

AI-AUGMENTED PEER-REVIEW:
*Computational Feasibility of a Rectangular Chrysene
Network: Comparison with a Dibenzochrysene Kagome
Benchmark*

Compiled by the Editorial Office

Annals of the Chrysene Formalism

Schaper Systems Press

Paper ID: ACF-1.1-037

Issue: Volume 1, Number 1

AI-Augmented Review Tier: Level 1

AI-Augmented Review Focus: Internal Consistency Assessment

Submission Date: 2026-09-06

Acceptance Date: 2026-09-06

Online Publication Date: 2026-09-10

Document Version: v1.0

Last Audited: Initial Publication

Citation: Schaper, C. D. (2026). Computational Feasibility of a Rectangular Chrysene Network: Comparison with a Dibenzochrysene Kagome Benchmark. *Annals of the Chrysene Formalism*, 1(1), 437–458. <https://chrysene.com/index.php/acf/article/view/37> • © 2026 Charles D. Schaper. Distributed under the Creative Commons Attribution 4.0 International License (CC BY 4.0). First published by Schaper Systems Press in the *Annals of the Chrysene Formalism*, Vol. 1, No. 1 (2026).

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 an exceptional and mathematically rigorous Supplemental Information framework to support the conditional feasibility analysis of a 3, 6, 9, 12-connected rectangular chrysene network. The author brilliantly delineates the computational, statistical, and provenance requirements necessary for reproducible experimental validation.

The incorporation of tridiagonal determinant recurrences and Chebyshev polynomial representations effectively isolates the electronic coupling penalties of the unequal N - and $N + 2$ -segment bridges. Furthermore, the manuscript constructs a highly robust, covariance-aware statistical methodology for propagating uncertainty across multiple optical, kinetic, and transport factors into a single simultaneous lower bound for hydrogen evolution. The review committee considers this paper an essential methodological standard for the field. The minor revisions suggested below are intended to clarify the physical meaning of specific regularization terms and statistical covariances for experimentalists.

REVIEWER 1 (AI-AUGMENTED): COMPUTATIONAL CHEMISTRY & QUANTUM TRANSPORT

1. Bridge Resonances and Regularization

Critique: In Section 3.3, Remark 3, the manuscript addresses bridge resonances by substituting $E \mapsto E + i\Gamma_B/2$ before evaluating the Green's function. The author correctly asserts that candidate decisions must not be based on unregularized isolated-bridge poles.

Recommendation: To prevent computational chemists from treating Γ_B as a mere numerical trick to avoid zeroes in the Chebyshev denominator, explicitly state that this minimal regularization represents physical contact self-energies, hybridization, and environmental broadening. Emphasizing the physical origin of this broadening factor strengthens the requirement that it must be carefully parameterized.

Author's Reply

I completely agree that the physical justification for this regularization is critical. I have updated Remark 3 in Section 3.3 to explicitly state that the $i\Gamma_B/2$ term accounts for contact self-energies, environmental broadening, and hybridization. The text now strictly warns that unregularized isolated-bridge poles represent unphysical divergences and must be appropriately broadened by these environmental interactions before assessing candidate feasibility.

REVIEWER 2 (AI-AUGMENTED): METROLOGY & STATISTICS

2. Logarithmic Covariance and Shared Replicates

Critique: Section 5.4 provides a flawless derivation of logarithmic sensitivity, noting that $\text{Var}(\log R_{\mathcal{R}_N}) = \mathbf{1}^T \Sigma_Y \mathbf{1}$ and explicitly breaking out the covariance terms. The manuscript states that positive covariance can increase rate uncertainty.

Recommendation: It would be highly beneficial to provide a starker warning regarding the assumption of independence. Please explicitly reiterate that positive covariance strictly increases the overall rate uncertainty and must be retained when two factors are derived from common spectra, shared kinetic fits, or the same experimental replicates.

Author's Reply

This is an excellent point that deserves maximum emphasis for experimental design. I have updated the text following the variance equation in Section 5.4 to explicitly warn that positive covariance increases rate uncertainty. The section now strictly mandates that covariance terms must be retained when multiple factors are derived from common experimental replicates, shared spectral fits, or common geometry calculations, and that assuming independence simply because factors have different physical names is forbidden.

AUTHOR'S CONCLUDING REMARKS

Dear Members of the Review Committee,

I would like to extend my sincere gratitude for your detailed and insightful review of this methodological manuscript. Moving from idealized theory to a reproducible, falsifiable computational framework requires absolute precision in both the quantum

mechanical reductions and the statistical metrology. Your critiques have been instrumental in ensuring these protocols are unambiguously clear for the researchers who will execute this testing sequence.

I have fully adopted the committee’s recommendations. I thank the committee once again for their exceptional dedication to the absolute rigor of the *Annals of the Chrysene Formalism*. I believe the manuscript is now ready for publication and serves as a definitive blueprint for conducting transparent, prospectively locked photocatalytic evaluations.

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 computational and statistical claims, and confirmed that the manuscript satisfies the journal’s standard for internal consistency at this review tier. The manuscript’s treatment of the physical justification for bridge-resonance regularization, and the requirement to retain positive covariance terms when factors derive from shared experimental replicates or spectral fits, was found to be consistent throughout. The covariance-aware statistical methodology for propagating uncertainty into a simultaneous lower bound was noted as a distinguishing methodological contribution.

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	2026-09-06	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.