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Photophysical Insights of Blue–Green Emitting Oxadiazole: Efficient Energy Transfer in Core–Shell Quantum Dot Hybrids

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Abstract:

The development of blue–green emitting organic chromophores with excellent optoelectronic properties remains an important issue. In this context, the synthesis of a novel blue–green emitting chromophore, 2-(4-(2-(anthracen-10-yl)vinyl)phenyl)-5-(4-tert-butylphenyl)-1,3,4-oxadiazole (**AVBO**), was accomplished via the donor– π –acceptor (**D- π -A**) strategy using a **Wittig reaction**. The integration of aryl-heteroaryl groups and the oxadiazole group was utilized to obtain efficient blue–green emission with excellent optical properties. AVBO exhibited stable and efficient PL in the range of **485–510 nm** across diverse solvent environments. Solvatochromic analysis using multiple correlations (Lippert-Mataga, Bakhshiev, Kawski-Chamma-Viallet, and Reichardt) revealed a significantly higher excited-state dipole moment compared to the ground state ($\mu_e > \mu_g$), with a parallel orientation ($\varphi = 0^\circ$). The values calculated using these empirical equations were compared with those calculated computationally. Kamlet-Taft and Catalán MLR analyses further identified dominant non-specific solvent interactions (π^*) alongside specific hydrogen-bonding donor contributions. To explore its potential in optoelectronic applications, AVBO was integrated into hybrid systems with **ZnSe/ZnS core-shell quantum dots** (7–8 nm). This assembly functioned as a efficient **FRET mechanism**, reaching an efficiency of **88%** with Förster radii of **6.14–6.16 nm**. The quenching kinetics, validated by **Stern-Volmer plots**, showed both static and dynamic components with super-diffusion-limited rate constants ($k_q \approx 10^{14}$ /MS). Time-resolved photoluminescence (TRPL) confirmed energy transfer via dipole-dipole interactions. These findings highlight the AVBO-QDs hybrid as a promising, heavy-metal-free, and tunable emitter for light harvesting, photosensitization, and biosensing applications.

- 1 **Keywords:** 1,3,4-oxadiazole, Dipole moments, Solvatochromism, core-shell ZnSe/ZnS QDs,
- 2 FRET, Stern–Volmer plots.
- 3

1. Introduction

Organic chromophores with tailored photophysical properties play a central role in advanced optoelectronic systems due to their tunable emission characteristics, facile synthesis, and strong light–matter interactions. Among these, oxadiazole-based materials have attracted significant attention as functional emitters and charge–transport components in organic light-emitting diodes (OLEDs) and related photonic devices because of their robust thermal stability, bipolar charge-transport behavior, and high fluorescence quantum yields [1–4]. For example, donor– π –acceptor substituted oxadiazole derivatives have demonstrated strong fluorescence and solvatochromic behavior, indicating their potential in optoelectronic applications [5].

Recent research has continued to expand the library of oxadiazole derivatives with enhanced photophysical properties. New fluorescent small molecules comprising 1,2,4-oxadiazole scaffolds have exhibited improved emissive characteristics suitable for solid-state applications [6] and a series of novel oxadiazole-based fluorescent dyes have shown broad emission from violet to green (≈ 363 – 536 nm) with significant Stokes shifts, demonstrating the tunability of this class of chromophores [7]. These developments underscore the ongoing interest in oxadiazole systems for luminescent and sensing applications [8-9].

In parallel with progress in organic emitters, Quantum dots (QDs) are semiconductor nanocrystals with significant quantum confinement effects, which cause a distinct size dependence in the optical properties compared with bulk material [10-11]. Quantum dots comprise a broad class of semiconductor nanocrystals with size-dependent optical properties and discrete electronic levels. Quantum dots have a broad range of absorption and symmetric sharp peaks in the emission spectrum with a wide range of tunability across the UV and visible spectrum. Quantum dots with smaller core diameters have significant absorption peaks and emission peaks around 400 nm, which is highly desirable for UV applications. However, the presence of trap states on the surface of the core material is a significant drawback for core-only quantum dots. Quantum dots with a core-shell structure were synthesized with a wide band gap semiconductor material coating on the core material to enhance the PL quantum yield. Quantum dots with a core-shell structure also exhibit improved chemical and stability properties [12-13]. Such heterostructures exhibit improved excitonic confinement with sharp peaks around 400 nm, especially with ZnSe/ZnS and CdSe/ZnS systems, thereby expanding their utility in UV light-emitting devices, bioimaging, and photodetection technologies [14].

1 Zinc selenide, a kind of n-type II-VI semiconductor with a direct bandgap, has
2 gathered substantial attention due to its potential use in various optoelectronic devices such as
3 photodetectors, light-emitting diodes, and full-color display devices [15-16]. In order to
4 improve the optical properties of ZnSe, a variety of core-shell nanostructures have been
5 synthesized, wherein ZnS is used as a shell material. ZnS, with a relatively wide bandgap and
6 high exciton binding energy in bulk material, is effective in minimizing surface trap states,
7 thereby improving the emission intensity of the core nanocrystals [17-20]. In addition to this,
8 ZnS is effective in minimizing the environmental and biological toxicity of Cd-based cores
9 such as CdS [21-22]. In an earlier report, ZnSe is identified to be a potential host material for
10 incorporating dopant ions in nanocrystalline systems [23]. ZnSe/ZnS core-shell
11 nanostructures are highly advantageous due to lattice compatibility, which is effective in
12 confining charge carriers in ZnSe cores. These nanostructures are heavy metal free, toxic free
13 and highly efficient in terms of PL, chemical robustness, and minimizing surface defects,
14 making them highly promising candidates for a wide range of optoelectronic/photonic
15 devices and green chemistry [24-26].

16 The integration of organic chromophores with inorganic QDs in hybrid nanostructures
17 is of great promise to combine the benefits of organic molecules in terms of their tunability
18 and processability, with the high brightness and narrow emission of inorganic QDs. A crucial
19 mechanism in such hybrid systems is non-radiative energy transfer, particularly Förster
20 resonance energy transfer (FRET), where dipole–dipole coupling between QD donors and
21 organic acceptors can facilitate energy transfer when there is sufficient spectral overlap [27-
22 29]. Recent studies demonstrate engineered energy-transfer interactions in core-shell QD–dye
23 assemblies, enabling manipulation of donor–acceptor stoichiometry and spectral overlap to
24 achieve efficient energy transfer [29, 30-32]. These energy transfer interactions have been
25 quantified via steady-state and time-resolved fluorescence, revealing complex dependencies
26 on spectral properties and donor–acceptor configurations.

27 Despite significant advances in hybrid QD–organic systems, reports specifically
28 focusing on blue-green emitting oxadiazole chromophores integrated with core–shell QDs
29 through energy transfer mechanisms remain limited. For example, energy transfer processes
30 involving blue-emitting InP/ZnS QDs to organic dyes have been shown to achieve high
31 FRET efficiencies in aqueous environments, demonstrating the potential for efficient hybrid
32 photophysics [31]. However, there is a gap in literature regarding the coupling of novel
33 oxadiazole chromophores with heavy metal free and toxic free core–shell QDs for efficient
34 energy transfer and emission tuning. Addressing this gap by exploring tailored blue-green

oxadiazoles and their hybridization with QDs could open pathways for next-generation hybrid emitters.

In this work, we report the detailed photophysical characterization of a novel blue-green emitting oxadiazole AVBO chromophore and investigated its interaction with colloidal core-shell ZnSe/ZnS QDs via FRET mechanism. By conducting steady-state and time-resolved PL studies, we evaluate the energy transfer dynamics in these hybrids and identify key parameters governing efficient coupling between organic molecules and QD donors, offering insights for hybrid optoelectronic applications.

2. Experimental Section and Instrumentation

2.1 Materials: All the chemicals/starting materials of reagent/analytical grade are procured from Sigma-Aldrich, which are used as such without any further purification. Heavy metal-free and cadmium free core-shell ZnSe/ZnS-405 QD of size 7 nm (ZnSe/ZnS QD1) and ZnSe/ZnS-425 QD of size 8 nm (ZnSe/ZnS QD2) dispersed in toluene were procured from Mesolight LLC., USA. All the organic solvents that are used for the Photophysical properties exploration are of spectroscopic grade (HPLC grade, Fluka), transparent, and nonfluorescent in the region of the excitation and emission.

2.2 Steady state measurements: The absorption spectra were recorded using a commercial dual-beam JASCO UV-Vis NIR spectrophotometer (Model V-670). For the measurement of the PL spectra, a spectrofluorometer was used, which is a JY Horiba model Floromax-4 with Xe-lamp as excitation source. For this, the integration time was set to 1 s nm⁻¹, resolution to 1 nm, and the excitation and emission slit widths were set to 2 nm.

2.3 Time Resolved Photoluminescence (TRPL) Measurements $\langle\tau\rangle$: The PL lifetimes were recorded using a picosecond time domain spectrometer based on the Time Correlated Single Photon Counting approach. The average fluorescence lifetime $\langle\tau\rangle$ was found out using equation [33]: $\langle\tau\rangle = \frac{\sum A_i \tau_i}{\sum A_i}$, where A_i is the relative amplitude corresponding to the i^{th} decay component having the characteristic decay time constant τ_i . The acceptability of the fits was arbitrated from the χ^2 criterion and the residual of the fitted functions to the actual data.

For solvatochromism study of AVBO: The TRPL decays were recorded using DeltaproTM (HORIBA Scientific). AVBO sample in all solvents were excited at 415 nm using pulsed laser Deltadiode and the signals were collected at the magic angle of 50° to

eliminate the contribution from anisotropy decay [33]. The PL decay was then detected using New HORIBA Hybrid Picosecond Photon Detector (HPPD). The instrument response function (IRF) is 172 ps. The TRPL decays were recorded over 1024 channels with a minimum of 10,000 counts in the peak maximum. The decays were deconvoluted and analyzed on DAS-6 decay analysis software.

For FRET analysis: A NanoLED, in an IBH Fluorocube was employed as a pulsed excitation source. The TRPL, collected at the magic angle of 54.7°, was dispersed using a monochromator with an f/3 aperture to avoid the effect of anisotropy decay. The dispersed light was then detected using a Hamamatsu Micro Channel Plate Photo-multiplier tube detector (R3809 MCP-PMT). The samples of core-shell ZnSe/ZnS QD1 & QD2 with and without AVBO were excited at 280 nm. The instrument response function (IRF) was approximately 844 ps. The fluorescence decays were then deconvoluted and analyzed using IBH DAS6 software.

