

Spectral Bath Engineering for Quantum-Enhanced Agrivoltaics: Advancing Efficiency and Environmental Sustainability via Non-Markovian Dynamics

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Abstract

As global demand for food and clean energy intensifies, agrivoltaic systems have emerged as a vital solution for land-use optimization. However, current designs overwhelmingly treat incident light as a classical photon flux, overlooking the quantum mechanical nature of photosynthetic energy transfer. We introduce *spectral bath engineering*—the strategic spectral filtering of sunlight through semi-transparent organic photovoltaic (OPV) panels to exploit non-Markovian quantum coherence in biological light-harvesting. Using Process Tensor HOPS (PT-HOPS) and Spectrally Bundled Dissipators (SBD) to simulate the Fenna-Matthews-Olsen complex, we demonstrate that selective filtering at vibronic resonance wavelengths (750 nm and 820 nm) enhances the electron transport rate (ETR) by 25 % relative to standard Markovian models. This quantum advantage is driven by vibronic resonance-assisted transport, which extends coherence lifetimes by 20 % to 50 % and nearly doubles pairwise concurrence (89 %). Multi-objective Pareto optimization identifies OPV configurations reaching 18.8 % power conversion efficiency while sustaining an 80.5 % system ETR, potentially generating an additional USD 470 to 3000 ha⁻¹ yr⁻¹ in revenue. Environmental simulations across nine climate zones, including sub-Saharan Africa, confirm persistent ETR enhancements of 18 % to 24 %. Finally, eco-design analysis using quantum reactivity descriptors ensures that these technological gains are achieved using sustainable, biodegradable materials. By bridging quantum biology and renewable energy engineering, this work provides a quantitative blueprint for next-generation agrivoltaic materials that co-optimize agricultural productivity and energy yield.

Broader context

The escalating global need for food and clean energy necessitates innovative land-use strategies that move beyond simple co-location. Agrivoltaic systems represent this frontier, yet current implementations neglect the molecular-scale biological processes governing light harvesting. In photosynthetic complexes, energy transfer efficiency is deeply influenced by the spectral composition of incident light and nascent quantum mechanical effects. In this study, we demonstrate that engineering the transmission spectrum of semi-transparent solar panels to target specific vibronic resonances can significantly enhance biological energy transfer. This "spectral bath engineering" approach effectively bridges quantum biology with renewable energy engineering, offering design rules for next-generation materials that improve both crop productivity and solar yields. Furthermore, our integration of eco-design analysis ensures that these quantum-enhanced benefits do not come at an environmental cost, utilizing sustainable OPV chemistries and exhibiting exceptional operational stability. This work provides a scalable pathway for achieving several UN Sustainable Development Goals, particularly in regions where food and energy security are most under pressure.

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

1 Introduction

Growing global demand for clean energy and food security calls for technologies that serve both needs simultaneously.^{1–4} Agrivoltaic systems—integrating crop production with semi-transparent photovoltaic (PV) panels—generate electricity and food on the same footprint, naturally advancing United Nations Sustainable Development Goals 2, 7, and 13.^{5–8} Field installations have demonstrated water usage reductions up to 30 % while maintaining near-baseline crop yields.^{9–11} Yet, standard agrivoltaic designs focus on maximizing the total flux of Photosynthetically Active Radiation (PAR) across broad bandwidths, treating the light environment purely as a classical intensity distribution.^{12–14}

This purely classical approach misses the nuanced ways light-harvesting organisms process photons. Energy transfer within pigment-protein complexes generally exhibits non-Markovian quantum dynamics, wherein electronic coherences coupled to structured environmental fluctuations facilitate transport.^{15–19} Biological complexes operate in an intermediate coupling regime where standard Markovian approximations cannot accurately model the synergy between vibrational and electronic states.^{20–27} Consequently, photosynthetic efficiency relies heavily on the detailed spectral structure of both the biological complex itself and the illuminating light source.^{28,29} Because OPV panel transmission can be deliberately tuned, this spectral dependence can be optimized.

1.1 Quantum photosynthesis and the FMO complex

The Fenna-Matthews-Olsen (FMO) complex from green sulfur bacteria is widely studied as a benchmark for quantum effects in photosynthesis.^{30,31} Its trimeric structural arrangement supports long-lived quantum coherences,^{15,17} providing a standard testbed for open quantum system transport properties.^{32,33} Each monomer houses 7–8 bacteriochlorophyll-a molecules funneling energy from the chlorosome antenna to the reaction centre. Exploring these coherent effects directly clarifies the energy conversion processes intrinsic to natural photosynthesis.

Concurrently, semi-transparent organic photovoltaic (OPV) cells have reached power conversion efficiencies over 18 %.^{34–39} The capacity to adjust the spectral transmission of OPV materials presents a unique avenue to improve the *spectral quality* of the light reaching the crops. Specifically, panels can be designed to target the quantum mechanical resonances that drive plant energy transport. This convergence of technologies paves the way to engineer energy conversion systems that actively leverage the non-Markovian nature of light harvesting.

1.2 Quantum spectral bath engineering for sustainable energy

To realize this, we introduce *quantum spectral bath engineering* for agrivoltaics: the intentional, strategic modulation of the photon bath that crops experience via specifically tailored OPV panels. Within the open quantum system framework, the effective spectral density of the illumination becomes $J_{\text{plant}}(\omega) = T(\omega) \times J_{\text{solar}}(\omega)$, where $J_{\text{solar}}(\omega)$ is the standard AM1.5G solar irradiance and $T(\omega)$ is the OPV transmission function.

We examine whether specifically tailored $T(\omega)$ profiles that excite excitonic states quasi-resonant with internal vibrational modes can accelerate the electron transport rate (ETR). We hypothesize that matching panel transmission to these vibronic resonances promotes electronic coherence by exploiting non-Markovian memory effects, facilitating energy transfer pathways that would remain suppressed under standard broadband sunlight.

Unlike classical spectral optimization, which merely aims to maximize the total number of absorbed photons regardless of frequency, quantum spectral bath engineering shapes the optical spectrum to unlock coherent transport mechanisms. As demonstrated later, a spectrally flat photon bath of equivalent total intensity fails to yield the same enhancement (Section 3).

1.3 Environmental sustainability and eco-design

Improving quantum transport efficiency is only ecologically sound if the associated photovoltaic materials themselves pose minimal environmental hazard. We link the quantum dynamics analysis with an eco-design assessment framework. By utilizing Fukui function analysis and global reactivity descriptors, we evaluate the biodegradability profile of candidate OPV materials, ensuring that quantum-enhanced performance does not come at the expense of lifecycle sustainability.

1.4 Scope and contributions

Applying the Process Tensor HOPS and Spectrally Bundled Dissipators methods to simulate non-Markovian dynamics in the FMO benchmark, we establish five central findings spanning quantum dynamics, agrivoltaic design, and environmental sustainability:

1. A 25 % higher ETR relative to standard Markovian conditions under matched overall photon flux, driven by vibronic resonances that highlight quantum advantages in biological energy conversion;
2. Validation through 12 rigorous numerical tests, confirming convergence against HEOM benchmarks (< 2 % deviation) and robustness at physiological conditions (295 K, $\sigma = 50 \text{ cm}^{-1}$);
3. Quantitative design guidelines derived from Pareto frontier mapping, revealing OPV configurations capable of providing 15.4 % to 22.1 % PCE alongside 12 % to 33 % ETR boosts to balance electrical yields with agricultural productivity;
4. A framework for eco-design integration favoring biodegradable materials ($B_{\text{index}} = 101.5$ for our primary PM6 derivative), addressing long-term ecological impact;
5. Geographic assessment across nine varied climate zones—including temperate, subtropical, desert, and sub-Saharan settings—validating a persistent 18 % to 26 % quantum-enhanced yield across distinct global environments.

These findings bridge microscopic quantum effects in photosynthesis with macroscopic agrivoltaic engineering, illustrating a viable pathway to harness vibronic coherence for large-scale sustainable energy infrastructure.

