC 9R14 Processor
Cores	96 cores

Quantum Algorithm Selection and Optimisation

Algorithm	Convergence	Accuracy	Runtime
Vanilla VQE	Poor	Low	High
UCCSD Ansatz	Good	Medium	Medium
ADAPT-VQE	Excellent	High	Medium
Stateful ADAPT-VQE	Excellent	High	Low

- **ADAPT-VQE advantages**:
  - Gradient-based operator selection
  - Dynamically constructed ansatz
  - Reduced circuit depth
- **Warm-starting technique**:
  - State preparation from previous calculations
  - Faster convergence for similar systems
  - 5-6$\times$ speedup demonstrated

Corrosion inhibition case study: System Setup and Classical Computational Details

Establish a baseline benchmark by using the DFT code CP2K to solve the problem classically then compare with the hybrid calculation using both CP2K and Qiskit

- System: Al(111) surface with triazole inhibitor and vacuum gap of 25 Å in the z-direction. The supercell is 4×4 size to avoid interactions between repeated cells
- PBE functional with D3 dispersion correction
- Binding energy calculation:

$$E_{\text{binding}} = E_{\text{supercell}} - (E_{\text{substrate}} + E_{\text{inhibitor}})$$

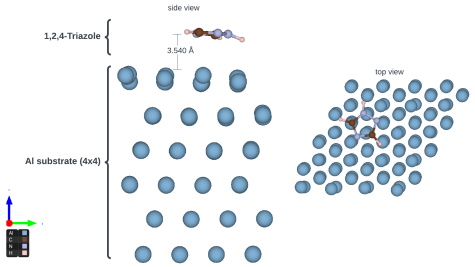


Figure: From [12]

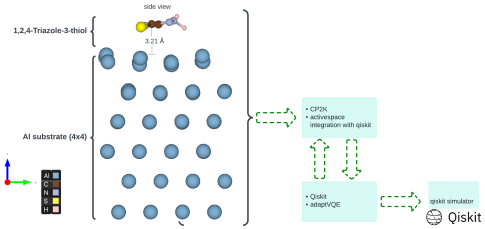
Complete Computational Parameters Summary

Method/Component	Details
Classical Calculations	
Geometry Optimization	ASE with orb-d3-v2 model
Dispersion Corrections	Grimme's D3 (integrated into neural network potential)
Surface Model	Al(111) 4×4 supercell
DFT Calculations	
Functional	PBE with GGA implementation
Basis Set	DZVP-MOLOPT-GTH (double-zeta valence polarized)
Method	GPW, plane-wave cutoff: 500 Ry, relative cutoff: 60 Ry
van der Waals	DFT-D3 with PBE reference functional
Vacuum Gap	25 Å (z-direction)
SCF Convergence	1.0E-6 Ha, Broyden mixing ($\alpha = 0.1$, $\beta = 1.5$)
Active Space Parameters	
Configuration	2e, 5o (2 active electrons in 5 orbitals)
Selection Method	ActiveSpaceTransformer (Qiskit implementation), canonical orbital energy ordering selection
Quantum Calculations	
Primary Algorithm	ADAPT-VQE from Qiskit, StatefulAdaptVQE from qiskit-nature-cp2k
Qubit Mapping	Parity with two-qubit reduction
Convergence Criteria	Energy threshold: 1e-6 Hartree, gradient norm: 1e-4
Classical Optimizer	SPSA (learning rate: 0.005, perturbation size: 0.05, max iterations: 1000)
Quantum Hardware & Simulation	
Simulators	Qiskit local and Aer

Corrosion inhibitors choice (Classical)

Inhibitor	MW (g/mol)	Temp (K)	pH Range	Eff. (%)
1,2,4-Triazole	69.07	298	8-10	90
1,2,4-T-3-thiol	101.13	298	4-10	70-90
Benzotriazole	119.12	298	7-10	90-98
2-MBI	150.2	298	4-10	90
THC	227.24	303	7	91-95
T-methionine	502.70	298	7	95-99