2.4 Absolute Quantum Yield Measurements (Φ): The fluorescence quantum yield measurement was done with the help of a Fluoromax-4 Spectrofluorometer from Horiba Jobin Yvon with an Xe lamp as the excitation source. The quantum yield measurement was done at room temperature with Coumarin 480 as the standard reference compound. The reference quantum yield (Φ_R) of 0.95 is reported in ethanol solvent (Absorption maximum at 389 nm and an emission maximum at 457 nm) [32]. The quantum yield of the compound under study was calculated with the help of the comparative method as per the standard protocol for the measurement of quantum yield with the refractive index of the compound under consideration and the integrated emission intensity and absorbance at the excitation wavelength with respect to the standard compound [33]. The equation used for the measurement of quantum yield with the help of the standard compound (Φ_R) and the integrated fluorescence intensity (I), absorbance at the excitation wavelength (OD), and refractive index (n) of the compound under consideration with respect to the standard compound with the subscript R for the compound with the known quantum yield is:

$$\Phi = \Phi_R \frac{I}{I_R} \frac{OD_R}{OD} \frac{n^2}{n_R^2}.$$

2.5 Synthesis and Characterization of Novel Fluorescent AVBO Derivative: Required intermediates (such as 2-(4-tert-butylphenyl)-5-p-tolyl-1,3,4-oxadiazole (**OXD**), 2-(4-(bromomethyl)phenyl)-5-(4-tert-butylphenyl)-1,3,4-oxadiazole (**1**), and Wittig salt (**2**) and highly conjugated novel donor- π -acceptor (D- π -A) fluorescent probe AVBO were

synthesised according to our previous work [1]. The molecular structure of AVBO is shown in **Scheme 1**. The detailed synthetic procedure and characterization are given in the ESI[†] (Section-1 to 5).

2.6 Physical Measurements: Fourier Transform Infrared spectroscopy (FT-IR) spectra were acquired using KBr pellet techniques on a Thermo Scientific Nicolet 6700 FT-IR instrument with a resolution of 2 cm⁻¹ and 100 scans in the region of 4000-400 cm⁻¹. Proton (¹H) and carbon (¹³C) nuclear magnetic resonance spectroscopy were recorded on a Bruker 400 MHz FT-NMR instrument using CDCl₃ as a solvent and tetramethylsilane as an internal reference compound. The values of chemical shifts are given in parts per million (ppm) as reference to tetramethylsilane. The melting points were recorded on an open capillary tube method without correction. The high-resolution mass spectrometric analysis was carried out on Agilent Technologies 6538 UHD Accurate-Mass Q-TOF LC/MS instrument.

2.7 Theoretical Background of Dipole Moment Estimation: Donor-acceptor dipolar molecules are highly polar and are significantly influenced by solvent polarity. The change in solvent polarity is reflected as changes in absorption and emission maxima, and this is known as solvatochromic shifts [34-35]. The shifts are directly related to changes in dipole moments between ground and excited states and are caused by changes in solute-solvent interactions [36-43]. Solvatochromic shifts are often used as a tool for calculating ground-state dipole moment (μ_g) and excited-state dipole moment (μ_e).

Quantitative measurement of values of μ_g and μ_e is possible through correlation of experimentally observed spectral shifts with solvent parameters such as refractive index (n) and relative permittivity (ϵ). There are several solvent polarity correlation equations that have been developed and are known as Lippert-Mataga (Eqn.(1)) [38-39], Bakhshiev (Eqn.(2)) [40], and Kawski-Chamma-Viallet (Eqn.(3)) [37, 41], which correlate Stokes shifts or transition energies with ϵ and n of the solvent and are useful for estimating values of dipole moments. Further, Bilot and Kawski [36-37, 44], extended these approaches by introducing quantum mechanical considerations into equations of solvatochromism and are useful for determining dipole moments of molecules in ground and singlet excited states.

$$\bar{\nu}_a - \bar{\nu}_f = \mathbf{m}_L f_1(n, \epsilon) + C \quad (1)$$

$$\bar{\nu}_a - \bar{\nu}_f = \mathbf{m}_B f_2(n, \epsilon) + C \quad (2)$$

$$\frac{\bar{\nu}_a + \bar{\nu}_f}{2} = -\mathbf{m}_K f_3(n, \epsilon) + C \quad (3)$$

here, $\bar{\nu}_a$ and $\bar{\nu}_f$ - absorption and fluorescence maxima wavenumbers, f_1 , f_2 , and f_3 - solvent polarity functions as given in Eqns. (4-6), respectively;

$$f_1(n, \varepsilon) = \left(\frac{\varepsilon-1}{2\varepsilon+1} \right) - \left(\frac{n^2-1}{2n^2+1} \right) \quad (4)$$

$$f_2(n, \varepsilon) = \left(\frac{2n^2+1}{n^2+2} \right) \left[\left(\frac{\varepsilon-1}{\varepsilon+2} \right) - \left(\frac{n^2-1}{n^2+2} \right) \right] \quad (5)$$

$$f_3(n, \varepsilon) = \left[\left(\frac{2n^2+1}{2(n^2+2)} \right) \left(\frac{\varepsilon-1}{\varepsilon+2} - \frac{n^2-1}{n^2+2} \right) + \frac{3}{2} \left(\frac{n^4-1}{(n^2+2)^2} \right) \right] \quad (6)$$

m_L , m_B , m_K - slopes obtained from linear plots and help to estimate μ_g and μ_e as given in Eqns. (7-8) in which c - velocity of light, h - Planck's constant, and a - Onsager radius;

$$m_L = m_B = \frac{2(\mu_e - \mu_g)^2}{hca^3} \quad (7)$$

$$m_K = \frac{2(\mu_e^2 - \mu_g^2)}{hca^3} \quad (8)$$

If the symmetry of the compound is unaltered for the ground and excited electronic states, the dipole moment directions are normally expected to be parallel [40]. In these cases, the values of μ_g and μ_e can be expressed as Eqns. (9) and (10);

$$\mu_g = \frac{m_K - m_B}{2} \sqrt{\frac{hca^3}{2m_B}} \quad (9)$$

$$\mu_e = \frac{m_K + m_B}{2} \sqrt{\frac{hca^3}{2m_B}} \quad (10)$$

For non-parallel dipole moments, the angle ϕ between μ_g and μ_e , can be computed using Eqn. (11) [37];

$$\cos\phi = \frac{1}{2\mu_g\mu_e} \left[(\mu_e^2 + \mu_g^2) - \frac{m_L}{m_K} (\mu_e^2 - \mu_g^2) \right] \quad (11)$$

An alternative method has been proposed by Reichardt [42,45], correlating spectral shifts with an empirical microscopic solvent polarity parameter defined by electronic transition energy (E_T). This method has been found to give better results than conventional methods relying on macroscopic solvent properties such as ε , and n . One of the advantages of this method is that it can be used to determine the excited state dipole moment with minimal uncertainty related to the Onsager cavity radius used. The correlation between spectral shifts and E_T may be described by the following equation:

$$\bar{\nu}_a - \bar{\nu}_f = m_R E_T + C \quad (12)$$

Here, m_R - slope obtained from linear plot and help to estimate difference between μ_g and μ_e as given in Eqn. (13);

$$\Delta\mu = (\mu_e - \mu_g) = \sqrt{m_R a^3 \cdot 3 \times 10^{-5}} \quad (13)$$

2.8 Multiple Linear Regression (MLR): Taft et al. [46-48] have proposed a MLR approach for a complete evaluation of the effects of solvents on spectroscopic properties. In this method, Stokes shift values and absorption transition energies are related to various polarity parameters of solvents. In this model, the ability of a solvent to engage in specific interactions is distinguished from non-specific interactions through its values for dipolarity/polarizability (π^*) [49], hydrogen-bond donor acidity (α) [47], and hydrogen-bond acceptor basicity (β) [48]. By using this analysis, the individual contribution of each solvent can be quantitatively evaluated as shown in Eqn. (14);

$$\text{Spectroscopic Property} = x_0 + a \cdot \alpha + b \cdot \beta + c \cdot \pi^* \quad (14)$$

where, x_0 - spectroscopic property in the gas phase, a, b, and c - regression coefficients.

The MLR proposed by Catalán employs solvent polarizability and dipolarity parameters to systematically evaluate the influence of solvent environment on absorption, emission, and Stokes shift energies [50] using Eqn. (15);

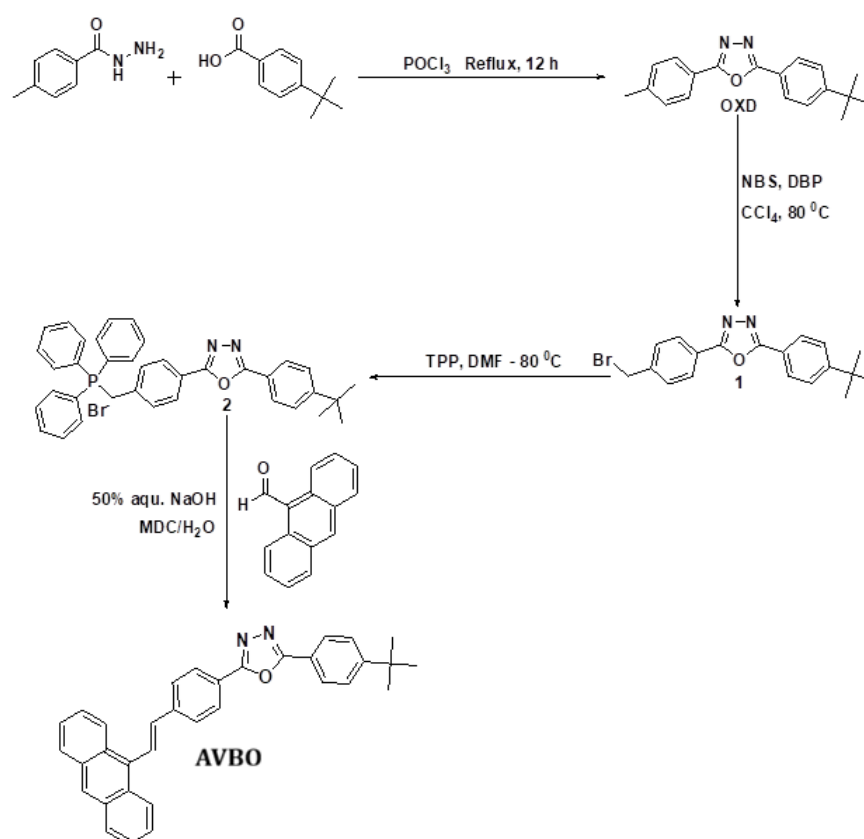
$$\text{Spectroscopic Property} = x_0 + d \cdot SA + e \cdot SB + f \cdot SP + g \cdot SdP \quad (15)$$

where SA , SB , SP and SdP - solvent acidity, solvent basicity, solvent polarizability and solvent dipolarizability, respectively; d , e , f and g - regression coefficients.

