Checkpoint 2

Project: Quantum-Enhanced Mapping of Battery Degradation Pathways

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Project snapshot

We're building a reliable, reproducible hybrid pipeline that turns chemistry (geometries → polarizabilities → Hamiltonians) into measurable optical signals and quantum-subspace energy estimates which are aimed at accelerating battery degradation insight.

What we've accomplished (highlights)

- Completed a focused literature + tooling scan (QSD theory, Qiskit Nature, PySCF, ASE, PyBaMM).
- Working control pipeline: Rodrigo implemented an ASE + NEB workbench and produced a robust control case ($2\ H_2 + O_2 \rightarrow 2\ H_2O$) to validate methods and tooling.
- Optics bridge: Samar created alpha.csv and a functioning chemistry→optics chain ($\alpha \rightarrow \varepsilon_r \rightarrow n \rightarrow \Delta\varphi$) and an MZI intensity model that converts tiny computed phase shifts into realistic detector signals.
- Fixed several thorny API/attribute issues and hardened code paths so notebooks run end-to-end in synthetic/fallback mode.
- Produced reproducible artifacts (Rho_Problem1.ipynb, Samar_mzi_py.ipynb) that demonstrate the full data flow.

What's working really well

- Pragmatic tooling choice: ASE + PySCF + small manual workflows give reliable, reproducible results faster than brittle automation packages. That's a big win for deliverability.
- Modular design: The pipeline cleanly separates geometry generation, polarizability computation, optical conversion, and QSD work making parallel workstreams easy for Rodrigo and Samar.
- Sensor integration mindset: Translating polarizability to MZI signals gives a tangible, experimental validation path — a strong differentiator for the project.
- Fallback resilience: Synthetic fallbacks ensure demos & CI runs succeed even if heavy libs aren't present; excellent for mentoring demos and workshops.

Key insights

- Trying AutoTST/pyGSM early saved us time: we learned they're fragile and that a simpler, maintainable stack is strategically better for MVP.
- The control $H_2/O_2 \rightarrow H_2O$ NEB run proved the NEB → TS workflow end-to-end, giving confidence we can port the approach to battery fragments.
- The optics mapping is not only feasible but gives immediate experimental design guidance (what thickness, density, visibility, and photon budget are needed to detect predicted changes).

Challenges (brief) and how we addressed them

- Tool fragility (AutoTST, pyGSM): Decoupled from MVP; switched to ASE + manual/NEB image generation.
- Chemistry target ambiguity: Ethylene glycol was a weak fit for Li-battery context — we're pivoting to battery-relevant species (EC, LiEC, Li-oxide fragments).
- PySCF API quirks: Implemented a robust finite-field fallback and wrapped calls with defensive logic and unit checks.

These are manageable, and each change improved reliability and clarity.

Current status (where we stand today)

- Notebooks run end-to-end in fallback mode; classical baselines and optical mapping are in place.
- Preliminary polarizabilities.csv exists and is producing $\Delta\varphi$ and SNR estimates.
- QSD prototype / classical-subspace fallback is ready; only Hamiltonian construction for battery fragments remains to be plugged in.

Path to MVP — clear, achievable milestones (target: Jan 30)

A : Finalize chemistry target (by Jan 5) Pivot to Ethylene Carbonate (EC) and a Li-containing fragment for domain relevance.

B: Geometry & classical baselines (by Jan 10) Create 3–7 images per pathway (ASE/NEB or controlled scans) and compute def2-SVP single-point energies; validate one point at def2-TZVP.

C : Polarizability & optics CSV (by Jan 14) Compute α (analytic or finite-field fallback), export SI units, ε_r, n, $\Delta\varphi$ into polarizabilities.csv.

D : MZI SNR maps (by Jan 16) Produce detectability heatmaps over (V, M, L) so experiments can pick tradeoffs.

E : Hamiltonians & QSD runs (by Jan 22) Build compact active-space Hamiltonians (Qiskit-Nature/PySCF) for EC/Li fragment and run QSD/EC prototype.

F : Benchmarking & figures (by Jan 26) Compare QSD energies to DFT baselines, compute MAE, create reaction coordinate plots, and correlate with MZI signals.

G : Final notebook & deliverables (by Jan 30) Single mvp_notebook.ipynb, polarizabilities.csv, figures, README, and CI smoke-test script.

Conclusion

- Connecting computed polarizabilities to MZI observables gives an immediate, testable path to validate quantum predictions which is uncommon and high-impact for industry partners.
- Synthetic fallbacks and CI-friendly notebooks mean we can demo reliably in workshops (QAMP/QCE) and scale to collaborators.
- The pipeline is directly relevant to OEM R&D (EV makers, battery labs). A successful pilot could reduce experimental cycles and DFT cost for failure-mode analysis.
- A well-documented QSD + sensor-fusion pipeline is a publishable artifact and a potential open-source toolkit for battery quantum simulations.