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Editorial Office  
Energy & Environmental Science  
Royal Society of Chemistry  
Thomas Graham House  
Science Park, Milton Road  
Cambridge CB4 0WF  
United Kingdom

Dear Editor,

We are pleased to submit our manuscript, “**Spectral Bath Engineering for Quantum-Enhanced Agrivoltaics: Advancing Efficiency and Environmental Sustainability via Non-Markovian Dynamics,**” for consideration as an original research article in *Energy & Environmental Science*.

Optimizing agrivoltaic systems—co-locating solar energy generation with agricultural production—is essential for enhancing global food and energy security. While conventional designs typically treat incident light as a classical photon flux, we show that leveraging the quantum mechanical nature of photosynthetic energy transfer can provide substantial productivity gains. Our framework of *quantum spectral bath engineering* utilizes non-Markovian coherence effects to optimize the spectral quality of light reaching the photosynthetic unit.

**(1) Quantifiable quantum advantages for the energy-food nexus.** Strategic spectral filtering through semi-transparent organic photovoltaic (OPV) panels enhances the photosynthetic electron transport rate (ETR) by 25 % via vibronic resonance-assisted transport. These quantum gains are robust under realistic environmental conditions, with pairwise concurrence nearly doubling (89 %) and linear entropy decreasing by 38 %. This improvement in agricultural productivity is achieved while maintaining 15 % to 18.8 % power conversion efficiency.

**(2) Rigorous computational validation and geographic relevance.** Our comprehensive framework achieved 100 % success across 12 independent numerical benchmarks, including comparisons with numerically exact HEOM. Geographic simulations across nine climate zones—including five sub-Saharan African sites—confirm persistent quantum advantages of 18 % to 28 %, demonstrating global applicability and particular relevance to regions where energy and food security are most critical.

**(3) Sustainable materials and operational stability.** Using eco-design analysis with quantum reactivity descriptors, we identify OPV materials with high biodegradability ( $B_{\text{index}} = 101.5$  for PM6 derivatives), ensuring end-of-life environmental compatibility. Year-long environmental stress simulations confirm an exceptional 0.17 % annual degradation rate, supporting the 20-year operational lifetimes required for commercial agrivoltaic deployment.

**(4) Quantitative design specifications for practical implementation.** Using Pareto frontier analysis, we establish precise engineering specifications for next-generation OPV materials—dual-band transmission at 750 nm and 820 nm with 70 nm FWHM. These specifications balance electrical power conversion with biological energy transfer enhancement, providing actionable targets for materials scientists working on sustainable energy technologies.

**(5) Experimental verification and deployment readiness.** We provide specific, testable pre-

dictions for validation using existing ultrafast spectroscopy techniques, with potential for immediate field trials. This bridges the fundamental quantum science with practical energy and environmental applications.

### Alignment with EES scope and mission

This manuscript directly addresses the core mission of *Energy & Environmental Science* by advancing sustainable energy technologies with clear environmental benefits:

- **Sustainable energy systems.** Our quantum-enhanced agrivoltaics contribute to sustainable land use by maximizing both energy and food output per unit area, directly addressing UN SDG 7 (Affordable and clean energy) and SDG 2 (Zero hunger). This is particularly relevant for sub-Saharan Africa and other regions facing food-energy nexus challenges.
- **Energy-environment nexus.** By demonstrating that quantum effects can enhance both energy conversion and biological productivity simultaneously, we address the critical interface between energy production and environmental impact, a core focus of EES.
- **Computational materials science.** We employ non-Markovian quantum dynamics methods (Process Tensor HOPS and Spectrally Bundled Dissipators) that offer significant computational advantages while maintaining accuracy, enabling modeling of complex energy conversion processes relevant to photosynthesis and solar energy.
- **Environmental sustainability.** Our eco-design framework using quantum reactivity descriptors ensures that the proposed technologies have minimal environmental impact at end-of-life, with biodegradable materials that support circular economy principles.
- **Global environmental applicability.** The demonstrated effectiveness across diverse climatic zones, particularly in sub-Saharan Africa, addresses environmental science applications where they are most critically needed.

### Broader impact and future directions

Beyond agrivoltaics, this study establishes a general methodology for quantum biomimetic engineering: identifying quantum-enhanced processes in natural systems and engineering artificial environments to maximize their efficiency. This approach has potential applications in artificial photosynthesis, quantum-dot solar cells, molecular electronics, and other sustainable energy technologies. The integration of quantum reactivity descriptors with eco-design principles provides a roadmap for environmentally sustainable quantum technologies.

### Suggested reviewers

We respectfully suggest the following expert reviewers, who possess complementary expertise spanning the interdisciplinary scope of this work:

1. **Dr. Gregory Scholes**  
Department of Chemistry, Princeton University, USA  
Email: gscholes@princeton.edu  
*Expertise: Quantum coherence in photosynthetic systems, ultrafast spectroscopy*
2. **Dr. Alexandra Olaya-Castro**  
Department of Physics and Astronomy, University College London, UK  
Email: a.olaya@ucl.ac.uk  
*Expertise: Quantum biology, open quantum systems, biological energy transfer*
3. **Dr. Jenny Nelson**  
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*Expertise: Organic photovoltaics, solar energy conversion, device physics*
4. **Dr. Akihiko Yamaguchi**

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*Expertise: Non-Markovian dynamics, process tensor methods, quantum simulation*

5. **Dr. Brenda Farnum**

Department of Chemistry, James Madison University, USA

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*Expertise: Artificial photosynthesis, solar fuels, sustainable energy*

## Manuscript details

- **Main text.** Approximately 5,000 words across 5 sections with 4 main figures
- **Tables.** 1 main text table (quantum metrics comparison)
- **Supporting Information.** Comprehensive SI including environmental models, biodegradability assessment, full validation suite, parameter sets, and 8 supplementary figures (S1–S8)
- **References.** Balanced across energy science (35%), quantum dynamics (30%), photosynthesis (25%), and computational methods (10%)

## Declarations

We confirm that this manuscript represents original research that has not been published previously and is not under consideration for publication elsewhere. All authors have approved the manuscript and agree with its submission to *Energy & Environmental Science*. We declare no conflicts of interest.

The work was conducted in accordance with ethical research practices. We confirm compliance with all data availability and reproducibility standards as outlined in EES guidelines.

## Closing statement

This work demonstrates that quantum mechanical principles derived from photosynthetic energy transfer can be systematically leveraged to improve sustainable agrivoltaic systems, addressing both clean energy and food security challenges. The combination of theoretical validation, quantitative design specifications, environmental applicability across diverse climate zones, and experimental verification pathways makes this work highly relevant to the broad readership of *Energy & Environmental Science* and its mission of advancing sustainable energy technologies with clear environmental benefits.

We would be honored to have this work considered for publication in EES. Thank you for your time and consideration.

Sincerely,

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