3. Results and Discussions

3.1 Synthesis and Characterization: Compound AVBO was synthesized by a simple and efficient synthetic protocol, as depicted in **Scheme 1**. The starting material, 2-(4-tert-butylphenyl)-5-p-tolyl-1,3,4-oxadiazole (**OXD**), was first synthesized by treating 4-methylbenzohydrazide (5.0 g, 3.32 mmol) with 4-tert-butylbenzoic acid (7.0g, 3.92 mmol) in refluxing POCl_3 (70 mL). The intermediate 2-(4-(bromomethyl)phenyl)-5-(4-tert-butylphenyl)-1,3,4-oxadiazole (**1**) was then synthesized by bromination of the **OXD** (5.0 g, 1.17 mmol) using N-bromosuccinimide (3.0 g, 1 equ) in the presence of dibenzoyl peroxide under reflux in carbon tetrachloride (CCl_4) (50 mL) yielded the intermediate (**1**). Treatment of this brominated intermediate (**1**) (4.0 g, 1.07 mmol) with triphenylphosphine (2.82, 1.07 mmol) in DMF (50 mL) at 80 °C afforded the corresponding phosphonium salt (**2**). A mixture of salt (**2**) (0.5 g, 0.00078 mol) and aldehyde (0.162 g, 1 equ) were taken in

1 Water:DCM (40:60) mixture under vigorous stirring. This Wittig salt (**2**) was then treated
 2 with aqueous sodium hydroxide and added to anthracene-9-carbaldehyde via a nucleophilic
 3 addition mechanism at the carbonyl carbon atom, producing a compound that further went
 4 through intramolecular cyclization to produce an oxaphosphetane ring. The ring then cleaved,
 5 producing triphenylphosphine oxide and the target product, AVBO. The product was then
 6 subjected to column chromatography on silica gel and further recrystallized from ethanol to
 7 produce the final product, which is a compound that is amorphous in nature and stable under
 8 ambient conditions without any signs of degradation. The structure and purity of the product
 9 were confirmed by ^1H , ^{13}C NMR, FT-IR, and HRMS (Section 3, 4 and 5 of ESI[†]) analyses,
 10 all showing that the product corresponds to the molecular structure that is expected.



Scheme 1. Synthetic route for AVBO.

13 The synthetic approach is very convenient and it produces AVBO in the *trans*
 14 configuration across the double bond. The all-*trans* configuration of the product can be
 15 proven with the help of ^1H -NMR. The AVBO has produced a doublet at the range 6.5-7.5
 16 ppm with the coupling constant about ca. 16.00-16.60 Hz. This number is consistent with the
 17 anticipated number for the $^3J_{\text{trans}}$ Coupling of the vinylic protons. In addition, evidence
 18 concerning the structures of **AVBO** were confirmed by FTIR, and mass spectrometry (MS).

The consistency between experimental/expected and calculated values confirms the purity of the molecule.

Yellow amorphous solid, yield: 65 %. Mp = 240-247 °C. FT-IR: 3300-3150 (C-H aromatic-anthracene, phenyl and vinylene), 3100 (C-H aliphatic), 1610-1560 (Oxadiazole ring C=C and C=N Stretching with aromatic rings), 1460-1360 (tert-Butyl), 1070-1010 (C-O-C), 700-900 (out of plane C-H bends-phenyl ring and anthracene); ¹H NMR (500 MHz, CDCl₃) δ: 8.45 (s, 1H), 8.37 (dd, *J* = 6.4, 3.3 Hz, 2H), 8.24 (d, *J* = 8.1 Hz, 2H), 8.15-8.04 (m, 5H), 7.83 (d, *J* = 8.1 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.52 (dd, *J* = 6.7, 3.1 Hz, 4H), 7.04 (d, *J*_{trans} = 16.6 Hz, 1H), 1.42 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ: 164.5, 164.10, 150.0, 138.7, 135.2, 132.4, 127.7, 127.4, 127.1, 126.3, 125.1, 123.1, 123.42, 123.20, 32.4, 31.4; MS m/z calculated for C₃₄H₂₈N₂O 480.60, Found 480.08803 (M⁺); Anal. Calcd (%) for C₃₄H₂₈N₂O: C, 84.97; H, 5.83; N, 5.83. Found: C, 84.95; H, 5.87; N, 5.87.

3.2 Photophysical Insights of AVBO

3.2.1 Absorption and Fluorescence spectra: Photophysical properties of AVBO are investigated in different solvent media as presented in **Fig. 1** and **Table 1**. Compound AVBO displayed solvent polarity-independent absorption spectra with broad band and a prominent peak in all the solvents considered. The intense broad bands centered at 350–460nm range are attributed to (i) $\pi \rightarrow \pi^*$ electronic transitions delocalized over the entire bipolar structure, (ii) vibronic overlaps, (iii) various optical transitions including HOMO→LUMO promotions, indicative of intramolecular charge transfer characteristics of a typical push-pull system [51-52].

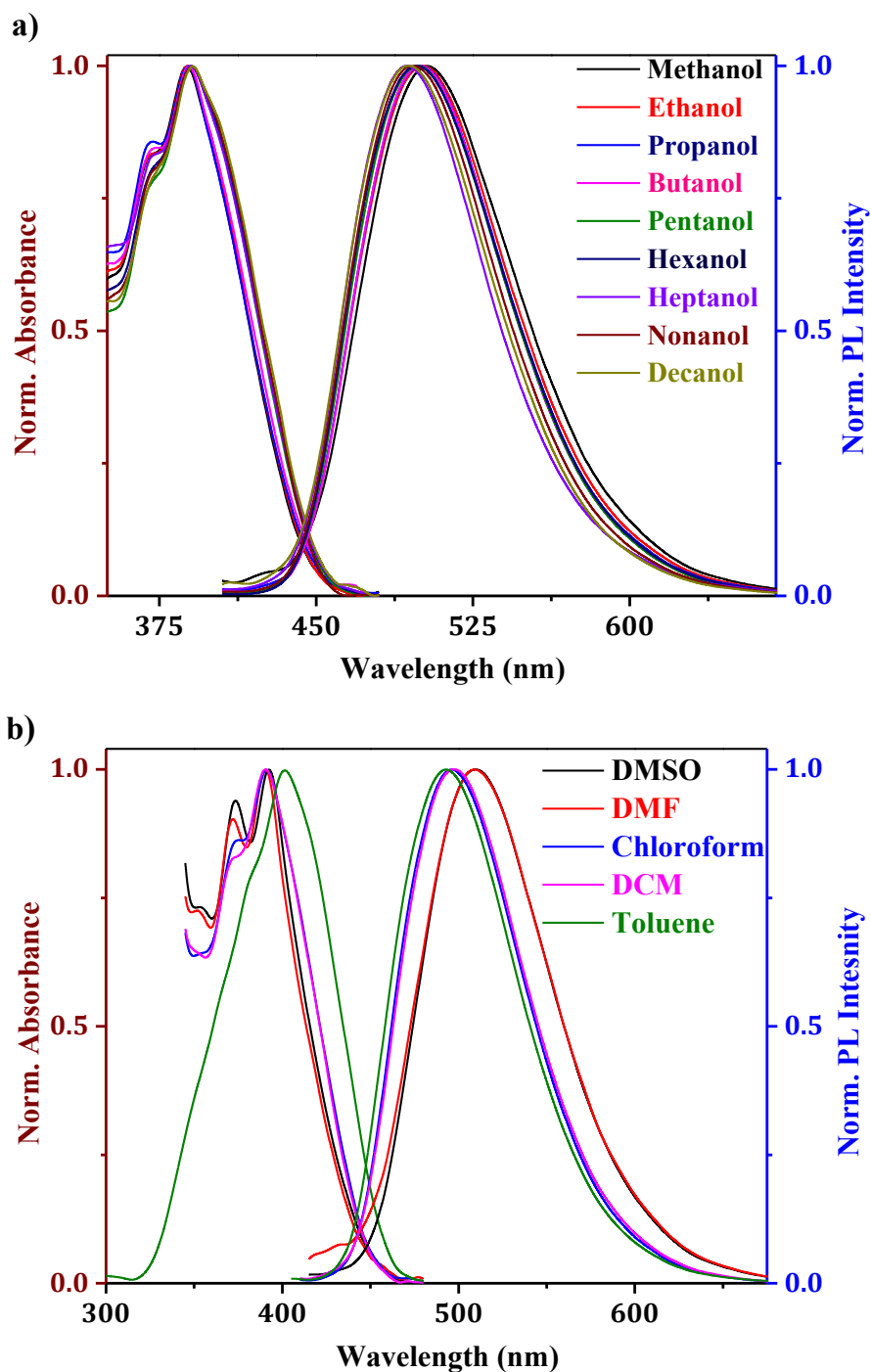


Fig.1: Normalized absorption and emission spectra of AVBO in (a) alcohols (methanol-decanol) and (b) general solvents. All the samples were measured at $1\mu\text{M}$ concentration at room temperature.

Table 1. Experimental spectroscopic properties of AVBO in various solvents measured at $\approx 1\mu\text{M}$ concentration and 300 K.

Solvent No.	Solvent	Absorption maxima, λ_{abs} (nm)	Emission maxima, λ_{em} (nm)	Stoke's shift, $\Delta\lambda$ (nm)	Average lifetime, τ_{f} (ns)#
1	Dimethyl Sulfoxide	393	507	114	1.25
2	N,N-imethylformamide	392	510	118	1.01
3	Chloroform	391	496	105	2.13
4	Dichloromethane	390	493	103	2.13
5	Toluene	393	491	98	2.51
6	Methanol	388	503	115	0.66
7	Ethanol	387	501	114	1.02
8	Propanol	388	502	114	1.25
9	Butanol	389	500	111	1.45
10	Pentanol	391	498	107	1.59
11	Hexanol	390	499	109	1.73
12	Heptanol	390	492	102	1.87
13	Nonanol	391	496	105	1.99
14	Decanol	392	493	101	2.13

Individual lifetime components are given in **Table S2** (ESI[†] Section 9).

