

Team Name: Quantum HQ

Team Participants: [Anusha Agarwal](#), [Neha Chandran](#), [Sophia Hou](#), [Surbhi Singla](#) (contact emails linked)

Academic Cohort: Thomas Jefferson High School Research QLab

High Level Overview: Our team developed a hybrid quantum-classical simulation pipeline to model the chemical aging of complex molecules found in asphalt binders. Using advanced quantum algorithms such as the Variational Quantum Eigensolver combined with second-order Suzuki-Trotter time evolution and integrating classical electronic structure methods, we simulated key aging processes such as oxidation, crosslinking, and π - π stacking with high chemical accuracy. Our framework enables efficient time evolution of molecular wavefunctions on near-term quantum hardware simulators, providing novel molecular-level insights into aging pathways and identifying critical reactive sites. These results demonstrate significant computational speedups over classical methods and establish a scalable approach to predict material degradation, with broad applicability to various aging-prone materials in industry and technology. We plan to extend this framework to multi-molecular systems and integrate experimental data-driven perturbations, aiming to enable predictive quantum simulations for real-world material design and accelerated aging mitigation in both asphalt and other diverse industries.

Link to Github Repository: <https://github.com/mastermercury18/mitre-gic>

Simulation Execution

We ran our simulation on the four component molecules that were chosen to represent each of the saturates, aromatics, resins, and asphaltenes in SARA. The main observables that we kept track of were the HOMO-LUMO (highest occupied molecular orbital - lowest unoccupied molecular orbital) gap, the dipole moment (by way of the electronic charge distribution), and the C=O bond mode.

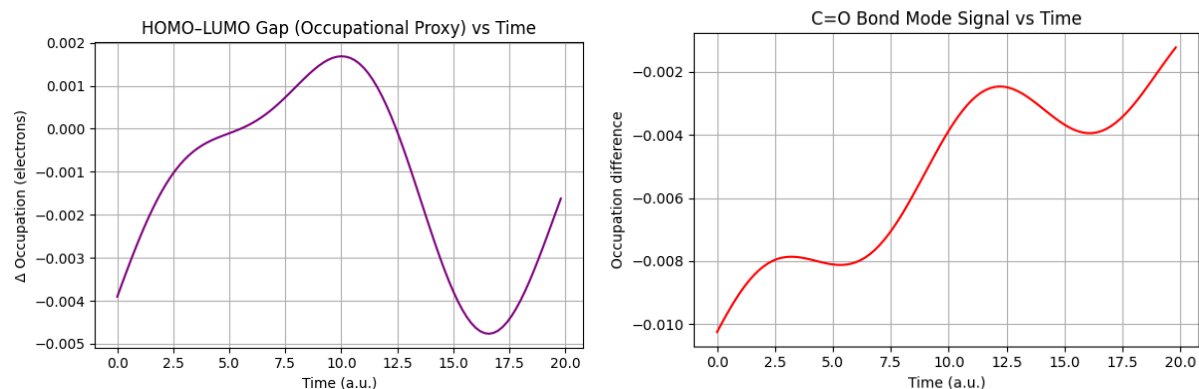
Our second-order Suzuki-Trotter expansion builds upon the variational quantum eigensolver (with a linear entanglement EfficientSU2 ansatz on an 8-qubit system representing the active molecular orbitals) to display time evolution which occurs over atomic time intervals, enabling precise simulation of the system's wavefunction evolution through unitary operations expressed as imaginary powers of Euler's number, resulting in characteristic oscillatory behavior. However, in reality, asphalt ages in an open, noisy environment, where interactions with the surroundings lead to dissipation and decoherence. To capture this, we introduced the master Lindblad equation alongside macroscopic curve fitting, which allowed us to extend our results to realistic time scales on the order of years. Thus, the short-term quantum oscillations observed in closed-system simulations transition into longer-term, smooth aging trends consistent with experimental observations.

Finally, in order to capture the molecular structure's impact on the aging of the molecule itself, we used a ranked system to organize the molecular orbitals as well as the atoms (based on a Fermionic numbering system) according to their respective contributions to the perturbation Hamiltonians representing different aging processes. This ranking allowed us to identify which orbitals and atomic centers are most involved in oxidation, crosslinking, and other chemical transformations driving degradation. By correlating these high-impact orbitals and atoms with their chemical environment and spatial position within the molecule (e.g., core vs. surface), we gained molecular-level insights into how structural motifs influence aging pathways. This information can inform targeted material design strategies by highlighting key reactive sites and bonding interactions critical to asphalt stability and longevity.

