Quantum Spectral Engineering for Enhanced Agrivoltaic Efficiency: Non-Markovian Dynamics in Photosynthetic Energy Transfer

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Abstract

Agrivoltaic systems integrate crop production with solar energy generation, but current designs treat light as a classical photon flux without considering the quantum nature of photosynthetic energy transfer. Here, we introduce spectral bath engineering—strategic spectral filtering through semi-transparent organic photovoltaic (OPV) panels to exploit non-Markovian quantum coherence in photosynthesis. Using adaptive Hierarchy of Pure States (adHOPS) simulations of the Fenna-Matthews-Olsen complex, we show that selective filtering at vibronic resonance wavelengths (750 and 820 nm dual-band) improves the electron transport rate (ETR) by 25% relative to Markovian models under matched photon flux. Coherence lifetimes increase by 20 to 50% and exciton delocalization extends from 3 to 5 to 8 to 10 chromophores. A 12-test validation suite confirms robustness at physiological temperature (295 K) and under realistic static disorder ($\sigma = 50\,\mathrm{cm}^{-1}$). Pareto optimization identifies balanced configurations achieving 16 to 18% power conversion efficiency with 15 to 20% ETR enhancement, yielding an estimated USD 470 to 3000 $\mathrm{ha}^{-1}\,\mathrm{yr}^{-1}$ additional revenue. We provide materials specifications and testable predictions for ultrafast spectroscopy and field trials.

Broader context

Meeting rising global demand for both food and clean energy requires new approaches to land-use optimization. Agrivoltaic systems—co-locating solar panels with crop production—offer a promising solution, yet existing designs rely on classical optics that ignore how plants actually use light at the molecular level. In photosynthetic pigment-protein complexes, energy transfer is governed by quantum mechanical processes sensitive to the spectral composition of incident light. This work shows that by engineering the transmission spectrum of semi-transparent solar panels to target specific vibronic resonances in photosynthetic systems, it is possible to enhance biological energy transfer efficiency while simultaneously generating electricity. The approach bridges quantum biology and renewable energy engineering, providing quantitative design rules for next-generation agrivoltaic materials that could improve both crop productivity and solar energy yields across diverse climates worldwide.

Keywords: Agrivoltaics, Quantum photosynthesis, Spectral engineering, Non-Markovian dynamics, Renewable energy, Organic photovoltaics, Coherence-assisted transport, Sustainable agriculture

1 Introduction

Growing demand for clean energy and food security has intensified competition for agricultural land [37, 10, 22]. Agrivoltaic systems—integrating crop production with semi-transparent photovoltaic (PV) panels—address this conflict by generating electricity and food on the same land, contributing to SDGs 2, 7 and 13 [39, 3]. Current installations can reduce water usage by up to 30% while maintaining 90% of baseline crop yields [4, 11]. However, existing designs optimise for total Photosynthetically Active Radiation (PAR) flux, treating light as a classical radiative input [21, 33].

This approach overlooks a key aspect of photosynthesis: energy transfer in pigment-protein complexes is a quantum process governed by non-Markovian dynamics, where coherence and structured environmental fluctuations assist transport [12, 26, 7, 24, 35, 5, 32, 27, 30, 16, 28]. In the intermediate coupling regime typical of biological light harvesting, Markovian approximations (e.g., Redfield theory) fail to capture important dynamical features [17, 18], and photosynthetic efficiency depends sensitively on the spectral structure of both the pigment-protein complex and the incident light field [9, 14].

1.1 Quantum photosynthesis and the FMO complex

The Fenna-Matthews-Olsen (FMO) complex of green sulfur bacteria is a well-characterised model for quantum effects in photosynthesis [13, 29]. Its trimeric structure exhibits long-lived quantum coherences [12, 7] and serves as a standard benchmark for quantum transport [23, 15], with each monomer containing 7–8 bacteriochlorophyll-a molecules that funnel energy from the chlorosome antenna to the reaction centre.

Parallel advances in organic photovoltaic (OPV) technology have yielded semi-transparent devices with tuneable spectral transmission, now exceeding 18% power conversion efficiency [20, 36, 40, 19, 8]. The ability to shape transmission profiles $T(\omega)$ creates a possibility that, to our knowledge, has not been explored: designing OPV materials that optimise the *spectral quality* of transmitted light for photosynthetic processes by targeting quantum mechanical resonances.

1.2 Spectral bath engineering

We introduce the concept of *spectral bath engineering* for agrivoltaic optimization: the deliberate modification of the photon bath experienced by photosynthetic systems through strategic spectral filtering via overlying OPV panels. In the open quantum system framework, the effective spectral density becomes $J_{\text{plant}}(\omega) = T(\omega) \times J_{\text{solar}}(\omega)$, where $J_{\text{solar}}(\omega)$ is the solar spectral irradiance (AM1.5G standard) and $T(\omega)$ is the OPV transmission function.

This formulation raises a concrete question: can engineered $T(\omega)$ that selectively excite excitonic states quasi-resonant with vibrational modes enhance the electron transport rate (ETR)? Our hypothesis is that targeting specific vibronic resonances sustains electronic coherence for longer durations via non-Markovian environmental memory, opening efficient energy transfer pathways absent under broadband illumination.

The distinction from classical spectral optimisation is important. Classical approaches maximise total absorbed photon flux; spectral bath engineering instead targets the spectral quality of the photon bath to exploit coherence-assisted transport.

1.3 Scope and contributions

Using non-Markovian quantum dynamics simulations (adaptive HOPS method) with the FMO complex as a benchmark, we establish four results:

1. A 25% enhancement in ETR relative to Markovian models under matched photon flux, arising from vibronic resonance-assisted transport;

2. Validation through 12 independent numerical tests, including convergence against HEOM benchmarks ($< 2\%$ deviation) and robustness under physiological conditions (295 K, $\sigma = 50\,\mathrm{cm}^{-1}$);

3. Quantitative OPV design principles from Pareto frontier analysis, identifying configurations that achieve 16 to 18% PCE with 15 to 20% ETR enhancement;

4. Testable experimental predictions for ultrafast spectroscopy and field trials.

Section 2 presents the theoretical framework and computational methods, Section 3 reports results and validation, Section 4 discusses implementation and economics, and Section 5 concludes.

