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COMPUTATIONAL DESIGN OF NEXT-GENERATION MULTIPLE-RESONANCE TADF EMITTERS FOR HIGH-COLOR-PURITY OLEDS

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Abstract

Multiple-resonance thermally activated delayed fluorescence (MR-TADF) emitters are promising materials for organic light-emitting diodes (OLEDs) because they can combine narrow emission spectra with efficient exciton utilization. However, simultaneously achieving high color purity, favorable excited-state kinetics, strong radiative transitions, and long-term stability remains challenging. This article proposes an integrated computational framework for designing next-generation MR-TADF emitters through molecular architecture engineering, quantum-chemical calculations, excited-state analysis, and multi-objective optimization. The proposed workflow combines density functional theory (DFT), time-dependent DFT (TD-DFT), excited-state geometry optimization, reorganization-energy analysis, and selected higher-level electronic-structure methods. Molecular descriptors would be used to investigate the relationships among heteroatom connectivity, frontier-orbital distributions, singlet–triplet energy splitting, emission energy, oscillator strength, and structural relaxation. Additional screening would address aggregation sensitivity, environmental effects, synthetic feasibility, and computational uncertainty. Rather than selecting candidates using a single descriptor, the framework prioritizes molecules that offer a favorable balance of optical and photophysical properties. The expected outcome is a reproducible workflow for ranking candidate structures and selecting compounds for experimental validation. Since no new molecular calculations or experimental measurements are provided, the article reports a proposed methodology and expected analytical outcomes rather than completed research findings. The framework aims to improve the connection between computational molecular design, experimentally measurable photophysical properties, and high-color-purity OLED development.

1. Introduction

Organic light-emitting diodes have become important in advanced display technologies because of their self-emissive operation, high contrast, rapid response, and compatibility with thin-film device architectures. Their performance depends on the molecular properties of the emitting materials, including emission wavelength, spectral bandwidth, photoluminescence quantum yield, excited-state lifetime, and chemical stability. In high-resolution displays, narrow emission spectra are especially desirable because they enable more precise color reproduction and improve separation between display primaries.

Conventional fluorescent emitters predominantly utilize singlet excitons, while thermally activated delayed fluorescence (TADF)

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materials can potentially recover triplet excitons through reverse intersystem crossing (RISC). This process enables triplet excitons to contribute to delayed fluorescence without requiring conventional heavy-metal phosphorescent emitters. Nevertheless, many donor–acceptor TADF molecules exhibit broad charge-transfer emission, which can limit color purity (Eng & Penfold, 2020).

Multiple-resonance TADF provides an alternative molecular-design strategy. By incorporating electron-donating and electron-accepting atomic centers into rigid conjugated frameworks, MR-TADF materials can establish alternating frontier-orbital distributions while limiting excited-state structural relaxation. Hatakeyama et al. (2016) demonstrated the potential of this approach through ultrapure blue-emitting molecules. Subsequent research has expanded the structural diversity of MR emitters and investigated strategies for controlling emission bandwidth, intermolecular interactions, and excited-state dynamics.

Despite substantial progress, several challenges remain. Modifications intended to narrow emission can alter oscillator strength, excited-state energies, or charge transport. A small singlet–triplet energy difference does not independently guarantee rapid RISC, high photoluminescence efficiency, or long device lifetime. Moreover, molecular properties calculated in isolation may not accurately reproduce the behavior of materials in OLED films.

Computational chemistry offers a systematic approach to these problems. DFT and TD-DFT can provide initial estimates of molecular geometries, excited-state energies, orbital distributions, and optical transition strengths. More advanced methods can investigate selected excited states when conventional approximations are insufficient. These calculations can reduce the number of structures requiring synthesis, provided that their limitations and uncertainty are explicitly considered.

Research gap. Although established MR-TADF studies demonstrate promising molecular architectures and spectral-narrowing strategies, an integrated candidate-selection workflow that considers emission bandwidth, excited-state kinetics, radiative properties, environmental sensitivity, and stability together remains valuable. This article addresses that gap by proposing a multi-objective computational framework linked to experimental validation.

