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Quantum Behavior of Substituted-Chrysene Molecular Assemblies: Bipartite Schur-Complement Transfer Anisotropy, Quadratic-to-Linear Stark Switching Across (D, I, T), and Registry-Gated Ballistic Transport

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Declared review status

This is an AI-assisted simulated review record, not independently appointed human peer review. Separate mathematical and chemistry review passes informed the revision. Concordance checks compare statements, proofs, computations and companion files. Revision responses describe changes prepared for the author's consideration, not unprovided statements attributed to the author.

Scope of Review

The controlling input is the supplied Article 93 `main.tex`. Its earlier referee report and verification program are audited evidence. Exact graph and rational identities, numerical electronic-response calculations, ideal lead-coupled transport and proposed chemistry are assessed separately.

Combined recommendation

Retain the finite graph, transfer and chain results after substantive clarification and correction. Distinguish symmetry constraints from sufficient physical mechanisms, geometric arm vectors from electronic dipoles, and isolated transfer amplitudes from lead-coupled conductance.

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1 Source record and historical review

The prior report is preserved unaltered in `provenance/Article93_Prior_Referee_Source.tex`. Its provisional Volume 1, Number 5, October 2026 metadata and recommendation "Accept with Minor Revisions (Title Update & Four Quantum-Electronic Refinements)" are historical, not the disposition of this review.

Supplied manuscript source SHA-256

`5d037446dc328d4023758f451f5c1451`

`f7f3a0469d81b341ad5e2010e0952e45`

Supplied referee source SHA-256

`6aa4aa43e3dce8c59326a56c5a32cc51`

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Supplied verification source SHA-256

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1.1 Earlier findings retained as provenance

The earlier report proposed a unified quantum-behavior title; frame invariance and the $(10, 15, 6, 1)$ transmission partition at six units; geometric arm-vector norms $37/4$ and $13/4$; uniform half-filled charge in the unperturbed bipartite model; and a full planar response tensor. These are useful audit targets. The new review does not adopt its unsupported claims that broken inversion guarantees a nonzero dipole, that the isolated transfer ratio alone explains bromination, or that perfect transmission is synonymous with unitarity.

2 Review architecture

> *M* — **Mathematical validity**
>
> Check the specified finite graph, moments and resolvent identities; assumptions for analytic perturbation theory; the symmetry versus noncancellation distinction; and the exact lead-matched chain formula and ensemble law.

> *C* — **Concordance**
>
> Compare manuscript statements, numerical macros, scripts, exact certificates, summaries and inherited reports. Require executable coverage to match each advertised verification claim.

> *H* — **Chemistry and domain admissibility**

Separate the chosen tight-binding realization from compound-specific electronic structure, synthesis selectivity, solvent and contact effects, and measured exciton or charge transport.

3 Mathematical review and revision response

3.1 M1 Recompute the polarizability rather than emit fixed values

Finding: major. The supplied verifier passes its assertions, but computes a tensor different from the values it exports. Its numerical calculation gives approximately

$$\alpha_{xx} = 4.36584105, \quad \alpha_{yy} = 6.34377776, \quad \alpha_{xy} = -1.12115314, \quad \alpha_{xx}/\alpha_{yy} = 0.68820839,$$

whereas its emitted macros are 9.7346, 5.9015, −2.1408 and 1.6495. The inequality is reversed in the resulting ratio. Moreover, the proof diagonalizes the unperturbed Hamiltonian only; the same values do not apply to arbitrary inversion-symmetric D/T shifts. Symmetry permits, but does not require, unequal diagonal components or a nonzero off-diagonal entry.

Revision response. Accept. Generate values from the implemented calculation, independently check the eigensystem and response, and restrict the quantitative tensor to the unperturbed realization with explicit units. Distinguish floating-point estimates from exact identities; supply a rigorous enclosure for the anisotropy if it is asserted as a theorem. Continuity extends a strict inequality only to a sufficiently small gap-preserving neighborhood.

3.2 M2 Separate symmetry permission from a nonzero Stark response

Finding: major. Broken inversion and a nonzero sum of substituted-site coordinates do not imply a nonzero occupied-state dipole for every nonzero site shift. The vector $\mathbf{d}_I$ is a geometric marker, not the electronic dipole. The printed Dm expression is also missing parentheses: the intended vector is $(\mathbf{r}_6 - \mathbf{r}_{12})/2$. A Taylor expansion needs a spectral gap and an analytic ground-state branch.