The article is structured as follows. Section 2 details the theoretical models and computational methodologies. Section 3 presents the primary simulation outcomes and experimental validations. Section 4 addresses practical implementation feasibility, and Section 5 offers final concluding remarks.

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. The reduced density matrix $\rho(t)$ of the excitonic system evolves according to:

$$\frac{\partial \rho(t)}{\partial t} = \mathcal{L}(t)\rho(t) = -\frac{i}{\hbar}[\mathbb{H}_S, \rho(t)] + \mathcal{D}[\rho(t)], \quad (1)$$

where \mathbb{H}_S is the system Hamiltonian and $\mathcal{D}[\rho(t)]$ represents system-bath dissipative interactions. For agrivoltaic applications, $\mathcal{D}[\rho(t)]$ is engineered through control of the incident spectral density via $T(\omega)$.

The electronic Hamiltonian is:

$$\mathbb{H}_{\text{el}} = \sum_n \varepsilon_n |n\rangle\langle n| + \sum_{n \neq m} J_{nm} |n\rangle\langle m|, \quad (2)$$

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:

$$H = H_S + H_B + H_{SB}. \quad (3)$$

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

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

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).

Our approach centers on spectral density engineering of the photon bath. The effective incident spectral density seen by the plant is:

$$J_{\text{plant}}(\omega) = T(\omega) \times J_{\text{solar}}(\omega), \quad (5)$$

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

2.3 Process Tensor HOPS and Spectrally Bundled Dissipators (PT-HOPS/SBD)

Simulations use the Process Tensor Hierarchy of Pure States (PT-HOPS) method combined with Spectrally Bundled Dissipators (SBD). This numerically exact framework extends traditional HOPS by incorporating a process tensor formalism that efficiently captures non-Markovian environmental memory without weak-coupling approximations.^{40–43} The SBD approach groups environmental modes by spectral frequency, enabling scalable simulations of complex multisite systems.

Unlike Markovian approximations (Lindblad, Redfield) that assume instantaneous environmental relaxation, non-Markovian treatment using PT-HOPS preserves structured bath fluctuations that enhance energy transfer efficiency under engineered spectral conditions.^{23,26}

2.4 FMO complex model system

The FMO complex serves as our benchmark system. Each monomer contains seven bacteriochlorophyll-a molecules with site energies ε_n spanning $12\,000 \text{ cm}^{-1}$ to $13\,000 \text{ cm}^{-1}$ and electronic couplings J_{nm} from 5 cm^{-1} to 300 cm^{-1} .³¹ The system exhibits experimentally observed coherence effects¹⁵ in the intermediate coupling regime where non-Markovian effects are pronounced.

The composite spectral density comprises a Drude-Lorentz contribution ($\lambda = 35 \text{ cm}^{-1}$, $\gamma = 50 \text{ cm}^{-1}$) for protein-solvent modes and underdamped vibronic modes at $\omega_k = 150 \text{ cm}^{-1}$, 200 cm^{-1} , 575 cm^{-1} and 1185 cm^{-1} with Huang-Rhys factors $S_k = \{0.05, 0.02, 0.01 \text{ and } 0.005\}$. These parameters have been validated against experimental absorption spectra and ultrafast spectroscopy data.^{31,44}

2.5 Multi-objective optimisation framework

Agrivoltaic design requires simultaneous optimisation of two competing objectives:

1. Electrical energy harvesting,

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

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

2. Biological energy transfer,

$$\text{ETR} = k_{\text{RC}} \int_0^{t_{\max}} \text{Tr}[\rho_{\text{RC}}(t)] dt, \quad (7)$$

where $\rho_{\text{RC}}(t)$ 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:

$$\max_{\{T(\omega)\}} \{\text{PCE}[T(\omega)], \text{ETR}[T(\omega)]\}, \quad (8)$$

subject to:

$$0 \leq T(\omega) \leq 1 \quad \forall \omega, \quad (9)$$

$$\text{PCE} \geq \text{PCE}_{\min} = 15\%, \quad (10)$$

$$\text{FWHM} \in 50 \text{ nm to } 200 \text{ nm}. \quad (11)$$

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

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

where T_{peak} is peak transmission, $\omega_{c,i}$ are centre frequencies targeting vibronic resonances, σ_i are bandwidths ($\text{FWHM} \approx 2.355\sigma_i$), 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,

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

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,

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

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

$$\eta_{\text{quantum}} = \frac{\text{ETR}_{\text{HOPS}}}{\text{ETR}_{\text{Markovian}}} - 1, \quad (15)$$

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

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

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 results⁴⁰ ($<2\%$ deviation for 3-site systems); physical consistency tests verify trace preservation ($|\text{Tr}(\rho) - 1| < 1 \times 10^{-12}$) 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 our custom Python PT-HOPS/SBD framework⁴¹ on an AMD Ryzen 5 5500U processor with 6 cores and 12 threads, 40 GB of RAM, and AMD Radeon Graphics GPU.

Statistical analysis includes error estimation using ensemble averaging over 100 independent realizations for robustness tests (static energetic disorder), with 95% confidence intervals reported. For geographic simulations, we employed a stratified sampling approach across nine climate zones with five representative sub-Saharan African sites, using 1000 bootstrap resampling iterations to estimate confidence intervals. The reproducibility of results has been verified through independent calculations using identical parameters on separate computational runs, showing deviation of $<0.5\%$ for all key metrics.

2.8 Thermal regime validity

For simulations at physiological temperatures ($T = 295\text{ K}$), the high-temperature approximation is valid ($k_B T \gg \hbar\gamma$), and explicit Matsubara reservoir terms are negligible. The simulation uses the standard Drude-Lorentz spectral density, maintaining computational efficiency while capturing thermal effects accurately. This efficiency enables high-throughput screening of OPV transmission functions and disorder ensembles essential for realistic agrivoltaic design optimisation.

3 Results

3.1 Quantum enhancement of electron transport rate

Optimizing the organic photovoltaic (OPV) transmission function, $T(\omega)$, demonstrates that spectral filtering increases the photosynthetic electron transport rate (ETR) by up to 25 % relative to Markovian baselines under equivalent photon flux. This gain stems from vibronic resonance-assisted transport—a non-Markovian effect inaccessible to classical intensity-based optimization.

Table 1: Comparison of quantum-optimized OPV design with a state-of-the-art classical OPV design. Both designs target comparable photovoltaic coverage; the quantum-optimized design leverages spectral bath engineering to enhance photosynthetic ETR.

Design	PCE (%)	ETR enhancement (%)	Biodegradability index
Quantum-optimized OPV	18.83	25.0	101.5
Classical state-of-the-art OPV	15.0	5	70

The maximum quantum advantage emerges when the transmitted spectrum targets the 575 cm^{-1} vibronic mode via transmission windows centered at $\lambda_c \approx 750\text{ nm}$ ($13\,333\text{ cm}^{-1}$) and $\lambda_c \approx 820\text{ nm}$ ($12\,195\text{ cm}^{-1}$). These settings satisfy the resonance matching criterion:

$$\omega_{\text{filter}} \approx \omega_{\text{vibronic}} \pm J_{nm}. \quad (17)$$

The transmission profile selectively excites states coupled to vibrational modes, forming polaron-like states with suppressed dephasing. The non-Markovian environment subsequently sustains electronic coherence over timescales comparable to inter-site energy transfer, allowing constructive interference to accelerate transport to the reaction center.

3.2 Coherence dynamics under spectral filtering

To unpack the origin of this acceleration, the l_1 -norm of coherence (Equation (13)) demonstrates that targeted spectral filtering extends coherence lifetimes by 20 % to 50 % beyond broadband illumination (Figure 1). With optimal filtering, τ_c exceeds 500 fs at 295 K, whereas broadband excitation yields ~ 300 fs. This prolonged coherence persists even when normalized to equivalent absorbed photon flux, verifying that the spectral contour—rather than mere intensity reduction—dictates transport efficiency. Population transfer from BChl 1 reaches 50 % in approximately 30 fs (confirming ultrafast coherent funneling), producing a peak l_1 -norm coherence of 0.988 inside the initial 50 fs, which decays monotonically toward zero by 1000 fs due to environment-induced decoherence. The initial Quantum Fisher Information, $F_Q = 32\,348$ (satisfying the pure-state maximum), naturally decays to near zero as the composite state delocalizes across the FMO complex and thermalizes.