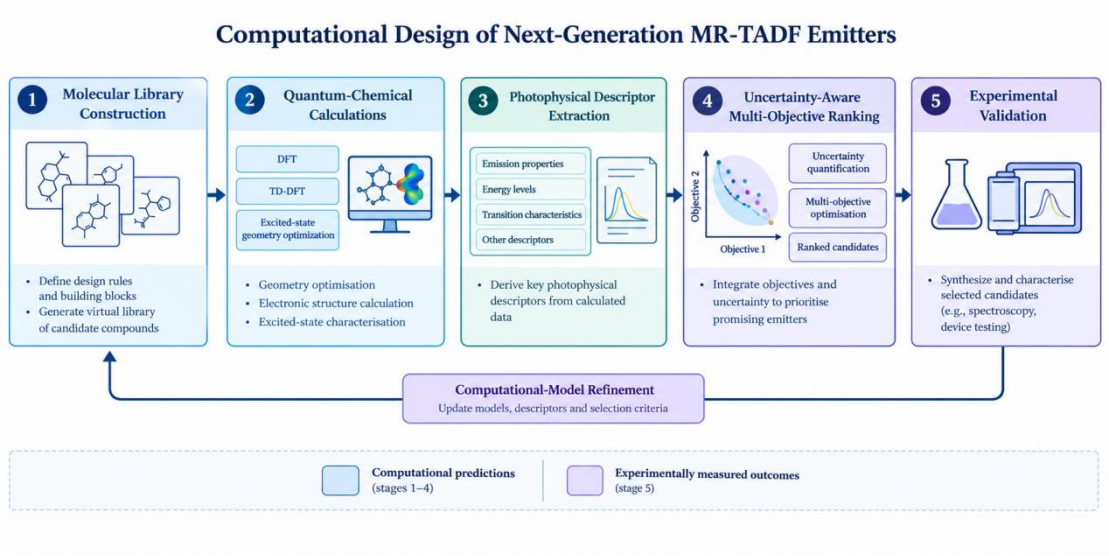
Aim and objectives. The aim is to develop a systematic approach for computationally prioritizing MR-TADF emitters for high-color-purity OLEDs. The objectives are to identify suitable molecular modifications, estimate relevant excited-state properties, evaluate competing design objectives, assess prediction uncertainty, and define a validation pathway connecting calculations with measured optical and device performance.

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Figure 1. Overall computational research framework



2. Literature Review

2.1. Molecular principles of MR-TADF

MR-TADF emission commonly arises from rigid conjugated structures in which electron-rich and electron-deficient atomic centers generate alternating frontier-orbital distributions. Boron–nitrogen-containing polycyclic aromatic frameworks are particularly prominent, although nitrogen–carbonyl and other heteroatom-containing systems have expanded the range of possible architectures.

The multiple-resonance effect depends on the spatial arrangement of these atomic centers and the resulting electronic structure, rather than simply the presence of particular heteroatoms. Appropriate orbital distributions can reduce exchange interaction while retaining sufficient transition strength for fluorescence. Molecular rigidity can also limit excited-state structural changes, reducing contributions to emission broadening.

Hatakeyama et al. (2016) established an important foundation for this field by demonstrating narrowband blue MR-TADF emission. Subsequent research has explored modifications to the aromatic core, conjugation, and steric environment to improve optical performance and molecular versatility.

A comprehensive review by Liu et al. (2025) discusses structural diversity across boron–nitrogen, nitrogen–carbonyl, and indolocarbazole MR frameworks. The review also identifies the difficulty of extending the range of emission colors without compromising the favorable properties of established structures.

2.2. Strategies for narrowing emission spectra

Emission bandwidth is influenced by excited-state structural relaxation, vibrational coupling, conformational flexibility, and interactions between neighboring molecules. Several complementary strategies are therefore relevant to computational molecular design.

First, molecular rigidification can limit geometric changes between ground and excited states. Second, controlled conjugation extension can modify emission energy and potentially improve spectral characteristics. Third, steric protection can reduce unfavorable intermolecular contacts and concentration-dependent quenching. Fourth, intramolecular interactions may stabilize molecular geometry, although their effects depend on the specific structure.

He et al. (2025) review spectral-narrowing strategies involving conjugation extension, molecular rigidity, bulky substituents, and intramolecular hydrogen bonding. Ni et al. (2025) discuss steric wrapping as an approach to reducing concentration-induced quenching and spectral broadening.

These strategies should not be treated as universally beneficial. Increased conjugation may change emission color or alter excited-state character, while bulky substituents can affect molecular packing and charge transport. Computational screening should therefore