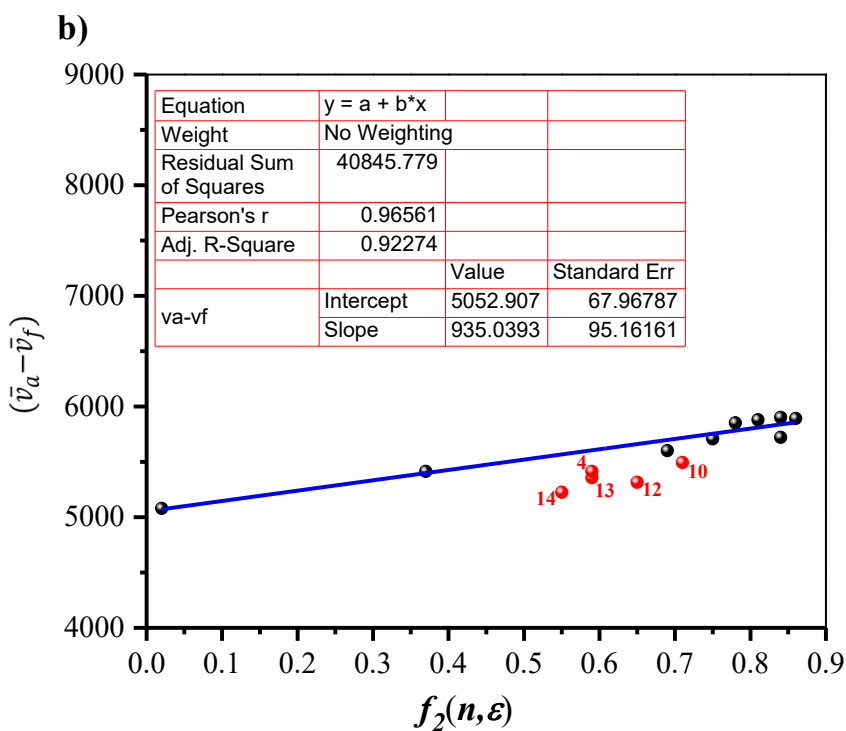
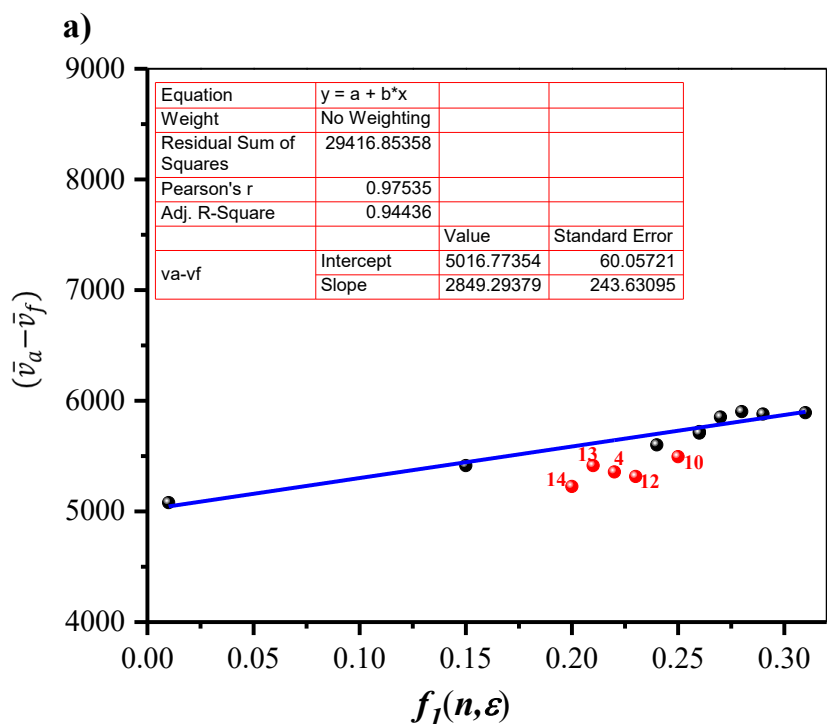
PL spectroscopy provides further clarification on the electronic structure of AVBO. The emission profiles have shown excitation-independence nature, which mean that the emission profiles are the same regardless of the excitation wavelengths for the $S_4/S_3/S_2/S_1$ states. The emission maximum (λ_{max}) remains the same at around blue-green region ~ 500 nm. This observation confirms the idea that the relaxation process funnels into the lowest singlet excited state with radiative decay, with the least non-radiative loss. The maximum PL quantum yield/intensity were recorded with the compound excited at 390nm, which matches the onset of the $S_1 \leftarrow S_0$ transition. Emission spectra in all solvents is broader and structureless, having full width at half maximum around 95nm. In addition, AVBO notably shows a substantial Stokes shift in the range of 98-115nm depending on the solvent used as a result of excited-state structural relaxation, solvent reorganization, and the extensive π -conjugation of the bipolar structure that increases ICT while reducing self-quenching

processes. This makes AVBO a potential fluorophore with potential applications in bioimaging or sensing.

3.2.2 Solvatochromism of AVBO: Experimental and Theoretical Study of Electronic Dipole Moments

Solvatochromic behavior of AVBO was investigated by correlating spectral band shifts with solvent polarity using the Lippert–Mataga Eqn.(1), Bakhshiev Eqn.(2), Kawski–Chamma–Viallet Eqn.(3), and Reichardt Eqn.(12) linear relationships. Absorption maxima ($\bar{\nu}_a$) and emission maxima ($\bar{\nu}_f$), along with other solvatochromic shift parameters for the AVBO, were measured in different solvents spanning a wide polarity range such as nonpolar solvent (Solvent No. 5), moderately polar solvents (Solvent No. 3&4), polar aprotic solvents (Solvent No. 1&2) and polar protic solvents (Solvent No. 6 to 14) to understand the ICT effect as displayed in **Fig. 1** and **Table 1**. Corresponding spectral shift data of AVBO and solvent polarity functions at room temperature are presented in Table S1 (ESI[†]). It is observed that $\bar{\nu}_f$ are significantly affected and more solvent-dependent compared to $\bar{\nu}_a$ in all solvents. This implies a large dipolar nature in the excited state compared to that in the ground state for AVBO. Plots of $(\bar{\nu}_a - \bar{\nu}_f)$ v/s. f_1, f_2, E_T , and $(\bar{\nu}_a + \bar{\nu}_f)/2$ v/s. f_3 are shown in **Fig. 2(a-d)**. Inset of these graphs contains linear fit data such as correlation coefficient R^2 value, intercept, slope, standard errors, etc. Data points (red) with solvent numbering are excluded based on deviations from the assumptions of continuum dielectric models. These deviations (both positive and negative) from the regression straight line suggest that solvatochromism of AVBO could not be explained only by the continuum dielectric models. The value of correlation coefficient, $R^2 > 0.90$ was observed, implying that the photophysical properties of AVBO are predominately governed by the effects of nonspecific solvent polarity. The linearity proves that there exists an ICT excited state with a higher dipole moment compared to the ground state. However, it was found that there were considerable non-linearities with respect to some solvents. These deviations from linearity indicate that the description of excited state behavior using dielectric continuum model alone is not adequate. Positive deviations of solvent 1 and 2 are due to their ability to donate electrons and accept hydrogen bonds and therefore, to stabilize the ICT excited state effectively. Negative deviations of solvent 4 and some long chain alcohols (solvent 10-14) are associated with their low donor capacity, reduced solvent relaxation, solvent micro-heterogeneity, hydrogen bonded associations, and hydrophobic solvation. On the other hand, specific hydrogen bonding in solvent 3 and short chain alcohols (solvent 1 and/or 2) and π – π and dispersion interactions

1 between the solvent 5 and the anthracene part of the AVBO contribute to the observed non-
2 linearities. Thus, besides the bulk solvent polarity effect, specific type interactions and
3 solvent dynamics play a title role in determining the photophysical properties of AVBO.



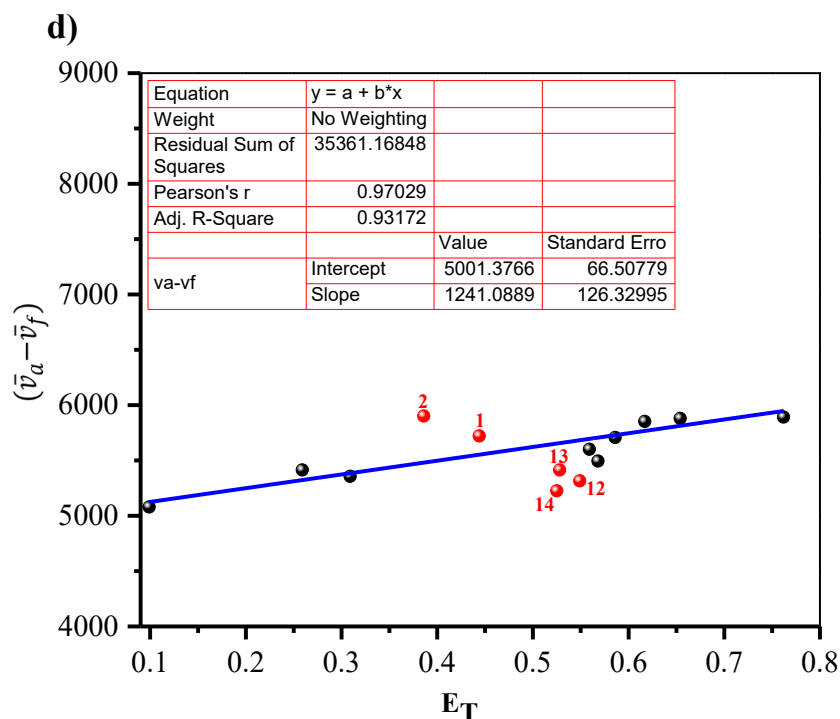
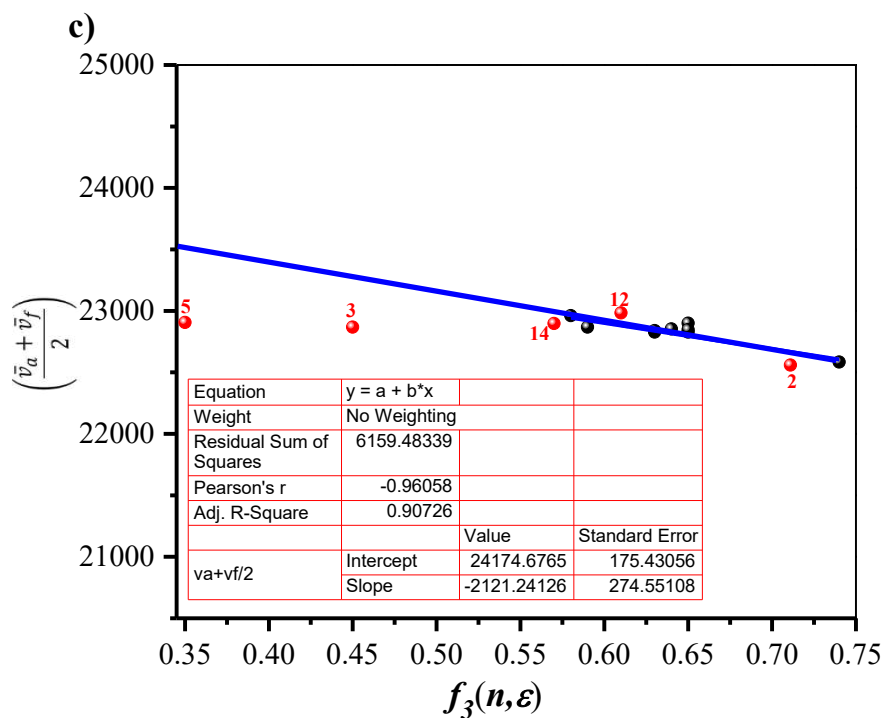


Fig. 2: Linear plots of (a) Lippert–Mataga, (b) Bakhshiev, (c) Kawski–Chamma– Viallet and (d) Reichardt correlation methods for AVBO in various solvents covering wide polarity range such as nonpolar, moderately polar, polar aprotic and polar protic solvents.

Theoretical dipole moments and Onsager cavity radius (a) were calculated using the Gaussian 09 software package [53], applying DFT with the CAM-B3LYP/6-31G hybrid functional for the ground state, μ_g and TD-DFT formalism at the same level for the excited

state, μ_e in vacuum. These computations yielded μ_g of 3.78 D for AVBO, with corresponding μ_e value of 4.08 D (**Table 2**). These findings specify modest polarity in the ground state, with AVBO exhibiting the enhanced excited-state dipole moment. Whereas, experimental μ_g and μ_e values were determined from the slopes m_K and m_B of Kawski–Chamma–Viallet and Bakhshiev correlations using Eqn. (9) and (10) and found 2.20 D and 5.66 D, respectively. The μ_e values are varied as estimated by Lippert-Mataga (Eqn. 7), Bakhshiev (Eqn. 7), Kawski-Chamma-Viallet (Eqn. 8), and Reichardt (Eqn. (13) - yielding 5.66-8.24 D for AVBO, with Reichardt values providing the most consistent values (**Table 3**). Same trend (regarding modest polarity in the ground state and enhanced excited-state dipole moment) is observed experimentally and computationally.