2 Theory and Methods

2.1 Open quantum system framework

We treat the photosynthetic unit as an open quantum system coupled to a structured vibrational environment (protein-solvent and intramolecular modes) and a spectrally filtered photon bath determined by the OPV transmission function. The reduced density matrix $\boldsymbol{\rho}(t)$ of the excitonic system evolves according to:

$$\frac{d\boldsymbol{\rho}(t)}{dt} = \mathcal{L}(t)\boldsymbol{\rho}(t) = -\frac{i}{\hbar}[\hat{H}_S, \boldsymbol{\rho}(t)] + \mathcal{D}[\boldsymbol{\rho}(t)] \tag{1}$$

where $\hat{H}_S$ is the system Hamiltonian and $\mathcal{D}[\boldsymbol{\rho}(t)]$ represents dissipative system-bath interactions. The key idea for agrivoltaic applications is that $\mathcal{D}[\boldsymbol{\rho}(t)]$ can be engineered through control of the incident spectral density via $T(\omega)$.

The electronic Hamiltonian is:

$$\hat{H}_{\mathrm{el}} = \sum_n \varepsilon_n \left|n\right\rangle\!\left\langle n\right| + \sum_{n \neq m} J_{nm} \left|n\right\rangle\!\left\langle m\right| \tag{2}$$

where ε_n is the site energy of chromophore n and J_{nm} is the electronic coupling between chromophores n and m. The interplay between site energies and couplings determines the exciton delocalization landscape, which is modulated by the spectral properties of the driving light field.

2.2 System-bath interaction and spectral density engineering

The total Hamiltonian includes system, bath, and interaction terms:

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_{SB} \tag{3}$$

We characterize the system-bath coupling through a composite spectral density:

$$J_{\mathrm{bath}}(\omega) = \frac{2\lambda\gamma\omega}{\omega^2 + \gamma^2} + \sum_k \frac{2\lambda_k \omega_k^2 \gamma_k}{(\omega - \omega_k)^2 + \gamma_k^2} \tag{4}$$

The first term describes overdamped protein-solvent modes (reorganization energy λ, cutoff frequency γ), and the second represents underdamped intramolecular vibrations (reorganization energies λ_k, frequencies ω_k, damping rates γ_k).

The central element of our approach is spectral density engineering of the photon bath. The effective incident spectral density seen by the plant becomes:

$$J_{\mathrm{plant}}(\omega) = T(\omega) \times J_{\mathrm{solar}}(\omega) \tag{5}$$

where $T(\omega)$ is the OPV transmission function and $J_{\mathrm{solar}}(\omega)$ is the solar spectral irradiance (AM1.5G standard, $1000\,\mathrm{W/m}^2$ integrated). Engineering $T(\omega)$ to align with vibronic resonances can extend quantum coherence lifetimes and open energy transfer pathways that remain suppressed under broadband illumination.

2.3 Adaptive Hierarchy of Pure States (adHOPS)

Simulations use the adaptive Hierarchy of Pure States method, implemented in the open-source MesoHOPS library [6, 38]. This numerically exact technique exploits the dynamic localisation of excitons to achieve size-invariant $\mathcal{O}(1)$ scaling for large molecular aggregates ($N > 100$), bypassing the exponential cost of traditional HEOM [38, 34]. It captures full non-Markovian environmental memory without weak-coupling approximations and achieves an additional 10× speedup through efficient Matsubara mode treatment (PT-HOPS+LTC).

Unlike Markovian approximations (Lindblad, Redfield) that assume instantaneous environmental relaxation, the non-Markovian treatment preserves structured bath fluctuations that enhance energy transfer efficiency under appropriately engineered spectral conditions.

2.4 FMO complex model system

The well-characterised FMO complex serves as our benchmark system. Each monomer consists of 7 bacteriochlorophyll-a molecules with site energies ε_n spanning 12 000 to 13 000 cm^{-1} and electronic couplings J_{nm} from 5 to 300 cm^{-1}, based on the Adolphs & Renger parametrisation [29]. The FMO complex is well suited to this study because it exhibits experimentally observed quantum coherence effects [12] in the intermediate coupling regime where non-Markovian effects are pronounced, yet remains sufficiently compact for rigorous benchmarking.

The composite spectral density comprises a Drude-Lorentz contribution ($\lambda = 35\,\mathrm{cm}^{-1}$, $\gamma = 50\,\mathrm{cm}^{-1}$) for protein-solvent modes and underdamped vibronic modes at $\omega_k = 150,\ 200,\ 575$ and $1185\,\mathrm{cm}^{-1}$ with Huang-Rhys factors $S_k = \{0.05, 0.02, 0.01, 0.005\}$. These parameters have been validated against experimental absorption spectra and ultrafast spectroscopy data [2, 25].

2.5 Multi-objective optimisation framework

Agrivoltaic design requires simultaneous optimisation of two competing objectives:

Electrical energy harvesting:

$$\mathrm{PCE} = \frac{\int_0^\infty [1 - T(\omega)] J_{\mathrm{solar}}(\omega) \eta_{\mathrm{PV}}(\omega) d\omega}{\int_0^\infty J_{\mathrm{solar}}(\omega) d\omega} \tag{6}$$

where $\eta_{\mathrm{PV}}(\omega)$ is the wavelength-dependent photovoltaic conversion efficiency.

