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Triazole-containing electroactive compounds in organic light-emitting devices: A review

This article is dedicated to Prof. Juozas Vidas Gražulevičius on the occasion of his 75th birthday in recognition of his outstanding contribution in the field of organic optoelectronics.

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Organic light-emitting diodes (OLEDs) represent a rapidly developing class of optoelectronic devices widely employed in display and lighting technologies. The continuous improvement of OLED performance critically depends on the development of organic materials capable of efficient charge transport, effective exciton utilisation, and long-term operational stability. Among nitrogen-containing heterocyclic compounds, triazoles have emerged as versatile scaffolds in materials science due to their exceptional electron-transporting properties. Structurally, triazoles are classified as 1,2,3-triazoles and 1,2,4-triazoles, both of which can accommodate diverse substituents around the core, enabling fine-tuning of their electronic and photophysical characteristics. These features make triazole derivatives and their derivatives highly suitable as electron-transporting materials, hosts and emitters in optoelectronic applications, including OLEDs, photovoltaics and sensors. The incorporation of triazole units allows for efficient charge transfer, enhanced thermal and chemical stability, and improved device performance. This review highlights the structural aspects and functional roles of triazole-based compounds in electron-transporting systems. The application of triazole-based compounds as hosts and emitters provides a comprehensive perspective on their potential for next-generation optoelectronic devices.

Keywords: triazole, OLED, carbazole, electron transport

INTRODUCTION

An OLED is a double-charge injection semiconductor device, based on electroluminescence (EL) from organic material that is inserted between two electrodes. Light emission is generated via radiative relaxation of excitons that are formed by simultaneously supplied electrons and holes upon external voltage. Although EL from pure organic material was observed for the first time in 1955 [1], the breakthrough in OLEDs began more than 30 years later, in 1987, when Tang and van Slyke from Eastman Kodak reported the first bilayer OLED fabricated using modern thin-film deposition techniques [2]. That device consisted of 1,1-bis[(di-4-tolylamino)phenyl]cyclohexane (TAPC) utilised as a hole-transporter and 8-hydroxyquinoline aluminium (Alq_3) used for both electron transport

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and light generation. Those organic layers were sandwiched between indium tin oxide (ITO) anode and magnesium–silver alloy cathode. The device demonstrated a luminescence of approximately 1000 cd/m^2 at an applied voltage of 10 V and an external quantum efficiency (EQE) of 1%. This major advancement introduced the heterostructure concept in the OLED design. Tang and van Slyke demonstrated that single-layer OLEDs are inefficient due to an unbalanced charge carrier injection and transport, resulting in high operational voltages and a low efficiency of emission. The incorporation of charge-transporting layers improves device performance by enhancing carrier balance and increasing the probability of electron and hole recombination within the emissive region.

Over nearly 40 years of scientific and technological progress, OLEDs are capable of achieving an impressive EQE of 50% and 100,000 working hours [3], with further improvements anticipated. A major milestone following the pioneering work of Tang was the demonstration of electrophosphorescent OLEDs by Baldo et al., based on the organoplatinum complex [4]. It was demonstrated that the utilisation of phosphorescent emitters allows the harvesting of both singlet and triplet excitons, allowing internal quantum efficiencies of up to 100%. Subsequently, the development of thermally activated delayed fluorescence (TADF) materials provided an alternative strategy for triplet exciton harvesting without the use of heavy metals. In 2012, Adachi and co-workers utilised purely organic emissive materials capable of triplet exciton harvesting through TADF in sky-blue, green and orange OLEDs achieving EQEs of 8, 19 and 11%, respectively [5]. More recently, OLED based on the boron-containing multiple resonance TADF emitters have demonstrated record EQEs exceeding 40% while maintaining an excellent colour purity [6].

In parallel with scientific progress, OLED technology is rapidly being commercialised [7]. OLEDs dominate in the portable display industry and have rapidly saturated the arena of flat-panel displays. Their advantages include a high brightness, a wide viewing angle (ca. 170°), a high contrast ratio, a high resolution, a high picture quality, a fast response time, a low power consumption and lightweight qualities. In contrast, OLEDs as a lighting technology are much less developed compared to OLED displays, as inherent issues impose limitations on their practical utility [8]. OLEDs have been investigated as planar white light sources since the early stages of their development. In 1994–1995, the research group of Kido highlighted the OLEDs potential for lightweight and large-area illumination applications [9]. Key advantages of OLED lighting include a low heat generation, a high colour rendering index, the absence of ultraviolet emission, and the potential for operation without toxic heavy metals [10, 11]. Since the technology is still emerging, several limitations continue to hinder large-scale commercialisation, including a comparatively low luminance, a high cost of fabrication, a limited suitability for high-power illumination, challenges related to the large-area electrical interconnection, and the necessity to be operated with constant current [12].

The design and development of advanced organic materials remain a key challenge to overcome limitations and further improve OLED performance in both display and lighting applications.

TRIAZOLES AS ELECTRON-TRANSPORTING MATERIALS

Nitrogen-containing compounds serve as a central scaffold in the development of organic optoelectronic materials. The key factor that determines electronic properties of such heterocycles is the location of free non-bonding electrons on a nitrogen atom. In the case of the essential electron donor 9*H*-carbazole, the electron pair on *sp*^{3}-hybridised nitrogen atom participates in electron delocalisation, inducing the appearance of negative charges on carbon atoms, thus bearing the electron-donating ability of the compound [13]. In contrast, lone electron pairs of nitrogen atoms of pyridine and triazine are in the equatorial position to the ring. This restrains them from being involved in π-conjugation and causes the appearance of partly positive charges on carbon atoms [14], which makes them favourable acceptor constituents in the design of donor-acceptor type electroactive compounds.

Triazole is a five-membered heterocyclic aromatic system having two carbon atoms and three nitrogen atoms (Fig. 1). The geometry of the electron pair of the singly-bonded nitrogen atom is pyrrole-like while two others adopt pyridine-like configuration located in the same plane as the σ-bonds.

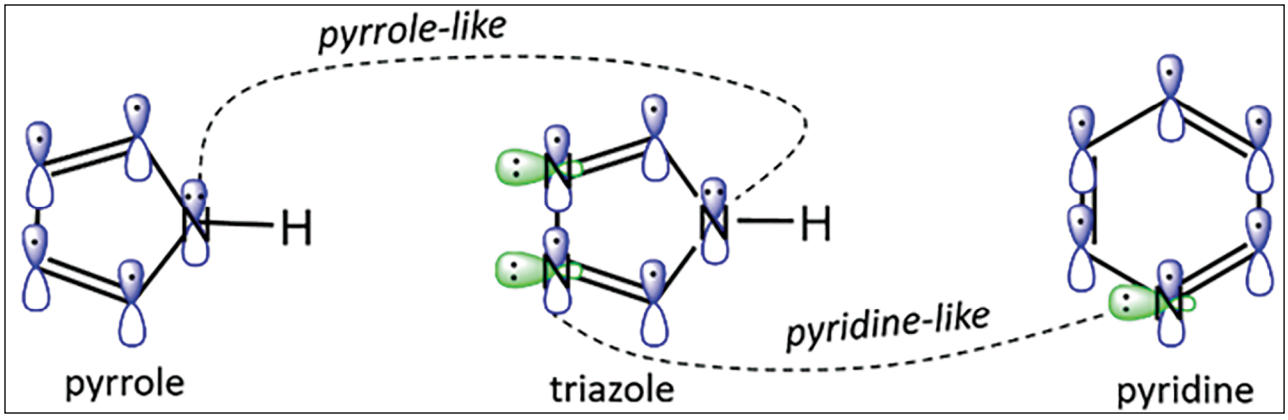

Fig. 1. Simplified visualisation of atomic orbitals of the nitrogen heterocycles discussed

This leads to an electron-accepting character of the triazole system which is by means lower than that of pyridine and triazine, but can be significantly reinforced by functionalising the triazole ring with various electron-withdrawing substituents.