- Shortlisted few inhibitor molecules
- Chosen two variations of Triazole inhibitors
- Geometry-optimized structures consistent with experimental observations



Binding Energy Comparison

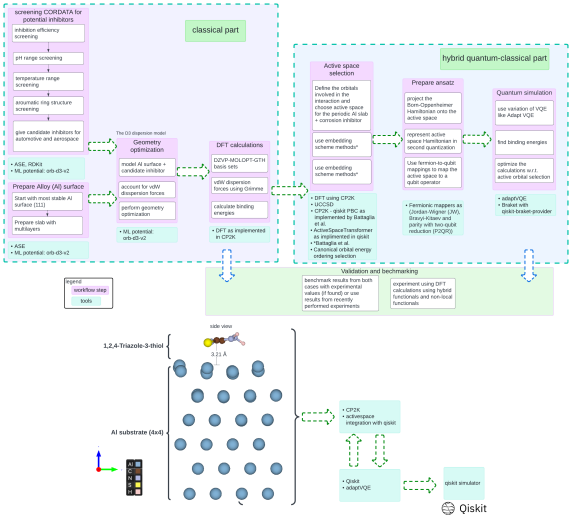
Method	Inhibitor	Binding Energy (eV)	Distance (Å)
Classical DFT	1,2,4-Triazole	-0.386	3.54
ADAPT-VQE	1,2,4-Triazole	-0.386	3.54
Classical DFT	1,2,4-T-3-thiol	-1.279	3.21
ADAPT-VQE	1,2,4-T-3-thiol	-1.279	3.21

Key Findings

- Agreement between classical and quantum methods
- Thiol derivative shows 3.3× stronger binding
- Results align with experimental observations where enhanced surface interaction of thiol derivative supports findings on sulfur's role in surface passivation
- Validates quantum approach for materials screening

Comments on VQE flavours

- **ADAPT-VQE shows good agreement with classical DFT**:
  - allowing more orbitals would enhance the results
  - the agreement with DFT shows good promise for the quantum workflow
- **Challenges with vanilla VQE**:
  - Convergence issues
  - Less accurate results
- **Active space limitations**:
  - Currently 2e, 5o
  - Future: expand to 10e, 20o



Performance analysis with simple example

- **Time distribution**:
  - CP2K: 62%
  - Quantum (Qiskit): 38%
- **Benchmarking results**:
  - Standard VQE: 3654s
  - ADAPT-VQE: 1552s
  - Stateful ADAPT-VQE: 272s
- **Key achievement**: 5-6× speedup with optimised implementation

Algorithm	Runtime (s)
VQE	3654
Stateful VQE	3134
ADAPT-VQE	1552
Stateful ADAPT-VQE	272

Table: Performance comparison on LiH benchmark

Computational Efficiency
Quantum embedding reduces quantum resource requirements

Computational Scaling and Resource Requirements

- **Current system size**:
  - Al(111) 4×4 supercell
  - 64 Al atoms total
  - 2 electrons, 5 orbitals (quantum)
- **Scaling challenges**:
  - Exponential growth with system size
  - Limited quantum coherence time
  - Classical-quantum communication overhead
- **Future targets**:
  - 10e, 20o active spaces
  - Larger surface models
  - Multiple inhibitor molecules

