Quantum Computing for Materials Science

quantum computer as another accelerator to HPC

Karim Elgammal

QAS2024

December 2, 2024

Overview

Motivation

- Quantum chemistry calculations are promising early applications of quantum computers
- Materials science simulations involve periodic systems and large numbers of atoms
- Current focus: Quantum-centric supercomputers with quantum accelerators
- Need for hybrid quantum-classical approaches for practical applications

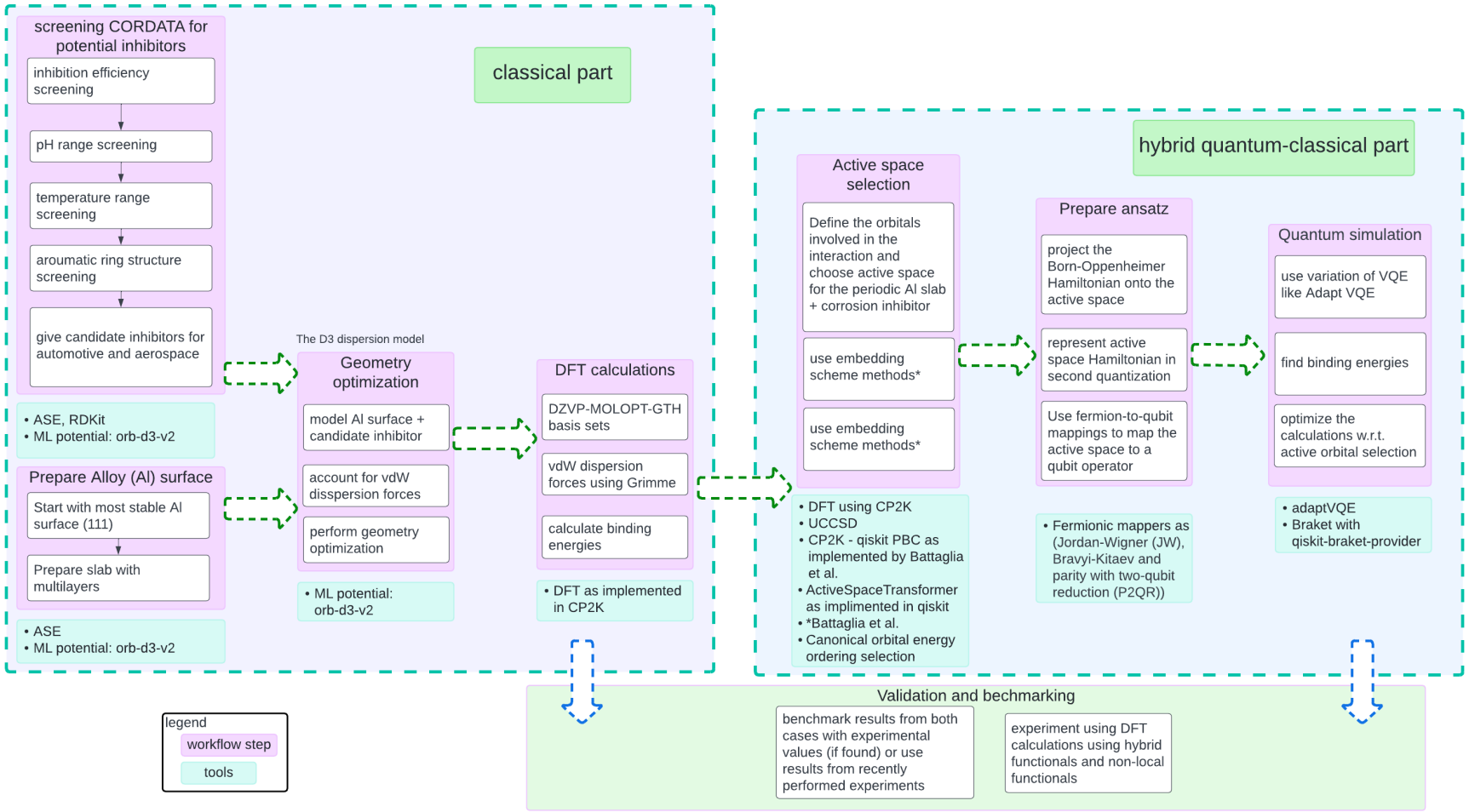
Why Quantum Computing for Materials?