Triazole was first reported in 1885 by Swedish chemist J. A. Bladin [15]. Throughout all the 20th century, the researchers' attention was devoted to the range of pharmacological properties of its derivatives, i.e. antioxidant, anti-inflammatory, antiviral, antimicrobical, antitubercular, anticancer, anticonvulsant, analgesic, etc. [16, 17]. In 1993, only six years after Tang and Van Slyke introduced the first OLED [2], a triazole-containing compound was utilised in the EL device for the very first time. A Japanese group of researchers lead by Okuyama designed and synthesised compound **1** (Fig. 2) that was used as an electron-transporting material (ETM) in an electroluminescent cell of a very simple structure [18]. At that time, derivatives of oxadiazole gained the reputation of efficient organic ETMs [19]. The idea of Kido and co-workers [18] was to take the well-known oxadiazole-containing ETM **2** (Fig. 2) and to replace the electron-transporting oxadiazole core by 1*H*-1,2,4-triazole that could also have possessed good electron-transporting properties due to the electron-deficient aromatic system. The sp^3-hybridised nitrogen atom was functionalised with a phenyl ring that, according to the authors' expectations, should have improved the film-forming properties of **2** and increased its thermal stability. A device with the structure ITO/TPD/Alq_3/**1**/Mg:Ag demonstrated a green emission with the luminance of 5800 cd/m^2 at 14 V. TPD

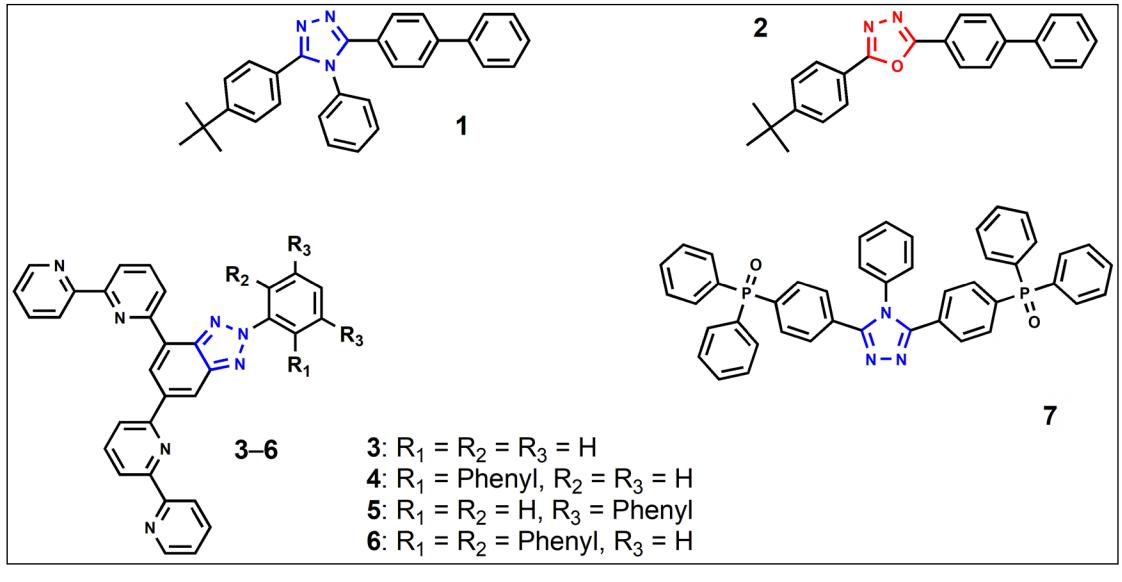

Fig. 2. Molecular structures of electron-transporting triazole and oxadiazole derivatives **1–7**

(*N*,*N*′-bis(3-methylphenyl)-*N*,*N*′-diphenylbenzidine) was used in the device as a hole-transporting material (HTM), Alq_3 as an emitter, and compound **1** as ETM.

Thanks to progress in computational chemistry, more than a decade later, Jansson et al. were able to conduct thorough density functional theory (DFT) calculations and to evaluate the electron-transporting properties of 1*H*-1,2,4-triazole derivatives not only quantitatively, but also to compare them with the ones of oxadiazoles and thiadiazoles by studying the influence of heteroatom [20]. Derivatives of thiadiazole and 1*H*-1,2,4-triazole were found to have reorganisation energies smaller than the ones of oxadiazoles that allowed the same rates of electron transfer for the first two groups of compounds. However, the obvious benefit of triazole over thiadiazole is a much larger structural tunability freedom due to the presence of the sp^3-hybridised nitrogen atom as an additional functionalisation site. Ichikawa et al. demonstrated [21] that isomeric 1*H*-1,2,3-triazole and 2*H*-1,2,3-triazole are more advantageous over their counterpart 1*H*-1,2,4-triazole since they are characterised by lower LUMOs (the lowest unoccupied molecular orbitals) and higher electron affinities (0.65 and 0.71 eV vs 0.48 eV, respectively). Therefore, the authors designed and synthesised a family of 2*H*-benzo[1,2,3]triazole-pyridine conjugates **3**–**6** (Fig. 2). Electron-deficient pyridinyl fragments were incorporated to improve the electron-transporting properties of a benzotriazole core. A series of OLEDs with the device structure ITO/NBP/Alq_3/**3**–**6**/LiF/Al were fabricated and the device without an additional layer of benzo[1,2,3]triazole derivatives was taken as a reference. NPB (*N*,*N*′-di(1-naphthyl)-*N*,*N*′-diphenyl-(1,1′-biphenyl)-4,4′-diamine) was used as HTM. Devices fabricated with **5** and **6** as ETMs demonstrated lower operational voltages in comparison to the reference device with Alq_3. It is worth noting that due to the C-C-fused benzotriazole system, the mentioned compounds suffered from relatively low triplet energy (E_T) levels (2.03–2.14 eV). Such feature is not desirable for organic ETMs since high E_T levels (ca. 3 eV) ensure a more efficient blocking of excitons. Maintaining both high E_T levels and a high thermal stability is one of the major challenges in the design of organic ETMs. Increasing the length of π-conjugation can enhance the thermal stability, but decrease E_T levels and shallow the energy bandgap (E_g). Zhuang et al. overcame the problem by appending the triazole central core with two diphenylphosphine oxide fragments (compound **7**, Fig. 2) [22]. The latter not only improved the electron-transporting and thermal properties of ETMs, but also did not lower the E_T levels as well as the band gap since they do not participate in the π-conjugation. By the introduction of two diphenylphosphine groups, all the characteristics of the parent compound **1** were significantly enhanced: the E_T level was increased (2.75 eV for **1** vs 2.86 eV for **7**), the band gap was expanded (3.71 eV vs 3.77 eV) and the glass transition temperature was also increased (70°C vs 133°C). OLED with **7** as ETM exhibited a higher efficiency and a lower driving voltage compared to the analogous OLEDs with the other known ETMs like **1**, TPBi (1,3,5-tris(1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzene) or BCP (2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline, also widely known as bathocuproine).