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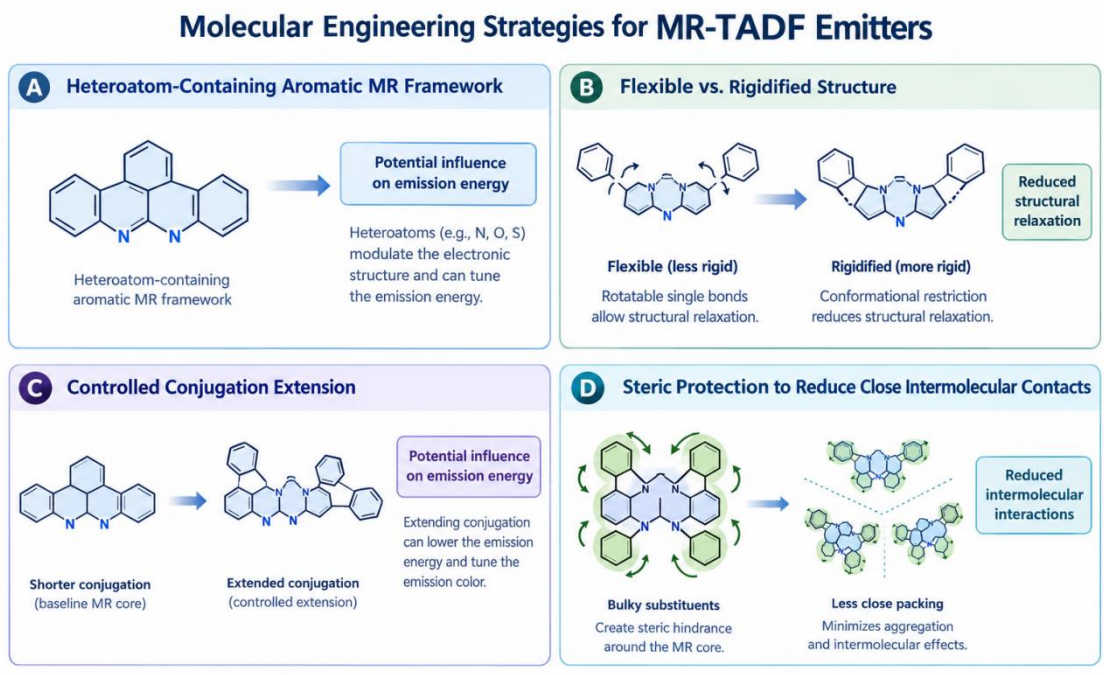
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evaluate the entire property profile of each candidate.

Table 1. Molecular design strategies and anticipated structure–property effects

Design strategy	Intended molecular effect	Properties to evaluate	Potential trade-off
Heteroatom-position engineering	Modify the multiple-resonance pattern	Orbital distribution, excited-state energies, oscillator strength	Loss of desired MR character
Core rigidification	Restrict structural relaxation	Geometry changes, reorganization energy, spectral width	Increased synthetic complexity
Controlled conjugation extension	Adjust emission energy	Excitation energies, oscillator strength, emission color	Broader emission or altered state character
Steric protection	Reduce unfavorable intermolecular contacts	Packing, aggregation sensitivity, concentration effects	Impaired charge transport
Intramolecular interaction engineering	Stabilize selected conformations	Conformational energies, geometry, spectral predictions	Additional conformers or unwanted electronic effects
Alternative MR scaffolds	Expand structural and color diversity	Electronic structure, stability, synthetic accessibility	Reduced reliability of existing predictive models

Figure 2. Molecular engineering strategies for narrowband emission



2.3. Excited-state energetics and delayed fluorescence

TADF relies on thermally assisted conversion of triplet excitons into emissive singlet states. The singlet–triplet energy difference, (\Delta E_{ST}), is therefore an important molecular descriptor. However, it cannot independently predict RISC rates or overall emission efficiency.

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Eng and Penfold (2020) explain that TADF performance depends on competing photophysical processes, including intersystem crossing, RISC, radiative decay, and nonradiative relaxation. Spin–orbit coupling, vibronic effects, excited-state character, and environmental interactions can all influence these processes.

A robust computational design should therefore combine energy-gap estimates with oscillator strengths, excited-state geometries, and kinetic descriptors where feasible. Candidates with favorable (\Delta E_{ST}) values should undergo further assessment rather than automatically being classified as high-performing emitters.

2.4. Computational approaches and predictive limitations

DFT is useful for optimizing ground-state geometries, while TD-DFT can estimate vertical excitation energies and transition strengths. Excited-state geometry optimization is important for evaluating emission and structural relaxation. However, predictions can depend on the functional, basis set, molecular conformation, and degree of charge-transfer character.

Ahmad et al. (2024) investigated mixed-reference spin-flip TD-DFT for MR emitters, addressing limitations associated with conventional linear-response TD-DFT. Their work supports using more advanced approaches for selected candidates when accurate excited-state ordering is essential.

Machine learning can accelerate candidate screening when sufficiently representative datasets are available. However, model predictions may become unreliable for molecular scaffolds that differ substantially from the training data. A combined approach rapid screening followed by quantum-chemical validation and experimental benchmarking is therefore preferable to reliance on a single method.

