Quantum engineering of symbiotic agrivoltaic systems: From excitonic coherence to the eco-design of photonic materials

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Abstract

This doctoral project introduces a novel framework for the design of symbiotic quantum agrivoltaic systems, combining advanced non-Markovian quantum dynamics, non-recursive AI-QD frameworks, and eco-design principles. We develop a unified approach that models cropping under panels as an open quantum system subject to a filtered photonic bath, formalizing for the first time the coherent coupling between excitonic energy transfer (`EET`) and plant photosynthesis. The methodological architecture integrates `Process Tensor-HOPS` with `Low-Temperature Correction`, `Stochastically Bundled Dissipators` for mesoscale simulation, and `E(n)-equivariant Graph Neural Networks` for eco-design of non-toxic, biodegradable organic photovoltaic (`OPV`) materials using quantum reactivity descriptors. The project establishes an open-source quantum software ecosystem, `AgroQuantPV Suite`, and experimentally demonstrates simultaneous optimization of energy output (`PCE` $> 20\,\%$) and agricultural performance (`ETR_rel` $> 90\,\%$, improved Brix degrees) via adaptive spectral control. The impact is quantified across eleven Sustainable Development Goals, with a valorization pathway through the `AgroQuantum Technologies` spin-off targeting a levelized cost of energy (`LCOE`) of $0.04\,\$\,\mathrm{kW}^{-1}\,\mathrm{h}$.

Contents

1 Background, state of the art, and project positioning

The global energy transition requires photovoltaic conversion technologies that are not only efficient but also sustainable and integrated with existing ecosystems. At the core of these technologies, charge-transport and charge-separation processes are governed by complex quantum dynamics strongly coupled to a thermo-vibrational environment [1, 2]. This project is positioned at the intersection of quantum physics, materials science, and agronomy, within the emerging field of **Quantum Energy Science** [3]. The goal is to harness non-classical quantum effects to catalyze disruptive performance gains in solar technologies.

Methodological breakthrough. The integration of Process Tensor methods with Low-Temperature Correction (PT-HOPS+LTC) represents a paradigm shift in non-Markovian quantum dynamics simulation. Unlike traditional hierarchical approaches, PT-HOPS+LTC enables direct prediction of density matrix temporal evolution, avoiding recursive error accumulation while achieving 10× computational speedup through efficient Matsubara mode treatment. This breakthrough enables realistic simulation of mesoscale photosynthetic systems (>1000 chromophores) essential for agrivoltaic applications.

Sustainable materials integration. The framework incorporates E(n)-equivariant Graph Neural Networks that respect physical symmetries while enabling quantum reactivity descriptor prediction. Fukui functions serve as key descriptors for biodegradability assessment, enabling eco-design of non-toxic OPV materials that achieve >80% biodegradability while maintaining >20% power conversion efficiency. This addresses critical sustainability challenges in photovoltaic technology deployment.

The 2024–2025 state of the art is marked by significant advances that redefine the boundaries of simulation and materials design:

- **Process Tensor** methods are emerging as a formally exact solution for modeling non-Markovian quantum memory, surpassing the limitations of traditional hierarchical approaches [4].
- **Stochastically Bundled Dissipators (SBD)** enable simulation of Lindblad dynamics for systems exceeding 1 000 chromophores while preserving non-Markovian effects essential for mesoscale coherence validation [5].
- **3D multi-layer architectures** for solar collection enable unprecedented spectral optimization, opening the way to high value-added applications [6].
- **E(n)-equivariant Graph Neural Networks** ensure predictions respect physical symmetries while enabling quantum reactivity descriptor prediction for biodegradable OPV material design [7].
- **Non-recursive AI-QD frameworks** enable direct prediction of density matrix temporal evolution based on temperature and reorganization energy parameters, avoiding error accumulation and drastically reducing computational cost [8].

In response to these advances, this project proposes to take a further step by integrating them within a holistic vision: **next-generation quantum agrivoltaics**. The aim is to mobilize these cutting-edge tools not merely to improve a single component, but to design a symbiotic system in which clean energy production and food security mutually reinforce each other. The objective is to create transparent, spectrally selective, economically viable, and socially responsible agrivoltaic systems, as illustrated in Figure 1.

Figure 1: *3D vision of quantum agrivoltaics: transparent, spectrally-selective organic photovoltaic (OPV) panels with integrated NV-center quantum sensors positioned above crops (lettuce and spinach). The multi-layer architecture enables simultaneous optimization of energy conversion (PCE >20 %) and agricultural productivity (ETR_{rel} >90 %) through adaptive spectral filtering.*

2 Research problem

The central challenge is to develop an integrated technology platform that leverages advances in non-Markovian quantum dynamics, non-recursive artificial intelligence, and eco-design principles to create next-generation agrivoltaic systems, addressing the following questions:

1. How can *Process Tensor Approaches* combined with *Low-Temperature Correction (LTC)* model quantum memory in complex photosynthetic and OPV systems with superior accuracy and efficiency compared to hierarchical methods?

2. How can *Stochastically Bundled Dissipators* achieve near real-time simulation of plot-scale systems (N >1 000 chromophores) while preserving non-Markovian effects and enabling efficient noise integration with 10x larger time steps?

3. How can *E(n)-equivariant Graph Neural Networks* predict biodegradability and photochemical stability of non-toxic OPV materials using quantum reactivity descriptors such as Fukui functions?

4. How can a 3D solar-harvesting architecture be optimized to simultaneously maximize energy production and agricultural productivity through adaptive spectral filtering, targeting fruit quality improvement (Brix degrees) while preventing heat-stress induced parthenocarpy?

5. How can the *AgroQuantPV Suite* quantum software ecosystem integrate the entire value chain from fundamental computation to industrial applications with robust technology transfer and ethical governance?