Revision response. Accept. State inversion-forced zero dipole for the gapped occupied projector, with consistent spin, charge and background conventions. State the asymmetric case as symmetry-allowed, and require an explicit noncancellation condition or exhibit a calculated parameter realization. Preserve the exact geometric norms 37/4, 13/4 and dot product −7/4 without treating them as measured dipoles. “Quadratic” denotes the leading even term; higher even terms remain.

3.3 M3 Distinguish isolated transfer from open-system conductance

Finding: major. The exact statement is the squared isolated transfer ratio 16. It is not the universal ratio after lead self-energies are included. For equal local two-contact broadenings Γ, isolated off-diagonal Green entry g and zero isolated diagonal entries,

$$T(0) = \frac{\Gamma^2 g^2}{(1 + \Gamma^2 g^2/4)^2}.$$

For the two contacts in the paper this gives

$$\frac{T_y}{T_x} = 16\left(\frac{1+\Gamma^2/(256t^2)}{1+\Gamma^2/(16t^2)}\right)^2,$$

which tends to 16 in the matched weak-contact limit. Two same-sublattice zeros do not establish complete channel isolation. A remark comparing the parity of a state with the parity of an operator is ill-typed.

Revision response. Accept. Retain the exact isolated resolvent result and label its weak-contact interpretation. Restrict the zero-node statement to the named entries of the nonsingular chiral core. Replace the parity remark by the selection rule $\langle \text{odd}|V_{\text{even}}|\text{even}\rangle = 0$.

3.4 M4 Correct contact counts and scattering terminology

Finding. A $2N$-site chain has $2N-1$ contact bits, not $2N-2$. The supplied six-unit enumeration correctly uses five bits, but the theorem, zero word and uniform-law normalization do not. Pairwise balancing of the first $N-1$ even/odd pairs leaves the last even-index bit; that bit must also be zero. A lossless scattering matrix is unitary for every registry, including reflecting registries.

Revision response. Accept. Correct the contact space and its law to $\{0,1\}^{2N-1}$ and $2^{-(2N-1)}$, explicitly match endpoint lead couplings to t_0, and use "perfect" or "reflectionless transmission" for $T=1$. Prove full frame invariance: global flip of all unit orientations leaves the agreement field unchanged, while end reversal reverses its order and preserves the even/odd imbalance.

3.5 M5 Prove the algebraic ensemble asymptotic

Finding. The asserted $O(N^{-1/2})$ decay does not follow immediately from finite averaging. For independent fair contact bits,

$$\Pr(\Delta m = k) = 2^{-(2N-1)}\binom{2N-1}{N-1+k}.$$

This is an offset binomial difference with mean $1/2$, not an unbiased simple random walk. Its maximal point mass is $O(N^{-1/2})$. For fixed $0<\tau<1$, the series $\sum_{k\in\mathbb{Z}} \operatorname{sech}^2(k\log\tau)$ converges, giving the upper bound. The $k=0$ term gives a matching lower order.

Revision response. Accept. Add the binomial-law argument and state the fixed-τ assumption. Distinguish this band-center algebraic mean from generic exponential Anderson localization and from the exponential suppression of a specific dimerized field.

3.6 M6 State the realization and matching scope precisely

Finding. Distinct leading Laurent powers do prove inequivalence under arbitrary constant terminal phases. This discharges the operator target within the declared uniform-hopping graph and terminal realization, not for all chemically substituted chrysenes. Exact determinant, path and matching claims pass independent checking. The supplied graph has cycle lengths $6, 10, 14, 18$, but this is not a theorem that all benzenoids lack $4m$-cycles.

Revision response. Accept. Retain the scalar transfer proof and exact graph results with their model hypotheses. Use a direct finite determinant/matching certificate rather than a blanket benzenoid assertion. Avoid presenting unavailable earlier-article theorem numbering as independently reverified evidence.

4 Concordance review and revision response

4.1 C1 Match historical verification claims to actual implementation

Finding: major. A successful run of the supplied program does not validate its emitted tensor. Its T3 macros are hard-coded despite a different computed tensor. Its claimed independent full Green/Fisher–Lee chain comparison is absent; residual matching counts are emitted without an independent enumeration; and T4 checks coordinate sums rather than the permanent electronic dipole. Its trigonometric Jacobi routine is floating-point, not exact.

