Quantum Computing for Materials Science

quantum computer as another accelerator to HPC

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Overview

Motivation

- Quantum chemistry calculations are promising early applications of quantum computers
- Materials science simulations involve periodic systems and large numbers of atoms
- Hybrid quantum-classical approach offers potential advantages

Objectives

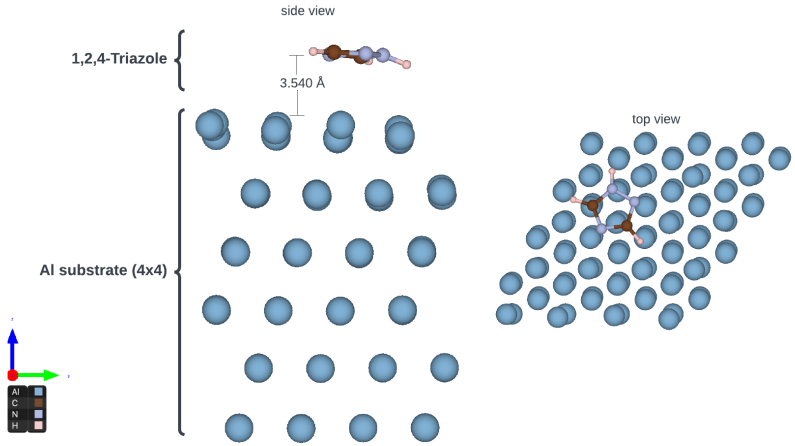
- Demonstrate hybrid quantum-classical calculations for materials
- Study binding energy of inhibitor molecules on metal surfaces
- Compare classical DFT with quantum-enhanced calculations

Classical DFT Approach

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

System Setup

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



System Description

- Optimized geometry of 1,2,4-triazole on Al(111)
- Periodic boundary conditions in XY plane
- Vacuum gap in Z direction
- Total system size: 8 atoms (inhibitor) + substrate

Quantum Computing Implementation

- Active space embedding approach
- ADAPT-VQE algorithm
- 2 electrons in 5 orbitals active space

Integration Strategy

- Socket-based communication between CP2K and Qiskit
- Self-consistent embedding iterations
- Multiple VQE implementations tested

Binding Energy Results

- Classical DFT: -0.385512 eV
- AdaptVQE: -0.385508 eV
- Vanilla VQE: -2.325986 eV

Conclusions

- AdaptVQE shows good agreement with classical DFT
- Demonstrates feasibility of hybrid approach
- Future work: larger active spaces and error mitigation