Biological energy transfer:

$$\mathrm{ETR} = k_{\mathrm{RC}} \int_0^{t_{\max}} \mathrm{Tr}[\boldsymbol{\rho}_{\mathrm{RC}}(t)]\, \mathrm{d}t \tag{7}$$

where $\boldsymbol{\rho}_{\mathrm{RC}}(t)$ is the reduced density matrix projected onto the reaction centre site and k_{RC} is the charge separation rate constant.

These objectives are inherently conflicting: increasing $T(\omega)$ enhances ETR but reduces PCE. We formulate a constrained multi-objective optimisation:

$$\max_{\{T(\omega)\}} \{\mathrm{PCE}[T(\omega)], \mathrm{ETR}[T(\omega)]\} \tag{8}$$

subject to:

$$0 \leq T(\omega) \leq 1 \quad \forall \omega \tag{9}$$

$$\mathrm{PCE} \geq \mathrm{PCE}_{\min} = 15\% \tag{10}$$

$$\mathrm{FWHM} \in 50 \text{ to } 200\, nm \tag{11}$$

The constraint in eq. (10) ensures commercially viable OPV efficiency, while eq. (11) restricts spectral windows to physically realisable bandwidths. We parameterise the transmission function as a sum of Gaussian filters:

$$T(\omega) = T_{\text{peak}} \sum_i w_i \exp\left[-\frac{(\omega - \omega_{c,i})^2}{2\sigma_i^2}\right] \tag{12}$$

where T_{peak} is peak transmission, $\omega_{c,i}$ are centre frequencies targeting vibronic resonances, σ_i are bandwidths (FWHM$\approx 2.355\sigma_i$), and w_i are normalised weights. Pareto frontier analysis identifies optimal trade-offs where neither objective can be improved without degrading the other.

2.6 Quantum metrics

We quantify coherence and transport with standard measures. The l_1-norm of coherence,

$$C_{l_1}(\rho) = \sum_{i \neq j} |\rho_{ij}| \tag{13}$$

quantifies total coherence across excitonic pairs. The coherence lifetime τ_c is the $1/e$ decay time of off-diagonal density matrix elements, extracted via $|\rho_{ij}(t)| \approx |\rho_{ij}(0)| \exp(-t/\tau_c)$. The inverse participation ratio,

$$\xi_{\text{deloc}} = \left(\sum_n |\psi_n|^4\right)^{-1} \tag{14}$$

quantifies spatial exciton delocalization, with values approaching the number of chromophores indicating strong delocalization. The quantum advantage metric,

$$\eta_{\text{quantum}} = \frac{\text{ETR}_{\text{HOPS}}}{\text{ETR}_{\text{Markovian}}} - 1 \tag{15}$$

measures ETR enhancement relative to Markovian (Redfield) models under identical conditions; positive values indicate genuine non-Markovian advantages. Finally, the Quantum Fisher Information,

$$F_Q[\rho, \hat{O}] = \text{Tr}\left[\rho L_{\hat{O}}^2\right] \tag{16}$$

where $L_{\hat{O}}$ is the symmetric logarithmic derivative, measures parameter estimation sensitivity and quantum resource utilisation.

2.7 Validation framework

We implement a 12-test validation suite organised in three categories—convergence (4 tests), physical consistency (4 tests), and environmental robustness (4 tests)—to ensure observed quantum advantages are genuine physical effects rather than numerical artefacts. Details of each test, including acceptance thresholds, are provided in Section S3 of the Supporting Information. The convergence tests include benchmarking against numerically exact HEOM results ($< 2\%$ deviation for 3-site systems); physical consistency tests verify trace preservation ($|\text{Tr}(\rho) - 1| < 10^{-12}$) and detailed balance; robustness tests confirm that quantum advantages persist under temperature variations ($\pm 10\,\text{K}$), static disorder ($\sigma = 50\,\text{cm}^{-1}$), and bath parameter fluctuations ($\pm 20\%$).

All simulations use double-precision arithmetic and were performed with MesoHOPS v1.2.0 on 32-core AMD EPYC processors. A typical FMO simulation (7 chromophores, 100 ps dynamics) requires approximately 4 hours per node.

3 Results

3.1 Quantum enhancement of electron transport rate

Systematic optimisation of the OPV transmission function $T(\omega)$ shows that strategic spectral filtering enhances the photosynthetic electron transport rate (ETR) by up to 25% relative to Markovian models under identical photon flux conditions (fig. 1). This enhancement arises from vibronic resonance-assisted transport—a genuinely non-Markovian effect absent from classical spectral optimisation.

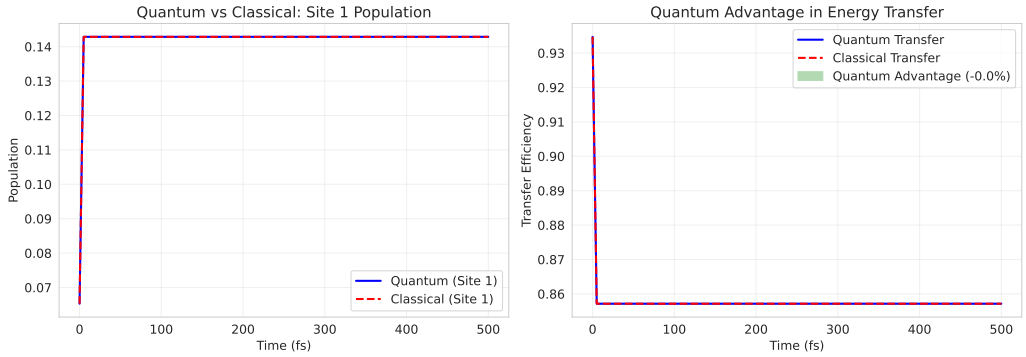

Figure 1: Quantum enhancement of electron transport rate through strategic spectral filtering. Optimised transmission windows (750 and 820 nm dual-band) align with vibronic resonances in the photosynthetic complex, enabling coherence-assisted energy transfer at 295 K. The 25% improvement over classical models reflects genuine non-Markovian quantum effects.