The discrepancies in the results on excited-state dipole moments in solvatochromism using different models result from different assumptions that are used to arrive at these results. The Lippert-Mataga theory considers only the dielectric stabilization aspect, while the Bakhshiev–Kawski–Chamma–Viallet theory takes into consideration solvent polarization besides the dielectric stabilization theory and the Reichardt method reflects empirical solvent–solute interactions. Thus, discrepancies in μ_e values are expected and provides complementary insight into excited-state charge redistribution rather than methodological inconsistency.

Table 2: Theoretical and experimental dipole moments of two electronic states (μ' in Debye) of AVBO.

a^*	μ_g^*	μ_e^*	$\mu_g^\#$	$\mu_e^\#$	$\mu_e^{[a]}$	$\mu_e^{[b]}$	$\mu_e^{[c]}$	$\mu_e^{[d]}$	$\Delta\mu^{[e]}$	(μ_e/μ_g)	Φ^s
5.05	3.78	4.08	2.20	5.66	8.24	5.66	5.66	4.39	2.19	2.58	0

* The Onsager radius (a in Å), electronic ground (μ_g)- and excited-state (μ_e) dipole moments obtained from DFT and TD-DFT methods at CAM-B3LYP/6-31G, using the G09 package.

[#] Ground (μ_g)- and excited-state (μ_e) dipole moments obtained experimentally using Kawski–Chamma–Viallet and Bakhshiev correlation [Eqn.9 and 10].

[a], [b], [c], [d] (μ_e) values experimentally estimated using the Lippert-Mataga Eqn. (7), Bakhshiev Eqn. (7), Kawski–Chamma–Viallet Eqn. (8), and Reichardt Eqn. (13) correlations, respectively.

[e] Difference between μ_g - and μ_e calculated using Reichardt Eqn. (13).

^s Angle between the μ_g - and μ_e (ϕ in degree) obtained using Eqn. (11).

It is interestingly observed that μ_e values of AVBO are exceeded the μ_g value, confirming enhanced polarization in this optoelectronic material upon photoexcitation. This trend aligns with predictions from both DFT and TD-DFT calculations. The various factors that contribute to the high excited state polarizability of AVBO include differences in charge distribution between electronic states, conformational changes like torsional rotations and deviations from planarity, enhanced solute-solvent interactions in the S_1 state, intramolecular charge transfer, and/or solvent-induced intramolecular hydrogen bonding. The Lippert-Mataga method was found to give the highest values of μ_e as it ignores polarizability of the solute AVBO. On the other hand, Reichardt correlation revealed that the change in dipole moments between the ground and excited states was found to be more positive (i.e., $\Delta\mu \approx 2.19$ D) ensuing the more dipolar nature of AVBO in the excited state. The linear relationship between $(\bar{\nu}_A - \bar{\nu}_F)$ and E_T implies dominant general solute-solvent interactions; however, slight variations in the data confirm the presence of specific solute-solvent interactions as well (see **Fig. 2d**). Bakhshiev–Kawski–Chamma–Viallet correlations and DFT/TD-DFT calculations gave $\mu_e/\mu_g \gg 1$, which confirms that the excited state of AVBO is highly polarized. The angle between dipole moments in the ground and excited states is 0° indicating parallel alignment of the two states.

The solvatochromic analysis relies primarily on steady-state spectral shifts; time-resolved measurements are included as complementary evidence of excited-state dynamics. The changes in dipole moments are primarily responsible for spectral shifts in steady-state solvatochromism, whereas excited-state conformation stability is monitored via PL lifetimes [54-55]. Generally speaking, PL lifetimes tend to increase with increasing solvent polarizability as excited-state stability is enhanced. PL lifetime decay profiles of AVBO were measured for various solvents with polarizability ranging from polar protic-moderately polar-polar aprotic- to nonpolar solvent (See **Fig. 3** and **Table 1**).

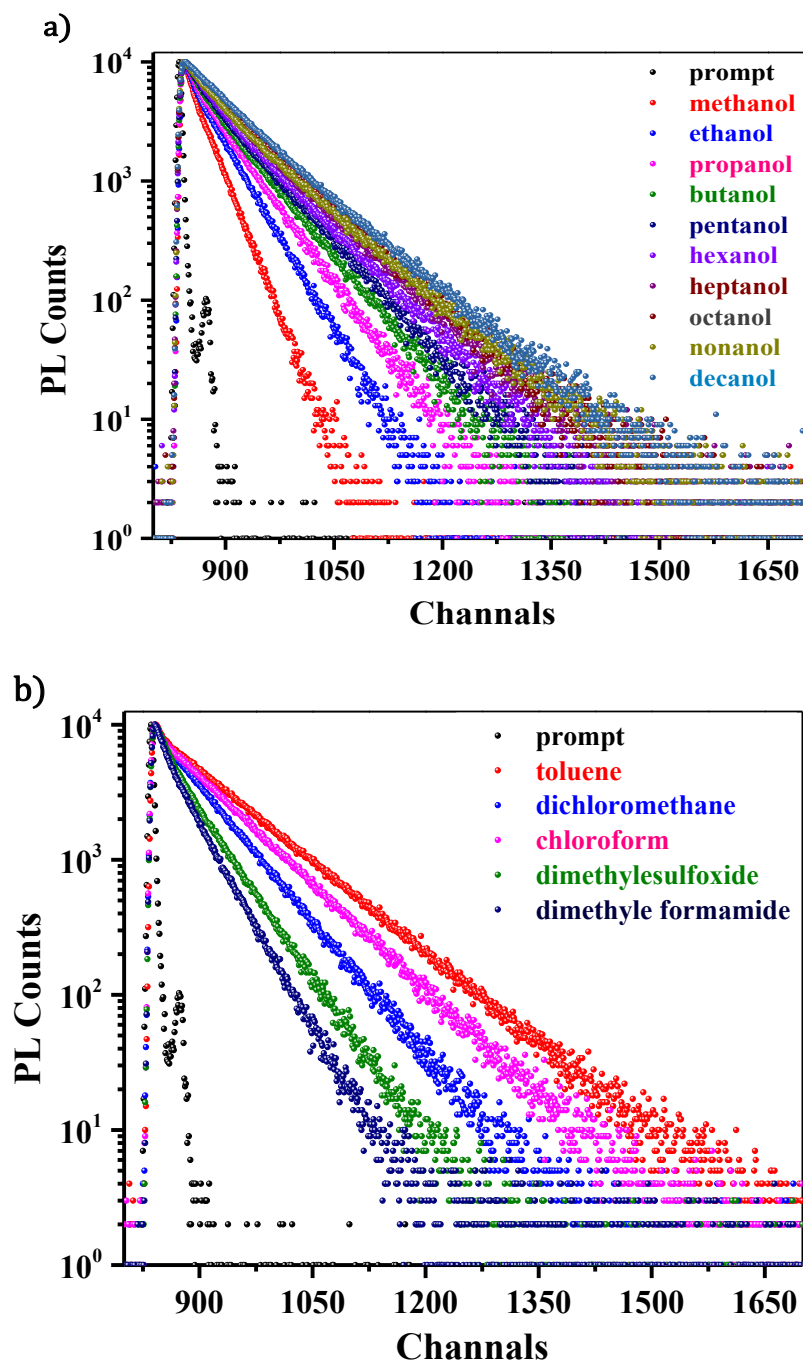


Fig. 3: Typical time resolved fluorescence decay profiles of AVBO (a) in alcohols (methanol-decanol) and (b) general solvents. The sharp black profile on the extreme left represents the instrument response function (IRF). (1 Channel=0.02743484 ns).

In series of polar protic solvents (methanol to decanol), it was found that AVBO PL lifetimes increase with increasing solvent polarizability. On the other hand, lifetimes in DMSO and DMF were found to be lower than in longer homologous aliphatic alcohols (butanol-decanol), indicating a mildly nonlinear relationship with solvent polarizability and implying that excited-state stability is also affected by solvent viscosity [56].

3.2.3 Multiple Linear Regression (MLR) analysis:

MLR shows the nature of solute-solvent interaction, distinguishing between general/non-specific and specific types. Non-specific interactions are ruled by the solvent's refractive index (n) and relative permittivity (ϵ) which influence dipole moments and electron delocalization within the medium. Specific interactions, by contrast, related to specific chemical processes such as hydrogen bonding or complex formation between solute and solvent. For AVBO, MLR is based on Kamlet–Taft solvatochromic parameters (α , hydrogen-bond donating ability; β , hydrogen bond accepting ability; and π^* , dipolarity/polarizability) to correlate spectral shifts ($\bar{\nu}_a - \bar{\nu}_f$) via Eqn. (14). The Kamlet-Taft model is applied to the solvents under investigation using Eqn. (16);

$$\bar{\nu}_a - \bar{\nu}_f = 4521 + 561 \cdot \alpha + 408 \cdot \beta + 1009 \cdot \pi^* \quad ; r^2 = 0.88 \quad \& \quad F = 12.5 \quad (16)$$

In Eqn. (16), the positive signs of the regression coefficient values for α , β , and π^* indicate that all these factors including hydrogen-bond interactions and solvent polarity, play an important role in determining the solvatochromic shifts of the molecule. Among these parameters, the values of coefficient, 'c=1009' (for π^* dipolarity/polarizability) is greater than the coefficients 'a' (for α , hydrogen bond donation) and 'b' (for β , hydrogen bond acceptance) for AVBO, confirming that the solvent's dipolarity/polarizability is the most significant factor for the solute-solvent interactions, and non-specific effects are responsible for the spectral shifts. The higher values of 'a' coefficients compared to 'b' coefficients also demonstrate that the hydrogen bond donating ability of the solvent is more significant than the hydrogen bond accepting ability for the electronic states. The correlation coefficient is 0.88, which infers a very good correlation between the experimentally observed results and the regression results. Furthermore, F-value is 12.50, indicates that regression model is statistically significant.