- Large solid-state systems require approximations in DFT
- Quantum computing can improve accuracy for critical subsystems
- Quantum embedding approach similar to QM/MM methods
- Potential for better description of electron correlation

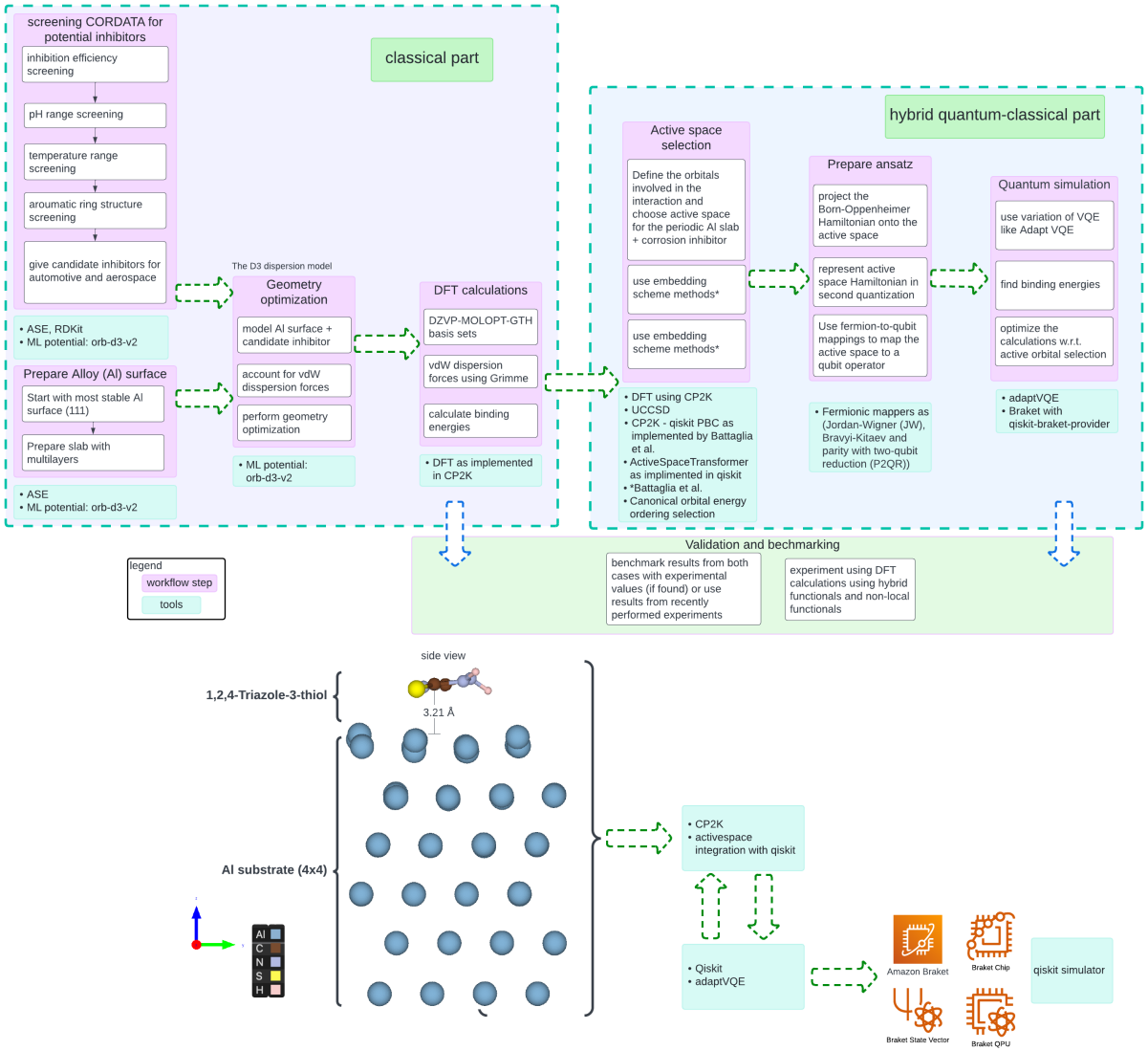
Our Approach - Core Methodology

- Simplify the problem and consider Aluminum substrate instead of alloys
- Approach the problem from DFT simulation workflow
- Introduce quantum computer as accelerator to the workflow
- Build Hybrid quantum-classical computational framework
- Focus on surface-adsorbate interactions