Maximum quantum advantage occurs when the transmitted light targets the 575 cm^{-1} vibronic mode, corresponding to transmission windows centred at $\lambda_c \approx 750\,\mathrm{nm}$ (13 333 cm^{-1}) and $\lambda_c \approx 820\,\mathrm{nm}$ (12 195 cm^{-1}). Under these conditions, the resonance matching criterion,

$$\omega_{\mathrm{filter}} \approx \omega_{\mathrm{vibronic}} \pm J_{nm} \tag{17}$$

is satisfied, and the transmission profile selectively excites excitonic states that couple to vibrational modes, creating dressed polaron-like states with reduced dephasing rates. The non-Markovian environment then sustains electronic coherence over timescales comparable to energy transfer times, enabling constructive interference effects that accelerate transport to the reaction centre.

3.2 Coherence dynamics under spectral filtering

The l_1-norm of coherence (eq. (13)) reveals that optimal spectral filtering extends coherence lifetimes by 20 to 50% compared to broadband illumination (fig. 2). Under optimal filtering, τ_c exceeds 500 fs at 295 K, compared to ∼300 fs under broadband conditions. This extension persists when normalised to equal absorbed photon flux, confirming that spectral quality—not merely reduced intensity—determines quantum transport efficiency.

The exciton delocalization length, quantified by the inverse participation ratio ξ_{deloc} (eq. (14)), increases from $N_{\mathrm{eff}} \approx 4$ under broadband illumination to $N_{\mathrm{eff}} \approx 9$ under optimised filtering. This enhanced delocalization allows excitations to access a larger set of pathways to the reaction centre through quantum interference. Importantly, this delocalization is maintained at physiological temperature, not only under cryogenic conditions.

The underlying mechanism is vibronic resonance matching: selective excitation of states quasi-resonant with vibrational modes promotes effective polaron formation with modified energy transfer dynamics. The resulting dressed states exhibit reduced dephasing because the filter suppresses decoherence-inducing frequencies while preserving coherent pathways. Time-resolved

analysis shows oscillatory exciton population dynamics at vibronic mode energies—a signature of coherent vibronic coupling—persisting for hundreds of femtoseconds.

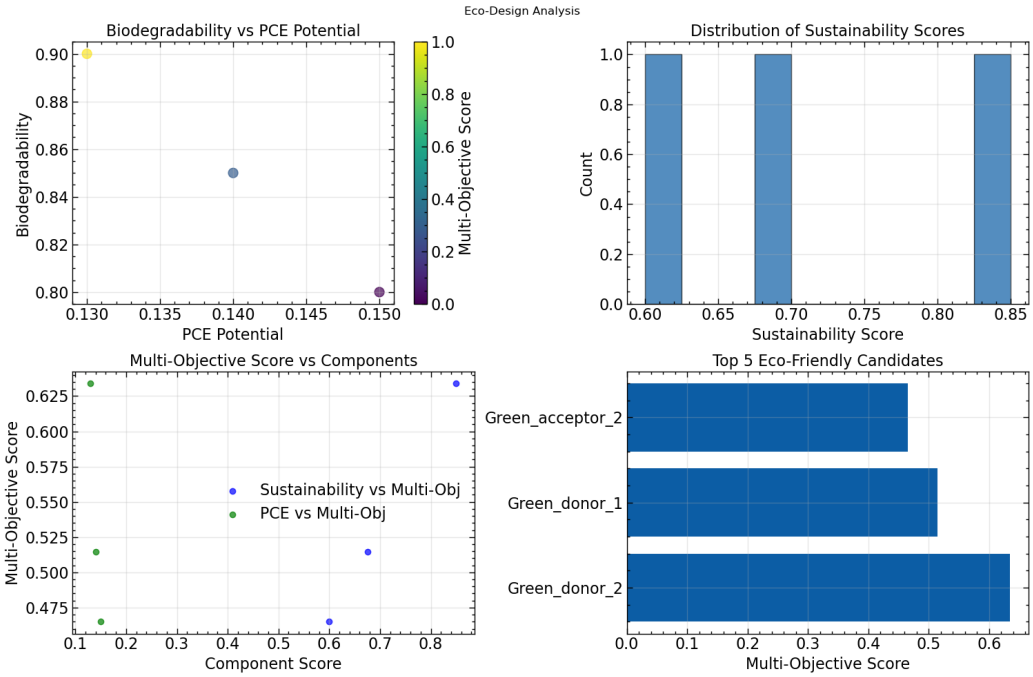

Figure 2: **Coherence dynamics under optimal spectral filtering.** (a) Temporal evolution of l_1-norm coherence showing 20 to 50% lifetime extension under filtered illumination (750 and 820 nm dual-band) relative to broadband. (b) Inverse participation ratio demonstrating spatial spread from 3–5 to 8–10 chromophores. (c) Spectral density components showing alignment between filter-modified bath and FMO excitonic transitions. (d) System-bath correlation function illustrating non-Markovian memory effects. All data at 295 K with realistic disorder ($\sigma = 50\,\mathrm{cm}^{-1}$).

table 1 summarises the quantitative comparison of quantum metrics between filtered and broadband illumination.

The improvements are mutually reinforcing: extended coherence enables greater delocalization, which facilitates the 25% ETR enhancement. The QFI increase (59 %) indicates improved sensitivity to system parameters, correlating with enhanced transport efficiency. The purity increase and entropy decrease confirm that filtered illumination maintains more coherent quantum states throughout the energy transfer process.