Table 2. Computational methods, applications, and limitations

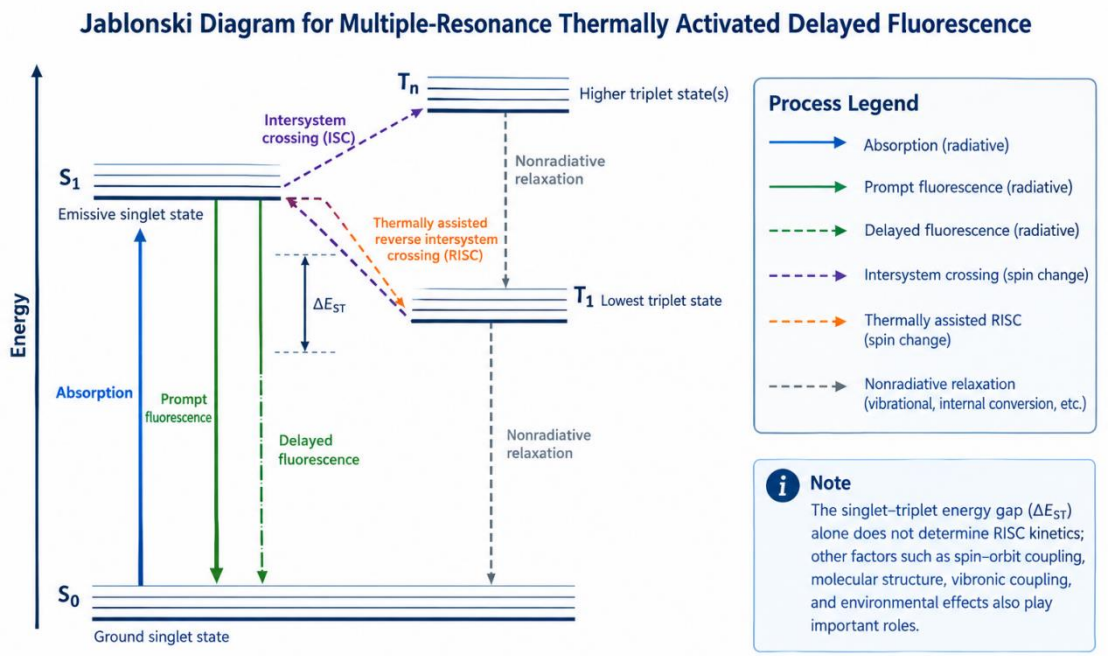
Method	Proposed application	Principal output	Main limitation
Ground-state DFT	Optimize molecular structures	Geometry, orbital energies, ground-state properties	Results depend on the functional and basis set
TD-DFT	Screen electronic transitions	Excitation energies and oscillator strengths	May misrepresent complex excited-state character
Excited-state optimization	Estimate emission properties	Relaxed excited-state geometry and emission energy	Higher computational cost
Vibrational/vibronic modeling	Estimate spectral shape and bandwidth	Simulated emission spectrum	Requires appropriate structural and vibrational treatment
Spin–orbit coupling analysis	Investigate spin-changing pathways	Coupling estimates for relevant states	Does not alone establish RISC kinetics
Spin-flip or multireference methods	Validate selected complex cases	Improved excited-state descriptions where appropriate	Computational expense and method-specific limitations
Molecular dynamics or conformer sampling	Examine flexibility and environment	Conformational distributions and sensitivity	Requires suitable sampling and environmental models
Machine learning	Prioritize large molecular	Rapid property predictions	Limited extrapolation beyond training data

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	libraries		

Figure 3. Excited-state processes governing MR-TADF



2.5. Solid-state effects and the remaining research gap

An isolated molecule may exhibit favorable calculated properties but perform differently in a solid film. Aggregation, host polarity, molecular packing, local electric fields, and intermolecular electronic coupling can influence emission energy, spectral width, and nonradiative decay.

Ni et al. (2025) emphasize concentration-dependent quenching and spectral broadening as continuing challenges for MR-TADF materials. These findings highlight the need to distinguish intrinsic molecular properties from environment-dependent behavior.

The unresolved problem is therefore not simply identifying a small energy gap or a rigid aromatic core. It is selecting molecules whose intrinsic excited-state characteristics remain favorable under realistic material and device conditions. This motivates a screening framework that combines molecular descriptors, uncertainty assessment, solid-state considerations, and experimental validation.

3. Conceptual Framework

The proposed framework links four levels of analysis.