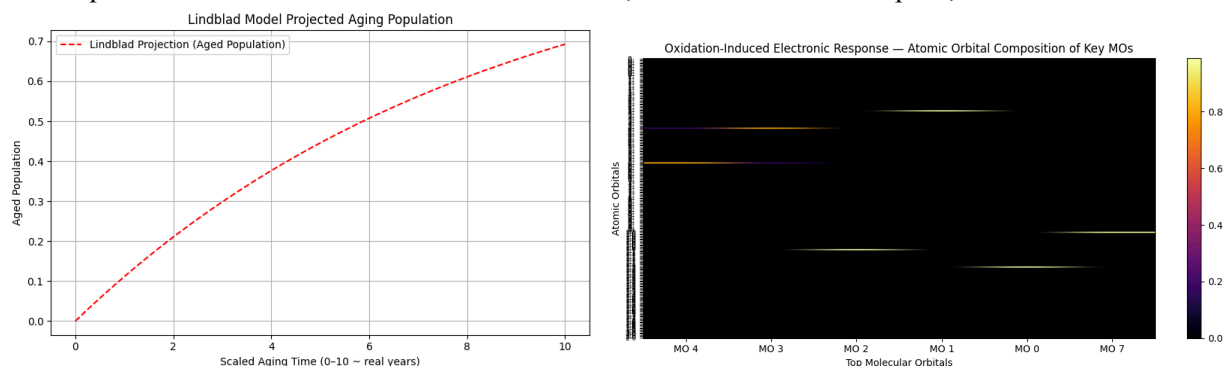
Results Interpretation

Example results are given for the resin component of SARA through the model molecule dibenzothiophene. Similar results are also available if the submitted notebooks are run for asphaltene (through model molecule violanthrone-79), aromatics (through model molecule naphthalene), and saturates (through model molecule squalene), however, in the interest of time, we are only explicitly presenting the numerical results for resins in this write-up (although, in later sections, other results may be

referenced). The VQE (<50 iterations) obtained ground state energy of the molecule before including aging Hamiltonian perturbations was -212.9491 Hartree and afterwards it was -213.9013 Hartree.



The graphs above show the Suzuki-Trotter short-term evolution of some observables of interest in dibenzothiophene. Comparatively, below, the Lindblad-Von Neumann long-term results for how the aged population increases from a ‘pristine’ population in the molecule over a 10 year period is shown. Again, similar plots were made for the three other molecules, but in the interest of space, are not included here.



The π - π stacking perturbation predominantly involves molecular orbitals MO 2 and MO 3 impacting surface carbon atoms such as C0 (55.2), C8 (52.4), and C5 (41.6). Water-induced polarization shows a strong effect in MO 1 and similarly targets surface carbons C0 (55.2), C8 (52.4), and C5 (41.6). Crosslinking affects MOs 4 and 5 and surface carbons C0 (46.4), C8 (44.6), and C1 (35.8) as primary contributors. In contrast, oxidation induces perturbations across MOs 0 to 4 (~0.02 each) and involves atoms like S12 (0.99), C11 (0.98), and conjugated carbons C4 (0.98) and C6 (0.98). Overall, stacking, water, and crosslinking perturbations strongly target surface aromatic carbons, while oxidation impacts heteroatoms and conjugated cores more subtly.

We used simulated perturbations to model the different chemical aging processes in our study, such as oxidation, crosslinking, and π - π stacking. While real perturbations could be derived by taking differences between reduced density matrices (RDMs) obtained from high-level electronic structure calculations on oxidized or otherwise modified species, we chose not to directly implement this approach in our current workflow. Instead, we have developed and tested CASSCF code within the notebook that can generate these reduced density matrices and extract perturbations by substituting just a few lines. The main reason for not using real RDM-based perturbations here is the significantly increased computational cost and complexity, which would require extensive additional calculations and data management. This would have made our initial exploration less efficient, whereas simulated perturbations allow us to systematically study and compare effects under controlled conditions. Additionally, this approach increases flexibility, as users of the notebook can input any SMILES geometry they want and quickly generate corresponding perturbations without needing to rerun expensive electronic structure calculations.