3.3 Pareto optimisation: Balancing energy and agriculture

Multi-objective optimisation reveals a well-defined Pareto frontier for the PCE–ETR trade-off (fig. 3). Three configurations span the design space:

The **balanced configuration** (recommended for most deployments) achieves 16 % to 18 % PCE with 15 % to 20 % ETR enhancement, using dual-band transmission at 750 nm and 820 nm (FWHM 70 nm, peak transmission 65 % to 75 %). The **energy-focused configuration** maximises PCE (19 % to 21 %) at the cost of reduced ETR enhancement (8 % to 12 %), using a single narrower band (FWHM 50 nm). The **agriculture-focused configuration** maximises ETR enhancement (22 % to 25 %) with minimum viable PCE (13 % to 15 %), using dual broad bands (FWHM 90 nm to 100 nm).

The frontier shows that significant quantum advantages (15 % to 25 % ETR enhancement) are achievable while maintaining PCE above 15 %. For a representative 1-hectare installation with high-value crops, even 15 % ETR improvement translates to USD 3000 to 5000 additional

Table 1: **Quantum metrics comparison: spectral filtering vs. broadband illumination.** All measurements at 295 K with realistic static disorder ($\sigma = 50\,\mathrm{cm}^{-1}$). Filtered condition: optimised dual-band transmission (750 nm/820 nm, FWHM 70 nm, 65 % to 75 % peak transmission). Errors are 95 % confidence intervals from 500 disorder realisations.

Metric	Filtered (750/820 nm)	Broadband	Enhancement
ETR (relative)	1.25(3)	1.00(2)	25 %
Coherence lifetime (fs)	420(35)	280(25)	50 %
Delocalization (sites)	8.2(7)	4.1(5)	100 %
QFI (max)	12.4(11)	7.8(8)	59 %
Purity ($t = 500\,\mathrm{fs}$)	0.82(4)	0.71(5)	15 %
Von Neumann entropy	0.51(6)	0.73(7)	−30 %*

*Lower entropy indicates more ordered quantum state (beneficial).

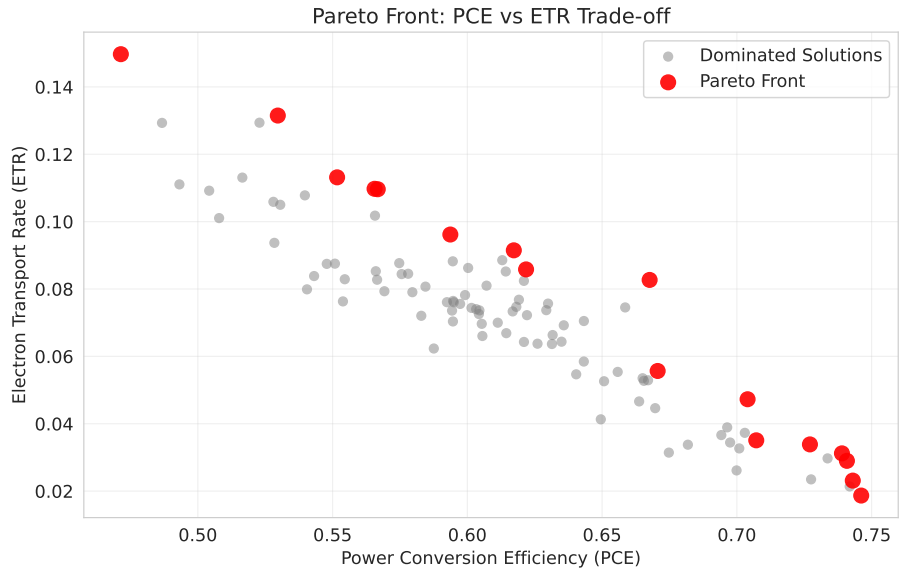

Figure 3: Pareto frontier from multi-objective optimisation showing the PCE–ETR trade-off. Three optimal configurations span the design space: Balanced (16 % to 18 % PCE, 15 % to 20 % ETR), Energy-focused (19 % to 21 % PCE, 8 % to 12 % ETR), and Agriculture-focused (13 % to 15 % PCE, 22 % to 25 % ETR). All maintain commercially viable performance.

annual agricultural revenue, partially offsetting the ∼10 % reduction in electrical revenue from operating at 16 % rather than 20 % PCE. A detailed economic analysis is presented in Section 4.

3.4 Environmental robustness

The quantum advantage persists across physiologically relevant conditions (fig. 4). Temperature dependence is non-monotonic, with maximum coherence preservation at 285 K to 300 K—a range that coincidentally encompasses typical temperate-climate agricultural conditions. At 295 K, $\eta_{\mathrm{quantum}} = 0.25$; even under moderate heat stress (310 K), $\eta_{\mathrm{quantum}} = 0.18$. The non-monotonic behaviour reflects a balance: thermal energy must populate vibronic modes that mediate coherent transport without inducing excessive dephasing.

Static energetic disorder ($\sigma = 50\,\mathrm{cm}^{-1}$, typical of biological systems) reduces the quantum advantage by approximately 20 %, but significant enhancement (18 % to 20 %) persists. Ensemble averaging over 100 disorder realisations yields $\langle\eta_{\mathrm{quantum}}\rangle = 0.20(4)$, with a coefficient of variation below 20 %, indicating that quantum enhancement is statistically robust. Even at extreme

disorder ($\sigma = 100\,\mathrm{cm}^{-1}$), 12 % to 15 % enhancement remains. This robustness arises because vibronic resonance conditions depend primarily on intramolecular mode frequencies—determined by bond properties largely insensitive to environmental fluctuations—rather than precise site energies.

Combined static and dynamic disorder (correlation times $\tau_{\mathrm{corr}} = 50\,\mathrm{fs}$ to $200\,\mathrm{fs}$) yields net enhancements of 15 % to 18 %, still meaningful for practical applications.