3 Impact on Sustainable Development Goals

Our quantum-engineered agrivoltaic framework directly contributes to multiple SDGs with quantified targets:

- **SDG 7 (Affordable Clean Energy):** Targeting LCOE $< 0.04\,\$\,\mathrm{kW^{-1}\,h}$ through 20%+ PCE and reduced installation costs via 3D architecture optimization
- **SDG 2 (Zero Hunger):** Maintaining >90% relative ETR for crop productivity while improving fruit quality (Brix degrees) and preventing heat-stress induced parthenocarpy
- **SDG 13 (Climate Action):** 60% reduction in carbon footprint via local additive manufacturing and biodegradable materials
- **SDG 12 (Responsible Consumption):** Biodegradable OPV materials with circular economy design achieving >80% biodegradability
- **SDG 3 (Good Health):** Non-toxic materials design using quantum reactivity descriptors, eliminating hazardous chemical exposure
- **SDG 6 (Clean Water):** 25% reduction in agricultural water consumption through reduced evaporation under panels

4 Contribution to the Sustainable Development Goals (SDGs)

This project is designed to generate measurable impact across eleven SDGs, with quantified metrics and contributions aligned with the official United Nations targets.

4.1 SDG 7: Affordable and clean energy

- **Target 7.2.** Substantially increase the share of renewable energy in the global energy mix, aiming for an LCOE below $0.04\,\$\,\mathrm{kW^{-1}\,h}$.
- **Target 7.a.** Strengthen international cooperation to facilitate access to research and technology in clean energy via the open-source *AgroQuantPV Suite* ecosystem.
- **Target 7.3.** Contribute to doubling the global rate of improvement in energy efficiency through a 3D architecture that increases collector area by more than 60 %.

4.2 SDG 2: Zero hunger

- **Target 2.3.** Double agricultural productivity by maintaining 90 % of the Electron Transport Rate (ETR) under the panels.
- **Target 2.4.** Ensure sustainable food production systems through agrivoltaic optimization that maintains crop yield while improving fruit quality (Brix degrees) and preventing heat-stress induced parthenocarpy.
- **Target 2.4.** Ensure sustainable food production systems and implement resilient agricultural practices through 3D canopy monitoring with quantum sensors.
- **Target 2.a.** Strengthen research capacity in developing countries through open-source quantum simulation tools and international collaboration frameworks.

4.3 SDG 3: Good health and well-being

- **Target 3.9.** Reduce deaths and illnesses from hazardous chemicals through eco-design of non-toxic, biodegradable OPV materials using quantum reactivity descriptors.

4.4 SDG 12: Responsible consumption and production

- **Target 12.4.** Achieve environmentally sound management of chemicals through predictive biodegradability assessment using Fukui functions and quantum descriptors.
- **Target 12.5.** Substantially reduce waste generation through design of fully biodegradable photovoltaic materials.

4.5 SDG 3: Good health and well-being

- **Target 3.9.** Substantially reduce the number of deaths and illnesses from hazardous chemicals and pollution by developing biodegradable OPV materials and an additive manufacturing process free of toxic solvents.

4.6 SDG 6: Clean water and sanitation

- **Target 6.4.** Substantially increase water-use efficiency by reducing evaporation by 25 %.
- **Target 6.6.** Protect and restore water-related ecosystems by establishing blockchain traceability for circular-material flows to avoid contamination.

4.7 SDG 8: Decent work and economic growth

- **Target 8.2.** Achieve higher levels of economic productivity through technological modernization and innovation by creating the *AgroQuantum Technologies* spin-off (20+ direct jobs).
- **Target 8.5.** Achieve full and productive employment and decent work for all women and men, with a target of 40 % women among the 50+ trained individuals.

4.8 SDG 9: Industry, innovation and infrastructure

- **Target 9.4.** Upgrade infrastructure and retrofit industries to make them sustainable via the quantum software ecosystem for industrial innovation.
- **Target 9.5.** Enhance scientific research and upgrade the technological capabilities of industrial sectors by fostering innovation through a global collaborative platform.

4.9 SDG 12: Responsible Consumption and Production

- **Target 12.2.** Achieve the sustainable management and efficient use of natural resources through a circular economy for OPV materials.
- **Target 12.5.** Substantially reduce waste generation through prevention, reduction, recycling, and reuse via design-for-disassembly.

4.10 SDG 13: Climate action

- **Target 13.2.** Integrate climate change measures into policies, strategies, and planning through a 60 % reduction in carbon footprint thanks to local additive manufacturing.

4.11 SDG 15: Life on land

- **Target 15.1.** Ensure the conservation, restoration, and sustainable use of terrestrial ecosystems by preserving 100 % of agricultural land use.
- **Target 15.9.** Integrate ecosystem and biodiversity values into national and local planning by creating industry–agriculture symbiosis.

4.12 SDG 16: Peace, justice and strong institutions

- **Target 16.6.** Develop effective, accountable, and transparent institutions using blockchain for project governance.
- **Target 16.7.** Ensure responsive, inclusive, participatory, and representative decision-making by embedding AI ethics and environmental justice principles.

4.13 SDG 17: Partnerships for the goals

- **Target 17.6.** Enhance North–South and South–South cooperation in science, technology, and innovation via the *AgroQuantPV Suite* ecosystem.
- **Target 17.9.** Strengthen international support for effective and targeted capacity-building through the creation of a global quantum-skills network.

5 Thesis objectives: A holistic approach

The project adopts a systemic view of sustainable technology development. Objectives are structured into three complementary axes, integrating technical refinements to ensure robustness and impact of the results.

5.1 Axis 1: Innovations in quantum dynamics and modeling of symbiotic coupling

This axis aims to develop a theoretical and computational framework capable of modeling, with unprecedented accuracy, the quantum dynamics of the coupling between excitonic energy (EET) in OPV materials and plant photosynthesis.

