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Quantum Computing Challenge: Simulating Asphalt Binder Aging with Quantum Algorithms

Quantum Chemistry: A Key Use Case for Quantum Computing

Quantum chemistry is poised to be one of the earliest and most impactful applications of quantum computing. The electronic structure problem, which involves solving the Schrödinger equation for molecules, is classically intractable for many systems of interest due to the exponential scaling of the Hilbert space with system size. Traditional methods such as Density Functional Theory (DFT) and Coupled Cluster (CCSD(T)) often struggle with strong electron correlation effects, particularly in reactive chemical environments.

Quantum computers, leveraging algorithms such as the Variational Quantum Eigensolver (VQE) and Quantum Phase Estimation (QPE), promise an exponential or polynomial speedup over classical methods in certain regimes [1,2]. These methods can capture electron correlation with fewer approximations, enabling more accurate modeling of complex chemical reactions, materials, and catalysts. Recent advances in quantum simulation techniques, including Sparse Quantum Dynamics (SQD) [3] and Krylov-based diagonalization methods [4], further extend the applicability of quantum algorithms to realistic molecular systems.

Specific use case problem: Quantum Simulations for Durable Asphalt Binders

Asphalt binders are critical components in modern infrastructure, with the U.S. alone spending $30-$50 billion annually on road maintenance. The primary challenge lies in their degradation due to oxidation, thermal cracking, and moisture damage, necessitating resurfacing every 10-15 years. Extending the lifespan of asphalt to 25-30 years would significantly reduce maintenance costs and environmental impact.

Computational studies help to design and develop asphalt with favorable properties. Simulating asphalt binders at the molecular level is computationally challenging due

to their heteroatomic composition, which includes sulfur-and nitrogen-containing polycyclic aromatic hydrocarbons (PAHs). Classical force fields struggle to accurately model oxidation pathways, charge transfer, and radical-driven reactions, which are essential to understanding aging mechanisms. Recent studies have demonstrated that quantum chemistry methods can better capture these effects [5].

Following observables and processes are relevant to develop better asphalt:

- **Oxidation energy barriers:** Understanding the activation energy of carbonyl (C=O) and sulfoxide (S=O) formation [6].
- **Charge transfer dynamics:** Investigating electron delocalization in aging reactions [7].
- **Binding energies of anti-aging additives:** Simulating interactions between asphalt and polymer/nanoparticle modifiers to enhance durability [8].

Quantum algorithms such as VQE and Krylov diagonalization provide a pathway to study these observables with higher accuracy than classical methods.

The Challenge

Participants will undertake a three-stage challenge to explore quantum simulations of asphalt binder degradation:

1. System Identification and Property Selection

- Identify a relevant molecular system and the key observable you want to study.
- Justify your choice based on quantum computational feasibility and chemical relevance.
- Explain why classical methods struggle with this problem and how quantum computing could help.

2. Model Hamiltonian Development

- Construct a Hamiltonian for the system using appropriate approximations and embedding techniques.
- Consider active space selection, qubit reduction techniques, or fragmentation methods.

- Relevant references: Molecular embedding techniques [9] Qubit encoding and reduction strategies [10]

3. Quantum Algorithm Implementation

- Implement a quantum algorithm (VQE, QPE, SQD, Krylov diagonalization, or other variations) to compute the chosen observable.
- Justify your algorithmic choices and discuss error mitigation strategies.
- Provide an analysis of expected quantum advantage, limitations, and potential improvements.

Judging Criteria

Participants will be evaluated on their execution across all three steps. While you are expected to cover all stages to some extent, **we encourage you to go deep into at least one area** (e.g., novel Hamiltonian construction, detailed quantum algorithm implementation, or rigorous physical system selection).

Scoring will be based on:

- Scientific Justification (30%): How well you motivated your system and observable choice.
- Modeling & Formulation (30%): The quality of your Hamiltonian development and approximations.
- Quantum Algorithm Design (40%): Correctness, efficiency, and novelty of your quantum implementation.

References

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This challenge presents a unique opportunity to apply quantum computing to a real-world industrial problem, pushing the boundaries of what is possible in materials science and chemistry. We look forward to your innovative solutions!