Molecular architecture determines heteroatom connectivity, conjugation, steric environment, and structural rigidity. These characteristics influence electronic structure, including frontier-orbital distributions, excited-state energies, and transition probabilities. Electronic structure influences photophysical behavior, including emission wavelength, spectral bandwidth, RISC feasibility, and nonradiative losses. These properties then interact with charge transport, host materials, molecular packing, and degradation processes to influence OLED-device performance.

The framework is iterative rather than strictly linear. Experimental measurements may reveal shortcomings in computational assumptions, prompting revised molecular models or screening criteria.

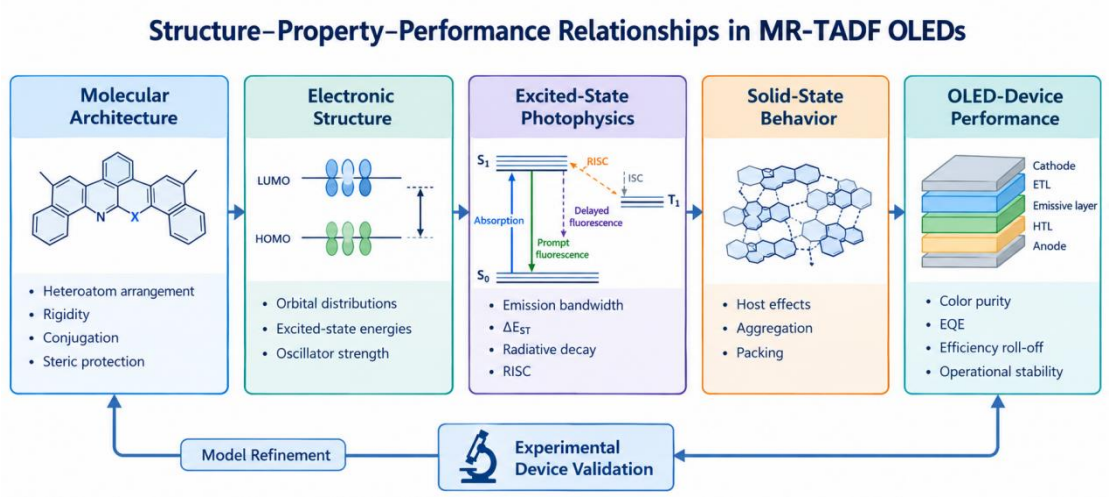
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Table 3. Conceptual framework variables and their roles

Framework level	Variables	Expected relationship	Validation approach
Molecular architecture	Heteroatom arrangement, rigidity, conjugation, steric protection	Establishes the electronic and structural characteristics of the molecule	Structural analysis and synthesis
Electronic structure	HOMO/LUMO distribution, excited-state energies, oscillator strength	Influences transition properties and state accessibility	DFT, TD-DFT, higher-level calculations
Photophysical behavior	Emission energy, bandwidth, RISC, radiative and nonradiative decay	Determines intrinsic emission characteristics	Spectroscopy and kinetic measurements
Solid-state environment	Host polarity, molecular packing, aggregation	Can modify emission and excited-state dynamics	Film spectroscopy and environment-aware modeling
Device performance	Color coordinates, EQE, efficiency roll-off, operational lifetime	Reflects combined optical, electrical, and degradation processes	OLED fabrication and device characterization

Figure 4. Structure–property–performance conceptual model



4. Results: Quantitative Synthesis of Recent Research

Recent experimental reports demonstrate that very narrow electroluminescence and high EQE can coexist in selected MR-TADF systems.

Study / molecular strategy	Reported photophysical result	Reported OLED result	Design implication
Zhou et al. (2026), B–N–B-embedded MR framework	PLQY 98–99%; solution FWHM 12–14 nm; kRISC 1.02–1.54 × 10^5 s^{-1}	EQEmax 37.9–38.3%; EL FWHM 15–17 nm; emissions at 453 and 499 nm	A hybrid B–N–B motif can combine narrow spectra, high PLQY, and enhanced spin conversion; environment and device architecture still matter.