TRIAZOLE DERIVATIVES AS HOSTS

In order to maximise the EQE of an OLED, a light-emitting material should possess as high as possible photoluminescence quantum yield (PLQY) and should be capable of harvesting triplet excitons. For example, solid state samples of conventional phosphorescent organoiridium emitters (Fig. 3) show PLQY values up to 100% [23–25]. Moreover, there are TADF exhibiting materials reported with the PLQY values of more than 90% [26, 27]. Nevertheless, OLEDs exploiting light-emitting layers of neat compounds often exhibit a poor performance due to an inherent aggregation-induced quenching of emission. In most cases, the layers of emitters dispersed in host matrixes show a considerably better performance. This observation highlights the necessity of a host environment for many organic light-emitting materials despite their intrinsically high luminescence efficiency and effective exciton-harvesting capability. Conventional fluorescent emitters utilise only singlet excitons. In contrast, TADF compounds harvest both singlet and triplet excitons, the latter possessing significantly longer lifetimes. As a result, triplet excitons are more susceptible to non-radiative energy loss processes

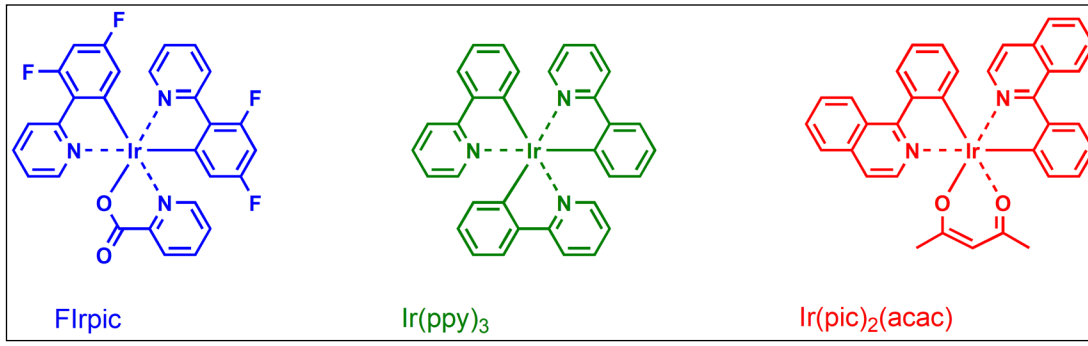

Fig. 3. Widely-used phosphorescent iridium (III) organic complexes: sky-blue emitting FIrpic, green-emitting $Ir(ppy)_3$ and red-emitting $Ir(pic)_2(acac)$

such as triplet–triplet annihilation and concentration quenching. In phosphorescent systems, triplet excited-state lifetimes are even longer since phosphorescence is a spin-forbidden transition with slower radiative kinetics. Consequently, triplet excitons in PhOLEDs are particularly vulnerable to external perturbations, making host–guest architectures essential for an efficient device operation [28–30]. Hosting strategy can prevent triplet energy dissipation by decreasing the triplet exciton lifetime. Host material with higher E_T can transfer its excitation energy to an emitter that facilitates the exciton formation. In that case, backward energy transfer (emitter → host) is diminished [31]. Another important feature for a host to possess is a considerable overlap of its emission spectrum with the absorption spectrum of the emitter in order to ensure energy transfer. So far, bipolar host materials exhibit a better performance in comparison to unipolar hosts since the former provide a balanced transport of charge carriers to the emitter thus increasing the probability of charge carrier recombination [32, 33].

Triazole is an appealing electron-transporting fragment in the design of bipolar hosts because it has excellent electron-transporting properties (discussed in the previous chapter), high E_T levels and thermal robustness. The bonding of the triazole ring with electron-rich hole-transporting moieties can form superior bipolar hosts with high and balanced hole-electron mobilities. Although there is practically no difference in the requirements of hosts for phosphorescent and TADF emitters, there are no reports of triazole-based compounds hosting the latter ones. On the other hand, there are plenty of examples of efficient electrophosphorescence utilising triazole-containing bipolar hosts (Figs 4–8) and common phosphorescent organoiridium complexes (Fig. 3).

Efficient blue electrophosphorescence is one of the most challenging tasks in the development of OLED display and lighting because blue phosphorescent emitters are characterised by much higher triplet states in comparison to green and red phosphor [34]. This subsequently restrains the molecular design of suitable host materials. Already limited pool of small, thermally stable organic molecules with bipolar charge transport is further restricted by the requirement for E_T levels around 3 eV. Recent studies showed that triazole moiety, while being covalently bonded to simple phenyl rings, can afford an excellent bipolar host for blue phosphorescent iridium complexes. Lee et al. reported bistriazole derivative **8** (Fig. 4) that consists of two electron-transporting 1,2,4-triazole moieties on a hole-transporting biphenyl core [35]. A sky-blue PhOLED based on the host-guest system of FIrpic and **8** as an emissive layer exhibited an impressive EQE of 30.2% with current efficiency (CE) of 65.9 cd/A and power efficiency (PE) of 62.8 lm/W. Compound **8** demonstrated a bipolar behaviour with electron and hole mobilities reaching $5.8 \cdot 10^{-5}$ and $2.9 \cdot 10^{-5}$ $cm^2 \cdot V^{-1}\ s^{-1}$, respectively, at a low electric field of $1.1 \cdot 10^6$ V cm^{-1}. However, electron transport prevailed at higher electric fields. The highly twisted geometry of **8** helps to avoid excimer and exciplex formation between the host and guest as well as between molecules from the neighbouring layers. A large E_g of 4 eV together with the high E_T of 3 eV ensure an effective energy transfer from the host to the emitter making compound **8** a universal host for triplet emitters of various colours.

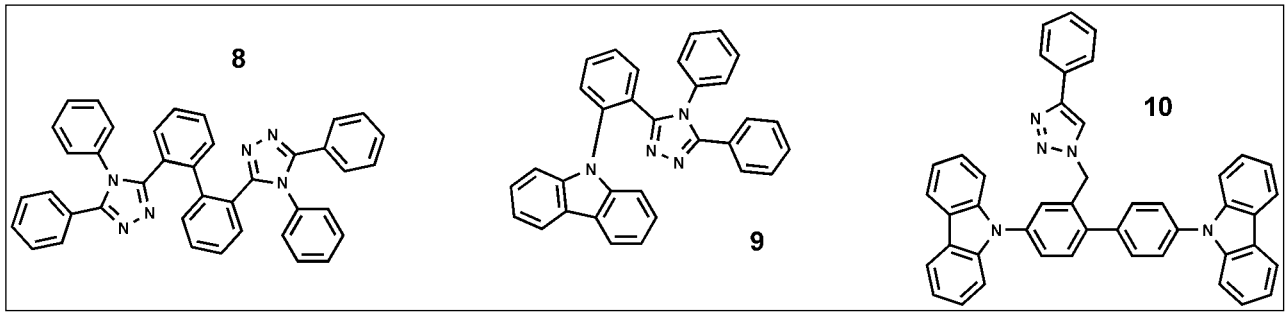

Fig. 4. Molecular structures of triazole-based host compounds **8–10**

Electron-rich 9*H*-carbazole is commonly used as a hole-transporting unit because of its low cost and the ability to tailor a broad range of properties via structural modifications [36–38]. Based on the known ETM compound **1**, Hung et al. reported bipolar carbazole–triazole conjugate **9** (Fig. 4) where the carbazolyl-fragment was connected to the *ortho*-position of triphenyltriazole [39]. Compound **9** was tested in the PhOLED hosting blue phosphor FIrpic, to afford CE_{max} of 46.06 cd/A PE_{max} of 39.8 lm/W and EQE of 21.78%.

In 2010, Kim et al. combined the electron-deficient triazole unit with the carbazole-based host CBP (4,4'-bis(*N*-carbazolyl)-1,1'-biphenyl) developing compound **10** (Fig. 4) in order to expand its E_g and enhance electron transport [40]. A blue FIrpic-based PhOLED using compound **10** as the host exhibited an EQE of 30% which is higher than that of a reference device with unmodified CBP. However, the new host showed a lower electrochemical stability, likely due to the methylene linker, resulting in reduced OLED stability compared to the CBP-based device.

The linking topology of *N*-phenylcarbazole and triphenyltriazole is the determinative factor of their hosting properties because of the opposite relationship between the E_{T1} and the degree of π-conjugation. Zhuang et al. reported four novel bipolar compounds of the donor–acceptor–donor (D–A–D) structure with *N*-phenylcarbazole fragments attached to the different sites of carbon-connected phenyl rings of triphenyltriazole [41]. Compounds **11** and **13** (Fig. 5) with *para-para* and *meta-para* linking patterns possessed lower E_{T1} of 2.7 and 2.76 eV, respectively. Their isomers **12** and **14** (Fig. 5) with *para-meta* and *meta-meta* linkages were found to have energies of the first triplet excited state (E_{T1}) as high as 2.7 and 2.76 eV.