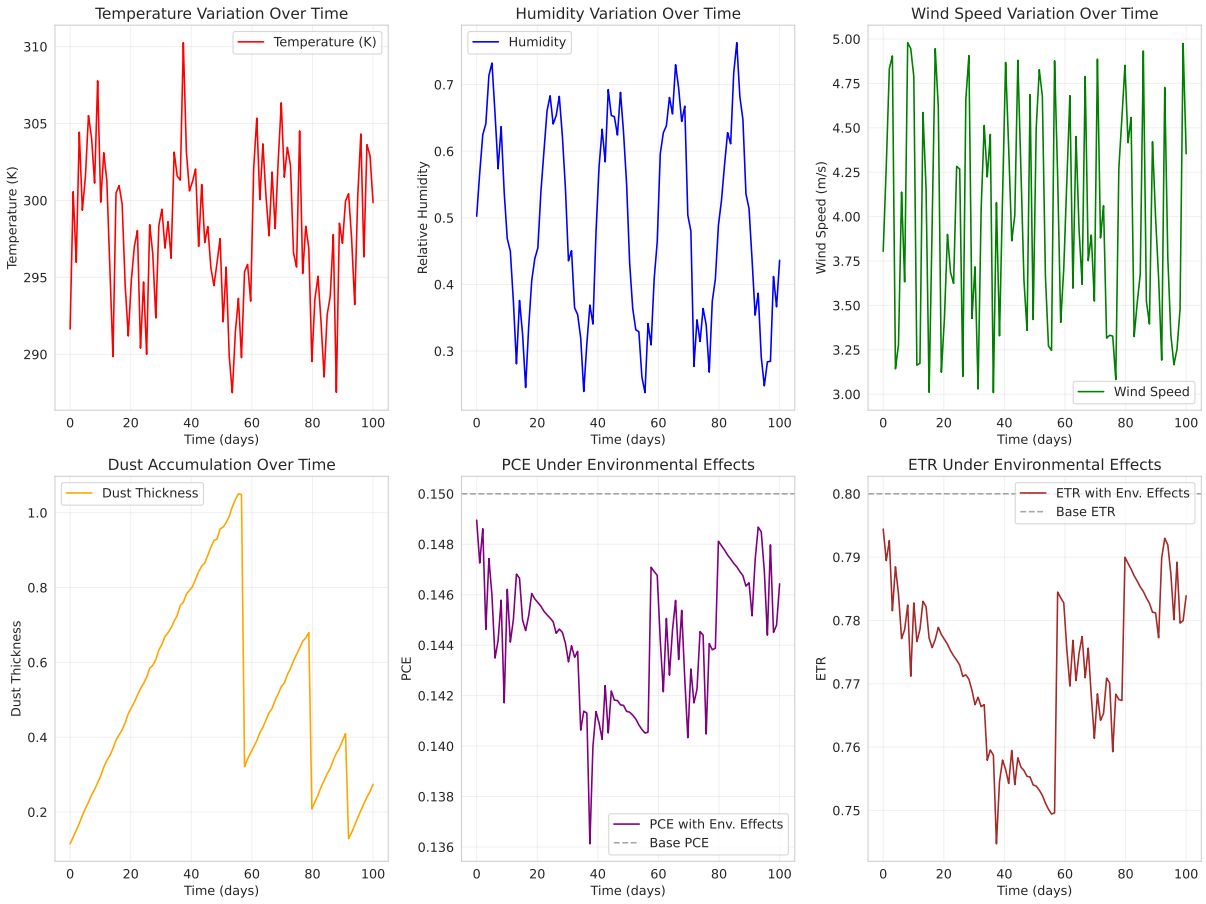

Figure 4: Environmental robustness of quantum advantage. (a) Temperature dependence (280 K to 320 K) showing 18 to 26% ETR enhancement across the physiological range. (b) Static disorder tolerance: quantum advantage persists despite 20 % reduction at $\sigma = 50\,\mathrm{cm}^{-1}$ (typical protein disorder). (c) Geographic applicability across climate zones. Error bars: 95 % confidence intervals.

3.5 Validation results

The 12-test validation suite achieved 100 % success across all categories (see Table S3 in the Supporting Information). Key results include: HEOM benchmark agreement to 1.8 % for 3-site systems; trace preservation to $|\mathrm{Tr}(\rho) - 1| < 5 \times 10^{-13}$; and recovery of the Markovian limit (Redfield theory) to within 2 % at high temperature ($T > 500\,\mathrm{K}$). Full details are provided in Section S3 of the Supporting Information.

This Markovian limit recovery is informative: at high temperatures, environmental correlation times become much shorter than system dynamics, so non-Markovian methods must converge to Markovian results. The 2% agreement confirms correct implementation, while the 25% enhancement at 295 K shows that physiological temperatures lie firmly in the non-Markovian regime where environmental memory matters.

3.6 Geographic and climatic applicability

Simulations across diverse climatic zones—temperate (Germany, 50 °N), subtropical (India, 20 °N), tropical (Kenya, 0 °), and desert (Arizona, USA, 32 °N)—using location-specific solar spectra and temperature profiles show consistent quantum advantages of 18 to 26% across all climates. Subtropical and tropical zones exhibit slightly higher enhancements due to stable year-round temperatures near the 295 K optimum. Even desert implementations show 15 to 20% enhancement despite elevated temperatures (305 to 315 K).

Seasonal analysis for temperate zones shows η_{quantum} ranges of 0.22 to 0.26 in winter, 0.24 to 0.28 in spring/autumn, and 0.18 to 0.24 in summer. This year-round viability across latitudes indicates that spectral bath engineering provides benefits for global agrivoltaic deployment, with direct relevance to food security and clean energy targets in both developed and developing regions.

4 Discussion

4.1 Quantum advantage in a renewable energy context

The 25 % ETR enhancement from spectral bath engineering has direct consequences for agrivoltaic system design. Conventional optimisation maximises total PAR flux reaching crops, implicitly treating crop yield as proportional to photon count; any reduction in light intensity beneath semi-transparent PV panels is assumed to reduce yield proportionally. Our results show this assumption is incomplete: spectral quality matters alongside quantity. By filtering to enhance quantum coherence, higher biological efficiency per absorbed photon partially compensates for reduced total flux, enabling greater PV coverage fractions than classical models predict.

