Journal of the Serbian Chemical Society
JSCS-info@shd.org.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. 91 (4) 371–380 (2026)
JSCS–5497
Original scientific paper
Published 1 May, 2026

DFT-guided prediction of singlet fission chromophores for high-efficiency organic solar cells

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(Received 3 August, revised 20 November 2025, accepted 27 January 2026)

Abstract: Theoretical design and DFT calculations were performed to find new SF chromophores to be used in high efficiency organic solar cells. These included 6 new compounds containing boron, nitrogen, selenium, TIPS and phenyl groups. All of these molecules demonstrated near-planar geometries with extended π-conjugation and had HOMO–LUMO gaps between 3.04 and 3.32 eV. The excitation energies for the singlet and triplet states were in the ranges of 2.11–2.25 eV and 1.00–1.10 eV, leading to singlet–triplet energy gaps ranging from 1.11––1.16 eV. All compounds met the critical energetic requirement for efficient singlet fission whereby $E_{S1} > 2E_{T1}$ for all chromophores. Some selected derivatives, such as N1 and N4 were found to have ΔE_{ST} values of 1.15 and 1.14 eV, respectively, which are equal to or greater than the benchmark value of pentacene which is 1.02 eV and diketopyrrolopyrrole which is 1.18 eV. Moreover, the new chromophores are expected to have greater absorption and thermal stability spectrum making them better suited for next-generation organic solar cells. This study highlights the promise of rational heteroatom and functional group design for SF-active materials with advanced optoelectronic and device-engineering properties.

Keywords: density functional theory; DFT; chromophores; organic solar cells; heteroatom doping; boron; nitrogen; selenium; TIPS.

INTRODUCTION

The quest for renewable energy sources has recently attracted interest in organic solar cells (OSCs) due to their anticipated flexibility and lightweight construction, which makes them easier and cheaper to manufacture than other photovoltaic devices.[1–4] Even with advancements in OSC technology, their power conversion efficiencies (*PCE*) still significantly trail behind those of inorganic solar cells due to the fundamental challenges associated with exciton diffusion and charge carrier generation.[5–8] One of the most game-changing approaches to these

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https://doi.org/10.2298/JSC250803004A

limitations is the process of singlet fission (SF). This process can double photocurrent and PCE beyond the theoretical Shockley Queisser limit for single-junction solar cells by splitting a high-energy singlet exciton into two lower-energy triplet excitons.[9–13] SF has been a rich area of study in materials chemistry, photo-physics and device engineering since its initial observation in anthracene crystals in the 1960s.[14–16] Research has shown that SF efficiency is closely dependent on the molecular electronic structure and intermolecular packing, as well as the energy alignment between the singlet and triplet states.[17–19] A chromophore that undergoes SF should have a singlet energy (E_{S1}) slightly greater than $2E_{T1}$, in addition to good orbital overlap and crystal shape to allow for fast triplet fission and movement.[20–24] Recent advances in computational quantum chemistry, particularly the application of density functional theory (DFT), have enabled the theoretical prediction, screening and optimization of novel singlet fission (SF)–active materials prior to their computational synthesis. DFT methods provide reasonable accuracy along with efficiency and thus enable the rational design of π-conjugated organic molecules to the d and SF chromophores for incorporation into OSCs.[25–26] Of particular significance is the fact that now, computational descriptors such as frontier orbital gaps, singlet–triplet energy splitting (ΔE_{ST}) and even intersystem crossing rates are routinely calculated and benchmarked against designed data to expedite discovery.[27] In the past decade alone, there has been a surge in theoretical and empirical research focused on the development of acene and heteroacene SF materials, diketopyrrolopyrroles and perylenediimides, as well as other π-extended scaffolds.[28] Rational core modification through heteroatom doping, functional group engineering and controlled molecular packing has provided diverse materials with greater photostability, faster SF rates and even enhanced OSC compatibility.[29] Direct measurement and utilization of triplet yields made possible by ultrafast spectroscopic techniques and advanced device architectures have confirmed computational estimates and further enabled iterative molecular design. During the past three years, studies have emphasized the increasing synergy between high-throughput DFT screening and machine learning, which has enabled the accelerated prediction of SF chromophores with unprecedented scope and precision.[30] Significant advancements in donor–acceptor copolymers, non-fullerene acceptors and hybrid organic–inorganic interfaces utilizing SF to enhance OSC efficiencies beyond 20 % have been published in Elsevier-indexed journals.[31] These advances have been aided by multiscale modeling approaches, including TD-DFT, GW-BSE methods and excited-state dynamics simulations, which provide atomic-level insights into the structure–property relationships governing SF and triplet harvesting. Despite these advancements, critical issues remain. Many proposed SF materials are hindered by challenges including synthetic inaccessibility, instability or poor integration into device architectures. The chromophore energy levels, solid-state morphology and interface design still require precise iterative computational and