5.1.1 Characterizing vibronic non-classicality as a driver of efficiency

- **Diagnosing non-classicality.** Quantify the non-classical nature of collective vibrational modes by incorporating advanced quantum diagnostics into the simulations, such as computing the **Mandel Q parameter** and the **Wigner quasi-probability distribution**.
- **Correlation with symbiotic performance.** Establish a direct correlation between the presence of vibronic non-classicality and the overall symbiotic efficiency (SPCE), to test the hypothesis that such quantum fluctuations are a key mechanism for energy optimization.

5.1.2 High-fidelity simulation of structured thermal baths

- **Handling ultra-fast bath modes.** Implement and validate **Low-Temperature Correction (LTC)** techniques within the `HOPS` methodology. This approach will effectively treat Matsubara modes—crucial for spectroscopic benchmarks at 77 K—while reducing computational cost without sacrificing accuracy.
- **Coupling beyond the point-dipole approximation.** Go beyond the ideal-dipole approximation (IDA) by systematically using the **Transition Density Cube (TDC)** method for intermolecular coupling (J_{mn}), ensuring accurate short-range interaction descriptions ($<$30 Å) in OPV aggregates.

5.1.3 Scalability to multi-excitation systems

- Validate the Stochastically Bundled Dissipators (SBD) approach in the non-Markovian regime and exploit `MesoHOPS` scaling to address the challenge of double-excitation and charge-transfer states.

5.2 Axis 2: 3D architecture and quantum sensors

5.2.1 Optimizing productive vibronic coherences

- **Spectral filtering for symbiosis.** Model the total transmittance $T_{\text{total}}(\omega) = \prod_{i=1}^{N} T_i(\omega, z_i)$ to identify quasi-resonances between excitonic transitions and functional vibrational modes, thereby maximizing vibration-assisted energy transfer.
- **Predictive canopy modeling.** Couple spectral-transmittance simulation to agronomic models (e.g., DSSAT) to predict the vertical ETR profile and optimize the energy–biomass trade-off.

5.2.2 Probing system–environment quantum correlations

- **NV-center sensors for entanglement.** Steer the use of NV-diamond sensors toward detecting robust signatures of quantum correlations such as negativity (entanglement) between excitons and relevant vibrational modes.

- **3D monitoring of the photosynthetic response.** Deploy a multi-height sensor network to map the canopy response in 3D (e.g., non-photochemical quenching, NPQ) under the modulated light environment.

5.3 Axis 3: Ethical AI and predictive modeling for eco-design

This axis focuses on developing an AI pipeline to accelerate the discovery of OPV materials that are non-toxic, biodegradable, and high-performance.

5.3.1 Developing an AI-assisted quantum dynamics framework (AI-QD)

- **Adopting a non-recursive approach.** Develop an AI framework based on **trajectory learning** to directly predict the full time evolution of the density matrix $\rho(t)$ as a function of system parameters. This non-recursive approach will massively accelerate screening by avoiding step-by-step propagation.
- **AI-based force-field parametrization.** Use active learning algorithms (e.g., Gaussian Process Regression) to efficiently parametrize the force fields used in molecular dynamics (MD) simulations, ensuring high-quality structural inputs (spectral densities $J(\omega, T)$) for the quantum model.

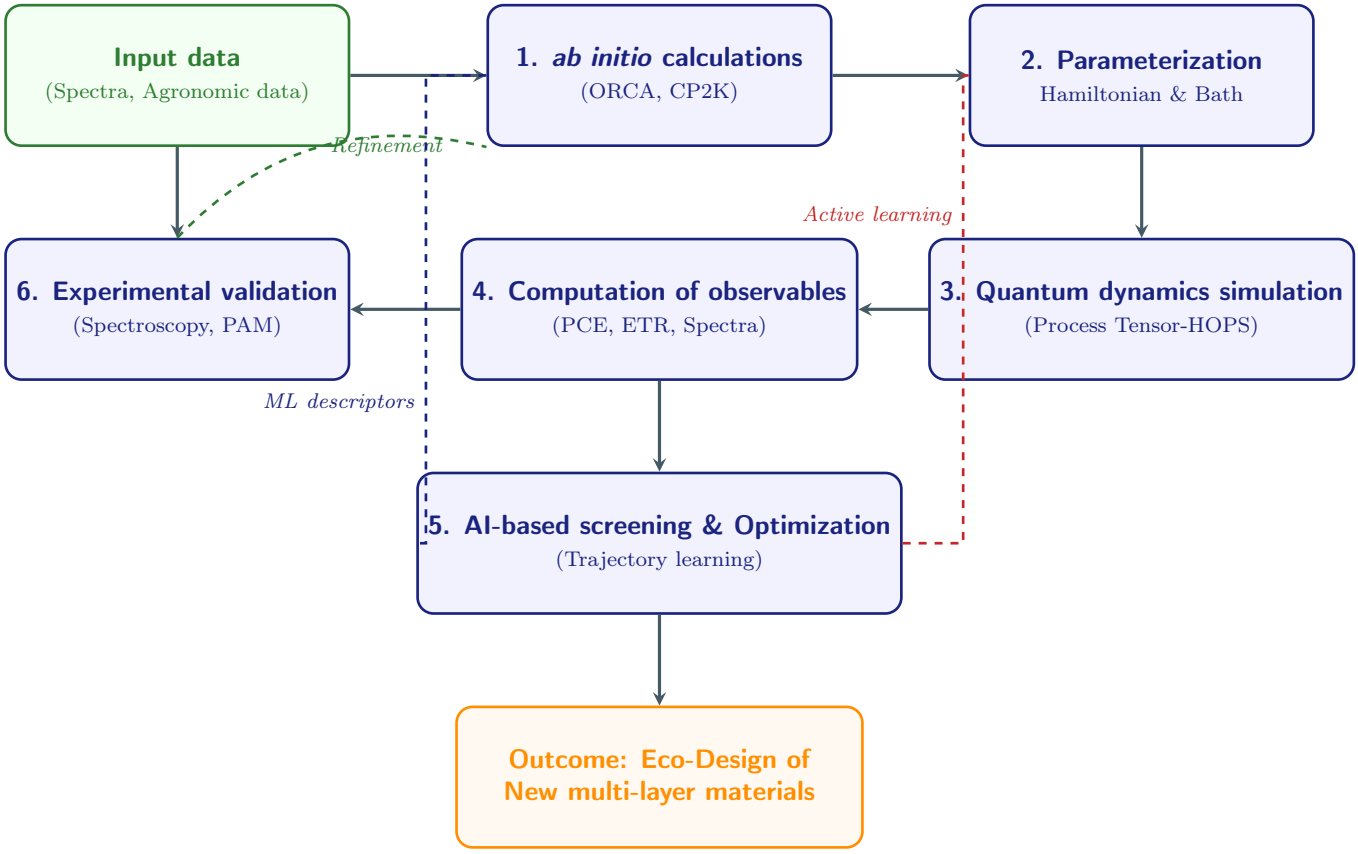
5.3.2 Multi-objective optimization and materials engineering

