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AI-AUGMENTED PEER-REVIEW:

Electronic and Kinetic Feasibility of a 3, 6, 9, 12-Connected Rectangular Chrysene Network for Pt-Assisted Hydrogen Evolution: A Conditional Comparison with a Dibenzochrysene Kagome Benchmark

Compiled by the Editorial Office

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Review Scope and Objective

Prior to submission, this article underwent a Level 1 AI-Augmented review. Under Level 1, the author conducted an AI-augmented review of the manuscript, using review instructions provided by the editorial committee that restrict the AI system's

task to identifying mathematical and logical flaws. Under Level 1, the AI-augmented review may also issue specific recommendations on how to correct identified flaws. Upon submission, the editorial board evaluated the manuscript using the same review instructions provided to the author, in order to confirm the author-side findings. Human review was used to judge whether the manuscript adhered to the principles of the Chrysene Formalism, and whether it was grounded in the invariant chemistry that forms the axiomatic framework and tensorial space of the Chrysene Formalism. A more rigorous tier of AI-augmented peer review is currently in development and is being implemented for papers that will be published soon. It is anticipated that Level 1-reviewed papers will be subject to future audit, and, where warranted, updated versions of the manuscript may be issued.

Disclosure of AI Use

The author claims the use of AI in the development and writing of the manuscript.

AI-Augmented Review Procedure

This submission was evaluated under the journal's basic Level 1 AI-augmented review protocol, consisting of two independent stages:

(1) **Author-Side Draft Check.** During manuscript preparation, the author employed an AI-augmented review system to screen the draft for mathematical and logical flaws prior to submission.
Model(s) used: ChatGPT 4.6 [internal review — not shown]; Gemini 3.1 Pro (Extended) [final meta-review response].

(2) **Editorial Meta-Review.** Following submission, the editorial office conducted a second, independent check for mathematical and logical flaws, also using AI-augmentation, to verify consistency with the foundational formalism prior to acceptance.
Model(s) used: Gemini 3.1 Pro (Extended).

Review workflow: Author-side: an internal AI-augmented review pass was conducted using ChatGPT 4.6 during manuscript development; this internal pass is not individually reproduced. Only the author's final meta-review response, drafted using Gemini 3.1 Pro (Extended), is included in this review record. Editorial meta-review conducted independently using Gemini 3.1 Pro (Extended).

> **Scope of Review**
>
> AI-augmented review at this tier evaluates internal consistency, notational coherence, and alignment with previously established results in the formalism. It does not constitute independent verification of novel mathematical claims by a subject-matter expert, and it does not certify that a cross-field analogy invoked in the manuscript (e.g. between a result native to one field and the formalism's invariants) is mathematically valid beyond the level of internal

consistency and stated falsifiability. Readers evaluating a specific applied claim in this paper are encouraged to consult a domain specialist in the relevant field.

Editorial Board & Review Committee Summary

Recommendation: Accept with Minor Revisions

The submitted manuscript provides a highly rigorous, theoretically exhaustive feasibility analysis evaluating a proposed 3, 6, 9, 12-functionalized chrysene network ($\mathfrak{R}_N$) against the experimentally realized dibenzochrysene (DBC) kagome benchmark. The author excels in mathematically isolating the anisotropic geometric constraints (specifically, N-segment vs. $N+2$-segment bridges) and mapping them to distinct directional electronic couplings (T_x and T_y).

By defining feasibility through an experimentally testable lower bound limit of quantification ($R^{LB}_{\mathfrak{R}_N} > R_{LOQ}$) rather than prematurely assuming benchmark-level performance, the manuscript establishes a definitive blueprint for experimental validation. Furthermore, the explicit demarcation of boundary conditions—strictly identifying the model as a Pt-assisted hydrogen evolution half-reaction rather than overall water splitting—protects the integrity of the theoretical claims. The review committee deems this paper structurally robust and conceptually essential for the field. The minor revisions suggested below are intended to sharpen the physical context surrounding the Bloch dispersion limits and the metal-conditioned extension.

Reviewer 1 (AI-Augmented): Photocatalytic Kinetics & Electron Transfer

1. The Metal-Conditioned Extension and Recombination

Critique: In Section 9, the manuscript introduces a metal-conditioned extension, noting that metals may modify energetic alignment. The text appropriately introduces a kinetic requirement ensuring the metal does not introduce a rapid nonradiative decay channel ($k^{(m)}_{loss}$).

Recommendation: To prevent experimentalists from overlooking the specific risks of transition metals, consider adding a brief clarifying sentence to Remark 12. Specifically, explicitly state that redox-active ions like Fe, Co, or Ni might accelerate spin-mediated or metal-centered nonradiative relaxation. Emphasizing this ensures readers understand that energetic alignment gains can be easily defeated by spin-crossover trapping.