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Lin et al. (2025), π-extension plus chalcogen effect	Peak at 453 nm; FWHM 17 nm; kRISC 3.0×10^6 s^{-1}	EQEmax 40.5%; EQE 38.4% at 100 cd m^{-2} and 28.2% at 1,000 cd m^{-2}; CIE (0.140, 0.059)	Combining transition-energy tuning with enhanced spin–orbit coupling can reduce the usual trade-off between color purity and RISC.
Li et al. (2025), indolocarbazole-embedded dual-boron MR emitters	Solution emission peak 490 nm; FWHM 18 and 19 nm	EQEmax 40.1% and 35.5%; EL FWHM 21 and 24 nm	Rigid alternative aza-polycyclic cores can provide blue–green emission below 500 nm with high device efficiency.
Hao et al. (2025), late-stage double borylation of B/N MR framework	ν-DABNA-M-B-Mes: PLQY 93%; FWHM 16 nm; kRISC 2.05×10^5 s^{-1}	EQE above 30%; sensitized device LT80 > 1,000 h at 100 cd m^{-2}	Synthetic accessibility, color tuning, and lifetime must be evaluated alongside narrowband emission.
Kim et al. (2025), longer-wavelength MR-TADF design	Study reports a narrow pure-green emitter; values depend on device/material configuration	PSF-OLED EQE 29.3%; LT95 6,019 h; TEOLED CIE (0.19, 0.76)	For longer-wavelength emitters, stability and color coordinates are as important as peak efficiency.
Cai et al. (2024), machine-learning-assisted DABNA-1 optimization	Top candidates predicted to show reduced reorganization energy and ΔEST; reported model R^2 0.77 and 0.72 for selected descriptors	No new device EQE established by the prediction exercise itself	Computational rankings can guide synthesis but must not be presented as experimentally validated device performance.
Shi et al. (2024), ML + VAE + DFT screening	Predicted high-PLQY blue-emitting candidates; predictions checked with quantum chemistry	Candidate discovery study, not proof that all proposed structures achieve device performance	Explainable and uncertainty-aware screening can expand the search space, but experimental validation remains essential.

4.1. Narrow bandwidth and high efficiency are increasingly compatible

The 2026 B–N–B-embedded system is especially relevant because it reports both high PLQY and narrow emission, then demonstrates that these molecular properties can translate into OLEDs with EQEs close to 38%. Its reported solution FWHM values of 12–14 nm and EL FWHM values of 15–17 nm show why solution spectroscopy alone is insufficient: device emission broadens relative to solution, although the bandwidth remains narrow. The study also reports RISC rates above 10^5 s^{-1}, supporting the need to assess excited-state kinetics alongside spectral shape (Zhou et al., 2026).

Lin et al. (2025) reported a deep-blue emitter with a 17 nm FWHM and an EQEmax of 40.5%, with comparatively high EQE retained at 100 and 1,000 cd m^{-2}. The reported RISC rate constant of 3.0×10^6 s^{-1} is a useful example of why a favorable ΔEST alone is not sufficient: molecular design can also target the spin–orbit coupling and state interactions that influence the conversion rate. These values are results from that specific molecular/device system and should not be generalized to every MR-TADF emitter.

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The indolocarbazole examples reported by Li et al. (2025) show that high EQE is not restricted to one canonical B/N scaffold. Their two emitters had solution emission at 490 nm with FWHM values of 18 and 19 nm, while their OLEDs achieved EQEs of 40.1% and 35.5% with EL bandwidths of 21 and 24 nm. This supports screening alternative rigid frameworks, particularly when the target color is near the blue–green boundary.

4.2. Color purity, kinetics, aggregation, and stability must be co-optimized

The studies collectively show that narrowing a spectrum is not an isolated molecular-design objective. The B–N–B work combines a rigid MR framework with helical distortion and reports high PLQY and RISC values, while the 2025 chalcogen strategy reports a high RISC rate with deep-blue emission. The late-stage borylation study by Hao et al. (2025) reports narrow emission alongside high PLQY and a long lifetime in a phosphor-sensitized device. These different approaches suggest that no single structural tactic is universally optimal; rather, the design depends on target wavelength, device architecture, synthetic constraints, and desired operational lifetime.

A further distinction is necessary between molecular photophysics and device performance. A molecule can have a high solution PLQY but show aggregation-induced broadening in a film, or it can show excellent peak EQE but strong roll-off at high luminance. Device lifetime depends on degradation pathways, charge balance, interfaces, and exciton density. The reported lifetime of a sensitized OLED should not be attributed to an isolated emitter alone.

4.3. What the literature implies for computational screening

The reviewed studies support a screening workflow with at least five simultaneous objective groups: (1) target color and FWHM; (2) radiative transition strength and PLQY-related indicators; (3) singlet–triplet energetics and RISC feasibility; (4) aggregation, packing, and environmental sensitivity; and (5) synthetic feasibility and device-relevant stability. Computational outputs should be assigned confidence levels based on method agreement, conformational sampling, and the similarity of each candidate to validated reference molecules. The evidence also highlights a critical gap: high-performing studies frequently combine molecular design with specific host materials, sensitizers, or device architectures. A model trained only on isolated-molecule descriptors may therefore rank the intrinsic emitter correctly but still fail to predict device EQE or lifetime. Device-level outcomes should be modeled only when sufficient matched data exist, and even then should be reported with uncertainty.