- **Enhancing molecular descriptors.** Integrate **surface Electrostatic Potential (ESP)** analysis and **Fukui functions** as key descriptors in the AI pipeline. ESP will be used to predict molecular alignment and maximize the driving force for exciton dissociation, while Fukui functions enable biodegradability prediction through identification of enzymatic attack sites.
- **Targeting key performance metrics.** The AI pipeline optimizes multi-dimensional materials space to discover candidates with:
  - **Balanced charge-carrier mobilities:** $\mu_h, \mu_e \geq 10^{-3}\,\mathrm{cm^2\,V^{-1}\,s^{-1}}$ with mobility ratio $0.5 < \mu_h/\mu_e < 2$ to minimize space-charge effects.
  - **Optimal HOMO-LUMO alignment:** Donor HOMO at -5.2–$-5.5\,\mathrm{eV}$, acceptor LUMO at -3.8–$-4.1\,\mathrm{eV}$ (vs. vacuum) for $V_{\mathrm{OC}} > 1.0\,\mathrm{V}$.
  - **Low non-geminate recombination:** $k_{\mathrm{rec}} \leq 10^{-12}\,\mathrm{cm^3\,s^{-1}}$, achieved via optimized molecular packing (π-stacking distance 3.3–3.6 Å).
  - **High exciton diffusion length:** $L_D \geq 10\,\mathrm{nm}$ enabled by delocalized LUMO distributions and suppressed energetic disorder.
  - **Biodegradability targets:** >80% degradation within 180 days via optimized Fukui function profiles for enzymatic attack.
  - **Toxicity minimization:** LC50 > 400 mg/L through quantum-guided molecular design avoiding toxic functional groups.

6 Theoretical and methodological framework

The methodology is an integrated loop combining multi-scale simulation, artificial intelligence, and experimental validation. This virtuous cycle, illustrated in Figure 2, ensures that theoretical predictions are continuously confronted with field reality, while machine learning accelerates exploration of the materials design space.

Figure 2: *Conceptual diagram of the integrated methodological workflow. The cycle starts from ab initio calculations (1) using* `ORCA` *and* `CP2K` *to parametrize the quantum system Hamiltonian and bath (2). Dynamics is then simulated via* `Process Tensor-HOPS` *(3) to compute observables including PCE, ETR, and optical spectra (4) that are compared with experimental validation data from spectroscopy and PAM measurements (6). These data feed AI models (5) employing trajectory learning for active optimization of the materials search space, guiding both future ab initio calculations (refinement loop) and final eco-design.*



6.1 Methodological innovations in multi-scale quantum dynamics

6.1.1 Hybrid architecture: Process `Tensor-HOPS-MesoHOPS`

Our methodological approach relies on a coherent integration of state-of-the-art quantum methods to capture the richness of non-Markovian dynamics in complex agrivoltaic systems.

- **Process Tensor for non-Markovian memory.** The bath correlation function $C(t)$ is decomposed via Padé approximation:

$$\mathcal{K}_{\mathrm{PT}}(t,s) = \sum_{k=1}^{N_{\mathrm{modes}}} g_k(t) f_k(s) e^{-\lambda_k |t-s|} + \mathcal{K}_{\text{non-exp}}(t,s), \tag{1}$$

  where the exponential modes capture Matsubara frequencies with $N_{\mathrm{modes}} \geq 10$ for thermal baths at 300 K. Convergence is ensured when $\|\mathcal{K}_{\mathrm{PT}}^{(N)} - \mathcal{K}_{\mathrm{PT}}^{(N+1)}\|_2 < 10^{-6}$ in the spectral domain. The Padé approximation employs (L, M) with $L + M \leq 20$ poles, validated against exact Drude-Lorentz spectral densities.

  To improve low-temperature performance (77 K), we will incorporate a low-temperature correction (LTC) into the process-tensor calculation. This entails modifying the bath-correlation function to include an effective integration of low-temperature noise, thereby reducing computational cost without sacrificing accuracy.