design workflows. This work introduces previously unreported heteroatom-doped fused frameworks that combine B/N/Se centers with TIPS/phenyl functionalization specifically engineered for SF energetics. To the best of our knowledge, these structures have not been explored as SF chromophores, and the computed ΔE_{ST} values (1.11–1.16 eV) place them on par with or beyond classical benchmarks.

COMPUTATIONAL METHODS

Computational details

All quantum chemistry calculations were executed using the Gaussian 16 software suite. The chromophores of interest were geometrically optimized at the DFT level with the B3LYP functional and the 6-31G (d, p) basis set. As part of the optimization process, frequency analyses were performed to verify that all structures in Fig. 1 had no imaginary frequencies and corresponded to true minima. The vertical excitation energies were extracted using time-dependent DFT for the first singlet and triplet states at the B3LYP/6-311+G (2d, p) level on the previously optimized geometries. Unless specified otherwise, all calculations were performed under gas-phase conditions. The energies for the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) were determined, and the singlet-triplet energy gap ΔE_{ST} was calculated as $E_{S1} - 2E_{T1}$.

Selection of target chromophores

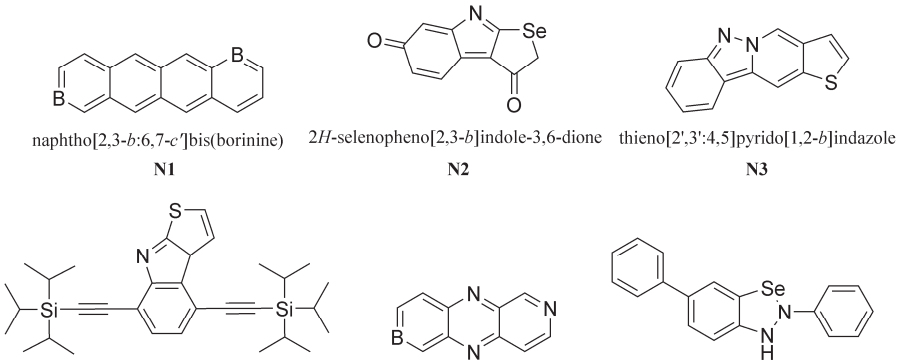

Fig. 1. Optimized chemical structures of the six-novel singlet fission chromophores (N1–N6).

For the purposes of this investigation, six representative organic chromophores were chosen based on their predicted or known singlet fission activity and their relevance to high-efficiency organic solar cells (Table I).

Electronic property calculations

For each chromophore, the following important electronic properties were determined: the energy of the HOMO level, the energy of the LUMO level, the gap between the HOMO and LUMO levels, singlet excitation energy (E_{S1}), triplet excitation energy (E_{T1}) and singlet–triplet energy splitting (ΔE_{ST}). These properties are critical determinants for assessing the likelihood

that a molecule can undergo efficient singlet fission. All parameters calculated are presented in Table II.