Reproducibility and Algorithm Traceability

Our submission includes a zip file containing four annotated Jupyter notebooks (.ipynb) alongside numerous auxiliary files (.xyz, .npz, .chk) generated during various runtime sessions. Many of these extra files store relevant metrics and intermediate data that illustrate aging mechanism results. However, for the clearest and most consistent output, a clean run of the notebooks within the qBraid environment is recommended, as it ensures all dependencies and runtime configurations are properly managed and the analysis proceeds smoothly from start to finish. The notebooks for aromatics and resins should have a maximum runtime of an hour in total (heavily impacted by DFT calculations), however, the saturates' and asphaltenes' notebooks have runtimes closer to five hours due to the molecular complexity (squalene has 80 atoms and violanthrone-79 has 102). For algorithm traceability, we provide the pipelines below: Classical Pre-Processing: SMILES → Geometry → DFT → ML Optimization → DFT → CASSCF → Quantum Pipeline

Quantum Simulation: Classical Integrals & RDMs → Fermionic Hamiltonian Construction (OpenFermion) → Definition of Aging Perturbations (oxidation, water, π - π stacking, crosslinking) → Mapping to Qubit Operators (Jordan-Wigner Transform) → Variational Quantum Eigensolver (VQE) for Ground State Preparation → Time Evolution via Second-Order Suzuki-Trotter Decomposition (TEBD-inspired) → Calculation of Time-Dependent Observables (HOMO/LUMO occupations, dipole moment, bond modes) → Post-Processing: Kinetic Model Fitting & Lindblad Master Equation Projection → Orbital and Atomic Contribution Analysis to Aging Perturbations

Quantum Advantage and Benchmarking

Asphalt, especially the asphaltene fraction, is a notoriously complex and heterogeneous mixture characterized by large molecular sizes and chemical diversity. Classical computational chemistry methods face significant challenges in this domain, particularly for time-evolution simulations that require repeated density functional theory (DFT) calculations, often resulting in prohibitively long runtimes - even the classical initialization of our notebooks in some cases took upwards of 800 minutes. Trying to time-evolve the system classically, and explore aging mechanisms in a time-dependent environment would require immense computing power. To overcome these limitations, we developed a novel hybrid approach that strategically integrates classical and quantum methods. Initial DFT calculations were performed sparingly to obtain accurate molecular geometries, followed by accelerated geometry optimizations using machine learning potentials from torchani, dramatically reducing classical computational costs.

Strengths	Weaknesses
> Accuracy in strongly correlated electronic states	Classical pre-processing is still needed!!
Efficient time-evolution with Suzuki-Trotter	Limited qubit count and coherence times
Include environmental effects via Lindblad eqs.	Noise and error rates
Direct Chemical Info from Quantum-Generated Operators	Resource and complexity scaling
More Accurate, Correlated Perturbations (from RDMs)	Require empirical knowledge for RDMs

The core innovation lies in leveraging quantum computing algorithms - specifically, the Variational Quantum Eigensolver (VQE) combined with second-order Suzuki-Trotter expansions and Lindblad master equation techniques to simulate the electronic structure and time evolution of aging-related molecular perturbations. Through active space reduction and frozen core approximations, the problem

was condensed into an eight-qubit representation that balances chemical accuracy with the constraints of near-term quantum hardware. This enabled simulations on IBM quantum simulators with runtimes under 10 minutes, representing an exponential speedup over classical methods. Importantly, our work includes hardware-ready code optimized for execution on real quantum devices, facilitating immediate experimental validation.

This flexible and scalable framework represents a first-of-its-kind application of quantum computing to model complex chemical aging pathways in asphaltene, paving the way for future studies of material degradation that were previously infeasible. Additionally, the empirical matching versus simulated perturbation data is fully adaptable depending on the use case. For instance, the current notebook uses empirical (SMILES) data to build molecular geometries, optimize structures, and determine base wavefunctions; however, because aging is an environmentally dependent process, the perturbations are modeled based on physically reasonable approximations of fundamental aging mechanisms.