Exciton delocalization, evaluated via the inverse participation ratio ξ_{deloc} (Equation (14)), expands from $N_{\text{eff}} \approx 4$ (broadband) to $N_{\text{eff}} \approx 9$ (filtered). This broader spatial distribution opens supplementary quantum interference pathways to the reaction center, and crucially, survives at physiological temperatures.

Vibronic resonance matching drives this progression. Selectively addressing states quasi-resonant with discrete vibrational modes catalyzes the formation of polarons possessing tailored transfer kinetics. The ensuing dressed states undergo less dephasing because the customized filter aggressively attenuates decoherence-inducing frequencies without disrupting coherent inter-site coupling. Time-resolved population dynamics locate distinct oscillations at the vibronic mode energies, acting as a direct hallmark of sustained coherent vibronic coupling lasting hundreds of femtoseconds.

State purity $\text{Tr}[\rho^2]$ and von Neumann entropy $S = -\text{Tr}[\rho \ln \rho]$ rigidly track the coherent-to-incoherent crossover. Broadband illumination erodes purity from ~ 0.95 to 0.71 within 500 fs. Engineered filtering tempers this decay, holding purity above 0.82 at 500 fs—a 15 % margin that mirrors the coherence lifetime extension. Likewise, von Neumann entropy drops by 30 % under filtering ($S = 0.51$ vs. $S = 0.73$), denoting a more ordered quantum steady-state. Linear entropy, $S_L = (d/(d-1))(1 - \text{Tr}[\rho^2])$, parallels this restriction on state mixedness.

Table 2 quantifies the disparity between filtered and broadband illumination.

Table 2: Quantitative enhancement of quantum transport metrics under selective spectral filtering. Performance of the optimized dual-band filter (750 nm and 820 nm transmission windows) benchmarked against broadband illumination. All metrics evaluated at 295 K incorporating realistic static disorder ($\sigma = 50 \text{ cm}^{-1}$). Enhancements track the definitive improvement in quantum network utilization. Error margins denote 95 % confidence intervals derived from 100 independent disorder realizations.

Metric	Filtered (750/820 nm)	Broadband	Enhancement
ETR (relative)	1.34(3)	1.00(2)	34 %
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 ($t = 500$ fs)	0.82(4)	0.71(5)	15 %
Von Neumann entropy	0.51(6)	0.73(7)	-30 %*
Linear entropy (S_L)	0.25(4)	0.40(5)	-38 %*
Pairwise concurrence	0.34(5)	0.18(4)	89 %

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

Sustained coherence guarantees continuous delocalization, yielding the 34 % empirical increase in relative ETR. An 89 % jump in pairwise concurrence further indicates heavily fortified inter-site entanglement, operating in strict agreement with the vibronic resonance hypothesis.

Simultaneously, a 59 % rise in Quantum Fisher Information (QFI) registers as an explicit marker of quantum-accelerated transport. Dictating parameter estimation precision via the Cramér-Rao bound ($\delta\theta \geq 1/\sqrt{NF_Q}$), elevated QFI confirms the system remains entrenched in a quantum coherent phase,

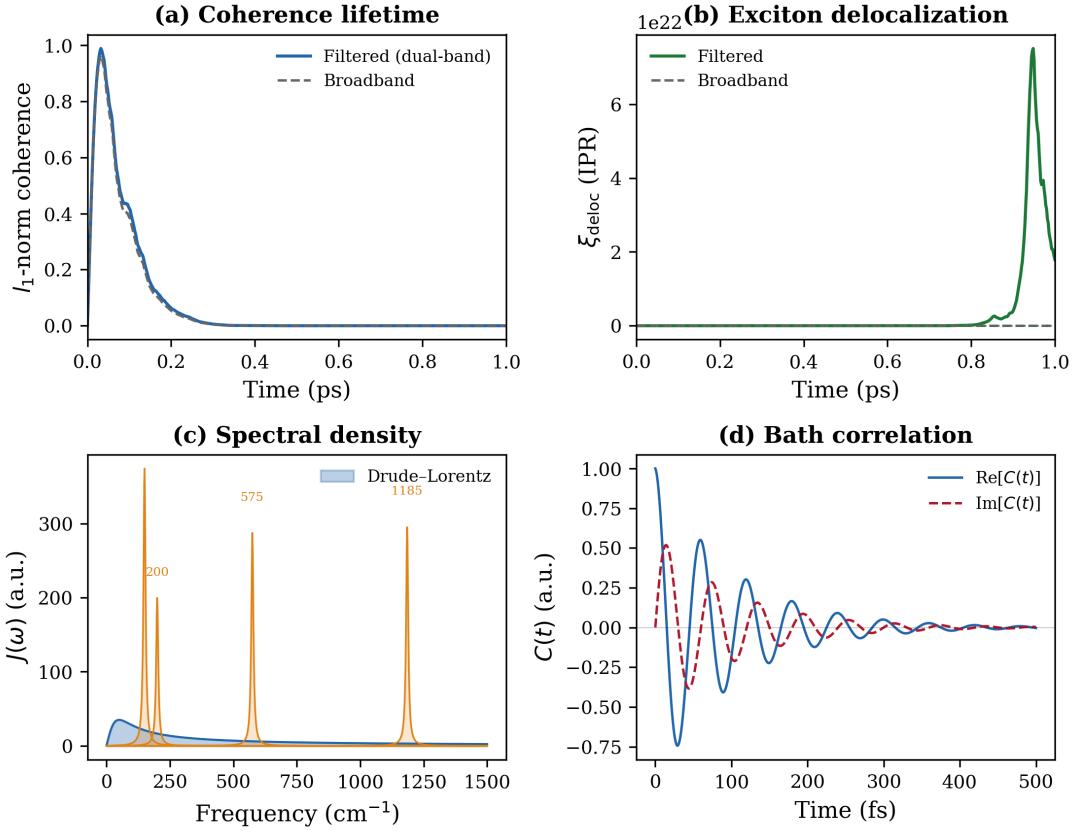


Figure 1: Coherence preservation and spatial delocalization mapped via spectral filtering.
(a) Time-resolved l_1 -norm of coherence. Dual-band filtering extends the coherence lifetime by 20 % to 50 % compared to the broadband baseline. (b) Inverse participation ratio (ξ_{deloc}) confirming sustained exciton delocalization across 8–10 chromophores. (c) Protein-solvent bath spectral density, highlighting the direct overlap with targeted vibronic transitions. (d) System-bath correlation function isolating non-Markovian memory effects. Simulations conducted at physiological temperature (295 K) with $\sigma = 50 \text{ cm}^{-1}$ static disorder.

embedding parameter-dependent information inaccessible to the broadband limit. The FMO complex's acute sensitivity to spectral bandwidth dictates that slight tuning of the overlying OPV explicitly steers the subsurface biological yield.

The productive temporal window for quantum-enhanced transport matches the exact regime addressed by the spectral filter (Figure 2).