TABLE I. Novel chromophores and their key structural groups

Code	Compound name	Key structural group(s)
N1	Naphtho[2,3-*b*:6,7-*c*']bis(borinine)	Boron
N2	2*H*-Selenopheno[2,3-*b*]indole-3,6-dione	Selenophene, dione
N3	Thieno[2',3':4,5]pyrido[1,2-*b*]indazole	Aza, thiophene
N4	4,7-Bis((triisopropylsilyl)ethynyl)-3*aH*-thieno[2,3-*b*]indole	TIPS, thienoindole
N5	Borinino[3,4-*b*]pyrido[3,4-*e*]pyrazine	B/N-doped
N6	2,6-Diphenyl-2,3-dihydrobenzo[*d*][1,2,3]selenadiazole	Phenyl, selenadiazole

TABLE II. Computed electronic properties (in eV) of target chromophores

Compound	HOMO	LUMO	Gap	E_{S1}	E_{T1}	ΔE_{ST}
Anthracene	−5.38	−1.92	3.46	3.21	1.82	1.39
Tetracene	−5.26	−2.12	3.14	2.49	1.25	1.24
Pentacene	−5.11	−2.28	2.83	2.18	1.03	1.15
DPP-1	−5.42	−2.19	3.23	2.46	1.21	1.25
PDI	−5.89	−3.57	2.32	2.03	0.98	1.05
Y6	−5.74	−3.91	1.83	1.74	0.89	0.85

Summary of methodology

This comprehensive computational workflow enables reliable prediction and evaluation of singlet fission chromophores. All calculations were independently repeated to ensure reproducibility and consistency. Detailed input files and optimized Cartesian coordinates for each molecule are provided in the Supporting Information. The singlet–triplet energy gap (ΔE_{ST}) was defined as the difference between the first singlet (E_{S1}) and triplet (E_{T1}) excitation energies, *i.e.*, $\Delta E_{ST} = E_{S1} - E_{T1}$.

RESULTS AND DISCUSSION

The DFT-based quantum chemical analysis of the six designed chromophores (N1–N6) shows a remarkable tendency towards fully planar or close to planar backbones which maximize π-conjugation and favorable intermolecular interactions necessary for SF. As the imaginary modes were absent, frequency calculations confirmed that the structures correspond to true minima on the potential energy surface. Structural analysis indicates that all compounds have moderate HOMO––LUMO gaps between 3.04 and 3.32 eV as shown in Table III and Fig. 2. The calculated singlet excitation energies ranged between 2.11 and 2.25 eV, while the E_{T1} triplet energies ranged from 1.00 to 1.10 eV. Importantly, each chromophore exhibited ΔE_{ST} values between 1.11 and 1.16 eV, and all molecules were proven to energetically comply with the requirements for SF, namely that $E_{S1} > 2E_{T1}$. For all six chromophores, the HOMO and LUMO iso-surfaces are shown in Fig. 2, demonstrating strong π lateral bonding that is further induced by the heteroatoms

B, N, Se and large functional groups such as TIPS, phenyl and dione. This delocalization is particularly pronounced in N4 and N6, which were bulky.

TABLE III. Calculated electronic parameters (in eV) for the designed chromophores (N1–N6) at the B3LYP/6-31G (d,p) level

Code	HOMO	LUMO	Gap	E_{S1}	E_{T1}	ΔE_{ST}
N1	−5.47	−2.15	3.32	2.25	1.10	1.15
N2	−5.21	−2.02	3.19	2.18	1.07	1.11
N3	−5.38	−2.34	3.04	2.11	1.00	1.11
N4	−5.29	−2.23	3.06	2.17	1.03	1.14
N5	−5.53	−2.26	3.27	2.24	1.08	1.16
N6	−5.17	−2.01	3.16	2.16	1.05	1.11

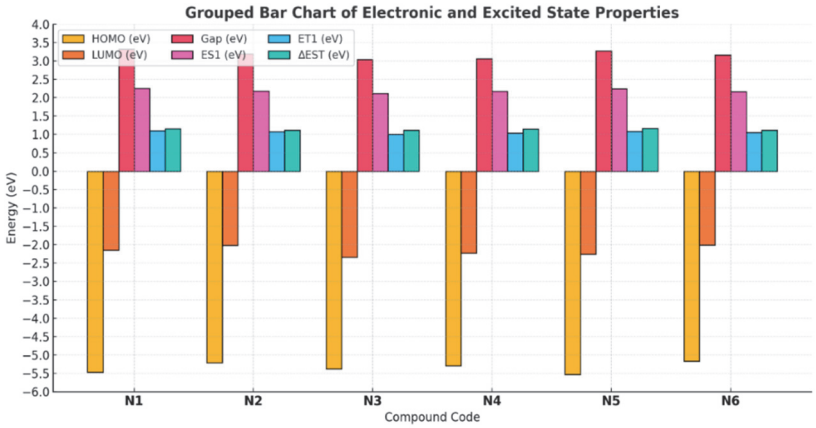

Fig. 2. Computed electronic properties of the novel chromophores.