The hosting properties of all four compounds were tested in green-emitting PhOLEDs with

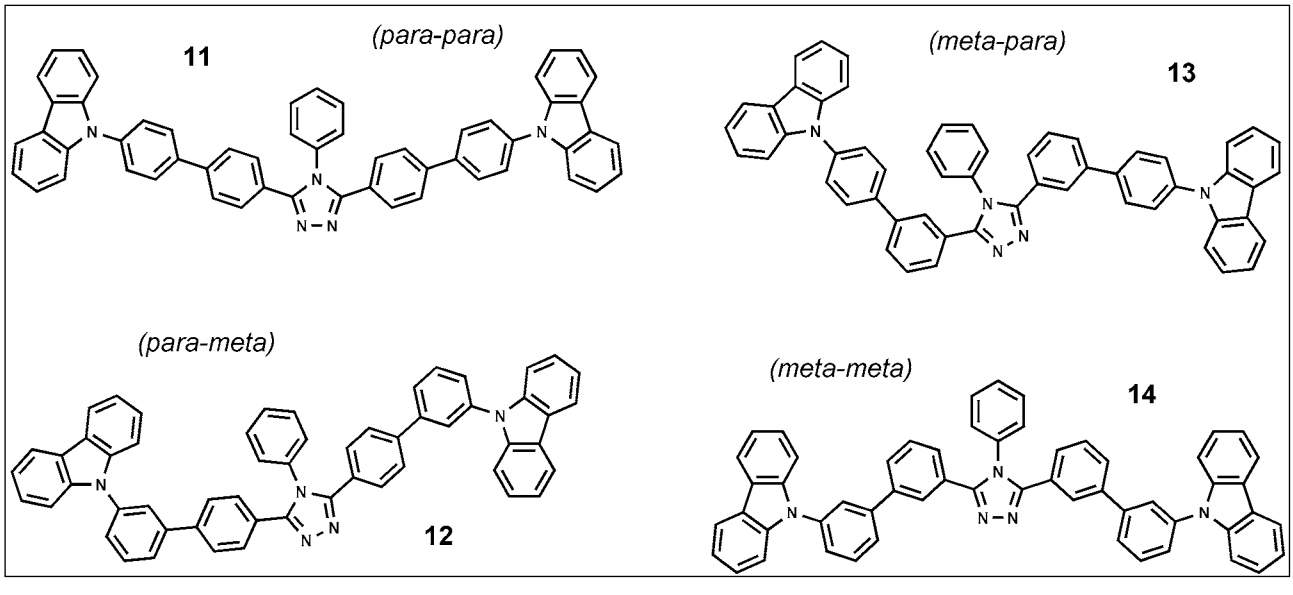

Fig. 5. Triphenyltriazole and *N*-phenylcarbazole compounds **11–14** with different linking topology

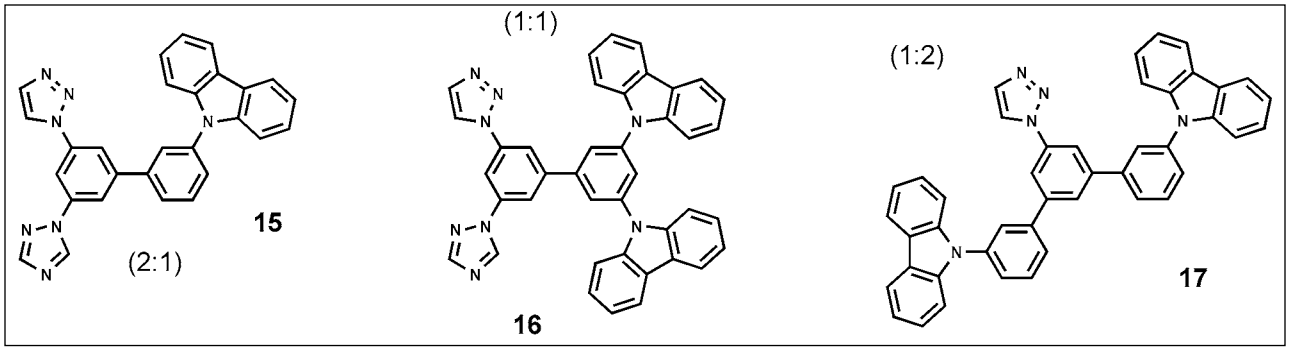

Fig. 6. Derivatives of biphenyl **15–17** with a different ratio of electron-accepting triazole and electron-donating carbazole units

the structure ITO/NPB/host **11**–**14**: $Ir(ppy)_3$ guest/TPBI/LiF/Al using green phosphor $Ir(ppy)_3$ as a dopant. All the devices were characterised by lower turn-on voltages compared to the reference device with a widely used CBP as a host. Inspired by the obtained results, the authors further fabricated blue-emitting PhOLEDs with the structure ITO/TAPC/ host **11**–**14**: FIrpic guest /BCP/ LiF/Al. Because compound **11** and **13** possessed E_{T1} lower than that of the FIrpic, utilising them as hosts resulted in extremely low device performances. However, compound **14** with the highest E_{T1} in the series afforded the most efficient device performances for both green and blue PhOLEDs. Blue OLED with compound **14** and the Firpic host-guest mixture demonstrated the CE_{max} of 21.1 cd/A and the PE_{max} of 18.7 lm/W. These results signify that upon designing bipolar host compounds, direct *para*-linkage should be avoided.

Meanwhile, not only the linking pattern, but also the ratio of n-type to p-type structural moieties plays a vital role in the efficiency of bipolar hosts. Liu et al. developed three bipolar compounds **15**–**17** (Fig. 6) with triazole-to-carbazole ratio of 2:1, 1:1 and 1:2 [42]. The abovementioned compounds were found to be the first examples of C-unsubstituted triazole used in the design of host materials. Biphenyl was selected as a π-spacer between electron-donating and electron-accepting groups.

PhOLED, based on **17** and FIrpic host-guest system, exhibited a low turn-on voltage of 3.1 V, CE_{max} of 44 cd/A, PE_{max} of 39.5 lm/W and EQE of 25%. For a comparison, hosts **15** and **16** provided a much inferior performance with CE_{max} = 21.8 and 17.3 cd/A, PE_{max} = 22.4 and 15.5 lm/W and EQE = 12.5 and 10.0%. It appears that a triazole–carbazole ratio of 1:2 is the most beneficial in that case. Authors attribute the low efficiency of devices based on **15** and **16** to the excessive electron current within the emitting layer that appears as a consequence of a too high ratio of electron-accepting triazole fragments in the hosting molecules.

Three years later, the same group of researchers proposed improved 1*H*-1,2,4-triazole-containing hosts **18**–**20** (Fig. 7) by introducing an auxiliary electron-deficient part of pyridine [43]. Due to a smaller molecular weight, the glass-transition temperature of compounds **18**–**20** is only 69–72°C. The respective hole and electron mobilities of the investigated compounds are of 10^{-6} and 10^{-7} cm^2 $V^{-1}s^{-1}$ orders of magnitude. Compound **18** with the *ortho*-linkage was found to possess the highest E_{T1} as well as the most balanced charge carrier mobilities. Its electroluminescent properties were tested in blue and green

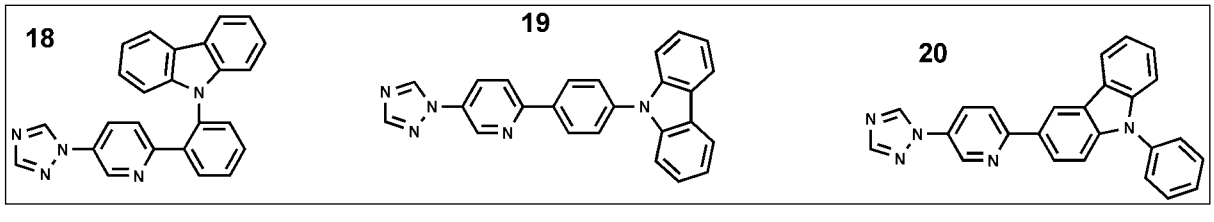

Fig. 7. Triazole-pyridine-carbazole hosts **18–20**

light emitting PhOLEDs with the device architecture ITO/PEDOT-PSS/TAPC/TCTA/**18**: FIrpic or $Ir(ppy)_3$/TmPyPb/LiF/Al. The blue and green-emitting devices showed the respective EQE values of 22.25% (CE_{max} = 41.98 cd/A) and 29.08% (CE_{max} = 96.98 cd/A) that are among the best PhOLED characteristics so far.