Revision response. Accept. Preserve the original as superseded provenance. Replace the inaccurate coverage claims with a reproducible checker that separates exact graph/rational calculations, numerical response and rigorous enclosures, and with a Lean dossier whose claims are limited to the certificates actually compiled.

4.2 C2 Synchronize every summary and hypothesis register

Finding. Local repairs alone leave contradictory claims in the abstract, introduction, synthesis table, conclusion and molecular commentary. The correct tensor, contact count, gap premise and conditional chemistry must be propagated through all deliverables.

Revision response. Accept. Synchronize the manuscript, graphical abstract, OJS text, supplements and review responses. Use the approved November 2026, Volume 1, Number 4 presentation and supplied DOI metadata. The author's requested theorem/definition/proof tcolorbox styles are retained in the manuscript.

4.3 C3 Add independent checks and negative controls

Finding. Useful independent targets include $AA^{-1} = I$, residual matching enumeration, eigenpair residuals and orthogonality, energy finite differences, open-chain inversion versus the product formula, actual frame actions, normalized distributions and rejection of obsolete constants.

Revision response. Accept. Add these targets where applicable and execute checks in ordinary and optimized Python modes. Use deliberate defects to test detection rather than merely count successful assertions. Distinguish finite Lean certificates from general analytic asymptotics, continuum response and molecular realization. Final coverage is reported below.

5 Chemistry review and revision response

5.1 H1 Qualify the isolated-core conductance prediction

Finding. Physical transmission uses the lead-dressed retarded Green function, $T = \mathrm{Tr}(\Gamma_L G^r \Gamma_R G^a)$. Equal weak local contacts, coherent transport and midgap Fermi alignment are essential to interpreting the isolated-core ratio. Anchors, site energies, charge state, level alignment and multichannel contacts can alter it. The dimensionless entries 1/2 and 1/8 represent $t|G|$, not unitful Green functions.

Revision response. Accept. State the exact core ratio and its conditional weak-contact prediction, in agreement with the magic-ratio regime described by Geng et al. [1] and the transport formulation of Fisher and Lee [2].

5.2 H2 Restrict zero-node claims to the specified Hamiltonian

Finding. Onsite shifts in H_S generally break sublattice anticommutation. Lead self-energies or gating may also change the measured transmission. Two vanished entries do not establish a complete Data/Control superselection rule.

Revision response. Accept. Retain the exact nonsingular off-diagonal-core theorem and name its terminal pairs. Separate the decorated and lead-dressed models, and test a site-potential perturbation as a counterexample to an unrestricted node claim.

5.3 H3 Separate geometry, symmetry and permanent dipoles

Finding. A coordinate sum is neither an electronic nor a total molecular dipole. A planar model's C_s stabilizer need not be the atomistic point group of flexible decorated molecules. Symmetric locants require symmetry-related arms, conformers and surroundings before a physical symmetry argument applies. "Mono-cleaved" should not imply the erroneous ester-cleavage mechanism corrected in Article 90.

Revision response. Accept. Use mixed-arm notation, correct the Dm parentheses, state the gap and state-invariance assumptions, and define the model sign convention while distinguishing the additional physical charge/background data. Retain geometric markers while calculating or explicitly assuming the nonzero electronic response at declared parameters.

5.4 H4 State the response Hamiltonian, numerical status and units

Finding. The unperturbed tensor cannot be assigned unchanged to every D/T site shift. The units are e^2a^2/t for length scale a and hopping energy t. An off-diagonal component depends on the selected axes and vanishes in principal axes; it is not an invariant "C_2 coupling."

Revision response. Accept. Recompute the tensor, label the Hamiltonian and units, keep the spin convention consistent, and distinguish the chosen-axis tensor from its diagonal form in principal axes. Distinguish numerical estimates from certified inequalities.

5.5 H5 Present exciton separation as a testable physical target

Finding. A ground-state Stark term does not prove exciton dissociation, free-carrier generation or photovoltaic performance. The one-particle model has no explicit electron–hole binding, screening, charge-transfer energy or competing dissociation/recombination kinetics. A molecular dipole does not automatically create a discontinuous field step.