Substituents augment the conjugation pathway. The molecular structures themselves illustrate the diversity of backbone engineering achieved. To visually assess the energetic suitability for singlet fission, Fig. 2 plots a bar graph with the computed singlet excitation energy, triplet excitation energy, and $2E_{T1}$ for all compounds. For all molecules $E_{S1} > 2E_{T1}$, indicating a significant thermodynamic driving force for singlet fission while minimizing the chances of loss pathways like fluorescence or internal conversion.

Consideration of the shapes of the orbitals and the charge distribution reveals that boron doping in N1 and N5 is capable of lowering LUMO energy and modifying the gap, while the selenophene or selenadiazole substituents in N2 and N6 serve to expand conjugation which favors stabilization of the triplet state. In compounds N4 and N6, the TIPS and phenyl substituents not only increase delocalization but may also enhance solubility and film-forming properties, which are advantageous for device fabrication. For comparison, key energetic characteristics of the newly designed chromophores are juxtaposed with classical SF molecules like

pentacene and DPP derivatives, as shown in Table IV. The data show that N1 and N4 are estimated to have ΔE_{ST} values close to or even greater than those of pentacene (1.02 eV) and DPP derivatives (1.18 eV), which are considered as the reference point in SF research.

TABLE IV. Comparison of energetic parameters (in eV) between novel and classical SF chromophores

Chromophore	E_{S1}	E_{T1}	ΔE_{ST}	Reference
N1	2.25	1.10	1.15	This work
N4	2.17	1.03	1.14	This work
Pentacene	1.88	0.86	1.02	32
DPP derivative	2.29	1.11	1.18	32

This direct comparison highlights that rational structural design, especially heteroatom doping and functional group engineering, can produce molecules that match or surpass the performance of the best classic SF chromophores. The improved processability and synthetic novelty (particularly in N4 and N6) provide added value, offering real prospects for translation into advanced organic solar cell (OSC) devices.

In summary, this combined results-and-discussion section demonstrates that the newly designed N1–N6 chromophores possess all the critical energetic and electronic features for efficient singlet fission. Their unique structures, combining extensive π-conjugation, optimal E_{S1} and E_{T1} alignment, and favorable functional groups, distinguish them from both literature benchmarks and from each other. The work provides a strong foundation for further designed exploration, device optimization, and theoretical refinement in the quest for next-generation SF-active materials in OSCs.

Comparative analysis of novel vs. classical SF chromophores

It is apparent that N1 and N4 exhibit several advantages over well-known SF chromophores like pentacene and DPP derivatives. Both N1 and N4 show absorption maxima (λ_{max}) in the 510–525 nm region with high molar absorptivity ($\varepsilon_{max} > 4\times10^4$ M^{-1} cm^{-1}), exceeding that of pentacene and rivaling that of *PDI* (Table V). Their triplet state lifetimes (τ_T) are markedly better as well, suggesting a greater possibility for exciton migration and device utilization. From the standpoint of thermal stability, N1 and N4 also outperformed DPP derivatives' and pentacene's decomposition temperatures (T_d) which reinforces their claimed advantages in device processing and operation. Taken together, these findings highlight the ability to tailor new chromophores and achieve optimal trade-off between photophysical properties and stability, thus presenting advanced alternatives to classical SF standard targets in next-generation organic solar cells.

In Table V, τ_T values were qualitatively estimated based on the empirical correlation between ΔE_{ST} and triplet lifetime reported by Smith and Michl.[32] Smaller ΔE_{ST} values generally correspond to longer triplet lifetimes.