Workflow Overview



Workflow with Example System



Problem Simplification

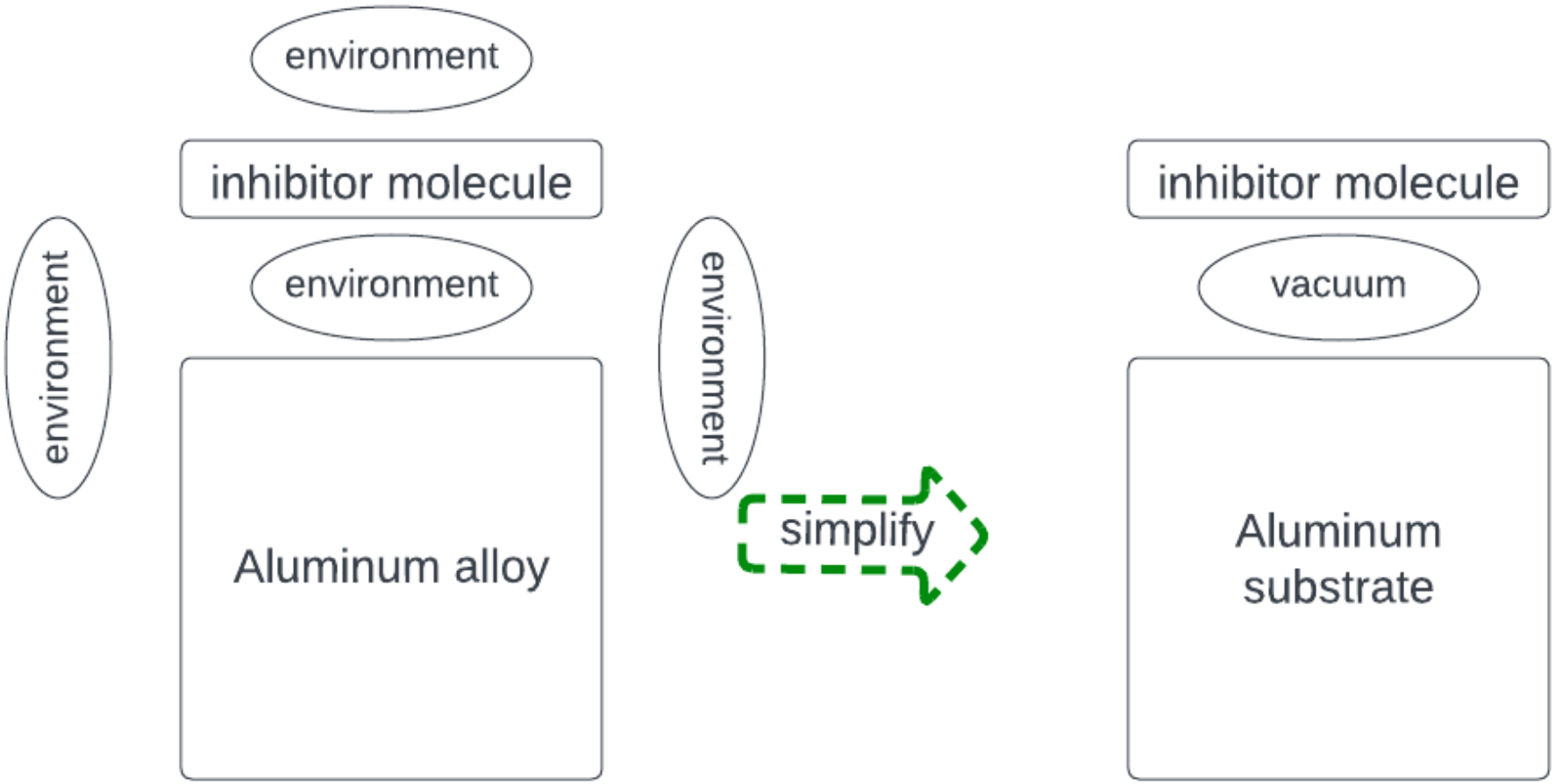


Figure: Simplifying the system from alloy to pure aluminum substrate

Research Goals

- Demonstrate hybrid quantum-classical calculations for materials
- Study binding energy of inhibitor molecules on metal surfaces
- Compare classical DFT with quantum-enhanced calculations
- Establish workflow for quantum-centric supercomputing