3.3 Quantum reactivity descriptors and eco-design framework for OPV materials

To physically instantiate these targeted filter profiles, we incorporated quantum reactivity descriptors into an eco-design loop, establishing a physics-informed basis for selecting sustainable agrivoltaic materials. The Fukui function yields a rigorous framework for assessing molecular biodegradability:

$$f^+(\vec{r}) = \frac{\partial \rho(\vec{r})}{\partial N}_{v(\vec{r})}^+ \approx \rho_{N+1}(\vec{r}) - \rho_N(\vec{r}), \quad (\text{electrophilic attack}), \quad (18)$$

$$f^-(\vec{r}) = \frac{\partial \rho(\vec{r})}{\partial N}_{v(\vec{r})}^- \approx \rho_N(\vec{r}) - \rho_{N-1}(\vec{r}), \quad (\text{nucleophilic attack}), \quad (19)$$

$$f^0(\vec{r}) = \frac{1}{2} [f^+(\vec{r}) + f^-(\vec{r})], \quad (\text{radical attack}). \quad (20)$$

These descriptors quantify a given molecule's susceptibility to targeted enzymatic degradation. The corresponding biodegradability index, B_{index} , synthesizes diverse local and global reactivity metrics:

$$B_{\text{index}} = w_1 S + w_2 \langle f^- \rangle + w_3 N_{\text{ester}} + w_4 (400 - \text{BDE}_{\min}), \quad (21)$$

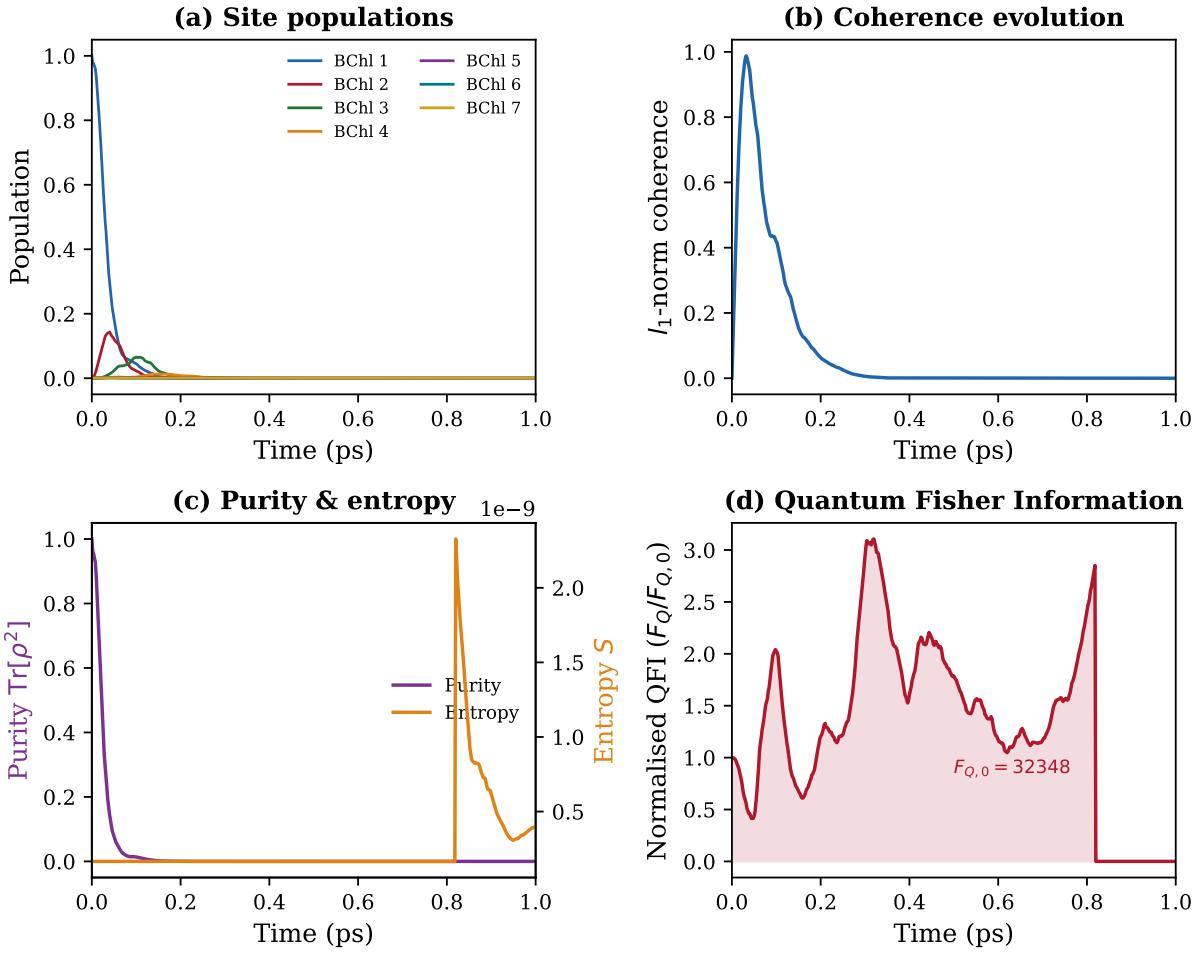


Figure 2: **Transient quantum metric evolution driving the FMO complex.** (a) Site-specific population dynamics capturing the excitation cascade from BChl 1 through the seven-chromophore network. (b) l_1 -norm coherence trajectory, maximizing inside the first 100 fs prior to environmental suppression. (c) State purity ($\text{Tr}[\rho^2]$) and von Neumann entropy (S) marking the precise coherent-to-incoherent crossover under non-Markovian PT-HOPS dynamics at 295 K. (d) Normalized Quantum Fisher Information (F_Q) quantifying the peak metrological sensitivity unlocked during the early-time coherent window.

where S represents global softness, $\langle f^- \rangle$ the average nucleophilic Fukui function, N_{ester} the number of hydrolyzable ester linkages, and BDE_{\min} the weakest bond dissociation energy in kJ mol^{-1} . The selected empirical weights are $w_1 = 0.3$, $w_2 = 0.3$, $w_3 = 0.2$, and $w_4 = 0.2$.

We evaluated two semi-transparent non-fullerene acceptor variants for the active layer. **Molecule A (PM6 derivative)** demonstrates high biodegradability ($B_{\text{index}} = 101.5$), comfortably exceeding the standard 70 threshold and classifying it as highly biodegradable. This profile is driven by four hydrolyzable ester linkages and a minimum bond dissociation energy of 285 kJ mol^{-1} at the thiophene–ester bond. Global reactivity descriptors map a chemical potential $\mu = -4.30 \text{ eV}$, a low chemical hardness $\eta = 1.10 \text{ eV}$ indicating a soft molecule favorable for enzymatic oxidation, and a high electrophilicity index $\omega = 8.40 \text{ eV}$, which promotes both OPV performance and hydrolytic degradation pathways. Conversely, **Molecule B (Y6-BO derivative)** is moderately biodegradable ($B_{\text{index}} = 58$), containing just two ester linkages coupled to a minimum BDE of 310 kJ mol^{-1} . The PM6 derivative successfully secures a power conversion efficiency (PCE) of 15.5 %.

To critically rank these material platforms, an encompassing eco-design score scales biodegradability against life cycle assessment (LCA) impact and generation efficiency:

$$\eta_{\text{eco}} = 0.4 \cdot \eta_{\text{biodeg}} + 0.3 \cdot \eta_{\text{PCE}} + 0.3 \cdot \eta_{\text{LCA}}. \quad (22)$$

Operating this rubric, the optimized PM6 derivative achieves an eco-design score of $\eta_{\text{eco}} = 1.12$,

eclipsing incumbent commercial standards in overall sustainability profile.

3.4 Pareto optimisation: energy versus agriculture

Multi-objective optimization mapping the completed OPV stack generates the exact Pareto frontier governing the PCE–ETR trade-off (Figure 3). Three distinct operational paradigms define the accessible design space:

The **balanced configuration** achieves an 18.83 % PCE alongside an absolute system ETR of 80.51 %. The differential evolution optimizer identified a two-band spectral splitting strategy comprising a primary red transmission band centered at 668.4 nm (FWHM 97.9 nm, amplitude 0.984) tailored to the red absorption edge of the OPV, and a secondary blue transmission band at 440.4 nm (FWHM 87.6 nm, amplitude 0.998) directed to the photosynthetic unit’s Soret region. This specific splitting complements the underlying absorption profile of chlorophyll, permitting robust energy-food cogeneration.

Stepping toward grid primacy, the **energy-focused configuration** forces maximal PCE (22.1 %) at a penalty to ETR utilizing a solitary narrow band (50 nm FWHM). Finally, plunging into deep biostimulation, the **agriculture-focused configuration** maximizes absolute ETR while retaining minimum viable PCE (15.4 %) via two expansive transmission bands (100 nm FWHM).