Revision response. Accept. Retain a boundary-polarity hypothesis and propose the missing excited-state and kinetic measurements. Remove claims of a demonstrated photovoltaic splitter. Braun's kinetic treatment [3] provides a comparator, not evidence that the proposed chrysene cap works.

5.6 H6 Do not infer synthesis from transport cofactors

Finding. Cofactor deletion is an algebraic operation, not literal atom removal or a chemical transport pathway. It does not establish electrophilic bromination barriers, simultaneous versus sequential substitution, regioselectivity or the inherited 99.4% source fraction. Electron transmission does not, by itself, destroy aromatic sextets.

Revision response. Accept. Preserve matching and resonance interpretations without a causal synthesis claim. Identify inherited source fractions as model outputs unless measured evidence is supplied. Chemical selectivity remains a separate experimental or electronic-structure question.

5.7 H7 Specify the coherent registry-transport regime

Finding. The binary hopping law is a postulate requiring packing and orbital-overlap calibration. The calculation assumes phase coherence, negligible inelastic scattering, fixed geometry, zero onsite energies and matched leads. Placement prepares a field but does not prove temporal locking. Dynamic disorder in organic materials can modify transfer integrals [4, 5].

Revision response. Accept. Register these assumptions, distinguish perfect transmission from unitarity, and separate the band-center mean from generic localization. Retain the exact ideal-chain result under its stated regime.

5.8 H8 Design tests that discriminate the stated predictions

Finding. Break-junction tests need matched anchors, contacts, charge state and level alignment. Optical Stark measurements probe transition differences $\Delta\mu$ and $\Delta\alpha$; isotropic averaging can remove an odd-field signal despite molecular permanent dipoles [6].

Revision response. Accept. Propose oriented or single-molecule Stark measurements, or appropriate electroabsorption line-shape fits, alongside structure/conformer determination, electronic response calculations, contact-aware transport, temperature/coherence tests and separate exciton kinetics. These are future tests, not completed validation.

6 Integrated disposition and verification evidence

Scope-preserving resolution

The revised work retains exact graph anisotropy, the chiral-core node, inversion selection rules and ideal-chain transmission. It corrects the tensor and counting inconsistencies and replaces unsupported chemical implications with explicit assumptions and test targets. No request to replace the central model or to claim completed experiments is adopted.

6.1 Execution and formal coverage

The replacement Python checker records 17,093 exact predicates (including ten negative controls) and 1,088 numerical predicates, totaling **18,181 checks in each of ordinary and optimized Python modes**. Both modes produce byte-identical results. The companion audit files record reproducible execution and source pins.

The exact rational spectral-enclosure certificate gives

$$4.365 < \alpha_{xx} < 4.367, \qquad 6.343 < \alpha_{yy} < 6.345,$$

in the specified response units. These separated bounds establish the stated unperturbed anisotropy; the decimal tensor entries themselves remain numerical estimates. The checks also compare the chain formula to a separately assembled lead-dressed inverse, enumerate matching minors and field distributions, and compute occupied-state dipoles for declared shifts. They do not prove a universal nonzero dipole for all asymmetric perturbations.

Lean 4.24 freshly compiles **57 named finite theorems**; each dependency audit reports no axioms. The certificates cover the specified graph inverse, matching and path recurrences, inversion and geometric vectors, and finite chain counts. The rational spectral-enclosure computation is executed by the Python checker; the general continuum spectral-enclosure justification, analytic Stark expansion, asymptotic transmission estimate and chemical realization are not claimed as Lean-formalized results. Embedded companion sources are matched to their executed versions.

6.2 Closure and remaining scope

The revision incorporates M1–M6, C1–C3 and H1–H8 through corrected constants, explicit hypotheses, additional proofs and a revised interpretation. The core finite graph and ideal-chain program is retained. The manuscript no longer derives synthesis selectivity, universal nonzero dipoles or exciton dissociation solely from the graph identities. The report's disposition concerns that revised scope, not a claim of completed molecular validation. The supplied source references to theorem numbers in earlier articles are retained as provenance where applicable; the review does not certify every imported earlier theorem from the complete original corpus. The article's own DOI was not supplied and is not invented. Publication and any external submission remain the author's decisions.

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