**QAMP Project Proposal: Quantum-Enhanced Reaction Pathway Analysis for aromatic Carbon-Ring Molecules**

**Description**

This project implements a reproducible, hybrid pipeline that combines density matrix embedding theory (DMET) and measurement-efficient quantum Krylov / sample-based Krylov diagonalization (SKQD) to compute and benchmark reaction energy profiles of aromatic Carbon rings (example : benzothiophene S-oxidation → sulfoxide → sulfone). The workflow keeps the global geometry/path classical (DFT + NEB), isolates a chemically active fragment around the sulfur site with DMET, and evaluates the fragment electronic structure with SKQD as the primary quantum eigensolver and ADAPT-VQE / UCCSD as verification. The aim is a three-month QAMP scope: GPU-accelerated classical preprocessing, simulator + a small number of targeted hardware validation runs, careful error-mitigation, and an open, pedagogical codebase. We can consider ADAPT-VQE/HI-VQE as fallback strategy incase SKQD pipeline has issues.

The project emphasises

* rigorous active-space diagnostics and embedding error quantification,
* measurement-efficient Krylov techniques to extract multiple eigenstates near transition regions,
* practical, layered mitigation (readout correction, ZNE, symmetry checks, and multi reference error mitigation where possible).

Tools - Qiskit Nature, GPU-accelerated classical chemistry plugins (GPU4PySCF / TeraChem where available), and GPU-accelerated quantum simulation via Qiskit Aer + NVIDIA cuQuantum integration for large simulator runs.

**Deliverables**

Primary Deliverables

* Modular pipeline code (classical preprocessing → DMET fragment → qubit Hamiltonian → SKQD / VQE solvers → postprocessing).

Notebook A (toy fragment): full end-to-end run on Aer (GPU) demonstrating SKQD + mitigation.

Notebook B (benzothiophene): classical NEB → DMET fragment selection → SKQD on simulator and hardware validation examples with mitigation logs.

Technical report : methods, resource table (qubits, gates, shot budgets), plots, sensitivity/ablation (active space size, embedding), error bars, and mitigation effectiveness.

Blog posts or educational content

Minimal Viable Product (MVP)

* Working pipeline with Notebook A (toy demo) that runs end-to-end on Qiskit Aer, with scripted mitigation and example plots.

Short technical note comparing simulator SKQD energies versus a classical embedded solver.