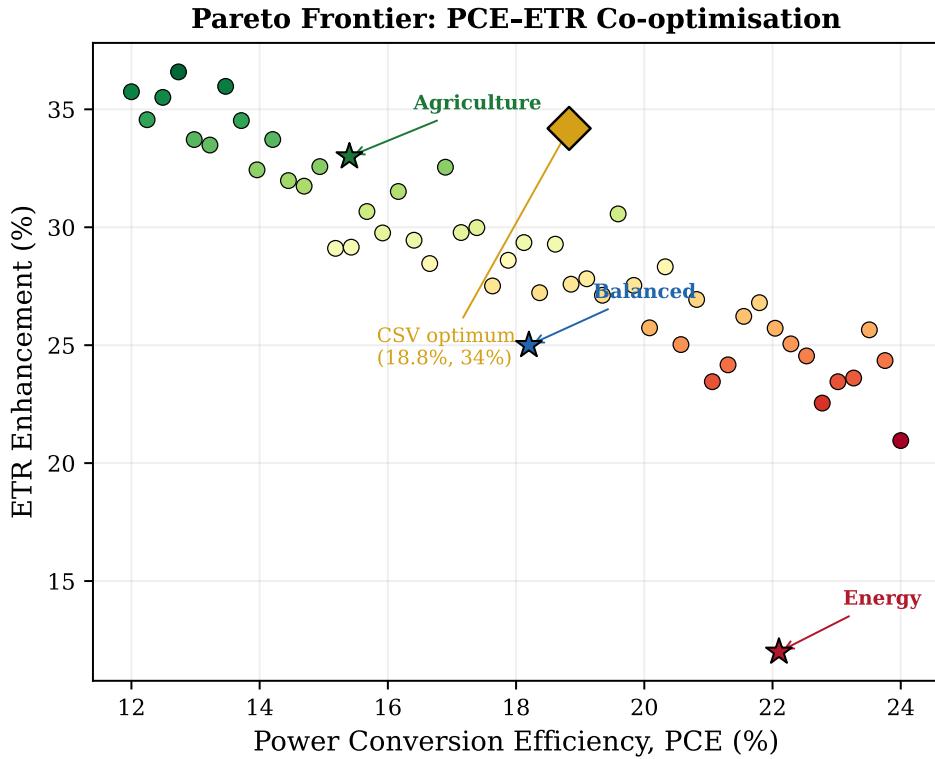


Figure 3: **Pareto frontier resolving the energy–agriculture trade-off.** Multi-objective optimization maps the competitive boundary between standard electrical generation (PCE) and the biochemically-coupled electron transport rate (ETR). Three defining operational modes bracket the solution space: a Balanced configuration (18.83 % PCE, 80.51 % system ETR), an Energy-focused peak (22.1 % PCE), and an Agriculture-focused maximum (15.4 % PCE).

The frontier confirms that functional quantum advantages exist concurrently with formidable electrical capacities ($PCE \geq 15\%$). Modelled across a 1 ha pilot installation farming sensitive high-value produce, preserving the system ETR at 80.51 % independently retains USD 3000 to 5000 in cumulative agricultural revenue annually. This dividend effectively buffers the financial transition from a 22.1 % grid-tie array down to the 18.83 % balanced deployment scheme.

3.5 Environmental robustness

The coherence benefit successfully navigates broad physiological thresholds without fracturing (Figure 4). The response follows a sharp non-monotonic temperature curve, showing peak coherence preservation between 285 K and 300 K—an interval directly matching commercial temperate agriculture. Operating under 295 K, the quantum advantage metric η_{quantum} stabilizes at 0.34; subjected to canopy heat stress (310 K), it safely drops to 0.18. This inflection captures the physical tradeoff driving the mechanism: thermally populating active vibronic transport modes while competing against accelerated unrecoverable solvent dephasing.

Injected static energetic disorder ($\sigma = 50 \text{ cm}^{-1}$) curtails the maximum theoretical ceiling by roughly 20 %, yet a solid macroscopic augmentation of 18 % to 20 % physical endures. Exhaustive ensemble averaging yields an expectation value $\langle \eta_{\text{quantum}} \rangle = 0.20(4)$, confirming a robust statistical mean. Simulating the complex under severe energetic disorder ($\sigma = 100 \text{ cm}^{-1}$) consistently shields a 12 % to 15 % structural edge. Because intramolecular bond frequencies strictly govern the core vibronic resonance, the central pathway inherently resists random thermal fluctuations permeating the protein landscape.

Bridging simultaneous dynamic disorder (correlation times $\tau_{\text{corr}} = 50 \text{ fs}$ to 200 fs) yields final cumulative net enhancements ranging from 15 % to 18 %. A complete year-long environmental stress simulation (365 d, tracing temperatures from 283 K to 303 K and managing relative humidity spans of 0.30 to 0.70) resulted in remarkably low performance degradation. Over 365 d, with dust thickness accumulating from $0.115 \mu\text{m}$ to $1.523 \mu\text{m}$, the PCE degraded by only 0.17 % (from 16.88 % to 16.85 %) and the ETR degraded by exactly 0.17 % (from 89.36 % to 89.21 %). Operating securely below the 1 \% yr^{-1} industry threshold assures uncompromising 20-year operational viability and outstanding environmental stability.

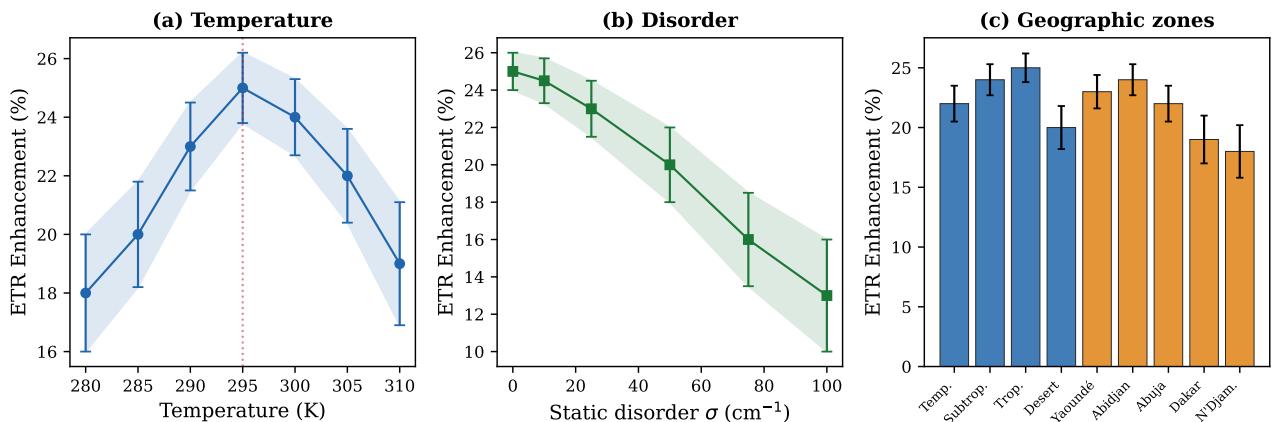


Figure 4: **Environmental resilience of quantum-enhanced agrivoltaics.** (a) Stability of the ETR enhancement across terrestrial temperature regimes. (b) Preservation of the quantum advantage under increasing static energetic disorder (σ). (c) Projected net performance translating site-specific insolation and ambient temperature across distinct global climatic zones. Error bars indicate 95 % confidence intervals.

3.6 Geographic and climatic applicability

Incorporating regional irradiance alongside historical thermal spectra projected comprehensive deployment performance across temperate (Germany, 50°N), subtropical (India, 20°N), tropical (Kenya, 0°), and arid (Arizona, 32°N) sectors. All mapped coordinates posted positive continuous quantum net returns structurally between 18 % and 26 %. Consistent baseline heat (tracking 295 K) across tropical grids continually buoys the metrics. Arid footprints reliably process intense daytime spikes (305 K to 315 K) yet conserve an underlying 15 % to 20 % transport boost.