Classical DFT Approach

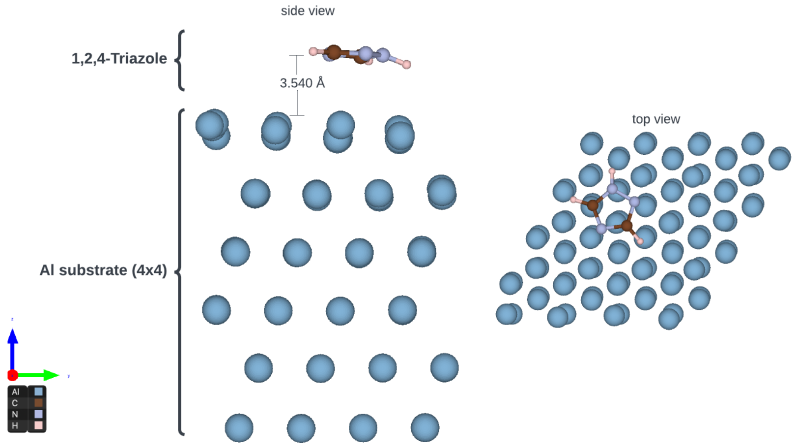
- Periodic DFT calculations using CP2K
- System: Al(111) surface with triazole inhibitor
- Geometry optimization using ML potentials

Case Study: Corrosion Inhibition

- Study of 1,2,4-triazole molecule on Al(111) surface
- Focus on metal-inhibitor interaction
- Goal: Calculate binding energy accurately

System Setup

- 4×4 Al(111) supercell
- PBE functional with D3 dispersion correction
- DZVP-MOLOPT-GTH basis sets



Computational Details

- GPW method (500 Ry plane-wave cutoff)
- Periodic boundary conditions with 25 Å vacuum gap
- Fermi-Dirac distribution (1000 K electronic temperature)
- DFT-D3 dispersion correction for van der Waals interactions

Workflow Steps

1. Supercell generation with ASE
2. Geometry optimization with ML potentials
3. DFT calculations for periodic system
4. Binding energy calculation:

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

Quantum Computing Implementation

- Active space embedding approach
- ADAPT-VQE algorithm with UCCSD ansatz
- 2 electrons in 5 orbitals active space
- Gradient threshold: 1e-4
- DFT embedding convergence: 1E-6

Active Space Configuration

- Self-consistent field (SCF) embedding
- Orbital selection: Canonical (energy-ordered)
- Maximum iterations: 100
- Full GPW method for electron repulsion integrals
- Periodic boundary conditions maintained

Integration Strategy

- Socket-based communication between CP2K and Qiskit
- FCIDUMP format for integral transfer
- Multiple VQE implementations:
  - Standard VQE with UCCSD
  - AdaptVQE with dynamic ansatz
  - StatefulVQE with warm-starting

Optimizer Configuration

- SPSA optimizer settings:
  - Maximum iterations: 1000
  - Learning rate: 0.005
  - Perturbation: 0.05
- Convergence criteria for embedding iterations
- Active space solver: Qiskit

Binding Energy Results

Method	Binding Energy (eV)	Distance (Å)
Classical DFT	-0.385512	3.54
AdaptVQE	-0.385508	3.54
Vanilla VQE	-2.325986	3.54

Analysis

- AdaptVQE shows excellent agreement with classical DFT
- Vanilla VQE shows significant deviation
- Binding distance remains consistent across methods
- Active space size limitations affect accuracy

Future Work

- Expand active space to include more orbitals
- Implement error mitigation techniques
- Improve convergence of AdaptVQE algorithm
- Study larger molecular systems
- Integration with quantum centric supercomputers

Conclusions

- Successfully demonstrated hybrid quantum-classical workflow
- AdaptVQE proves more robust than vanilla VQE
- Current limitations:
  - Active space size
  - Convergence challenges
  - Hardware constraints
- Promising path for quantum-accelerated materials science