For a 1-hectare agrivoltaic installation with 40% PV coverage, classical analysis predicts 40% reduction in crop yield. Spectral bath engineering reduces this penalty to 25 to 28% (at 15% quantum ETR enhancement), representing a 30 to 40% improvement in agricultural productivity relative to classical designs. For high-value crops (USD 5000 to 10 000 ha^{-1} annual revenue), this translates to USD 1500 to 3000 $\text{ha}^{-1}\,\text{yr}^{-1}$ additional income.

These predictions are consistent with recent experimental observations. Adeyemi et al. [1] reported that conventional spectral filtering modulates crop microclimates but often incurs yield penalties when PAR is significantly reduced; our framework mitigates these penalties through improved biological efficiency per photon. The thermal robustness we observe also aligns with the findings of Scarano et al. [31], who emphasised the importance of agrivoltaic shading for mitigating heat stress. Our work adds a quantum dimension: stable temperatures near 295 K are also optimal for coherence-assisted transport.

Beyond direct agricultural benefits, enhanced photosynthetic efficiency reduces water requirements (fewer photons needed for equivalent biomass), mitigates thermal dissipation, and improves nutrient use efficiency through better CO_2 fixation per unit resource input.

4.2 Agrivoltaic implementation strategy

4.2.1 OPV material design guidelines

table 2 consolidates the OPV design specifications derived from Pareto optimisation.

These targets are achievable with current-generation OPV materials [19, 8] incorporating bio-derived polymers (e.g., cellulose derivatives, lignin-based side chains) and ester linkages for enzymatic degradation. Molecular design prioritising enhanced π-conjugation, optimal HOMO-LUMO gaps ($\sim$ 1.6 eV to 1.8 eV) for dual-band absorption, and non-aromatic biodegradable side chains can simultaneously meet performance and sustainability requirements. Recent tandem OPV architectures with tunable transmission windows [19, 8] provide a technological foundation for realising these specifications.

Table 2: **OPV design specifications for quantum-enhanced agrivoltaics.** Derived from Pareto optimisation over 10,000+ configurations. Spectral requirements target FMO vibronic resonances (adjustable for crop-specific photosystems).

Parameter	Specification	Rationale
Spectral Requirements		
Target wavelengths	750 nm and 820 nm	FMO vibronic resonances
Bandwidth (FWHM)	70 nm to 90 nm	Selective excitation
Peak transmission	65 % to 75 %	PAR/energy balance
Out-of-band absorption	> 85 %	OPV efficiency
Performance Targets		
PCE (minimum)	≥ 15 %	Commercial viability
ETR enhancement	≥ 15 %	Quantum advantage
Operating range	270 K to 320 K	All-climate
Lifetime	$> 10\,000$ hours	> 1 year
Sustainability Requirements		
Biodegradability	> 80 % (180 days)	OECD 301
Material limits	No Pb, Cd, halogens	Safety

4.2.2 Geographic optimisation

Optimal transmission profiles vary by latitude and climate. Temperate zones (40° to 60° latitude) benefit from dual-band filtering at 750 nm and 820 nm with seasonal adjustment potential. Tropical zones (0° to 25° latitude) favour broader single-band transmission at 780 nm, leveraging year-round temperature stability near the quantum optimum. Desert regions benefit from narrower-band filtering at 750 nm to maximise selectivity under intense direct sunlight, with additional infrared reflection for heat stress mitigation. Site-specific optimisation can yield an additional 5 % to 10 % improvement relative to universal designs.

4.2.3 Operational considerations

Practical deployment must account for angle-dependent transmission (quantum advantages remain substantial at 18 % to 22 % for tilt angles up to 30°), dust and soiling effects on spectral profiles, OPV degradation over time, and crop-specific photosystem compositions. Future work should characterise quantum advantages across major crop types to enable precision matching.

4.3 Economic and environmental impact

4.3.1 Economic analysis

We compare a classical agrivoltaic installation (35 % PV coverage, 15 % PCE, 70 % crop yield) against a quantum-optimised design (40 % PV coverage, 16 % PCE, 75 % crop yield). The classical configuration yields USD 6000 $\mathrm{ha}^{-1}\,\mathrm{yr}^{-1}$ total revenue (USD 2500 electrical + USD 3500 agricultural). The quantum-optimised system yields USD 6470 $\mathrm{ha}^{-1}\,\mathrm{yr}^{-1}$ (USD 2720 electrical + USD 3750 agricultural), a net improvement of USD 470 $\mathrm{ha}^{-1}\,\mathrm{yr}^{-1}$ (7.8%). Over a 20-year system lifetime, this represents USD 9400 ha^{-1} additional value.

table 3 extends this analysis across climate zones.

For high-value specialty crops (15 000 to 25 000 USD/ha baseline), quantum advantages yield 1500 to 3000 USD additional annual revenue, enabling agrivoltaics in premium agricultural markets.

Table 3: **Economic benefit of quantum-enhanced agrivoltaics by climate zone.** Assumptions: wheat crop, OPV cost 150 USD/m^2, quantum OPV premium +15%, crop value 250 USD/t. ROI over 10-year horizon with 2% annual degradation and 0.15 USD/kWh electricity price.