Tao et al. studied the structure-hosting properties relationship in a triazole-triphenylamine series of compounds **21**–**28** (Fig. 8) [44]. Since a high E_T is not intrinsic to the triphenylamine fragment, consequently all the compounds exhibited E_{T1} values ranging from 2.37 to 2.57 eV. As expected, the highest E_{T1} was found for compounds with a *meta*-linkage pattern. Based on these values, authors selected red and green-emitting $Ir(ppy)_3$ and $Ir(pic)_2(acac)$ pigments with a respective E_T of 2.0 and 2.4 eV as emissive dopants for PhOLED fabrication. The device structure was ITO/MoO_3/NBP/host-guest/BCP/Alq_3/LiF/Al. Almost all devices with $Ir(pic)_2(acac)$ afforded an efficient deep-red electrophosphorescence (CIE coordinates x = 0.68,

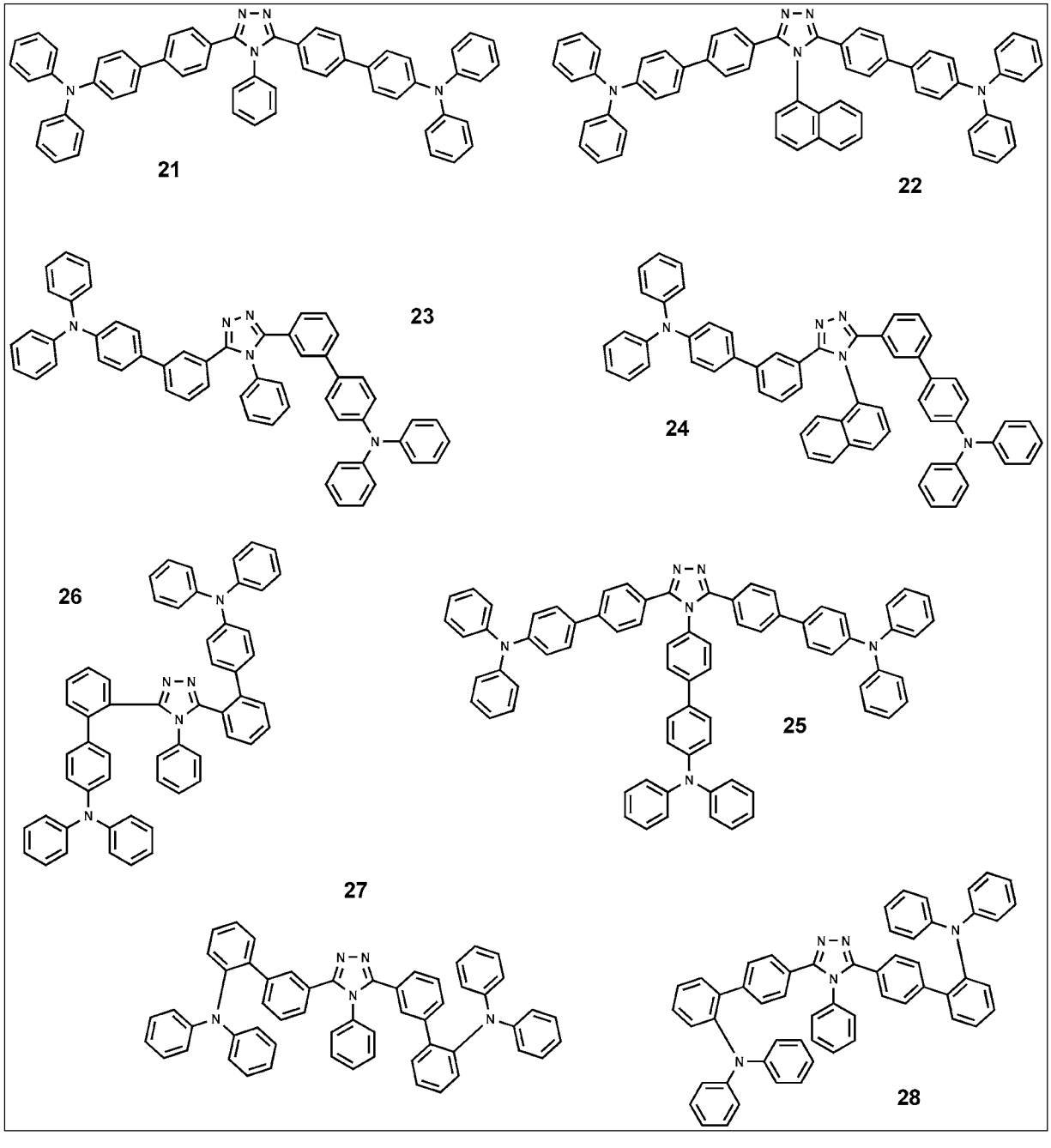

Fig. 8. Triazole-triphenylamine hosts **21–28**

y = 0.32) and were characterised by much lower turn-on voltages than the reference device utilising the CPB host. The authors attribute such a decrease in turn-on voltages to perfectly matched HOMOs (the highest occupied molecular orbitals) between the new hosts (–5.2–5.33 eV) and NBP as HTM (–5.4 eV). The device with compound **28** exhibited the best performance with EQE = 16.8% and CE_{max} = 12.4 cd/A. Green PhOLED based on $Ir(ppy)_3$ and compound **27** exhibited the highest luminance (L_{max}) of 48 618 cd/m^2, CE_{max} of 49.0 cd/A and PE_{max} of 52.7 lm/W. These values are 29968 cd/m^2, 50.7 cd/A and 38 lm/W for the device hosted by **27**.

TRIAZOLE DERIVATIVES AS LIGHT-EMITTING MATERIALS

Apart from being utilised as ETMs, derivatives of triazole can find application as efficient emitters in OLEDs if bipolar charge-transport is accompanied by a high PLQY in the solid state. Upon taking a look at the parameters of bipolar triazole-based host, one can particularly assume that such compounds could possess unique luminescent properties with emission maxima located in the short-wavelength spectral region and therefore, could be of great use for the application in near-ultraviolet (NUV) OLEDs. To date, there are only a few reports on NUV OLEDs, all of them exhibiting rather poor device performances that are far from the needs of practical application [45, 46]. Xue et al. reported triazole derivative **29** (Fig. 9) the analogues of which were previously studied as host materials to afford efficient NUV EL [47]. Compound **29** has not only high and balanced charge carrier mobilities reaching 10^{-4} cm^2/Vs order of magnitude, but also emits bright violet light with photoluminescence maximum (PL_{max}) of 401 nm with PLQY of 72% in crystalline powder state and PL_{max} of 414 nm with PLQY of 50% in an amorphous layer. Strong NUV fluorescence of **29** is attributed to the highly twisted structure that affords weak intermolecular π–π interactions and a weak intramolecular charge-transfer character. A non-doped OLED with the structure ITO/MoO_3/NPB/TCTA/**29**/TPBi/LiF/Al exhibited EL with a peak at 408 nm, a narrow full-width at half-maximum of 44 nm, and CIE coordinates (x = 0.17, y = 0.07). The device was characterised by a low turn-on voltage of 3.2 V, CE_{max} of 2.85 cd/m^2 and EQE of 6.57% which is among the highest reported values for NUV OLEDs.