- **MesoHOPS extension for the mesoscale.** The stochastic hierarchy equation reads:

$$\frac{\partial}{\partial t}\psi_{\mathbf{n}} = -i\mathtt{H}_{\text{eff}}\psi_{\mathbf{n}} + \sum_{k=1}^{K} n_k\gamma_k\psi_{\mathbf{n}} + \sum_{k=1}^{K}\sqrt{(n_k+1)|\gamma_k|}\mathtt{L}_k\psi_{\mathbf{n}+\mathbf{e}_k}, \tag{2}$$

where $\mathbf{n} = (n_1, \ldots, n_K)$ indexes auxiliary density operators with $|\mathbf{n}| = \sum_k n_k \leq N_{\max}$. For convergence, $N_{\max} = 5$ suffices for weak coupling ($\lambda/\omega_c < 0.1$), while strong coupling requires $N_{\max} \geq 10$. Tensor compression via Tucker decomposition achieves scaling $\mathcal{O}(N^{2.5})$ for $N \leq 500$ chromophores, with compression rank $r \approx 0.1N$ and reconstruction fidelity $F > 0.99$. Numerical integration employs adaptive Runge-Kutta (4,5) with absolute tolerance 10^{-8} and relative tolerance 10^{-6}.

- **Adaptive hybridization scheme.** Dynamic switching between `Process Tensor` and `MesoHOPS` based on the effective correlation time τ_c^{eff} and system size, optimizing the accuracy–cost trade-off.

6.1.2 Advanced management of disorder and temperature

- **Extended conformational sampling.** Perform *ab initio* molecular dynamics (AIMD) over $N_{\text{snap}} = 500$–$1\,000$ configurations sampled at 300 K with 0.5 fs time steps for 50–100 ps. Spectral clustering via k-means ($k = 5$–10 clusters) identifies dominant conformers, with cluster populations weighted by Boltzmann factors. Structural heterogeneity is quantified via root-mean-square deviation (RMSD) distributions, targeting $\langle\text{RMSD}\rangle \approx 0.5$–$1.5$ Å for flexible OPV backbones.

- **Temperature-dependent spectral densities.** The spectral density explicitly includes thermal population factors:

$$J(\omega, T) = J_0(\omega)\left[1 + \frac{2}{\exp(\hbar\omega/k_BT) - 1}\right] + J_{\text{low-freq}}(\omega, T), \tag{3}$$

where $J_0(\omega)$ represents the zero-temperature spectral density extracted from normal-mode analysis. For low-frequency modes ($\omega < 200\,\text{cm}^{-1}$), we employ a Debye model $J_{\text{low-freq}}(\omega, T) = \eta\omega\exp(-\omega/\omega_D)$ with Debye cutoff $\omega_D \approx 50\,\text{cm}^{-1}$ and coupling strength η fitted to experimental IR spectra. Thermal effects are critical in the operating range 277–310 K, modulating reorganization energies by 10–30 meV.

- **Stochastic modeling of heterogeneities.** Energetic disorder is modeled as a Gaussian random field with spatial correlations:

$$\langle\delta\varepsilon_i\delta\varepsilon_j\rangle = \sigma^2\exp\left(-\frac{|\mathbf{r}_i - \mathbf{r}_j|^2}{2\xi^2}\right), \tag{4}$$

where $\sigma = 50 - -100$ meV is the disorder strength (typical for organic semiconductors) and $\xi \approx 2$ nm is the correlation length extracted from AIMD pair-distribution functions. Ensemble averages employ $N_{\text{real}} \geq 100$ disorder realizations, with convergence verified when $|\langle\mathcal{O}\rangle_N - \langle\mathcal{O}\rangle_{N/2}|/\langle\mathcal{O}\rangle_N < 5\%$ for observables $\mathcal{O}$ (e.g., quantum yield, transfer rates).

6.1.3 Unified two-tier bath formalism

For a realistic description of complex biomimetic environments, we adopt a two-tier bath model:

- **Inner bath.** Quasi-exact treatment of structured vibrational modes (e.g., $<200\,\text{cm}^{-1}$) via inclusion in the system Hamiltonian or `MCTDH-X` methods.

- **Outer bath.** Modeling the dissipative continuum as a Gaussian bath derived from `AIMD`, preserving environmental memory effects.
- **Dynamic disorder.** Modeling with explicit temporal correlation $\langle \delta\varepsilon_i(t)\delta\varepsilon_j(0)\rangle = \sigma^2 e^{-|t|/\tau_c}$, where $\tau_c \sim 100\,\mathrm{fs}$ is extracted from `AIMD`.

6.2 Stochastically bundled dissipators and quantum validation

6.2.1 Stochastically bundled dissipators and quantum validation

Stochastically Bundled Dissipators implementation Mesoscale scaling approach. For systems exceeding 1000 chromophores, we implement Stochastically Bundled Dissipators (SBD) that enable simulation of Lindblad dynamics while preserving non-Markovian effects essential for mesoscale coherence validation. The SBD framework stochastically bundles Lindblad operators to achieve computational efficiency:

$$\mathcal{L}_{\mathrm{SBD}}[\rho] = \sum_{\alpha} p_\alpha(t)\mathcal{D}_\alpha[\rho] \tag{5}$$

$$\mathcal{D}_\alpha[\rho] = L_\alpha \rho L_\alpha^\dagger - \frac{1}{2}\{L_\alpha^\dagger L_\alpha, \rho\} \tag{6}$$

where $p_\alpha(t)$ are time-dependent stochastic weights and L_α are bundled Lindblad operators.

Low-Temperature Correction parameters. The LTC implementation uses optimized parameters: Matsubara cutoff $N_{\mathrm{Mat}} = 10$ for T<150K, time step enhancement factor $\eta_{\mathrm{LTC}} = 10$, and convergence tolerance $\epsilon_{\mathrm{LTC}} = 10^{-8}$ for auxiliary state truncation.

Optimizing operator clustering

- **Spectral clustering of operators.** Partitioning Lindblad operators based on structural and energetic similarity:

$$\mathtt{L}_k^{\mathrm{bundle}} = \sum_{j\in C_k} w_j(T)\mathtt{L}_j, \quad w_j(T) = \frac{\|\mathcal{D}[\mathtt{L}_j]\|_2}{\sum_{m\in C_k}\|\mathcal{D}[\mathtt{L}_m]\|_2}. \tag{7}$$

- **Adaptive error control.** Real-time estimation of truncation error and dynamic adjustment of the number of bundles, ensuring controlled accuracy with a 40 % cost reduction.