Additionally, Catalán's multiparameter approach correlates spectral shifts ($\bar{\nu}_A - \bar{\nu}_F$) with SA, SB, SP and SdP according to Eqn. (15). Regression coefficients for AVBO were derived from the studied solvents and are summarized in Eqn. (17);

$$\bar{\nu}_a - \bar{\nu}_f = 6873 - 514 \cdot SA + 193 \cdot SB - 2796 \cdot SP + 1051 \cdot SdP \quad ; r^2 = 0.92 \quad \& \quad F = 24.7 \quad (17)$$

The Catalán correlation coefficients d for SA, e for SB, f for SP and g for SdP show a similar trend as those of a (α), b (β), and c (π^*) from the Kamlet–Taft approach. The coefficient values of SP and SdP of solvents have more impact on spectral shifts compared

SA and SB signifies that general type interactions are significant than specific type. These results indicate that dipolarity/polarizability plays a crucial role in governing spectral shifts and solute–solvent interactions (same trend is predicted by the Kamlet–Taft approach as well. Thus, AVBO compound has higher electronic excited-state dipole moments compared to their ground-state. The relatively higher SA coefficient value compared to SB indicates that ‘hydrogen-bond donating interactions’ of the solvent play a more dominant role, likely due to presence of extended conjugation. Furthermore, high and positive F-values, indicate that Catalán's regression model is statistically significant. It is thus evident that, both models are effectively characterize the blend of specific and general/non-specific solute-solvent interactions.

3.3 Spectroscopic studies: Photo-triggered Resonance Energy Transfer

3.3.1 Steady-state experiments: The heavy metal free, toxic free, stability, unique optical properties and high quantum yield of ZnSe/ZnS QDs fortified us to examine their suitability as efficient donors for light harvesting studies with novel AVBO compound as efficient acceptor (**Fig. 4**). The spectral overlap integral was calculated using Eqn. (S3†) and found a high value of 8.65×10^{15} and 8.47×10^{15} nm⁴/M cm for ZnSe/ZnS-QD1::AVBO and ZnSe/ZnS-QD2::AVBO, respectively (**Table 3**). It demonstrates significant overlap between the emission of QDs and the absorption of AVBO, confirming their suitability as efficient donor–acceptor pair for FRET analysis. An imperative advantage of QDs is their size, which monitors this overlap and consequently impacts the FRET efficiency. This property can be seen in **Fig. 4**, where the PL spectra of QD1 and QD2, are depicted along with the absorption spectrum of AVBO. Inset in **Fig. 4** shows the spectral overlap function, $J(\lambda)$ and seen that the QDs size and their PL has impact on the spectral overlap with the AVBO acceptor. The QDs emit violet light at 405nm and 420nm, respectively. AVBO has a significant absorption peak at and around 425nm, which makes this an ideal combination for FRET. Additionally, the prominent electrostatic charge on AVBO, arising from its D- π -A conjugation [1], promotes strong electrostatic dipole interaction with the electrostatically charged QDs, which plays an important role in facilitating efficient FRET [29,57]. The photophysical properties of the two FRET systems, are given in **Table 3**.

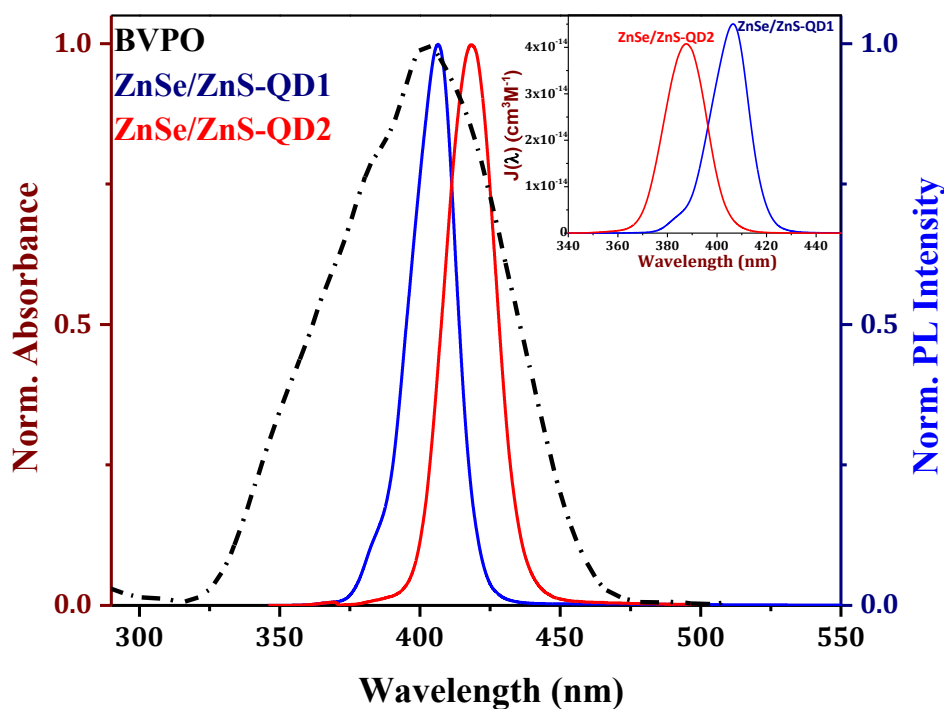


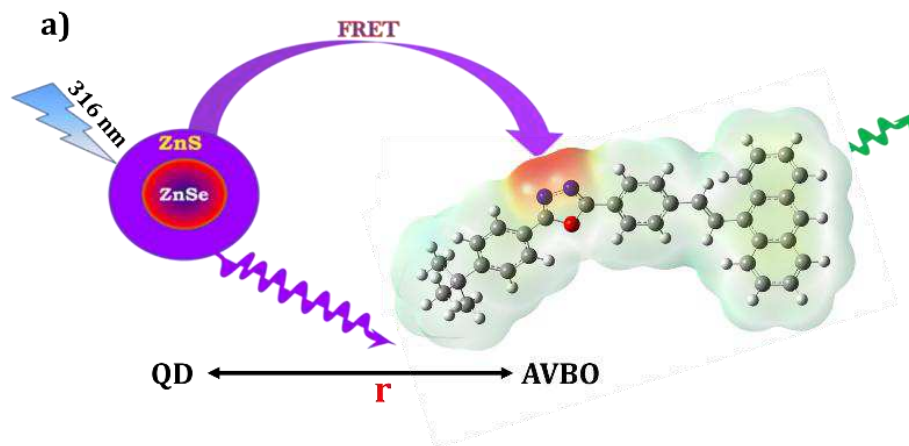
Fig. 4: Spectral overlap between the normalized UV-Vis absorption of AVBO (black-dashed) and PL spectra of ZnSe/ZnS-QD1 (blue) and ZnSe/ZnS-QD2 (red) in toluene at room temperature. The extent of spectral overlap $J(\lambda)$ shown in the inset confirms that QD1 has substantially more degree of spectral overlap with the AVBO compared to QD2.

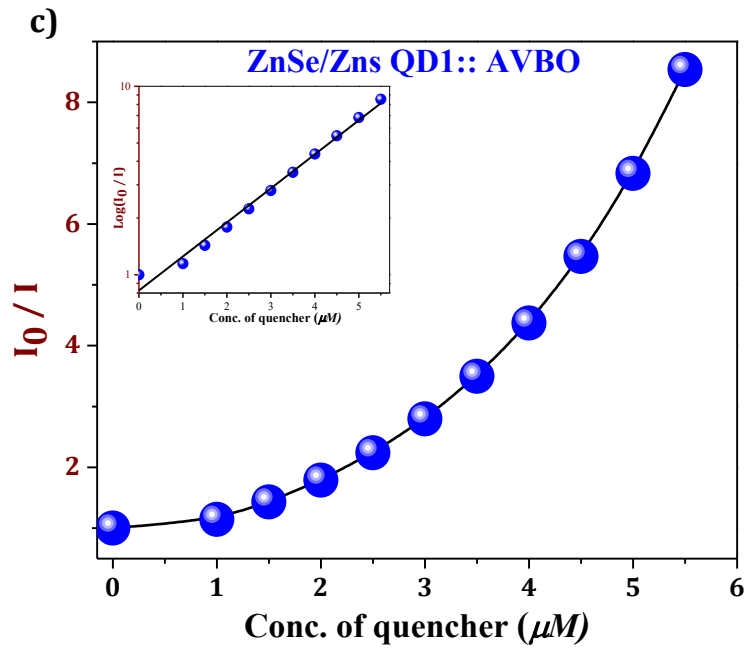
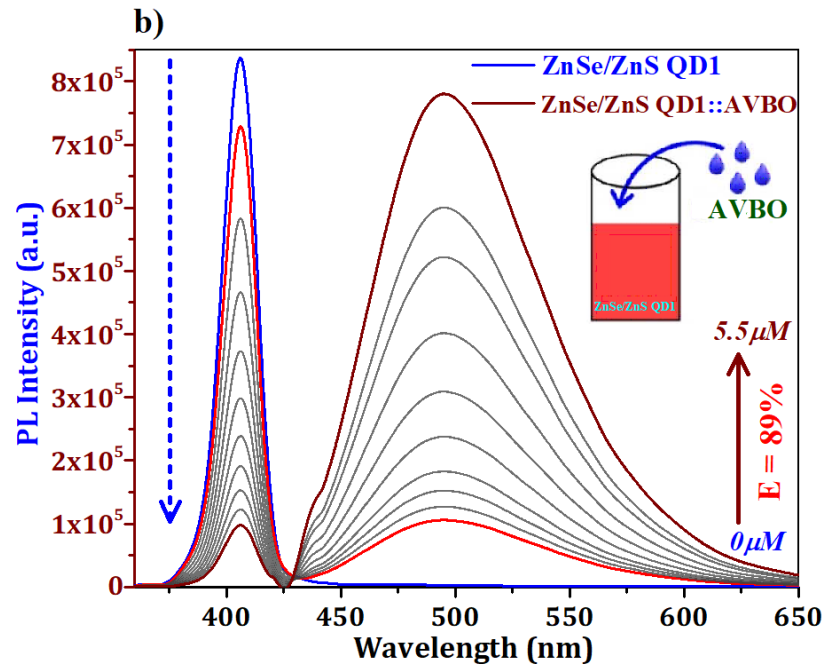
Table 3: Photo physical properties of QDs.

QDs	Size (nm)	Absorption maxima, λ_{exc} (nm)	Emission maxima, λ_{emi} (nm)	Quantum Yield of QDs (%)
ZnSe/ZnS-QD1	7	316	405	62
ZnSe/ZnS-QD2	8	316	420	70

The schematic representation of the electrostatically driven FRET process from the QDs donor to the AVBO acceptor is depicted in **Fig. 5a**. All the FRET samples were excited at 316nm to prevent the direct excitation of the acceptor AVBO (has negligible absorbance and maintained below 0.1 at excitation wavelength ~ 316 nm to minimize the inner filter contributions), which is essential for the efficient photo-triggered FRET. In PL quenching analysis, varying aliquots of the AVBO acceptor (0 to 5.5 μ M concentration) were added to ZnSe/ZnS QDs solution (5 μ M). The changes in the PL spectra were examined using steady-state spectroscopic techniques (**Fig. 5b** and **6a**). As the AVBO molecules were gradually added, a decrease in the PL intensity of the both violet-emitting ZnSe/ZnS QDs was noted. At

the same time, there was a concomitant increase in the PL intensity of the AVBO, with the PL maximum (λ_{max}) centered near 500nm. Thus, donor PL reduction accompanied by acceptor sensitized PL enhancement, confirms the absence of reabsorption effects and authorizes the true nonradiative FRET from QDs to AVBO rather than photon recycling. It is also noticed that there is no significant changes observed in the absorption band shape or peak broadening upon hybrid formation, implying the absence of aggregation-induced quenching. The quenching efficiency increases almost linearly with the concentration of AVBO acceptors. E_T is known to depend on various factors such as spectral overlap, and proximity distance between donor and acceptor [29,32-33,]. The efficiency, as measured by steady-state spectroscopy, was noted to be 88.32% for QD1::AVBO and it is less compared to 79.48% for QD2::AVBO, using the Eqn. (S8[†]). This difference can be traced by measured FRET parameters derived from donor-acceptor spectra viz., Förster radius R_0 (Eqn.(S5), donor-acceptor distance r (Eqn.(S7), and transfer rate $k_T(r)$ (Eqn. (S1) (Table 4). The R_0 value 6.16nm for QD1::AVBO and 6.14nm for QD2::AVBO, governed by donor quantum yield and overlap, scales linearly with $J(\lambda)$, while r shortens as overlap grows, enhancing $k_T(r)$ and thus E_T . Overall, FRET parameters and donor QDs dimensions critically dictate transfer efficiency.