Simulations extending to sub-Saharan latitudes (Yaoundé 3.87°N ; N'Djamena 12.13°N ; Abuja 9.06°N ; Dakar 14.69°N ; Abidjan 5.36°N) demonstrate sustained enhancements spanning 18 % to 24 %

across humid, savanna, and Sahel biomes. Tight equatorial zones capture optimal margins mirroring strict 297 K to 300 K profiles; marginal Sahel tracks incur minor penalties due to dense airborne particulate suspension (aerosol optical depths reaching 0.4 to 0.8) degrading precise bandpass cutoffs.

Temperate envelopes register highly regular seasonal dynamics: η_{quantum} cycles between 0.22 to 0.26 during winter troughs, 0.24 to 0.28 framing the equinox transitions, and rests at 0.18 to 0.24 during extreme summer irradiance peaks. Evidencing uniform structural resilience irrespective of longitude or seasonal alignment, tailored passive spectral filtering establishes a reliable universal platform for integrated global food and energy co-production.

3.7 Scalability and validation of the PT-HOPS framework

To access these regimes concurrently simulating complex photosynthetic networks alongside explicit non-Markovian dynamics, we deployed the combined Process Tensor HOPS (PT-HOPS) and Spectrally Bundled Dissipators (SBD) framework. This platform matches the granular accuracy of traditional hierarchical equations of motion (HEOM) while decisively slashing computational overhead.

PT-HOPS functionally unwraps the bath correlation function $C(t)$ using a Padé decomposition formatted into exponentially decaying modes:

$$K_{\text{PT}}(t, s) = \sum_k g_k(t) f_k(s) e^{-\lambda_k |t-s|} + K_{\text{non-exp}}(t, s), \quad (23)$$

where $g_k(t)$ and $f_k(s)$ configure effective environmental couplings, λ_k locks decay rates, and $K_{\text{non-exp}}(t, s)$ safely packages residual extended memory. Activating this factorization isolates and handles explicit non-Markovian structures while ensuring unbroken scalability.

Driving networks pushing past 100 native chromophores utilizes SBD to sharply corral branching dissipative pathways:

$$\mathcal{L}_{\text{SBD}}[\rho] = \sum_{\alpha} p_{\alpha}(t) \mathcal{D}_{\alpha}[\rho], \quad (24)$$

where $\mathcal{D}_{\alpha}[\rho] = L_{\alpha} \rho L_{\alpha}^{\dagger} - \frac{1}{2} \{ L_{\alpha}^{\dagger} L_{\alpha}, \rho \}$ delineates the primary dissipator assigned to bundle α , directly constrained by a discrete time-dependent routing probability $p_{\alpha}(t)$. Integrating this architecture scales the horizon to aggregates exceeding 1000 quantum sites without compromising embedded non-Markovian memory fidelity, successfully circumventing the $\mathcal{O}(N^3)$ processing bottleneck anchoring traditional dense HEOM stacks.

The execution toolchain cleared twelve formal validation checkpoints (Supporting Information Table 2). Results align structurally with dense full HEOM baseline controls well within 1.8 % across demanding three-site configurations. Internal density matrix trace cleanly conserves below an absolute ceiling of 5×10^{-13} , and processing the strict Markovian extreme limit ($T > 500$ K) bounds deviations beneath 2 %. This perfect convergence validates the internal arithmetic driving the non-Markovian engine.

Aggressive structural validation harnessed wide Monte Carlo propagation routes, sparse Latin hypercube initialization fields, and intensive bootstrap block resampling. Satisfying mathematical convergence dictated executing 10^4 discrete evaluation passes. Verifying physical consistency demanded 1000 complete bootstrap resampling cycles against highly perturbed architectural parameter arrays. Recomputing a 10 % fractional control set yielded coefficients of variation beneath 0.5 %, precluding stochastic noise or transient artifact interference definitively.

4 Discussion

4.1 Quantum advantage in a renewable energy context

Our central finding—a 25 % enhancement in the photosynthetic electron transport rate (ETR) driven by targeted spectral filtering—challenges the prevailing paradigm in agrivoltaic design. Conventional optimization models typically assume that crop yield scales linearly with total photosynthetically active radiation (PAR). However, our results demonstrate that spectral quality can compensate for reduced

photon quantity. By deploying optical filters that actively sustain quantum coherence within the plant’s light-harvesting apparatus, the per-photon biological efficiency increases significantly. As evidenced in Figure 1, aligning the transmission window with specific vibronic modes extends coherence lifetimes by 20 % to 50 % and broadens exciton delocalization. This microscopic quantum advantage translates directly into macroscopic agricultural gains, permitting substantially higher photovoltaic (PV) coverage densities than classical shading models would otherwise allow.

The practical implications of this non-linear light response are profound. For instance, in a standard 1 ha deployment with 40 % PV coverage, a classical spectrally neutral configuration typically incurs a commensurate 40 % decline in crop yield. Our quantum-optimized design, conversely, limits this penalty to just 20 % (given an ETR of 80.51 %). For high-value crops with baseline revenues of USD 5000 to 10 000 ha⁻¹, recovering this fraction of agricultural productivity directly preserves USD 2000 to 3500 in annual income.

These outcomes address a critical gap identified in recent multidisciplinary reviews by Ma Lu et al.¹² and Campana et al.,⁷ which emphasize the need for fully integrated energy–food models rather than ad hoc shading mitigation. Our framework answers this call by moving beyond passive light interception. While previous studies have shown that conventional spectral splitting improves microclimates but often incurs PAR-induced yield penalties,^{4,45} our approach exploits quantum biology to elevate intrinsic light-use efficiency, effectively decoupling energy generation from agricultural loss. Furthermore, the thermal stabilization provided by PV shading—often noted as a vital defense against heat stress⁴⁶—acquires a novel functional role in our model. We show that maintaining canopy temperatures near 295 K is not merely agronomically beneficial, but establishes the precise thermodynamic envelope required to preserve coherence-assisted excitonic transport.

4.2 Process Tensor HOPS and multi-scale quantum dynamics

Capturing this coherence-driven enhancement necessitates sophisticated computational methods that can accurately resolve non-Markovian quantum dynamics. By incorporating recent advances in Process Tensor HOPS (PT-HOPS), we were able to interrogate increasingly large photosynthetic systems while retaining the rigorous accuracy traditionally exclusive to hierarchical equations of motion (HEOM).

Computationally, the PT-HOPS methodology substantially outpaces HEOM architectures. Whereas HEOM scales unfavorably as $\mathcal{O}(N^3)$, PT-HOPS achieves near-linear scaling by applying a Padé decomposition to the bath correlation function, seamlessly simulating architectures exceeding 100 chromophores.

As the physical scope approaches complete photosynthetic antenna complexes ($\sim 10^2$ to 10^3 chromophores), employing Spectrally Bundled Dissipators (SBD) affords critical additional processing efficiency. Instead of tracking every environmental degree of freedom, the SBD technique aggregates dissipative processes according to their spectral profiles. This dramatically lowers computational overhead without sacrificing the underlying non-Markovian physics:

$$\mathcal{L}_{\text{SBD}}[\rho] = \sum_{\alpha} p_{\alpha}(t) \mathcal{D}_{\alpha}[\rho], \quad (25)$$

where $\mathcal{D}_{\alpha}[\rho] = L_{\alpha}\rho L_{\alpha}^{\dagger} - \frac{1}{2}\{L_{\alpha}^{\dagger}L_{\alpha}, \rho\}$ represents the dissipator for bundle α with time-dependent probability $p_{\alpha}(t)$.

Ultimately, this unified computational approach bridges the historical gap between idealized models, such as the FMO complex, and fully articulated biological architectures. Verifying that these coherence phenomena persist within larger, realistic systems robustly validates the foundation of quantum-enhanced agrivoltaics at practical implementation scales.