Considering deep-blue EL, triazole derivative **30** (Fig. 9) is an illustrative example. Cang et al. reported a novel deep-blue fluorescent molecule **30** consisting of anthracene as an electron donor and triazole as an electron acceptor [48]. Compound **30** showed NUV emission with a peak at 407 nm, the vibronic structure of which indicates the contribution of locally excited states into luminescence. The layer of the compound exhibited deep-blue emission with a peak at 448 nm. It was noteworthy that no charge-transfer (CT) component was observed in its S_1 (singlet) state. Interestingly, the emission of the solutions of compound **30** were characterised by quite short fluorescence lifetimes (τ = 2.85 ns in hexane, 3.01 ns in isopropyl ether, 3.39 ns in ether, 3.76 ns in tetrahydrofuran and 3.69 ns in acetonitrile) as well as its neat layer (τ = 4.24 ns). A non-doped blue OLED utilising **30** as an emitter demonstrated EQE of 3.3% with an EL peak at 429 nm and CIE coordinates of (x = 0.17, y = 0.13) located in the deep-blue region.

Cui et al. combined the tetraphenylethylene (TPE) fragment of a weak electron-donating character with

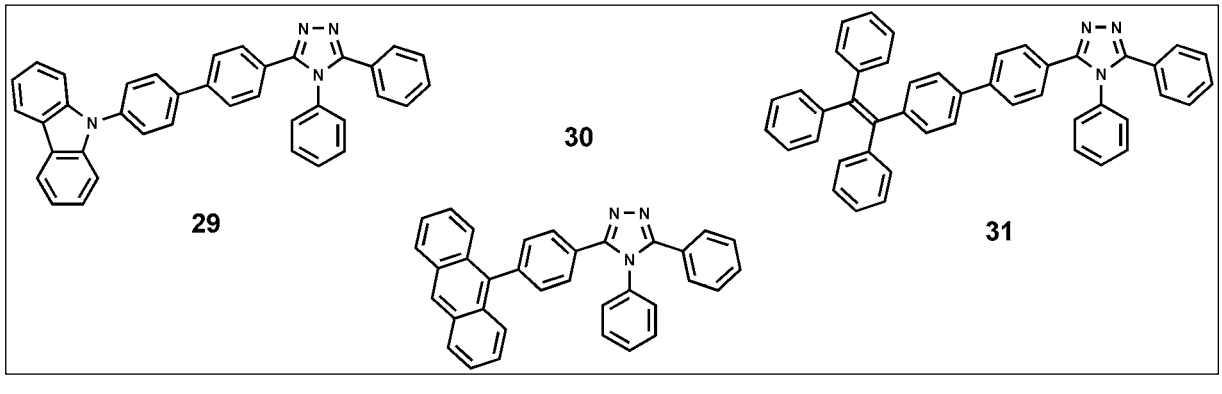

Fig. 9. Molecular structures of highly fluorescent triazole derivatives **29–31**

a triazine core [49]. TPE is a well-known moiety utilised to enhance PLQY in the solid state. The free rotation of the benzene rings of TPE moiety is not restricted in solutions. Therefore, almost all the excited state energy is wasted through the non-radiative decay channel resulting in the negligible PLQY of the solutions. Upon aggregation, the aforementioned rotation is severely ceased due to the spacious restraints imposed by the proximity of bulky phenyl rings that closes the non-radiative decay channels and promotes molecules to release excitation energy through the emission of light. Compound **31** (Fig. 9) is also characterised by a higher PLQY in its solid state compared to the one in the solution. Three mutually exclusive phenyl groups on the triazole ring could render molecular aggregates with weak π–π interactions. Indeed, the tetrahydrofuran solution of compound **31** was almost non-luminescent whereas the neat layer demonstrated impressive PLQY of almost 76%. Non-doped OLED utilising **31** as an emitter exhibited a good performance with EQE of 2.4%, luminance of 1020 cd/m^2 and EL_{max} at 468 nm.

As it was mentioned before, triazole-containing organic ETMs are more efficient in comparison to oxadiazole-containing ones. Lee et al. compared the luminescent properties of triazole- and oxadiazole-containing compounds [50]. As long as the authors aimed to realise TADF, they selected 10*H*-phenoxazine as one of the strongest electron-donating moieties used in the design of luminescent TADF compounds. Upon removal of oxygen, PL decays of the dilute toluene solutions of all the compounds **32–35** (Fig. 10) except **33** were characterised by prompt and delayed lifetime components suggesting that the exited states of these compounds relax via TADF. It was also observed that the deoxygenated solution of oxadiazole-containing compound **34** with a D–A–D structure exhibited significantly higher PLQY (43.1%) than its counterpart **32** with a D–A structure (29.8%). Such a sharp change was not observed for triazole-containing luminogens indicating the less significant participation of triplets in their emission.

Indeed, DFT calculations revealed that oxadiazole-containing compounds have a smaller singlet–triplet energy gap (ΔE_{ST}). The E_T levels were calculated to be the same for all of the compounds (2.83–2.84 eV). However, triazole-based luminogens possessed higher S_1 (3.8 eV for **33**, 3.69 eV for **35**) which means that in order to achieve efficient TADF, triazole needs to be covalently bonded with an electron donor of higher E_T levels. OLED possessing an emissive layer as the mixture of DPEPO (bis[2-(diphenylphosphino)phenyl]ether oxide) and **34** exhibited EQE of 14.9% which was remarkable at the time. A device of the same architecture with compound **35** exhibited EQE only of 6.4%.

The effect of a phenyl linker with different steric hindrance on luminescence properties on D–A–D triazole-based compounds was studied by Kim et al. [51]. The electron-accepting character of 1*H*-1,2,3-triazole was strengthened by the incorporation of a 4-cyanophenyl group through a facile nucleophilic aromatic substitution reaction. The series of luminophores **36–41** (Fig. 11) varying by the bulkiness of a *π*-linker and the strength of electron-donating moiety was synthesised. Empirical observation disclosed that the emission wavelength depended more on the donor strength rather than the steric hindrance of the π-spacer. *ortho*-Tolyl-

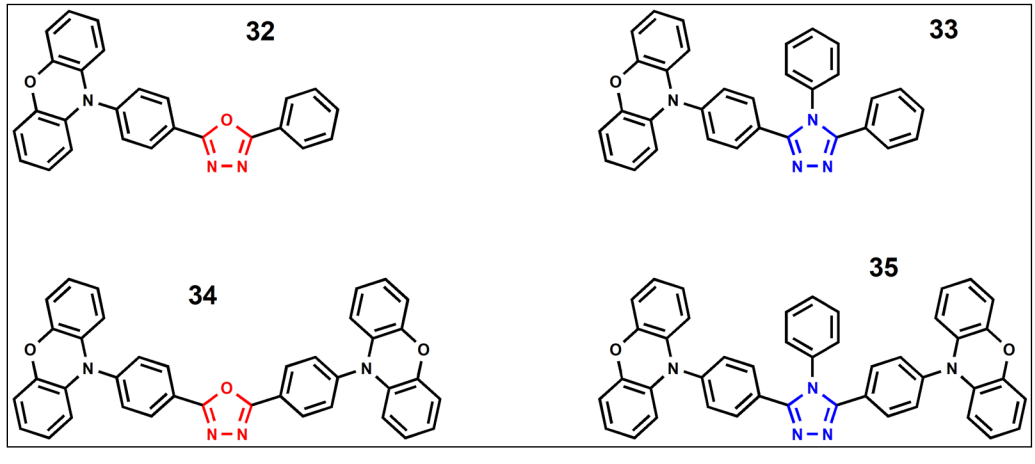

Fig. 10. Phenoxazine-substituted analogues of oxadiazole (**32**, **34**) and triazole (**33**, **35**)