5. Proposed Computational Workflow

5.1. Molecular library and validity checks

The proposed study should begin with a documented library of experimentally reported MR-TADF scaffolds and chemically plausible derivatives. Candidate modifications may include heteroatom-position changes, controlled π-extension, rigidification, steric shielding, chalcogen incorporation, and alternative aza-polycyclic frameworks. Each structure should be checked for valence, charge, plausible connectivity, conformational flexibility, and synthetic accessibility before expensive calculations are attempted.

5.2. Quantum-chemical calculations

Ground-state geometries should be optimized with DFT and checked for convergence; frequency calculations should be used where appropriate to confirm minima. TD-DFT can provide initial excitation energies and oscillator strengths, but more than one suitable functional should be tested on a representative subset. Selected promising or electronically complex candidates should receive excited-state geometry optimization and, where justified, spin-flip or multireference calculations. Vertical and adiabatic energy gaps must be labeled separately.

5.3. Spectral, kinetic, and environmental descriptors

The descriptor set should include emission energy, oscillator strength, HOMO/LUMO localization, ΔEST, geometry displacement, reorganization energy, conformational sensitivity, and—where feasible—spin–orbit coupling and RISC-related estimates. FWHM

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should be estimated through vibronic modeling or ensemble methods, not inferred from a single geometry. Solvent, host polarity, concentration, and aggregation should be considered for the most promising structures through suitable environmental models or molecular simulations.

5.4. Multi-objective ranking and uncertainty

Candidates should not be ranked by a single weighted score unless the weighting scheme is justified and sensitivity-tested. A Pareto-front approach can identify molecules that offer different trade-offs between color, bandwidth, transition strength, kinetics, stability indicators, and synthetic complexity. Method disagreement should lower confidence rather than be hidden by averaging. Machine-learning models should report held-out performance, scaffold-aware validation, uncertainty estimates, and applicability limits.

5.5. Experimental validation

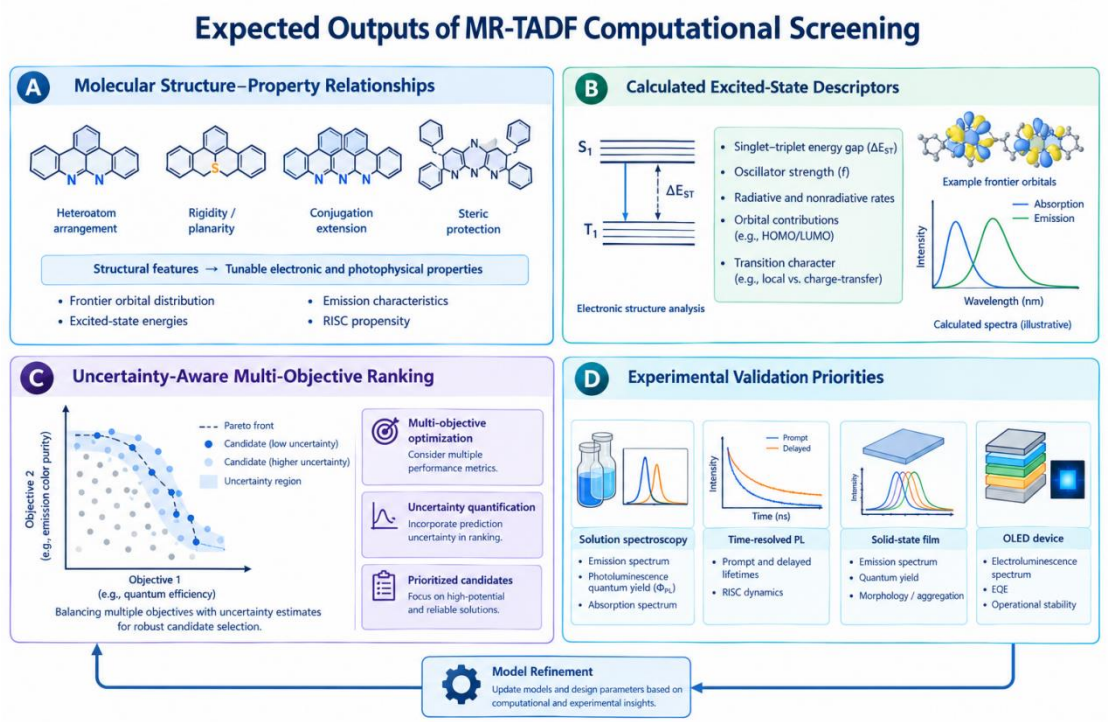
Validation should proceed from synthesis and structural characterization to solution absorption/emission, absolute PLQY, temperature-dependent time-resolved photoluminescence, and solid-film concentration studies. Only candidates that retain favorable properties in the relevant film environment should progress to OLED fabrication. Device testing should report EL peak, EL FWHM, CIE coordinates, EQE at multiple luminances, efficiency roll-off, maximum luminance, and operational lifetime under clearly stated conditions.