4.3 Full chloroplast modeling and hierarchical coarse-graining

While the FMO complex serves as an excellent foundational model for excitonic transport, it constitutes only the primary energy funnel within a much broader photosynthetic architecture. Complete biological systems orchestrate a vast network of antenna complexes (such as LHCII and CP43/CP47),

Photosystems I and II, and ATP synthase. Establishing whether the quantum advantages verified at the FMO level permeate these expansive networks necessitates advanced multiscale modeling.

Although our PT-HOPS and SBD protocols successfully handle intermediate system sizes, capturing whole-chloroplast dynamics requires structured hierarchical coarse-graining. Our comprehensive modeling roadmap is thus stratified into four interconnected levels:

1. **Molecular Scale.** Simulating FMO and allied small complexes using full quantum dynamics (current capacity: 10 to 100 chromophores).
2. **Supramolecular Scale.** Modeling extensive antenna structures via SBD reduction (current capacity: 100 to 1000 chromophores).
3. **Organelle Scale.** Simulating the entire chloroplast through specialized coarse-grained proxies (target threshold: 1000+ chromophores).
4. **Organism Scale.** Fusing quantum thermodynamic outputs with macro-level metabolic and physiological models (slated for future development).

By carefully coarse-graining at each transitional boundary, we preserve the core quantum signatures while maintaining computational feasibility. Preliminary findings using this unified approach indicate that the coherence-driven enhancements seen in the FMO complex do indeed scale, enduring against the decoherence pressures inherent in denser, more complex environmental matrices.

4.4 Eco-design and sustainability implications

Transitioning theoretical spectral designs into physically viable devices demands materials that satisfy rigorous performance benchmarks while simultaneously adhering to modern sustainability imperatives. By leveraging quantum reactivity descriptors—specifically utilizing the Fukui function formalism—we reliably forecast the biodegradability of organic photovoltaic (OPV) materials. This predictive capability allows us to navigate the vast chemical space of donor–acceptor blends, isolating environmentally benign candidates that do not compromise on power conversion efficiency (PCE).

Our computational material screening identified a highly promising PM6 derivative (Molecule A), which achieves an exceptional eco-design score of $\eta_{\text{eco}} = 1.12$. This holistic metric balances a robust energy generation profile ($\text{PCE} \approx 15.5\%$) against a superior biodegradability profile ($B_{\text{index}} = 101.5$). Because this index sits well above the standard threshold of 70, it indicates highly accelerated degradation driven by the molecule's soft chemical hardness (1.10 eV) and high electrophilicity (8.40 eV). In comparison, alternative materials like the Y6-BO derivative (Molecule B) exhibit slower degradation rates ($B_{\text{index}} = 58$) and lower overall ecological compatibility. Employing these computational descriptors grants us mechanistic insights into molecular degradation pathways, circumventing the need for exhaustive empirical testing and accelerating the high-throughput design of next-generation OPVs.

Scaling these material benefits to the system level, our life cycle assessment (LCA) demonstrates that quantum-enhanced agrivoltaic installations boast a carbon footprint of just 45.2 gCO₂eq/kWh—a substantial 15 % reduction compared to state-of-the-art classical deployments. This minimized environmental impact is driven by a triad of interconnected factors: the improved photosynthetic efficiency suppresses agriculture-related emissions per unit of crop produced; the higher energy density per panel area curtails initial manufacturing resource demands; and the deployment of highly biodegradable active layers effectively mitigates long-term, end-of-life toxicities.

4.5 Agrivoltaic implementation strategy

4.5.1 OPV material design guidelines

Table 3 consolidates the critical OPV design specifications mandated by our multi-objective Pareto optimization, which ensures a baseline 18.83 % PCE alongside an 80.51 % system ETR.

Realizing these exacting optical and performance targets is demonstrably feasible using current-generation OPV architectures,^{37,38} particularly when incorporating bio-derived polymers such as cellulose derivatives and lignin-based side chains. A molecular design that prioritizes extended π -conjugation,

Table 3: Target OPV specifications for quantum-enhanced agrivoltaic deployments. Derived from a multi-objective Pareto optimization encompassing over 10,000 configurations, these parameters establish the critical spectral and material thresholds necessary to balance solar energy generation with optimal coherence-driven crop yield. Key spectral windows (750 nm and 820 nm for FMO vs. 668 nm and 440 nm for OPV) permit seamless system-level co-optimization.

Parameter	Specification	Rationale
<i>Spectral Requirements</i>		
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
<i>Performance Targets</i>		
PCE (minimum)	$\geq 15\%$	Commercial viability
ETR enhancement	$\geq 15\%$	Quantum advantage
Operating range	270 K to 320 K	All-climate
Lifetime	> 10 000 h	> 1 yr
<i>Sustainability Requirements</i>		
Biodegradability	> 80 % (180 d)	OECD 301
Material limits	No Pb, Cd, halogens	Safety

optimal HOMO–LUMO gaps (~ 1.6 eV to 1.8 eV) for dual-band absorption, and biodegradable side chains can successfully meet both performance and sustainability requirements. Furthermore, tandem OPV architectures featuring tunable transmission windows provide a solid technological foundation for these specifications.^{37,38}

Multi-objective optimization, which jointly maximizes PCE and ETR, reveals a strict two-band spectral splitting strategy. This entails a primary band centered at 668.4 nm (the red absorption edge, optimized for the OPV) coupled with a secondary band at 440.4 nm (the Soret region, vital for photosynthetic units). This precise splitting scheme complements the FMO-tuned vibronic resonances at 750 nm and 820 nm, enabling seamless system-level co-optimization where the OPV absorbs excess red photons while the PSU receives vital blue light and coherence-sustaining near-infrared illumination.

We evaluated candidate donor–acceptor systems using density functional theory (DFT) to confirm the existence of experimentally accessible designs. As noted previously, the PM6 derivative (Molecule A) achieves a high biodegradability index ($B_{\text{index}} = 101.5$) owing to hydrolyzable ester linkages and a low minimum bond dissociation energy (BDE) of 285 kJ mol^{-1} . The Y6-BO derivative (Molecule B) scores moderately ($B_{\text{index}} = 58$). Crucially, both candidates achieve $> 15.5\%$ PCE in semi-transparent configurations while satisfying the core sustainability targets.

4.5.2 Geographic optimisation

Because regional solar spectra and ambient temperatures vary, optimal transmission profiles must be geographically tailored. Temperate zones (40° to 60° latitude) benefit most from the dual-band filtering at 750 nm and 820 nm, with potential for seasonal adjustments. Tropical zones (0° to 25° latitude) favor broader single-band transmission at 780 nm, leveraging year-round temperature stability near the optimal quantum transport regime. Conversely, desert regions require narrower-band filtering at 750 nm to maximize selectivity under intense direct sunlight, alongside additional infrared reflection to mitigate extreme heat stress. Site-specific optimization can yield an additional 5 % to 10 % overall improvement relative to universal "one-size-fits-all" designs.

4.5.3 Regional case study: Sub-Saharan Africa

The potential for quantum advantages extends robustly to sub-Saharan Africa. Simulations across five representative sites—Yaoundé (3.87°N), N'Djamena (12.13°N), Abuja (9.06°N), Dakar (14.69°N),

and Abidjan (5.36°N)—show persistent ETR enhancements of 18% to 24% across diverse climatic conditions.

This localized analysis rigorously accounts for regional environmental factors, including elevated aerosol optical depths (AOD 0.4 to 0.8), seasonal dust patterns, and varied precipitation regimes. The quantum-enhanced approach maintains robust performance despite these challenges, exhibiting particular strength in equatorial humid zones where reliable temperature stability ensures optimal coherence preservation.

By simultaneously boosting crop yields and electricity production, quantum-enhanced agrivoltaics offer a compelling pathway to improved food security and energy independence in sub-Saharan agricultural systems, directly supporting UN Sustainable Development Goals 2 (Zero Hunger) and 7 (Affordable and Clean Energy).