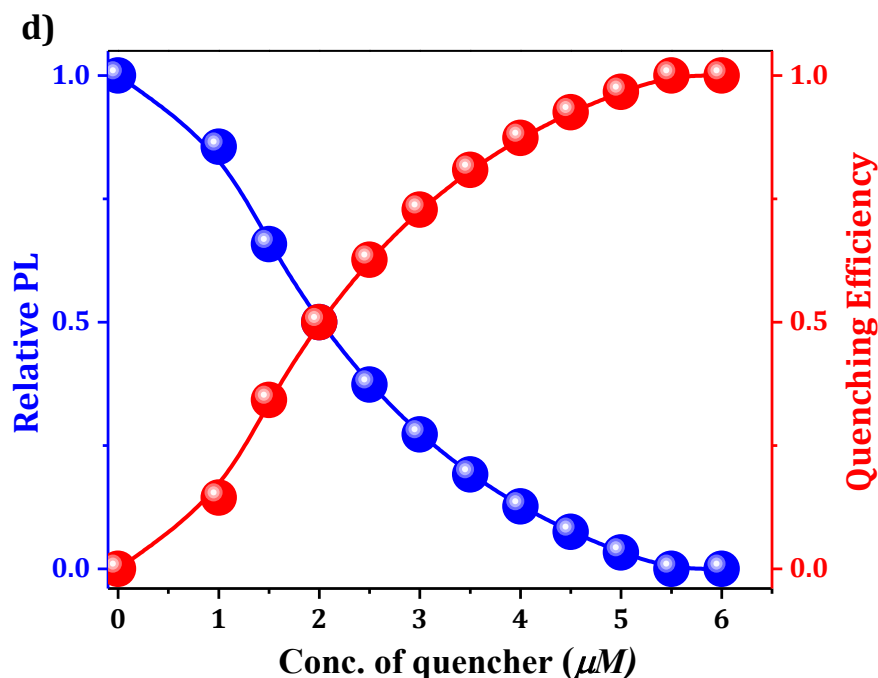


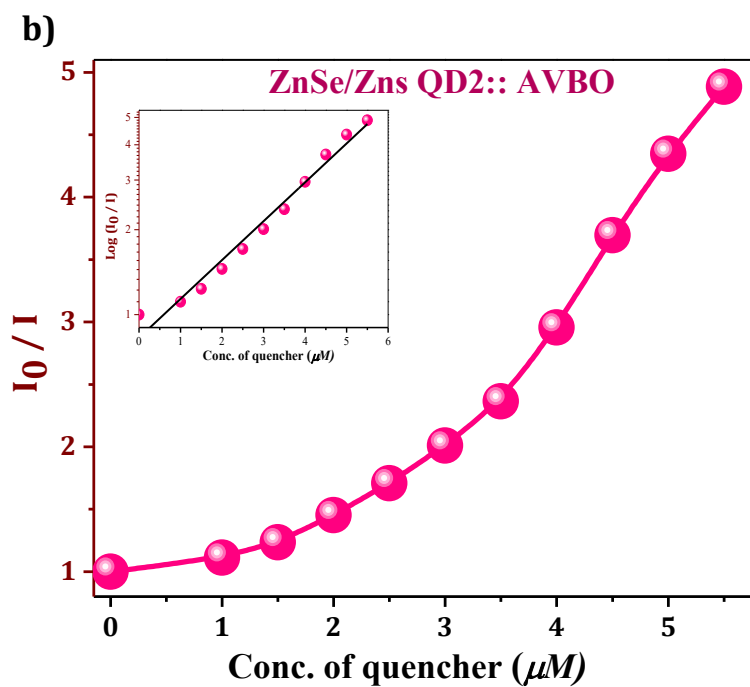
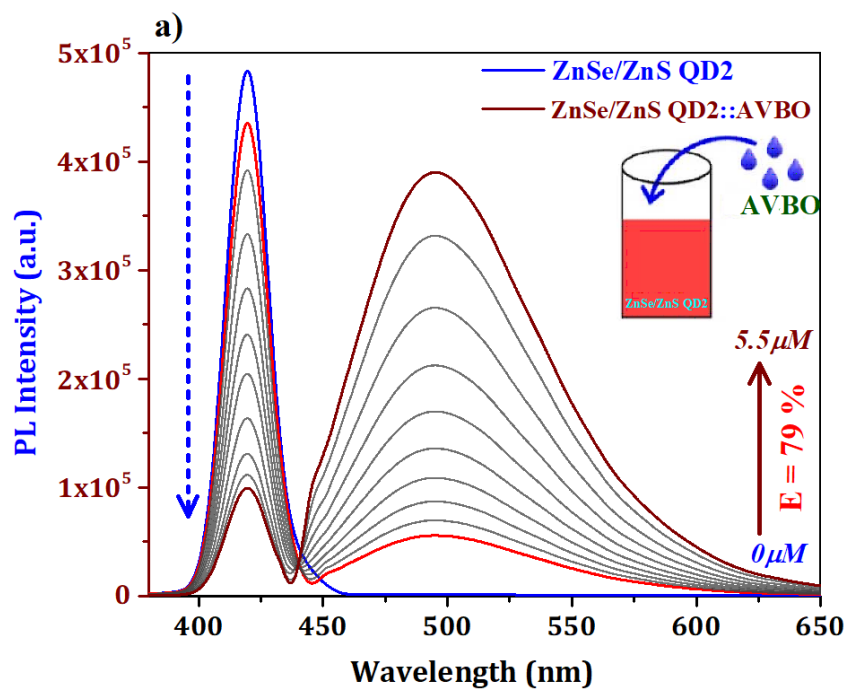
Fig. 5: Steady-state FRET studies in the ZnSe/ZnS QDs1:: AVBO donor-acceptor system. (a) Schematic representation of the electrostatically driven FRET process from the violet emitting ZnSe/ZnS QDs donor to the AVBO acceptor. (b) PL spectra changes in ZnSe/ZnS QDs1:: AVBO upon incremental addition of varying concentrations of AVBO ($\lambda_{exc}=316$ nm) chromophore. The PL peak around 500 nm corresponds to the AVBO results from FRET from the QDs1. (c) Stern–Volmer plot of concentration of quencher v/s I_0/I . **Inset graph:** The plot for $\log(I_0/I)$ vs $[C]$ of AVBO acceptor. (d) A saturation in both the relative PL intensity of donor ZnSe/ZnS QDs1 and the quenching efficiency was observed after ~ 6 μM addition of the acceptor AVBO dye.

Table 4: FRET parameters obtained from steady-state measurements.

FRET Pair	Spectral overlap, $J(\lambda)$ (nm^4/Mcm)	Förster radius, R_0 (nm)	Donor-Acceptor distance, r (nm)	FRET Efficiency (%)	Transfer rate $k_T(R)$ s^{-1}	Quenching volume, V (cm^3)	Quenching radius, r_q (nm)
ZnSe/ZnS-QD1::AVBO	8.65×10^{15}	6.16	4.40	88.32	11.06×10^8	3×10^{-16}	71.81
ZnSe/ZnS-QD2::AVBO	8.47×10^{15}	6.14	4.90	79.48	5.68×10^8	2×10^{-16}	65.66

The Stern-Volmer plot (I_0/I versus concentration of quencher $[C]$) indicates that there is a non-linear behavior, showing an upward exponential tail (**Fig. 5c** and **6b**). This indicates that both static and dynamic effects are present in the PL quenching mechanism. The dynamic effect occurs due to excited state interactions between donors and acceptors, while the static one originates from weak donor-acceptor interactions before excitation. Since, no significant changes in the band shape makes it clear that aggregation cannot be responsible for the effect under study, so that it is purely associated with the process of quenching. The SV constant (K_D) from the slope of these plots are found to be $1.34815 \times 10^6 \text{ M}^{-1}$, and $0.74187 \times 10^6 \text{ M}^{-1}$ for QD1::AVBO and QD2:: AVBO, respectively. The estimated bimolecular quenching constant (k_q) was determined to be $1.988 \times 10^{14} \text{ /MS}$ and $1.07 \times 10^{14} \text{ /MS}$ for these FRET conjugates, which are much larger than the typical diffusion-only controlled quenching process ($\sim 10^{10} \text{ /MS}$), predicted by Smoluchowski equation, $k_{diff} = 8RT/3\eta$ [58]. Higher k_q values of infer that FRET is not a diffusion controlled process alone instead supports strong donor-acceptor interaction-assisted energy transfer accompanied by static one resulting from weak donor-acceptor interactions before excitation. It also suggest the existence of closeness proximity between AVBO and QDs surface, facilitating efficient energy transfer. Thus, it is clear that the quenching phenomenon is best explained using a mixed approach that involves both static and dynamic mechanisms. This type of association behavior is normally seen in donor-acceptor hybrid systems based on QDs, wherein surface adsorption keeps the distance between donors and acceptors less than diffusion-controlled limits. The exponential rise in PL quenching can be analyzed using the Perrin model [33], where the logarithmic plot of the relative donor PL intensity varies linearly with the concentration of the acceptor (Inset graph of **Fig. 5c** and **6b**). For QDs::AVBO FRTE pairs, the quenching volume and radius are estimated and presented in Table 4. These substantial quenching spheres (3 and 2×10^{-16} for QD1 :: AVBO and QD2 :: AVBO, respectively), stemming from strong electrostatic interactions implies that any acceptor arriving this volume sphere can diffuse to the QD donor surface and involve in efficient FRET. In this case, quenching volume refers to the existence of an active volume or a "sphere of action" around the excited state QDs. Randomly quenching will happen in the system where there is a quencher in the sphere of action of the volume "V". In addition, relative PL of donor and acceptor, and FRET quenching efficiency are found to be saturated after adding $\sim 6 \mu\text{M}$ of AVBO (**Fig. 5d** and **6c**). It is noteworthy that the PL intensity of isolated AVBO ($\sim 7 \mu\text{M}$), under direct excitation at 312nm was found to much lesser than the intensity of the

- 1 QDs::AVBO hybrids, representing efficient FRET. The description of the Stern-Volmer and
- 2 Perrin model analysis are given in Section 7 of the ESI†.