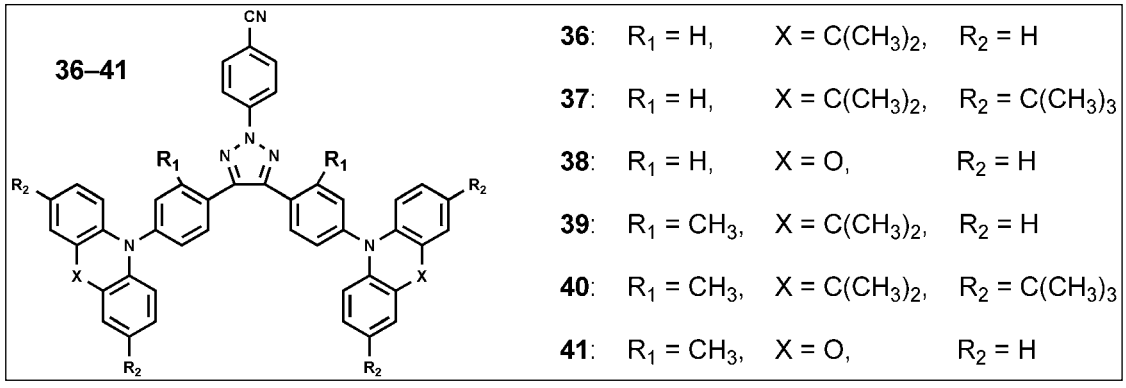

Fig. 11. Donor-substituted triphenyltriazoles (**36–38**) and their dimethyl-analogues (**39–41**)

substituted triazoles **39**–**41** were found to possess effectively separated HOMOs and LUMOs thus facilitating smaller ΔE_{ST} values and a reverse intersystem crossing, while the phenyl-substituted ones (**36**–**38**) were characterised by higher PLQY most likely due to a stronger electronic coupling between the donor and acceptor parts. Upon dispersion in the DPEPO host matrix, all the discussed luminogens afforded superior PLQY values ranging from 59 to 78%. It is worth mentioning that TADF of all the host-guest layers except **36** possessed short (<10 μs) delayed components which is profitable for the device stability. A series of OLEDs were fabricated with the following device architecture: ITO/NPB/*m*CP/DPEPO:**36**–**41**/DPEPO/TPBi/LiF/Al. All the OLEDs demonstrated high EQEs in the range from 15.6% for a sky-blue-emitting device to 20.7% for the green one.

Recently, C_3-symmetrical fused polyheterocycles became of special interest as electron acceptors for TADF emitters [52, 53]. The convenience of such structures is the option to bond them with electron-donating units to afford star-shaped D_3A luminophores. Star-shaped twisted compounds offer plenty of benefits over their linear analogues, comprising the advantages of small molecules and polymers, i.e. the facile solution processability, good film-forming properties and the high degree of chemical purity. Besides, a star-shaped structure leads to the suppression of intermolecular interaction in the solid state and affords a more efficient solid-state emission.

In recent years, tricyclic heptazine moiety featuring seven sp^2-hybridised nitrogen atoms was discovered to be among the strongest electron-accepting units reported [53]. In 2020, the research groups of Yang [54] and Zysman–Colman [55] almost simultaneously proposed a novel C_3-symmetrical star-shaped electron acceptor tristriazolotriazine (Fig. 12) consisting of fused 1,3,5-triazine and 1*H*-1,2,4-triazole motifs and having nine sp^2-hybridised nitrogen atoms.

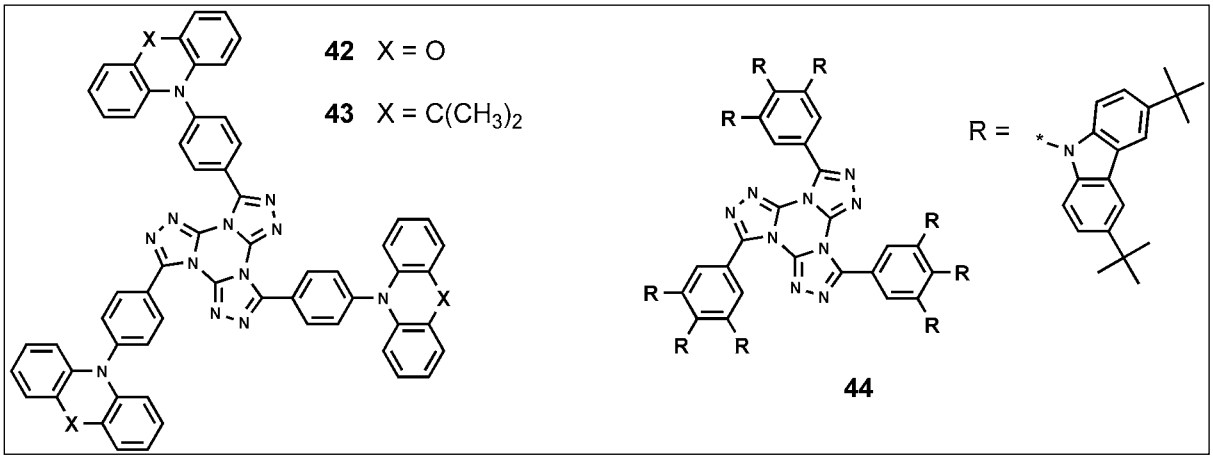

Fig. 12. Tristriazolotriazine-based compounds **42–44** with different electron-donating substituents

An interesting characteristic of two luminophores **42** and **43** (Fig. 12) is their behaviour upon aggregation. When traditional experiments for examining aggregation-induced emission enhancement (AIEE) properties with different water/organic solvent ratios were carried out, **42** exhibited blue-shifted emission while the emission peak of **43** appeared to be red-shifted. Authors attribute this to the differences in geometries of the luminophores that, in turn, cause the differences in reorganisation energies. The blue-shifted AIEE of **42** was attributed to the lower reorganisation energies in aggregates than in the solutions and the scarce π-π stacking caused by a highly twisted structure. On the other hand, the less twisted geometry of **43** stimulates π-π stacking and interaction between the molecules leading to the red-shift of emission. For the confinement of luminophores, the authors selected 9-(4-*tert*-butylphenyl)-3,6-bis(triphenylsilyl)-9*H*-carbazole (CzSi) as an appropriate host due to its wide E_g. Compound **42** possesses the ΔE_{ST} value of 0.2 eV, and compound **43** has the ΔE_{ST} value of 0.07 eV due to a stronger phenoxazine electron-donating motif and a more twisted structure.

Solution-processed OLEDs with a device architecture of ITO/PEDOT:PSS/CzSi:**42**–**43**/DPEPO/TmPyPB/Liq/Al were fabricated. The OLED containing **42** demonstrated a high luminance of 1898 cd/m^2, CE_{max} of 19.2 cd/A, PE_{max} of 5.2 lm/W and EQE of 14.5%. The performance of **43**-based OLED was much more inferior with L_{max} of 346.6 cd/m^2, CE_{max} of 4.1 cd/A, PE_{max} of 1.1 lm/W and EQE of 1.9%. The better performance of **42**-based device is attributed to a higher PLQY and a better TADF performance of compound **42**.

The group of Zysman–Colman [55] introduced a tristriazolotriazine acceptor decorated with carbazole units **44** (Fig. 12) and cross-compared its characteristics with those of compound **42**. While dispersed in the CzSi host, the novel compound **44** possessed a higher PLQY and a shortened excited state lifetime than the reference **42**. Nevertheless, the solution-processed OLED based on **44** afforded EQE only of 5.8%.

Recently, two compounds with triphenylamine as a central core and phenyltriazole side-arms **45**–**46** (Fig. 13) were published [56]. The PL of solutions of these compounds are characterised by a moderate solvatochromism: their PL peaks shift from 395 nm in non-polar toluene to ca. 430 nm in polar dimethyl sulfoxide (DMSO) or ethanol. The reported PLQY values for their dilute acetonitrile solutions are 78% for compound **45** and 28% for **46**.