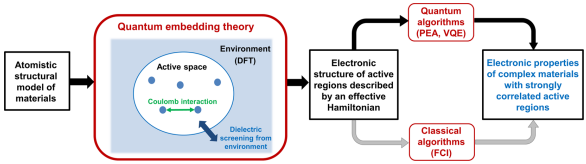


Figure: Quantum embedding scales efficiently

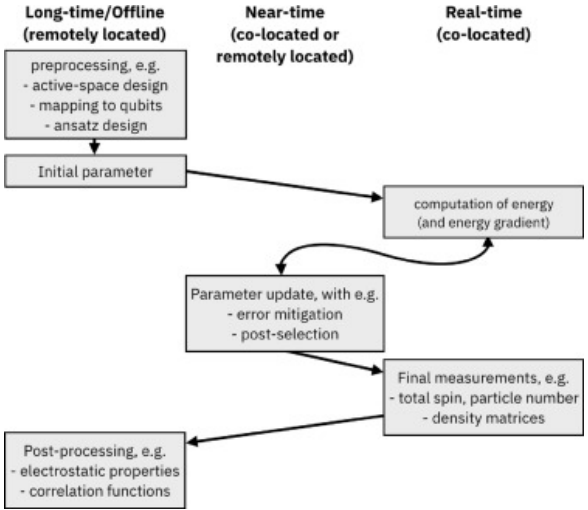
$$\text{Qubits} = 2 \times n_{\text{orbitals}} \tag{2}$$

$$\text{Classical cost} \propto N^3 \tag{3}$$

$$\text{Quantum cost} \propto 2^{n_{\text{active}}} \tag{4}$$

Broader Applications in Materials Science

- **Immediate applications**:
  - Carbon capture (MOFs)
  - Hydrogen storage materials
  - Battery electrode interfaces
  - Photovoltaic materials
- **Automotive industry**:
  - Lightweight alloy protection
  - Electric vehicle components
  - Smart coating development
- **Aerospace applications**:
  - High-temperature resistance
  - Space environment protection
  - Advanced composite interfaces



Comparison with Traditional Approaches (predictions)

Method	Accuracy	Cost	Time to Solution
Experimental screening	High	Very High	Months
Pure DFT	Medium	High	Days
Hybrid functionals	High	Very High	Weeks
Quantum-HPC hybrid	**High**	**Medium**	**Hours**

- **Traditional experimental approach**:
  - Synthesise and test hundreds of compounds
  - Expensive laboratory equipment
  - Long development cycles
- **Pure computational approach**:
  - Limited accuracy for complex systems
  - Scaling challenges for realistic models
- **Quantum-HPC approach**:
  - Best of both worlds: accuracy + efficiency
  - Rapid screening capabilities
  - Reduced experimental validation needs

Current Limitations and Technical Challenges

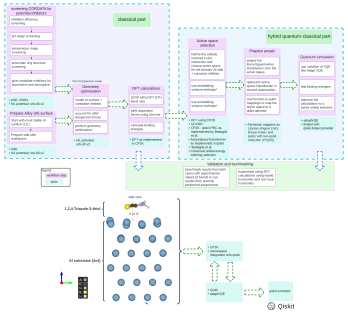
- **Quantum hardware limitations**:
  - Limited qubit counts (100-1000)
  - Short coherence times
  - High error rates
- **Software integration**:
  - Communication latency
  - Data format conversion
  - Synchronisation challenges
- **Active space selection**:
  - Manual orbital selection
  - System-dependent optimisation
  - Balance accuracy vs. resources
- **Validation challenges**:
  - Limited experimental benchmarks
  - Complex multi-physics interactions
  - Scale-up verification needed
- **Performance considerations**:
  - Queue times on quantum hardware
  - Cost optimisation
  - Workflow orchestration

Key Challenge
Balancing quantum advantage
with practical constraints

Summary and Impact

- **Achievement**: First quantum-HPC workflow for corrosion inhibition
- **Validation**: Quantum results match classical DFT
- **Efficiency**: ADAPT-VQE shows significant speedup
- **Practical impact**: Enables screening of green inhibitors

Paper: open here Code: GitHub repository [11] Materials Cloud Archive 2024.211 (2024) raw data to reproduce the workflow
Demo video on YouTube: video demo



Future Directions

- **Immediate goals**:
  - Expand active space (currently 2e,5o $\rightarrow$ 10e,20o)
  - Test the workflow using SQD on real quantum hardware (IQM)
  - Benchmark against FCI for accuracy validation
- **Long-term vision**:
  - Apply to other materials challenges:
    - Carbon capture (metal-organic frameworks)
    - Hydrogen storage (catalysis)
    - Battery materials
  - Integrate with HPC scheduling systems
  - Develop automated active space selection

Quantum-centric supercomputing is ready for materials science applications. Let's collaborate to accelerate material discovery!

