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AI-AUGMENTED PEER-REVIEW:

Directional Excited-State Polarization in a 3,6,9,12-Connected Rectangular Chrysene Network: A Range-Separated Fragment Comparison with a Dibenzochrysene 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 establishes a highly rigorous, falsifiable framework for evaluating directional excited-state polarization in a 3,6,9,12-connected rectangular substituted-chrysene network. The author effectively compares a finite rectangular fragment ($\mathfrak{R}_{2,y,f}$) against a dibenzochrysene (DBC) benchmark fragment ($\aleph_f$) using a Tamm-Dancoff approximation within a $6o/6v$ frontier space. The manuscript successfully identifies three optically allowed states with centroid separations between 3.946 and 5.301 Å.

Crucially, the author resists over-interpreting these results, correctly utilizing fragment-resolved populations to prove that the excitations remain predominantly bridge-centered ($h_B > 0.62$, $e_B > 0.74$) rather than achieving full opposite-core separation. The review committee deems the foundational calculations mathematically and structurally sound. The minor revisions suggested below are intended to sharpen the physical justifications for the selected computational constraints.

Reviewer 1 (AI-Augmented): Computational Quantum Chemistry

1. Auxiliary Basis Linear Dependence

Critique: Section 6.1 appropriately discloses that the Weigend auxiliary Coulomb metrics suffer from severe linear dependence, demonstrating reciprocal condition numbers of approximately 10^{-20}.

Recommendation: To fully satisfy the computational chemistry community, consider adding a brief clause in Section 9 (Conclusion) explicitly reiterating that this linear dependence prevents the assignment of quantitative spectroscopic accuracy until it is resolved by a better-conditioned auxiliary basis.

Author's Reply

I completely agree. The conclusion (Section 9) has been amended to explicitly recall the condition numbers of 1.62×10^{-20} and 3.54×10^{-20}. The text now formally states that confirmation with a better-conditioned auxiliary basis is required before assigning quantitative spectroscopic accuracy, reinforcing the necessity of computational Gate G_1.

2. In-Plane Geometry Constraints

Critique: During the GFN2-xTB geometry conditioning, the heavy-atom in-plane coordinates were fixed ($\Delta x_i = \Delta y_i = 0$), allowing only out-of-plane and hydrogen coordinates to relax.
Recommendation: Briefly expand in Section 3.1 on why this specific lattice constraint was necessary. Specifically, note that treating the heavy atoms as lattice constraints prevents the unconstrained finite dimer from undergoing unphysical planar folding that would be unavailable to an embedded node in an extended covalent network.

Author's Reply

This is a vital physical distinction. Section 3.1 has been updated to explicitly state that an unconstrained finite dimer can fold in a manner that is unavailable to a node embedded in an extended covalent network. The text now clarifies that treating the heavy-atom in-plane coordinates as lattice constraints prevents this unphysical folding behavior.

Reviewer 2 (AI-Augmented): Materials Design & Catalysis

3. Bridge-Centered Polarization vs. Catalyst Placement

Critique: Proposition 5 brilliantly demonstrates that optimizing for absorption and centroid displacement alone is insufficient, as both marginal distributions can remain trapped on the extended bridge.
Recommendation: In Section 7.1, when defining the localization functional $\mathcal{L}$, add a brief note emphasizing that a targeted inverse-design workflow intended for catalyst extraction must explicitly reward electron population at the designated catalyst-facing region.

Author's Reply

This is an excellent contextual addition. In Section 7, following Proposition 5, I have added explicit text stating that a design intended for catalyst extraction should reward electron population directly at the designated catalyst-facing region. This perfectly frames why an absorption-centroid objective is insufficient on its own.

4. Basis Set Limitations in Computational Gates

Critique: The manuscript wisely delegates the calculation of vertical ionization potentials and electron affinities to Gate G_3.
Recommendation: Explicitly clarify in the definition of Gate G_3 that the minimal STO-3G basis set currently utilized lacks the necessary diffuse flexibility to accurately describe diffuse charge-transfer states or electron affinities.

Author's Reply

Thank you for this precision. In Section 8, the description of Gate G_3 (Exciton and charge-separation energetics) has been updated to explicitly require a range-separated method with both polarization and diffuse flexibility. Furthermore, Section 6.2 (Uncertainty hierarchy) already explicitly acknowledges that STO-3G lacks sufficient polarization and diffuse flexibility for quantitative excited-state or charge-displacement analysis.

Author's Concluding Remarks

Dear Members of the Review Committee,

I would like to extend my sincere gratitude for your rigorous and constructive review of this manuscript. Establishing an unambiguous boundary between optical absorption and true charge separation requires strict analytical discipline, and your critiques have refined the manuscript's methodological justifications immensely.

I have fully adopted the committee's recommendations. I thank the committee once again for their exceptional attention to the methodological boundaries of this finite-fragment calculation. I believe the manuscript is now finalized and serves as a highly robust, falsifiable starting point for the inverse design of photosynthetic materials.

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-chemistry claims, and confirmed that the manuscript satisfies the journal's standard

for internal consistency at this review tier. The manuscript's treatment of the auxiliary-basis linear-dependence limitation, the physical justification for the in-plane geometry constraints, the distinction between bridge-centered polarization and catalyst-facing electron population, and the basis-set limitations acknowledged within the computational gate hierarchy was found to be consistent throughout. The separation of weak optical-directional polarization from persistent charge separation was noted as a central 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	2026-09-07	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.