

Department of Physics  
Faculty of Science  
University of Douala  
P.O. Box 24157  
Douala, Cameroon

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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, “**Quantum Spectral Engineering for Enhanced Agrivoltaic Efficiency: Non-Markovian Dynamics in Photosynthetic Energy Transfer**,” for consideration as an original research article in *Energy & Environmental Science*.

### Significance and novelty

This work addresses a central challenge in renewable energy and food security: the optimization of agrivoltaic systems that co-locate solar energy generation with agricultural production. Standard agrivoltaic designs typically treat light as a classical photon flux, overlooking the quantum mechanical aspects of photosynthetic energy transfer. We present a framework for *quantum spectral bath engineering*, which utilizes quantum coherence effects to improve both solar energy harvesting and agricultural productivity.

Key findings of this study include:

**(1) Quantifiable quantum advantages:** We demonstrate that spectral filtering through semi-transparent organic photovoltaic (OPV) panels can enhance the photosynthetic electron transport rate by 25% via vibronic resonance-assisted transport. Economic analysis indicates that this improvement can translate to USD 470 to 3000 in additional annual revenue per hectare, supporting the practical viability of quantum-informed design.

**(2) Rigorous computational validation:** Our framework achieved 100% success across 12 independent numerical tests, including benchmarking against numerically exact methods and robustness checks under physiological environmental conditions. This validation ensures that the observed effects are physically grounded and reproducible.

**(3) Actionable design principles:** Using Pareto frontier analysis, we establish quantitative specifications for next-generation OPV materials—specifically, dual-band transmission at 750 and 820 nm with 70 nm FWHM. These specifications balance electrical power conversion efficiency (15 to 21%) with biological energy transfer enhancement (8 to 25%).

**(4) Experimental verification pathway:** We provide specific predictions for verification using existing experimental techniques, including coherence lifetime extensions of 20 to 50% in ultrafast spectroscopy and 10 to 18% yield improvements in field trials.

### Alignment with EES scope

This manuscript is well-aligned with the interdisciplinary scope of *Energy & Environmental Science*:

- **Solar fuels:** Our results provide design principles for enhancing natural photosynthesis that are directly applicable to artificial systems.
- **Sustainable energy:** Agrivoltaics are key to sustainable land use, contributing to UN SDGs (Clean Energy, Zero Hunger, Climate Action).
- **Computational energy science:** We utilize a non-Markovian quantum dynamics method (adaptive HOPS) that offers a  $10\times$  speedup, enabling the modeling of complex energy conversion processes.
- **Interdisciplinary research:** This work integrates quantum biology, renewable energy engineering, and materials science.

## Impact and future directions

Beyond agrivoltaics, this study establishes a methodology for biomimetic quantum engineering: identifying quantum-enhanced processes in nature and engineering environments to maximize their efficiency. This has potential applications in quantum-dot solar cells, molecular electronics, and light-harvesting materials.

Our findings show that quantum coherence effects in biological systems are not just fragile laboratory phenomena but can serve as robust design principles for engineered sustainable energy technologies. These advantages are accessible with current materials and fabrication methods.

## 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

Department of Physics, Imperial College London, UK

Email: jenny.nelson@imperial.ac.uk

*Expertise: Organic photovoltaics, solar energy conversion, device physics*

### 4. Dr. Akihiko Yamaguchi

Graduate School of Science, Kyoto University, Japan

Email: yamaguchi@kuchem.kyoto-u.ac.jp

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

### 5. Dr. Brenda Farnum

Department of Chemistry, James Madison University, USA

Email: farnumbr@jmu.edu

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

## Manuscript details

- **Main text:** Approximately 7,000 words
- **Figures:** 6-8 main text figures (to be finalized)
- **Supporting Information:** Comprehensive SI including environmental models, biodegradability assessment, complete validation data, and parameter sets

- **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. Computational resources were provided by the African Institute for Mathematical Sciences. 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 used to improve practical agrivoltaic systems. The combination of theoretical validation, quantitative design specs, and experimental pathways makes this work relevant to the broad readership of *Energy & Environmental Science*.

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

Sincerely,

Steve Cabrel Teguia Kouam  
Department of Physics  
University of Douala, Cameroon  
Email:  
steve.teguia@facsciences-uy1.cm