Sample-based Quantum Diagonalization (SQD)

Classical post-processing of quantum samples to find eigenvalues/eigenvectors

- **Advantages**:
  - Noise robust, reduced qubit requirements
  - Large Hamiltonians (millions of terms)
  - Quantum + classical hybrid computing
- **Method**:
  - Sample quantum circuits
  - Refine configurations classically
  - Diagonalize in sampled subspace

Ref: arXiv:2405.05068

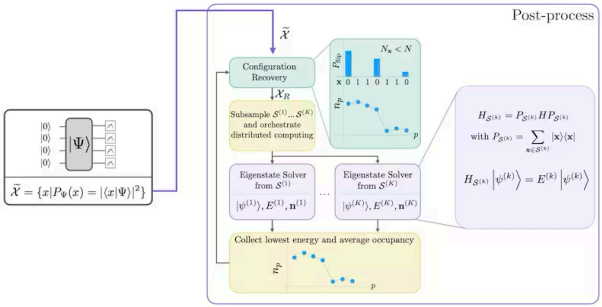


Figure: SQD workflow

Want to Learn More About SQD and Quantum Computing?

Quantum Autumn School 2025 - Information

Nov 3-7, 2025 | Stockholm, Sweden

- Introduction and how to build a Quantum algorithm
- SQD & variational quantum algorithms
- Quantum error correction (QEC)
- EuroHPC-JU quantum HW (VLQ)
- Industry: IQM, IonQ, NVIDIA

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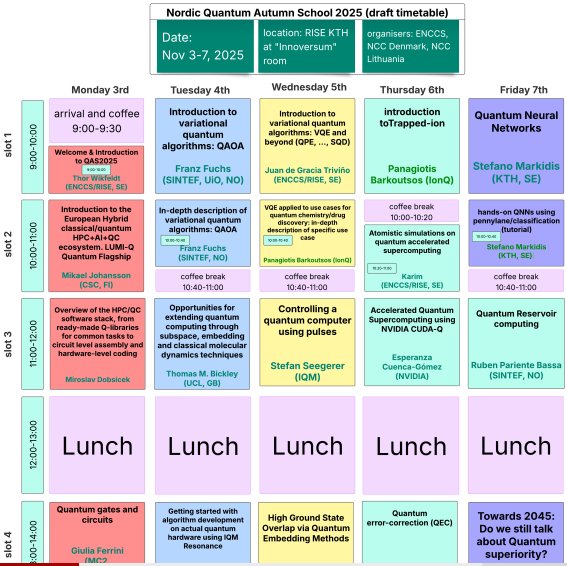
Quantum Autumn School 2025 - Detailed Program



Useful literature and resources

Learning resources

- For some recent VQE implementations: [14]
- A good review article on the topic of quantum-centric supercomputing: [3]
- For more insights, see the tutorial video lecture [15]
- NVidia blog post on ADAPT-VQE [9]

Qiskit Nature and CP2K resources

- Qiskit-nature-CP2K integration https://github.com/Qiskit/qiskit-nature-cp2k
- Qiskit-nature https://github.com/qiskit-community/qiskit-nature

Quantum Embedding tools

- A Python package for Bootstrap Embedding (BE) method for quantum embedding: [16], the related publication is [17]
- For more on quantum embedding: [18]

Acknowledgements

- AWS for Braket credits and EC2 AMD HPC instances
- Airbus and BMW experts for industrial insights
- Qiskit nature CP2K integration https://github.com/mrossinek/qiskit-nature-cp2k

Thank you! Questions?

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