Execution Environment and Challenges

Our implementation was carried out using Python 3.10.18, Qiskit 0.44.1, Qiskit Terra 0.25.1, IBM Provider 0.8.0, and OpenFermion, with all quantum simulations executed on IBM Quantum simulators. We primarily used the `statevector_simulator` for idealized, noiseless simulations and the `qasm_simulator` with 8192 shots to emulate realistic hardware behavior. While no real quantum processing units (QPUs) were used (except for proof-of-concept at the very end of the notebooks) as simulators gave better accuracy and convergence, all circuits were explicitly constructed to be hardware-compatible and require minimal adaptation for deployment on IBM quantum devices. Thanks to active space reduction and frozen core approximations, each molecular system was encoded using only eight qubits, keeping the simulation within the reach of near-term devices while preserving essential chemical accuracy. Circuit depths varied based on the complexity of the Hamiltonian and perturbations but typically reached 200–400 gates per Suzuki-Trotter time step. The EfficientSU2 ansatz used for VQE was kept intentionally shallow, ensuring fast convergence and tractable circuit depths even under noisy conditions. Full quantum simulations excluding classical pre-processing but including VQE optimization and 100-step time evolution ran in under 10 minutes, representing a significant speedup compared to the multi-day runtimes (which often crash due to memory requirements) that were seen in entirely classical environments.

During development, several challenges emerged due to ongoing updates and deprecations in the Qiskit and Qiskit Nature ecosystems. Many previously standard components (such as the `PySCFDriver`, `ElectronicStructureProblem`, and many legacy estimators) had been restructured or deprecated, forcing a shift to the newer primitives-based workflow. This required manually transforming `FermionOperators` into `SparsePauliOp` formats and resolving orbital ordering mismatches between OpenFermion and Qiskit conventions. Additionally, while we did not run on real hardware, our circuits were designed to anticipate practical hardware limitations such as noise, gate infidelity, and shot variance. We addressed these potential issues through noise-aware design choices like low-depth ansätze, linear entanglement patterns, and the use of grouped Pauli evolution terms to minimize overhead. Although real device access remains a limiting factor, this project demonstrates that quantum simulation of realistic aging processes in complex molecular systems is already viable at the simulator level - and scalable to hardware in the near future.

Industrial Relevance and Future Directions

The modular design of our quantum workflow opens up a transformative next stage: integrating all four SARA fractions into a single, unified simulation notebook. This will enable quantum modeling of intermolecular dynamics, such as additive–binder diffusion, synergistic aging across molecular classes, and surface-level interactions with aggregates, moisture, or external oxidants - phenomena that are impossible to fully capture in isolated molecular simulations. By expanding from single-molecule

perturbations to full-system environments, we can begin simulating real binder behavior under real-world conditions.

We also hope to work directly with experimental materials science labs to calibrate our perturbation operators using empirical data - oxidation rates, FTIR spectra, mass loss curves, and accelerated aging studies. These collaborations will allow us to turn abstract perturbations into physically grounded, data-driven operators that reflect how actual materials respond to aging stressors. In doing so, we shift the simulation pipeline from theoretical modeling to a predictive engine for binder performance.

Most significantly, the speed and modularity of our quantum simulation pipeline - particularly the VQE + second-order Suzuki-Trotter evolution - makes it realistic to embed within optimization feedback loops - this would otherwise be impossible to do both accurately and efficiently. These loops can iteratively adjust the binder's structure or composition to minimize quantum-measured aging signals, such as HOMO-LUMO collapse or carbonyl bond formation. Because our simulations complete in under 10 minutes and scale well under frozen core + active space compression, we are poised to build a quantum-accelerated inverse design workflow: structure in, durability out. This goes beyond observing degradation - it enables the active design of more resilient materials, *in silico*, and at quantum speed. We plan to implement these after the GIC challenge as well because the methods presented can be expanded not only to asphalt, but also to other aging-prone infrastructure materials such as biomedical device materials (implants), aerospace coatings, battery electrolytes, flexible electronics, etc. These materials all suffer from chemical degradation over time (for example, oxidation, UV damage, hydrolysis) and our quantum framework offers a generalizable and fast tool for simulating, quantifying, and minimizing these aging mechanisms at the molecular level. By embedding quantum observables like bond mode intensities or charge redistribution into optimization loops, we can iteratively improve the molecular composition and geometry of materials to enhance lifetime performance, reduce maintenance cycles, and increase reliability in extreme environments.

Selected References

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