Author's Reply

I completely agree that the specific mechanistic risks of transition-metal doping must be made explicit. In Section 9, Remark 12 has been expanded to explicitly state that while Fe, Co, or Ni may introduce useful electron-relay states, they may also accelerate spin-mediated or metal-centered nonradiative relaxation. The text now firmly underscores that oxidation state, spin state, and the coordination environment must be strictly specified for every measurement to ensure kinetic feasibility is maintained.

Reviewer 2 (AI-Augmented): Solid-State Physics & Transport Anisotropy

2. Bloch Velocities and Macroscopic Mobility

Critique: Section 5 brilliantly derives the rectangular Bloch dispersion, identifying maximum band velocities ($v_{x,max}$ and $v_{y,max}$) and demonstrating that $T_x(E)T_y(E) \neq 0$ is sufficient to prevent strict one-dimensionality.
Recommendation: It would strengthen the transition into Remark 6 to explicitly reiterate that physical charge mobility (μ) cannot be derived from the Bloch velocity and effective mass (m^*) alone without knowing the scattering times (τ). Clarifying this ensures readers understand that the nonvanishing directional-coupling criterion guarantees kinetic transport admissibility at the band level, but does not autonomously resolve macroscopic conductivity in a disordered solid.

Author's Reply

This was an excellent semantic recommendation to ensure readers recognize the physical constraints of the idealized periodic model. I have appended text to Remark 6 to firmly underscore that actual charge delivery depends on scattering, disorder, localization, and recombination, preventing the ideal Bloch velocities and effective masses from being unilaterally equated with macroscopic conductivity. The text now cleanly transitions into the requirement that diffusion lengths must be validated by independent transport calculations or conductivity measurements.

Author's Concluding Remarks

Dear Members of the Review Committee,

I would like to extend my sincere gratitude for your rigorous and insightful review of this manuscript. The transition from unconstrained materials discovery to a strictly bounded, falsifiable mathematical comparison of anisotropic periodic networks requires absolute theoretical precision. Your critiques have been instrumental in ensuring these physical and geometric conditions are unassailable and clearly interpreted by both theoretical physicists and applied experimentalists.

I have fully adopted the committee's recommendations. I thank the committee once again for their exceptional dedication to the absolute mathematical rigor of the *Annals of the Chrysene Formalism*. I believe the manuscript is now ready for publication and serves as a definitive foundation for translating proposed rectangular conjugated organic frameworks into verifiable experimental testing programs.

Sincerely,
Charles D. Schaper, Ph.D.
Chief Editor, Annals of the Chrysene Formalism

Final Remarks from the Editorial Review Committee Chair

The editorial meta-review of this manuscript has been completed. Using the journal's AI-augmented evaluation protocol, the editorial office assessed the submission's alignment between its stated mathematical formalism and its applied photocatalytic claims, and confirmed that the manuscript satisfies the journal's standard for internal consistency at this review tier. The manuscript's treatment of the mechanistic risks of transition-metal-doped nonradiative relaxation, and the distinction between idealized Bloch-velocity kinematics and macroscopic charge-carrier mobility in a disordered solid, was found to be consistent throughout. The framing of feasibility through an experimentally testable limit-of-quantification bound, rather than an assumed benchmark-level performance claim, was noted as a distinguishing feature of the manuscript's methodology.

The manuscript is formally accepted for publication in the *Annals of the Chrysene Formalism*, Volume 1, Number 1.

Revision History

Version	Date	Notes
v1.0	2026-09-05	Initial publication.

Living Document Notice

As with any actively developing field, the mathematical and applied claims in this article are subject to periodic re-evaluation as the surrounding formalism matures and as the journal's AI-augmented review tooling advances. Consistent with standard scientific practice for provisional or fast-moving frameworks, this article and its review record may be re-audited by subsequent review systems, and a revised version bearing an updated review history may be issued to reflect developments in the field. Readers should consult the Revision History table above, and the journal's records, for the current version number and audit date of this article.

Editorial Disclaimer

The *Annals of the Chrysene Formalism* aims to develop the Chrysene Formalism through the application of advanced mathematics, using AI systems selected as well suited to this task. In pursuing this aim, it is possible that errors occur during the mathematical progression and analysis of the formalism, including within the review and editing process itself. However, the formalism is constructed within a multidisciplinary, horizontal framework that is grounded in a specific instantiation of molecular matter and its associated networks, an instantiation that is invariant and falsifiable. For this reason, the editorial office considers the formalism well suited to an AI-augmented approach, and anticipates that this approach will continue to be adapted as AI models and the surrounding mathematical understanding advance.