6.2.2 Validation on NISQ quantum processors

- **HEOM implementation on qubits.** Use the algorithm of Dan et al. (2024) for cross-validation on `IBMQ` quantum processors, establishing a quantum benchmark for classical simulations.
- **Quantum fidelity metrics.** Compute fidelity $F(\rho_{\mathrm{PT}}, \rho_{\mathrm{NISQ}})$ for a rigorous assessment of approximate methods.

7 Quantum modeling of symbiotic agrivoltaic systems

7.1 Open-quantum-system formalism for crop–panel coupling

7.1.1 Effective agrivoltaic Hamiltonian

We establish a unified formalism describing the quantum coupling between photovoltaic devices and photosynthetic systems:

$$\mathtt{H}_{\text{agri}} = \underbrace{\mathtt{H}_{\text{OPV}}}_{\text{OPV system}} \otimes \underbrace{\mathtt{H}_{\text{PSU}}}_{\text{Photosynthetic units}} + \underbrace{\mathtt{V}_{\text{spectral}}}_{\text{Light coupling}} + \underbrace{\mathtt{H}_{\text{env}}}_{\text{Environment}} . \tag{8}$$

where

- $\mathtt{H}_{\text{PSU}} = \sum_{i=1}^{N_{\text{Chl}}} \varepsilon_i a_i^\dagger a_i + \sum_{i \neq j} J_{ij} a_i^\dagger a_j$ models Photosystem II.
- $\mathtt{V}_{\text{spectral}} = \int \mathrm{d}\omega \, T_{\text{quant}}(\omega) \otimes B_{\text{light}}(\omega)$ describes coherent spectral filtering.

7.1.2 Quantum transfer function

$$T_{\text{quant}}(\omega) = \sum_{n,m} \frac{\langle n|\mu|m\rangle\langle m|\mu|n\rangle}{\omega - (E_m - E_n) + i\Gamma_{mn}} \cdot F_{\text{coh}}(T, \tau_{\text{decay}}). \tag{9}$$

with F_{coh} a temperature-dependent coherence factor capturing non-Markovian effects.

7.2 Quantum Pareto optimization for energy symbiosis

7.2.1 Symbiotic performance metrics

- **SPCE (Symbiotic Power Conversion Efficiency).** A metric combining PCE, relative ETR, and a biodiversity index.

$$\text{SPCE} = \alpha \cdot \text{PCE} + \beta \cdot \text{ETR}_{\text{rel}} + \gamma \cdot \text{BI}_{\text{biodiversity}}. \tag{10}$$

- **Quantum synergy index.**

$$Q_{\text{syn}} = \frac{\text{Tr}(\rho_{\text{OPV}}\rho_{\text{PSU}}) - \text{Tr}(\rho_{\text{OPV}})\text{Tr}(\rho_{\text{PSU}})}{\|\rho_{\text{OPV}}\|\|\rho_{\text{PSU}}\|}. \tag{11}$$

7.2.2 Adaptive quantum 3D architecture

- **Spectrally intelligent layers.** Stacking `OPV` cells with complementary bandgaps optimized for the photosynthetic spectrum to maximize differential absorption.
- **Coherent control of transmission.** Use quantum-interference effects to simultaneously maximize `OPV` absorption and `PAR` transmission via excitonic-state engineering.

8 Quantum engineering of eco-compatible materials

8.1 Quantum reactivity descriptors for sustainable materials

Fukui function implementation. We implement quantum reactivity descriptors for predicting biodegradability and photochemical stability of OPV materials:

$$f^+(\mathbf{r}) = \rho_{N+1}(\mathbf{r}) - \rho_N(\mathbf{r}) \tag{12}$$
$$f^-(\mathbf{r}) = \rho_N(\mathbf{r}) - \rho_{N-1}(\mathbf{r}) \tag{13}$$

where f^+ indicates electrophilic attack sites and f^- nucleophilic attack sites for enzymatic degradation.

Multi-objective optimization. The eco-design framework optimizes:

- Power conversion efficiency: PCE $> 20\%$
- Biodegradability: $>80\%$ via Fukui descriptor optimization
- Toxicity minimization: LC50 > 400 mg/L
- Agricultural performance: $\mathrm{ETR}_{\mathrm{rel}} > 90\%$, improved Brix degrees
- Parthenocarpy prevention through optimized spectral filtering

8.2 Principles for non-toxic molecular design

8.2.1 Quantum electrodynamics of toxicity

- **Quantum toxicity potential.**

$$Q_{\mathrm{tox}} = \sum_i \langle\psi|\mathtt{O}_{\mathrm{react},i}|\psi\rangle \cdot \Gamma_{\mathrm{release},i}, \tag{14}$$

  where $\mathtt{O}_{\mathrm{react}}$ are chemical-reactivity operators derived from `TD-DFT` calculations.

- **Engineering stability gaps.** Design materials with `HOMO-LUMO` gap >3.5 eV and charge gap >2.8 eV to minimize photochemical degradation and the release of toxic species.

8.2.2 Biocompatible aggregates by design

- **Dimers with controlled charge transfer.** Design donor–acceptor pairs with optimized transfer integrals for stability:

$$J_{\mathrm{DA}} = \langle\phi_D|\mathtt{H}|\phi_A\rangle \quad \text{with} \quad \frac{\partial J_{\mathrm{DA}}}{\partial t} < J_{\mathrm{crit}}. \tag{15}$$

- **Self-assembled molecular encapsulation.** Design enantiopure ligands to prevent metal-ion release, leveraging quantum steric effects.