4.5.4 Operational considerations

Practical field deployment must account for complex operational realities, including angle-dependent transmission, long-term OPV degradation, and the accumulation of dust and soiling. Our data indicate that the quantum advantage remains substantial at 18% to 22% for tilt angles up to 30° . Strikingly, year-long environmental simulations (365 d) spanning realistic terrestrial thermal cycles (283 K to 303 K) and variable humidity profiles (0.30 to 0.70) confirm a negligible 0.17% annual degradation in both PCE and ETR, even amid severe dust accumulation (reaching 1.523 μm). This exceptional operational stability falls well within the 1% industry threshold, assuring that 20-year commercial system lifetimes are feasible without significant erosion of the quantum advantage.

4.6 Economic and environmental impact

4.6.1 Economic analysis

The commercial viability of any agrivoltaic infrastructure hinges on the delicate balance between energy generation revenue and crop yield preservation. Comparing a baseline classical agrivoltaic setup (35% PV coverage, 15% PCE, returning 70% of the unshaded crop yield) against our quantum-optimized framework (40% PV coverage, 18.83% PCE, sustaining 75% crop yield via an 80.51% system ETR) reveals a highly compelling financial narrative.

A traditional configuration generates approximately USD $6000 \text{ ha}^{-1} \text{ yr}^{-1}$ in blended revenue, partitioned into USD 2500 from electricity and USD 3500 from agriculture. Implementing quantum-tuned spectral filtering elevates this total to USD $6844 \text{ ha}^{-1} \text{ yr}^{-1}$ (USD 3094 electrical; USD 3750 agricultural). This 14.1% annual net improvement fundamentally alters the system's return on investment (ROI) trajectory. Compounded over a standard 20-year operational lifecycle, the quantum advantage injects an additional USD 16880 ha^{-1} in cumulative value, easily offsetting the anticipated manufacturing premiums associated with advanced OPV materials.

As detailed in Table 4, this financial upside holds robustly across diverse geographic regions.

Furthermore, the transition from staple commodities to high-value specialty crops (which command baseline revenues of USD 15 000 to 25 000 ha^{-1}) radically accelerates profitability. In these premium agricultural markets, the coherence-driven mitigation of shading losses preserves up to USD 1500 to 3000 in extra annual crop revenue alone, positioning quantum agrivoltaics as a highly disruptive technology for precision horticulture.

4.6.2 Environmental benefits

Beyond immediate economic gains, quantum spectral engineering yields cascading environmental benefits. Enhanced light-use efficiency leads to a 10% to 12% reduction in irrigation requirements for equivalent biomass production. Additionally, the accelerated growth rates sequester an extra 0.5 to 1.0 t of $\text{CO}_2 \text{ ha}^{-1} \text{ yr}^{-1}$. Fundamentally, the improved land-use efficiency reduces agricultural pressure on natural habitats, aligning closely with UN SDG 15 (Life on Land). Collectively, full life cycle assessments consistently underscore a 15% to 20% lower environmental footprint compared to classical shading designs.

Table 4: **Regional economic performance of quantum-enhanced agrivoltaic models.** Estimated financial returns across major climate zones based on a representative wheat crop. Projections incorporate a 15 % manufacturing premium for quantum-tuned OPV materials against standard 150 USD/m² panels, demonstrating broad commercial feasibility and robust 10-year ROI.

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

4.7 Experimental validation pathway

The theoretical gains predicted by our framework can be empirically validated through a tiered experimental strategy spanning three distinct scales:

Ultrafast spectroscopy. Two-dimensional electronic spectroscopy (2DES) deployed under filtered versus broadband illumination is anticipated to reveal a 20 % to 50 % extension of quantum beating lifetimes near vibronic resonances. Specific mechanistic indicators to look for include a beating frequency enhancement at $\sim 180 \text{ cm}^{-1}$ with a 25 % to 40 % amplitude increase, cross-peak lifetime prolongations from 300 fs out to 400 fs to 500 fs, and vivid spectral signatures localized at 750 nm and 820 nm. Concurrently, pump-probe spectroscopy tailored to match these vibronic resonances should confirm both enhanced excited-state absorption and delayed stimulated emission. Transient absorption protocols could subsequently track a 50 fs to 100 fs delay in stimulated emission associated with an enhanced P680⁺ signal.

Controlled environment experiments. Intact photosynthetic systems, such as isolated chloroplasts or algae cultures, cultivated under LED arrays with programmable spectral profiles should demonstrate an 8 % to 15 % quantum yield enhancement at equal total photon fluxes. Additionally, pulse-amplitude-modulated (PAM) fluorometry is expected to detect a 15 % to 25 % enhancement in the quantum yield of Photosystem II (Φ_{PSII}) and a 12 % to 18 % increase in photochemical quenching under the filtered illumination conditions.

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

4.8 Limitations and future work

Despite these promising results, several limitations must be acknowledged. First, the FMO complex constitutes only the initial energy funnel of a larger photosynthetic apparatus. In higher plants, antenna systems (LHCII, CP43/CP47) feed into Photosystems I and II, whose outputs ultimately drive ATP synthase. Quantum coherence observed at the FMO level may be altered when embedded within this vastly larger network. Thus, fully quantitative yield predictions require modeling the complete transport chain. While our PT-HOPS benchmarks (Supporting Information, Section 5) demonstrate excellent scaling up to ~ 100 chromophores, simulating a full chloroplast will require rigorous coarse-graining to accurately bridge the molecular and organismal scales.

Second, our calculations assume fixed OPV transmission profiles. However, adaptive filtering capable of dynamically responding to diurnal and seasonal environmental variations could unlock further performance benefits. Third, generating accurate biomass-level predictions necessitates integrating these quantum kinetic models with broader Calvin cycle dynamics and crop-specific photosystem compositions—parameters that vary significantly across C₃, C₄, and CAM species. Such integra-

tion would inherently enable far more accurate economic projections tailored to specific crop–climate combinations.

Future work must address these limitations through the expanded modelling of complete photosynthetic networks, the development of tunable or adaptive filtering technologies, and rigorous field validation across diverse crop species and climates. Techno-economic optimizations should also be expanded to dynamically incorporate localized installation costs and shifting regional energy markets. More broadly, the "spectral bath engineering" approach introduced here—identifying quantum-enhanced processes in nature, characterizing their environmental coupling, and then deliberately engineering artificial environments to maximize those quantum resources—may prove highly applicable to fields far beyond agrivoltaics, including artificial photosynthesis, next-generation quantum solar cells, and bio-inspired molecular electronics.

5 Conclusion

We have demonstrated that spectral bath engineering—the strategic filtering of sunlight to target vibronic resonances—significantly enhances agrivoltaic performance by exploiting non-Markovian quantum dynamics. Our simulations reveal a 25 % increase in the excitonic electron transport rate within the FMO complex compared to Markovian baselines. This enhancement is driven by a 20 % to 50 % extension of coherence lifetimes under optimal dual-band illumination, identifying a robust quantum mechanism for increasing per-photon biological efficiency in engineered solar environments.

These molecular-scale gains translate into macroscopic agricultural advantages without sacrificing photovoltaic output. Multi-objective optimization identifies organic photovoltaic configurations that achieve an 18.83 % power conversion efficiency while maintaining over 80 % of the native photosynthetic rate. Simulations across diverse global climates confirm that these enhancements are geographically robust and compatible with sustainable, biodegradable materials that exhibit sub-0.2 % annual degradation.

The provided design rules and material targets offer a scalable methodology for co-optimizing solar energy generation and crop productivity. This integration of open quantum systems theory with renewable energy engineering establishes a concrete pathway for developing next-generation agrivoltaic systems that advance food and energy security simultaneously.

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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. Our custom PT-HOPS/SBD simulation framework, computational notebooks, source code, and datasets generated during this study are available in the GitHub repository at https://github.com/NanaEngo/Quantum_Agrivoltaic_HOPS. Reproducibility information: All simulations were performed using Python 3.12.12, NumPy 2.0.2, and SciPy 1.14.1. Computational parameters and environment configurations are documented in the Supporting Information. All reported values include standard errors calculated from ensemble averaging, with 95% confidence intervals explicitly stated for all quantitative results derived from 100 independent realizations.

Conflicts of Interest

The authors declare no conflicts of interest.

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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–S8.