Stage	Main output	Decision criterion	Key caution
1. Chemical validation	Valid candidate structures	Plausible valence and synthetic route	Generated structures may be chemically inaccessible
2. DFT / TD-DFT	Geometries, state energies, oscillator strengths	Convergence and method agreement	Functional dependence and state-ordering errors
3. Excited-state refinement	Relaxed structures, emission estimates, ΔEST	Consistent state definitions	Do not mix vertical and adiabatic gaps
4. Spectral/kinetic analysis	FWHM estimates, reorganization, SOC/RISC indicators	Consistent multi-property profile	FWHM and RISC need more than a single descriptor
5. Environment assessment	Concentration/host sensitivity indicators	Properties remain plausible in films	Isolated-molecule predictions can be misleading
6. Pareto ranking	Shortlist with uncertainty	Competitive trade-offs and robust ranking	Avoid arbitrary single-metric optimization
7. Experimental validation	Measured spectra and device data	Agreement with predictions	Device EQE and lifetime are not computational facts

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Figure 5. Expected computational outputs



6. Discussion

Recent experimental work has moved MR-TADF development toward a regime in which very narrow emission and high EQE can be achieved simultaneously in selected systems. The 2026 B–N–B framework and the 2025 deep-blue and indolocarbazole examples illustrate that multiple molecular strategies can reach strong performance. The implication is not that one scaffold has universally solved the design problem, but that a broader search across molecular topology, heteroatom placement, rigidity, and spin-conversion pathways is justified.

The quantitative comparisons also clarify why headline values must be interpreted carefully. FWHM in solution, film photoluminescence, and electroluminescence are not interchangeable. EQEmax is not equivalent to EQE at high luminance, and a lifetime reported for a sensitized device is not a direct measure of intrinsic emitter stability. Cross-study comparison should therefore preserve device context and report several complementary metrics wherever possible.

Computational chemistry can help explain these results and prioritize follow-up candidates, but it cannot replace experiments. The 2024 machine-learning studies show that virtual screening can explore adjacent chemical space and suggest structures with favorable descriptors. They also show why prediction metrics and independent validation are important. The strongest workflow is hierarchical: inexpensive screening eliminates poor candidates, higher-level calculations investigate promising structures, and experimental results recalibrate the model.

The proposed framework advances the original concept by explicitly connecting molecular descriptors to the practical metrics used in published studies. It treats the emitter, solid-state environment, and OLED architecture as related but distinct layers. This separation is important for avoiding overclaiming: a predicted small ΔEST is a reason to investigate a candidate, not evidence that it will achieve a particular EQE, color coordinate, or operational lifetime.

7. Limitations and Future Research

This article is a focused narrative synthesis rather than a systematic review, and the selected studies do not represent every MR-TADF family or every result published by October 2026. Because the papers use different experimental protocols and device architectures, the values in Table 1 are illustrative rather than directly comparable under controlled conditions. The current article also does not

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report new DFT/TD-DFT calculations, a newly trained machine-learning model, or laboratory measurements.

Future work should establish a curated, machine-readable dataset that distinguishes solution, film, and electroluminescence measurements; records host, concentration, temperature, and device architecture; and links each value to the original paper and supporting information. Benchmarking should compare several quantum-chemical methods on a common subset. Models should be validated by molecular scaffold, and uncertainty should be propagated into the final candidate ranking. Promising candidates should be synthesized and tested in matched device architectures before device-level claims are made.

8. Conclusion

Recent MR-TADF research demonstrates that narrowband emission, high photoluminescence efficiency, fast RISC, and OLED EQEs approaching or exceeding 40% can coexist in selected molecular systems. The 2026 B–N–B-embedded platform, the 2025 chalcogen-assisted deep-blue emitter, and indolocarbazole-based emitters provide quantitative evidence that diverse molecular architectures can deliver high color purity and device efficiency. Machine-learning-assisted screening offers a complementary way to explore chemical space, provided its predictions are not mistaken for measured performance.

The most defensible next-generation design strategy is multi-objective and uncertainty-aware. It should assess spectral width, emission energy, transition strength, singlet–triplet energetics, RISC-related processes, environmental sensitivity, synthesis, and operational stability together. The framework presented here is intended to guide such work and make the connection between computational predictions and experimentally measurable OLED performance more transparent. Its proposed candidates and workflow must be validated through actual calculations, synthesis, spectroscopy, and device testing.

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