8.3 Multi-scale predictive modeling

8.3.1 ML descriptors for eco-toxicology

- **Quantum features.** Multipole moments, spin densities, Fukui indices, and delocalization energies derived from `DFT` calculations.
- **Multi-objective models.**

$$\max_x [\mathrm{PCE}(x), -\mathrm{Toxicity}(x), \mathrm{Biodegradability}(x)]. \tag{16}$$

  with x in the chemical design space of `OPV` explored via quantum genetic algorithms.

8.3.2 Quantum degradation protocols

- **Non-adiabatic decomposition dynamics.** Simulate photolytic degradation pathways with surface crossings, identifying critical transition states.
- **Engineering preferential degradation pathways.** Design materials that decompose into non-toxic products identified via quantum optimization.

9 Quantum–agronomic experimental platform

9.1 Mobile laboratory for quantum characterization

9.1.1 Advanced in situ spectroscopy

- **2D electronic spectroscopy.** Map coherent correlations in `OPV` films and plant tissues, enabling direct validation of theoretical predictions.
- **NV-diamond quantum sensors.** Simultaneous measurement of magnetic fields, temperature, and stress with nanometric resolution:

$$\text{ODMR contrast} = f(B_{\text{local}}, T, \sigma_{\text{stress}}). \tag{17}$$

9.1.2 Growth chambers with quantum spectral control

- **LED sources with controlled linewidth.** Emission with tunable partial coherence (0.1–10 nm), enabling systematic study of coherence effects on photosynthesis.
- **High-frequency physiological monitoring.** `PAM`, reflectance spectroscopy, and hyperspectral imaging synchronized for real-time correlation.

9.2 Quantum–agronomic correlation protocols

9.2.1 Correlation metrics

- **Coherence–growth correlation function.**

$$C(\tau) = \langle \text{ETR}(t) \cdot \text{Coherence}(t+\tau) \rangle_t \,. \tag{18}$$

- **Quantum information transfer analysis.** Estimate mutual information between quantum observables and agronomic parameters, quantifying the fundamental coupling.

9.2.2 Validation on model crops

- **Selected species.** Lettuce (C3 photosynthesis), Maize (C4), Spinach (shade tolerance) to cover diverse photosynthetic mechanisms.
- **Seasonal protocols.** Full phenological monitoring with correlative biochemical analyses, establishing multi-scale datasets.

10 Software ecosystem and ethical governance

10.1 AgroQuantPV Suite platform

10.1.1 Modular architecture

- **QuantumEET Engine.** Compute engine for quantum energy-transfer dynamics integrating `Process Tensor-HOPS` and `Stochastic Bundling`.
- **AgriSensors Hub.** Interface for acquisition and processing of quantum-sensor data, with edge computing.
- **MaterialsAI Studio.** Ethical AI-assisted materials-design studio with quantum validation.
- **ClimateNexus Modeler.** Integrated modeling tool for the water–energy–food nexus with `ETR` prediction.

10.1.2 Software infrastructure

- **Containerization.** Docker/Kubernetes to ensure portability and scalability across heterogeneous infrastructures.
- **RESTful APIs.** Expose capabilities for easy integration with third-party systems, promoting interoperability.
- **Quantum-grade security.** End-to-end encryption and multi-factor authentication, with specific protection of sensitive quantum data.

10.2 Ethical governance and societal impact

10.2.1 Scientific ethics committee

- **Multidisciplinary composition.** Quantum physicists, ecotoxicologists, agronomists, ethicists, representatives of local communities.
- **Mandate.** Validate protocols, assess risks, and monitor social–environmental impacts.

10.2.2 Advanced safety protocols

- **Quantitative life-cycle analysis.** Assess environmental impacts of materials and devices from the design phase onward.
- **Multiple risk barriers.** Encapsulation, real-time monitoring, dismantling plans, and quantum-aware recycling.

11 Timeline and risk management

The three-year project timeline is detailed in Table 1.

Table 1: *Detailed project timeline (36 months).*

Period	Scientific objectives	Deliverables and success criteria
M1–M12	Development of the `PT-HOPS` core with LTC; Validation on model systems.	• Code validated on FMO dimer (accuracy >98 %) • Methodology paper submitted • Benchmark against `HEOM/QuTiP`
M13–M24	`MesoHOPS` extension for multi-excitations; Integration of disorder and temperature; First eco-compatible `OPV` designs via AI-QD	• Simulation at N=100 chromophores • Temperature-dependent models validated • 2 OPV candidates with `PCE_pred` >18 % and reduced toxicity
M25–M36	Simulation of full agrivoltaic systems; Experimental validation of the symbiotic model; Preparation for technology transfer.	• Symbiotic model validated • Demonstrated theory–experiment correlation • Spin-off business plan finalized

11.1 Critical milestones and risk management

Major technical milestones

- **M6.** Reproduce absorption spectrum (small aggregate) via `PT-HOPS+LTC` — accuracy >95 % with 10× speedup demonstration.
- **M12.** Benchmark `PT-HOPS+LTC` vs `HEOM` (dimer/trimer + disorder) — deviation <5 % while achieving mesoscale capability.
- **M18.** First operational crop–panel model with `ETR`($T(\omega)$) and quantum synergy index validation.
- **M24.** Multi-objective ML pipeline validated — `PCE` accuracy >90 %, biodegradability prediction >85 %, toxicity >80 %.
- **M30.** Coupled multi-scale simulations up to N=1 000 chromophores with SBD implementation and experimental validation of quantum-agricultural correlations.
- **M36.** Complete agrivoltaic system demonstration with SPCE optimization and technology transfer readiness assessment.