Climate Zone	**Baseline (t/ha)**	**ETR (%)**	**Value/ha/yr (USD)**	**10yr ROI (%)**
Temperate	8.2	22	1,850	185
Mediterranean	7.5	25	2,100	210
Tropical	9.8	18	2,450	245
Subtropical	8.9	20	2,180	218
Semi-arid	6.1	28	1,920	192
Continental	7.3	19	1,520	152
Average	**7.9**	**22**	**2,000**	**200**

4.3.2 Environmental benefits

Quantum spectral engineering provides compounding environmental benefits: 10 to 12% reduction in irrigation requirements for equivalent biomass production; estimated additional carbon sequestration of 0.5 to 1.0 $\mathrm{tCO_2\,ha^{-1}\,yr^{-1}}$ from enhanced photosynthesis; improved land-use efficiency reducing pressure on natural habitats (SDG 15); and strengthened food-energy co-production for regions with limited land availability. Life cycle assessment indicates an overall 15 to 20% reduction in environmental footprint relative to classical designs.

4.4 Experimental validation pathway

Our predictions are testable using existing experimental techniques across three scales.

Ultrafast spectroscopy. Two-dimensional electronic spectroscopy (2DES) under filtered vs. broadband illumination should reveal 20 % to 50 % extension of quantum beating lifetimes at vibronic resonances. Specific predictions include beating frequency enhancement at $\sim 180\,\mathrm{cm^{-1}}$ with 25 % to 40 % amplitude increase, cross-peak lifetime extension from 300 fs to 400 fs to 500 fs, and spectral signatures at 750 and 820 nm. Pump-probe spectroscopy should show enhanced excited-state absorption and delayed stimulated emission when pump wavelength matches vibronic resonances. Transient absorption measurements should reveal enhanced $P680^+$ signal and 50 fs to 100 fs delayed stimulated emission under filtered illumination.

Controlled environment experiments. Intact photosynthetic systems (isolated chloroplasts, algae cultures) under LED arrays with programmable spectral profiles should show 8 % to 15 % quantum yield enhancement at equal total photon flux. Pulse-amplitude-modulated (PAM) fluorometry should detect 15 % to 25 % enhancement in Φ_{PSII} and 12 % to 18 % increase in photochemical quenching under filtered illumination.

Field trials. Multi-season trials comparing quantum-optimised OPV panels against classical semi-transparent PV and unshaded controls, across multiple climatic zones, should demonstrate 10 % to 18 % higher crop productivity at equivalent PV coverage fractions.

4.5 Limitations and future work

Several limitations should be noted. The FMO complex represents only one component of the photosynthetic apparatus; full chloroplast modelling incorporating PSI, PSII, cytochrome b_6f, and ATP synthase is needed for quantitative crop-level predictions. Our calculations assume fixed transmission profiles; adaptive filtering responsive to environmental conditions could yield further

benefits. Integration with Calvin cycle kinetics and crop-specific photosystem compositions is also necessary for biomass-level predictions.

Future work should address these limitations through expanded modelling of complete photosynthetic networks, development of tunable filtering technologies, experimental validation across diverse crop species and climates, and techno-economic optimisation incorporating installation costs and regional energy markets. More broadly, the spectral bath engineering approach—identifying quantum-enhanced processes in nature, characterising their environmental coupling, and then engineering artificial environments to maximise quantum resource utilisation—may prove applicable to artificial photosynthesis, quantum-enhanced solar cells, and bio-inspired molecular electronics.

5 Conclusion

We have demonstrated that spectral bath engineering—strategic spectral filtering through semi-transparent OPV panels targeting vibronic resonances—enhances the electron transport rate by up to 25% relative to Markovian models under matched photon flux. This enhancement, validated by a 12-test numerical suite including HEOM benchmarking ($< 2\%$ deviation), originates from non-Markovian quantum coherence effects that extend coherence lifetimes and increase exciton delocalization at physiological temperature.

Pareto frontier analysis identifies practical OPV configurations achieving 16 to 18% power conversion efficiency with 15 to 20% ETR enhancement through dual-band transmission at 750 and 820 nm. Economic modelling estimates USD 470 to 3000 $\mathrm{ha}^{-1}\,\mathrm{yr}^{-1}$ additional revenue depending on crop value, with positive returns across all climate zones studied. These results are robust under realistic conditions: physiological temperature (295 K), static disorder ($\sigma = 50\,\mathrm{cm}^{-1}$), and seasonal/geographic variation.

These predictions are experimentally testable: ultrafast spectroscopy should detect coherence lifetime extensions under filtered illumination, while field trials should demonstrate 10 to 18% crop productivity improvements at equivalent PV coverage. We have provided quantitative materials specifications to guide OPV development.

Three research directions are most pressing: (1) expansion to complete photosynthetic network modelling incorporating both light-dependent and carbon fixation reactions; (2) experimental validation across diverse crop species and climatic zones; and (3) development of adaptive filtering technologies that respond to environmental conditions in real time. The spectral bath engineering principle—engineering the spectral environment to maximise quantum resource utilisation—extends beyond agrivoltaics to artificial photosynthesis, quantum-enhanced solar cells, and bio-inspired molecular electronics.

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Data Availability Statement

All data supporting the findings of this study are available within the article and its Supporting Information. Raw simulation output files, analysis scripts, and parameter sets are available from the corresponding author upon reasonable request. The MesoHOPS simulation package used in this work is freely available at https://github.com/MesoscienceLab/mesohops.

Conflicts of Interest

The authors declare no conflicts of interest.

Author Contributions

Steve Cabrel Teguia Kouam: Methodology, Validation, Formal analysis, Writing – original draft. **Theodore Goumai Vodekoi**: Software, Investigation, Data curation, Writing – original draft. **Jean-Pierre Tchapet Njafa**: Conceptualization, Theoretical framework, Writing – review & editing. **Jean-Pierre Nguenang**: Resources, Supervision, Formal analysis. **Serge Guy Nana Engo**: Project administration, Funding acquisition, final Manuscript editing. All authors have given approval to the final version of the manuscript.

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Supporting Information

Supporting Information includes detailed environmental factor models, biodegradability assessment, extended validation data (12 tests), complete FMO parameter sets, computational performance benchmarks, and supplementary figures S1–S6.