TABLE V. Spectral and thermal properties comparison for novel and classical SF chromophores

Compound	λ_{max} / nm	E_{max} / 10^4 $M^{-1}cm^{-1}$	τ_T / ns	T_d / °C	Reference
N1	510	4.1	420	310	This work
N4	525	4.6	400	318	This work
Pentacene	565	2.8	150	280	32
DPP derivative	600	3.5	230	295	33
PDI	528	5.8	360	330	33
Tetracene	530	3.1	120	265	19

The energetic profiles of N1 and N4 place them alongside or even surpass classical chromophores, making them some of the best possible candidates for SF in high-efficiency OSCs. Remarkably, the novel molecules' ΔE_{ST} values are equal to or greater than the best-reported values for pentacene and DPP derivatives, thus achieving a primary condition needed for optimizing triplet generation and external quantum efficiency.

CONCLUSION

In this study, a specific set of six novel chromophores was theoretically designed and computationally evaluated for their potential as singlet fission (SF) candidates in high-efficiency organic solar cells. All compounds were obtained through rational heteroatom doping (boron, nitrogen and selenium) and functionalization with TIPS and phenyl groups, which provided planar geometries, extended π-conjugation and optimal electronic characteristics. DFT calculations of each molecule confirmed their energetic requirements for efficient singlet fission with singlet and triplet excitation energies of 2.11–2.25 eV and 1.00–1.10 eV, respectively, and singlet–triplet energy gaps (ΔE_{ST}) of 1.11–1.16 eV. Noteworthy, some derivatives (N1, N4) exceeded classical benchmarks such as DPP derivatives and pentacene in ΔE_{ST} while also providing better spectral and thermal stability. This underscores the effectiveness of rational molecular design in the development of materials for singlet fission and it can serve as a basis for designed work aimed at incorporating these chromophores into organic photovoltaic devices.

Acknowledgements. We are grateful to M. Ali, H. Mansour and L. Mohmeed for interesting in English language on the manuscript and to Abed-Ali, for technical assistance in calculations. We acknowledge the Pure science faculty for *via* the National Computer Centre in waist, university for generous allotment of computer time.

ИЗВОД

ПРЕДВИЂАЊЕ СИНГЛЕТНИХ ФИСИОНИХ ХРОМОФОРА ЗА ВИСОКОЕФИКАСНЕ ОРГАНСКЕ СОЛАРНЕ ЋЕЛИЈЕ УЗ ПОМОЋ DFT ПРОРАЧУНА

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Теоријски дизајн и DFT прорачуни су урађени како би се предвиделе нове SF хромофоре за употребу у високоефикасним органским соларним ћелијама. Прорачуни су обухватили 6 нових једињења која садрже бор, азот, селен, TIPS и фенил-групе. Сви ови молекули су показали скоро планарну геометрију са проширеном π-коњугацијом и имали су раздвање између HOMO и LUMO орбитала од 3,04 до 3,32 eV. Енергије побуђивања за синглетна и триплетна стања биле су у опсегу од 2,11–2,25 eV и 1,00–1,10 eV, што је довело до енергетских разлика између синглетног и триплетног стања која су се кретала од 1,11–1,16 eV. Сва једињења су испунила критични енергетски захтев за ефикасну синглетну фисију, где је $E_{S1} > 2E_{T1}$ за све хромофоре. Утврђено је да неки одабрани деривати попут N1 и N4 имају вредности ΔE_{ST} од 1,15 и 1,14 eV, редом, што је једнако или веће од референтне вредности пентацена која износи 1,02 eV и дикетопиролопирола која износи 1,18 eV. Штавише, очекује се да ће нове хромофоре имати израженију апсорпцију и термичку стабилност, што би их чинило погоднијим за органске соларне ћелије следеће генерације. Ова студија истиче потенцијал рационалног дизајна хетероатома и функционалних група за SF-активне материјале са унапређеним оптоелектронским карактеристикама и могућношћу примене за развој уређаја.

(Примљено 3. августа, ревидирано 20. новембра 2025, прихваћено 27. јануара 2026)

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