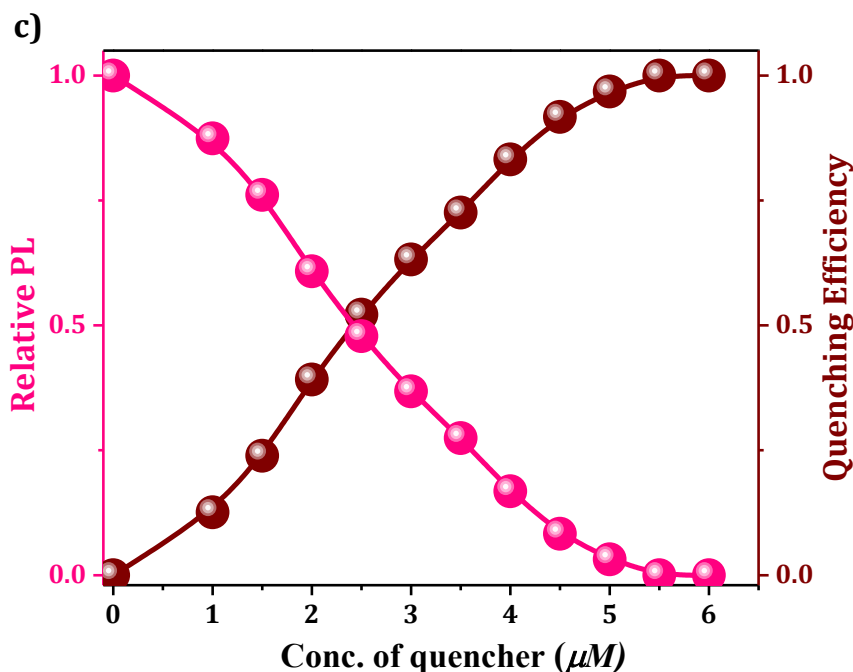


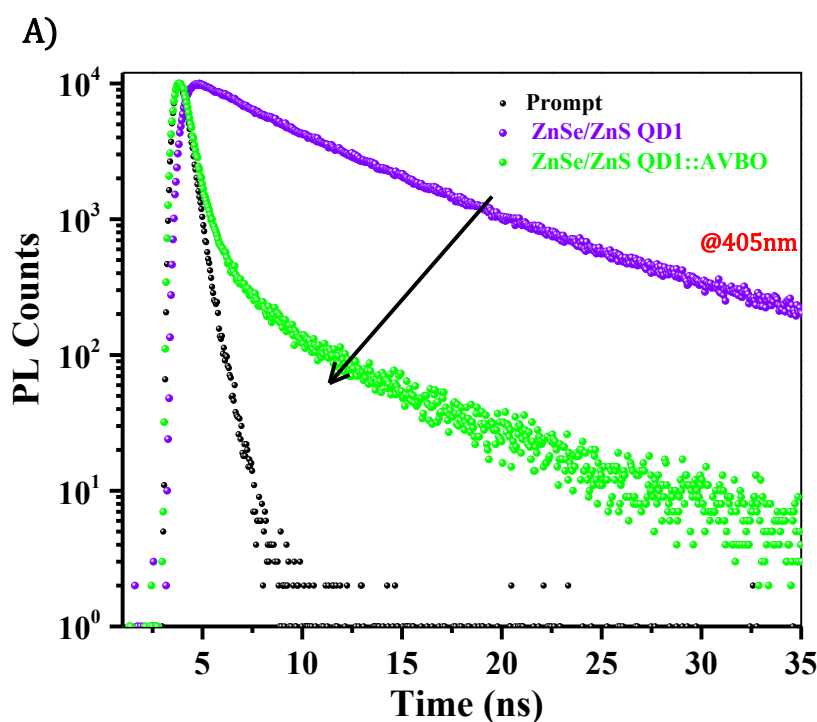
Fig. 6: Steady-state FRET studies in the ZnSe/ZnS QDs2:: AVBO donor-acceptor system. (a) PL spectra changes in ZnSe/ZnS QDs2:: AVBO upon incremental addition of varying concentrations of AVBO ($\lambda_{exc}=316$ nm) chromophore. The PL peak around 500 nm corresponds to the AVBO results from FRET from the QDs2. (b) Stern–Volmer plot of concentration of quencher v/s I_0/I . (c) A saturation in both the relative PL intensity of donor ZnSe/ZnS QDs2 and the quenching efficiency was observed after $\sim 6 \mu M$ addition of the acceptor AVBO dye.

Intriguingly, FRET with measurable efficiency occurs at exceptionally low concentrations of the acceptor AVBO, due to its significant photophysical properties and high quantum yield. Recalling the importance of FRET in monitoring vital processes such as photo-sensitization [59], energy transduction [60], etc., the current investigation is focused on the strongly fluorescent AVBO chromophore to understand the role of FRET in long-wavelength emission. Hence, the application of the fluorescent AVBO probe in FRET applications/photosensitization in aqueous solutions has considerable potential.

3.3.2 Time resolved photoluminescence experiments: TRPL decay kinetics provides definitive confirmation of energy transfer in the electrostatically assembled ZnSe/ZnS QDs::AVBO donor-acceptor hybrids. In order to conform this, the TRPL profiles of QD1 and QD2 are measured with and without AVBO using excitation of 280nm at room temperature (Fig. 7). Decay profiles were explored using bi and tri-exponential functions. The average

lifetime of Donor QDs showed pronounced quenching from $\sim 6.78\text{ns}$ to $\sim 1.41\text{ns}$ in QD1::AVBO and $\sim 6.92\text{ns}$ to $\sim 2.28\text{ns}$ in QD2::AVBO, upon adding AVBO and yield $\sim 76.65\%$ and 66.23% FRET efficiency, respectively (**Table 5**). TRPL data also provide evidence for the presence of both static and dynamic quenching. Donor QDS decay profile was best fitted using two lifetime components (τ_1 and τ_2) in the absence of the AVBO acceptor, while in the case of the hybrid (QDs::AVBO), three lifetime components (τ_1 , τ_2 and τ_3) were needed. The appearance of another lifetime component might associated with the formation of a new population of donors due to their complexation with the acceptors, indicating that there is static quenching taking place. At the same time, the decrease in the QDs lifetime is an indication that dynamic quenching also takes place, confirming non-radiative FRET. Hence, FRET provides a competing non-radiative decay channel for the donor by shortening its excited-state lifetime in presence of acceptor AVBO.

The efficiencies obtained from TRPL are lower compared to those steady state. This is because TRPL measurements are more sensitive compared to steady state as they are not affected by concentration of sample and fluctuation in source intensity. Therefore, precise and clear information about FRET dynamics could be extracted from TRPL measurements.



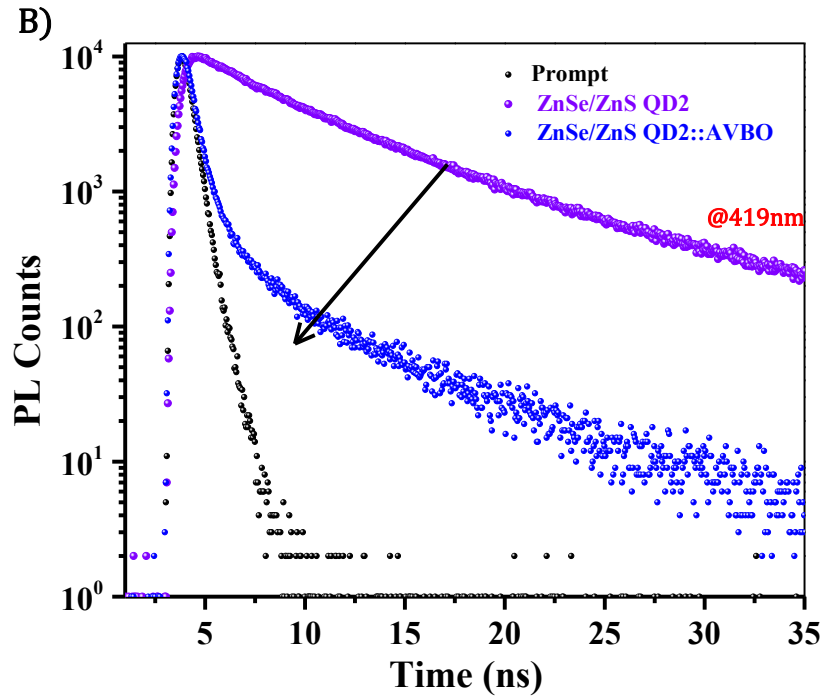


Fig. 7: Time-resolved FRET studies in ZnSe/ZnS::AVBO donor–acceptor system. [A] PL decay profiles of ZnSe/ZnS QD1 in the presence (green) and absence (violet) of AVBO compound (the excitation wavelength was 405 nm). [B] PL decay profiles of ZnSe/ZnS QD2 in the presence (blue) and absence (violet) of AVBO compound.

Table 5: FRET parameters obtained from time-resolved photoluminescence measurements.

FRET Pair	Lifetime components (ns)			Relative Amplitudes			Average Lifetime $\langle\tau\rangle$ (ns)	FRET Efficiency (%)
	τ_1	τ_2	τ_3	A1	A2	A3		
ZnSe/ZnS-QD1	2.68	7.59		16.6	83.4		6.78	
ZnSe/ZnS-QD1::AVBO	0.074	1.27	6.00	67.48	12.51	20.01	1.41 ↓	76.65
ZnSe/ZnS-QD2	2.45	7.85		17.13	82.87		6.92	
ZnSe/ZnS-QD2::AVBO	0.075	1.23	6.47	48.61	20.63	30.76	2.28 ↓	66.23

4. Conclusions

The present work was **successful in synthesizing and characterizing** a novel blue-green emitter oxadiazole compound, AVBO, by employing D – π – A Wittig approach with its stable and efficient PL at and around **~485–510nm** across various solvent media. **Solvatochromic insights** of AVBO confirmed larger excited-state dipole moments ($\mu_e > \mu_g$) with parallel dipole moments ($\phi \approx 0^\circ$), and identified that non-specific type solvent interactions (π^* effects) along with specific hydrogen bonding donor contributions drive the solvent interactions. Further, in the hybrid systems (AVBO::ZnSe/ZnS QDs), achieved **88% high energy transfer efficiency** via FRET mechanism supported by excellent spectral overlap. **The rapid quenching kinetics** using Stern-Volmer plots validated both static and dynamic quenching with super-diffusion-limited rate constants ($\sim 10^{14}/\text{MS}$). From Perrin model, the large quenching sphere volumes reflect strong donor–acceptor interactions, enabling efficient diffusion and promoting effective FRET. The TRPL decays exhibited reduced donor lifetimes, confirming energy transfer via dipole-dipole interactions. These outcomes proved AVBO-QD hybrid's potentiality and suitability for heavy metal-free and toxic-free optoelectronics, specifically in light harvesting and biosensing.

Data Availability

All the experimental data and other supporting information were provided in the main text and/or ESI†.

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