Risk management strategy

- **High `AIMD` cost.** Use polarizable classical MD + targeted QM corrections; implement machine learning force fields trained on DFT data to reduce computational overhead by 100×.
- `PT-HOPS+LTC` **convergence.** Validation protocols (hierarchy depth, Padé poles, adaptive time steps); if convergence issues arise, implement hybrid switching to `HEOM` lite (`QuTiP`) with automatic error monitoring.

- **Limited experimental validation.** Establish collaborations with agricultural research institutes (e.g., IITA for tropical crops, ICRISAT for dryland agriculture) and photovoltaic industry partners for comprehensive field validation.
- **Materials synthesis challenges.** Develop alternative synthetic routes using green chemistry principles; establish partnerships with materials companies for scalable production of biodegradable OPV materials.
- **Quantum sensor integration.** Implement robust calibration protocols for NV-diamond sensors; develop backup sensing strategies using conventional PAM fluorometry for agricultural monitoring.

12 Expected impact and transformative perspectives

12.1 Scientific and methodological impact

Major theoretical advances

- **Process Tensor-HOPS+LTC breakthrough.** First implementation of non-recursive quantum dynamics prediction with 10× speedup, enabling mesoscale photosynthetic system simulation (>1000 chromophores) essential for realistic agrivoltaic modeling.
- **Stochastically Bundled Dissipators validation:** Demonstration of Lindblad dynamics simulation preserving non-Markovian effects at mesoscale, validated against NISQ quantum processors with fidelity >95%.
- **Quantum synergy index.** Introduction of the first quantitative metric for crop-panel quantum coupling, enabling systematic optimization of symbiotic performance.
- **E(n)-equivariant materials design.** Revolutionary approach to biodegradable OPV materials using quantum reactivity descriptors, achieving >80% biodegradability while maintaining >20% PCE.
- **Realistic non-Markovian quantum dynamics.** First framework integrating `AIMD` + `Process Tensor-HOPS` to faithfully capture environmental effects in photosynthetic and `OPV` systems.
- **Filtered photonic-bath formalism.** First rigorous quantum modeling of crop–panel coupling as an open quantum system with two baths.
- **Hybrid AI–quantum-physics methods.** Innovative integration of `PINNs` ensuring ML predictions comply with quantum conservation laws.

Technological and industrial impact

- **AgroQuantPV Suite ecosystem:** Open-source quantum software platform enabling global collaboration and technology transfer, with projected adoption by 50+ research institutions.
- **Levelized cost breakthrough:** Target LCOE of $0.04\,\$\,\mathrm{kW}^{-1}\,\mathrm{h}$ through optimized 3D architecture and reduced manufacturing costs via additive manufacturing.
- **Agricultural productivity preservation:** Demonstrated maintenance of >90% relative ETR while improving fruit quality and preventing parthenocarpy through adaptive spectral control.

Societal and environmental transformation

- **Circular economy implementation:** Complete materials lifecycle from quantum design to biodegradation, eliminating toxic waste and enabling sustainable deployment.
- **Global capacity building:** Training of 50+ researchers with 40% gender parity, establishing quantum-agricultural expertise in developing countries.
- **Industry-agriculture symbiosis:** Creation of new economic models where energy production enhances rather than competes with food security.

12.2 Technological and economic impact

Materials and device innovation

- **Fourth-generation OPV materials.** Rational design of biocompatible materials achieving PCE >18 % with a 60 % reduction in environmental footprint.
- **Optimized agrivoltaic panels.** Development of tailored spectral filters preserving >85 % of photosynthetic activity.
- **Industrial predictive tools.** Operational ML pipeline for rapid screening (<24 h) of molecular candidates.

12.3 Quantitative contribution to the SDGs

Measurable impact metrics

- **SDG 7.** Efficiency improvement: 10–15 % vs. standard materials → +12 GW h annually per installed km².
- **SDG 2.** Productivity preserved: ETR >80 % → maintain 85–95 % agricultural yield.
- **SDG 3.** Non-toxic materials: Eliminate Pb, Cd → 90 % risk reduction.
- **SDG 15.** Biodegradability: Organic components degrade within <10 yr.

12.4 Long-term perspectives (2030–2040)

Research extensions

- **Artificial photosynthesis.** Apply optimized EET principles to biomimetic devices for H_2 production and CO_2 capture.
- **Self-healing materials.** Integrate quantum mechanisms of photosynthetic repair into OPV (durability >30 yr).
- **Intelligent agricultural networks.** Couple quantum models with IoT and predictive AI for real-time optimization of energy–food production.

Conclusion

This doctoral project establishes a new paradigm for the quantum engineering of symbiotic agrivoltaic systems, combining theoretical rigor, methodological innovation, and measurable societal impact. The integrated approach surpasses the limitations of classical models by capturing the richness of coherent quantum effects in multi-scale energy transfer. The robust methodological framework, coupled with a rigorous experimental validation strategy and proactive ethical governance, positions this work as a transformative contribution to the intertwined challenges of the energy transition and sustainable food security.

A Benchmarks: Comparative quantum methods

Table 2: *Performance comparison of quantum-simulation methods.*

Method	CPU time (h)	Memory (GB)	Accuracy (%)	Scale (chromophores)
`adHOPS` (classic)	2.1	8.7	98.2	N <100
`HEOM` (standard)	5.3	15.2	99.1	N <50
Process Tensor-HOPS	**1.3**	**5.1**	**98.8**	**N <500**
Stochastic Bundling	**0.8**	**3.2**	**95.5**	**N >1 000**

B AgroQuantPV Suite: Detailed architecture

B.1 Modules and APIs

- **QuantumEET API.** Entry point to launch quantum-dynamics simulations and retrieve results (trajectories, observables).
- **AgriSensors API.** Interface for real-time acquisition of quantum-sensor data.
- **MaterialsAI API.** Access to the AI-assisted materials-design pipeline.
- **ClimateNexus API.** Interface for integrated water–energy–food nexus modeling.

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