Interestingly, in their neat state (powder), compounds **45** and **46** show a very broad emission covering nearly the whole visible spectrum. The most intensive bands of this emission are significantly red-shifted (with peaks around 600 nm) compared to the corresponding solutions. However, when these compounds were incorporated in the poly(dimethylsiloxane) matrix (PDMS), their PL made a significant blue-shift and the samples emitted sky-blue light with the most intensive peaks in the region of ca. 400–500 nm. The PL of the neat compounds was only moderate compared to their solutions. CIE 1931 colour coordinates with an *x* ranging from 0.29 to 0.36 and *y* from 0.31 to 0.40 are close to those of white light (x = 0.33, y = 0.33). These properties make such molecular structures attractive as potential white

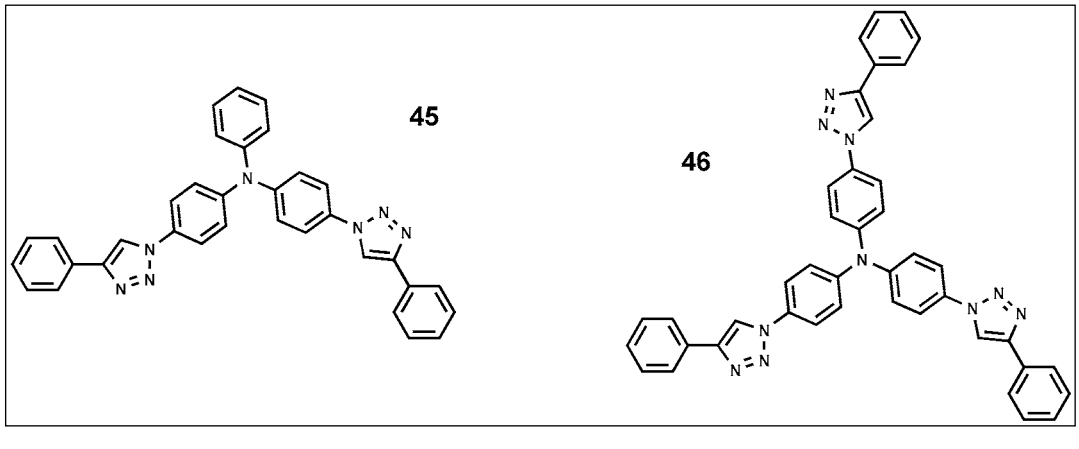

Fig. 13. Phenyltriazole-substituted triphenylamines **45–46**

light emitters. Besides, due to the presence of triazole units, compounds **45** and **46** show reversible acid sensitivity. When their samples (either solid or liquid) are exposed to a vapour of acid, changes in both absorption and emission spectra are observed which be seen as a colour change by an eye. The bands of both absorption and PL shift backwards when the samples are exposed to an alkali vapour (e.g. triethylamine). Such properties make these materials to be used as acid detectors as well.

In a very recent study, eight new derivatives of triazole **47**–**54** (Fig. 14) and their properties are presented [57]. The main interest of the study was the impact of triazole connectivity on the photophysical properties of donor–acceptor emitters. Compounds **47**–**54** were divided into two groups where the electron donor was connected either to the triazole's N^1 nitrogen atom ('donor-N') or C^4 carbon atom ('donor-C').

'N-connected' compounds **47**–**50** were obtained by one-pot synthesis from ethynyl-substituted quinoxaline, sodium azide, and an appropriate donor-substituted phenylboronic acid catalysed by copper (II) acetate. The yields of compounds **47**–**50** were from 54 to 87%. 'C-connected' compounds **51**–**54** were obtained from the condensation of tetrazoloquinoline with appropriate donor-substituted phenylacetylenes catalysed by copper. The yields of the latest were somewhat lower (between 44 and 70%).

The positions of fluorescence bands of compounds **47**–**54** depend on donor substituents and shift from ca. 400 nm (carbazoles) to 500 nm (diphenylamine and phenoxazine). PL bands of 'C-connected' compounds are somewhat red-shifted compared to their 'N-connected' analogues. Interestingly, all these compounds exhibit nearly identical and wide phosphorescence bands (recorded at 80 K with a delay).

'N-connected' derivatives exhibit higher singlet and lower triplet energies compared to their 'C-connected' counterparts. The HOMO–LUMO gaps are larger for 'N-connected' derivatives as well. These trends are attributed to disrupted donor–acceptor conjugation through the nitrogen linkage, thereby rendering the acceptor less electron-deficient in the 'N-connected' series. Most of the compounds among **47**–**53** favour room-temperature phosphorescence (RTP) due to large singlet–triplet energy gaps (ΔE_{ST} = 0.4 eV), while 'C-connected' phenoxazine (**54**) uniquely exhibits TADF attributed to its small ΔE_{ST} of 0.1 eV. Despite all the interesting features described above, PLQY values of compounds **47**–**54** (1% in zeonex polymer matrix) are only up to 20%.

SUMMARY

Along with growing human population and accelerating technological progress, the urge of humanity for semiconductors is increasing constantly. The expanding replacement of inorganic semiconductors to organic ones is dictated by the ease of their synthesis, a wide variety of

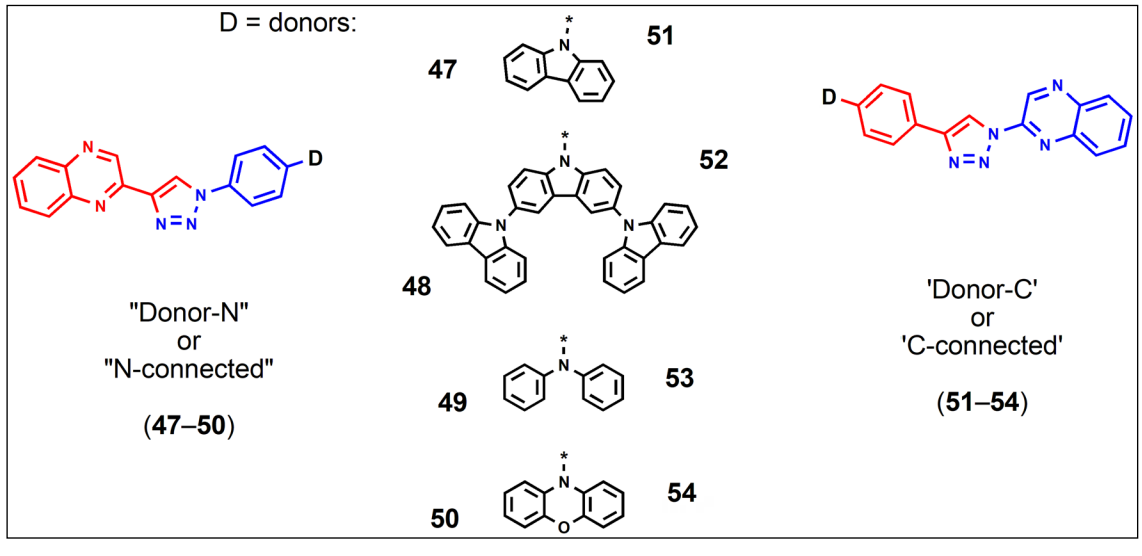

Fig. 14. Triazole derivatives **47**–**54** with differently connected donor units

properties achievable, and environmental friendliness. The field of OLEDs is the dominant area of utilisation of organic semiconductors to date. It comprises two big segments: OLED display and OLED lighting technologies. The former has been successfully commercialised and widely utilised for a long time, whereas the latter is still emerging and is hindered by severe shortcomings that need to be addressed before commercialisation. By a smart design of organic π-functional systems that has advanced the theoretical basis, researchers are now capable of achieving diverse properties of organic semiconductors. This review is mainly focused on the advantages of triazole-based fragments as the ones with the most promising electron-deficient moieties utilised in the engineering of organic semiconductors. Despite being scarcely investigated, triazolyl-based compounds are of great use for organic optoelectronics due to the following reasons:

1. Derivatives of triazole can be obtained via easy and cost-effective synthetic procedures.

2. Triazole has three sites that can be easily functionalised: two carbon and one nitrogen. It predetermines a wide structural tunability and makes triazole more advantageous over other five-membered heterocycles, such as oxadiazole and thiadiazole.

3. Triazole is an electron-deficient aromatic system with low-lying LUMO levels, that makes it suitable for the design of electroactive compounds of a donor–acceptor structure.

4. Due to its electron deficient character, triazole is a perfect candidate for a highly efficient organic electron-transporting materials.

5. Triazole is highly thermally and electrochemically stable.

6. High triplet energy level values (ca. 3 eV) make triazole of high use in the design of bipolar host-compounds for organic triplet emitters, exhibiting either TADF or phosphorescence.

All the above-mentioned characteristics make triazole a promising electron-accepting unit in the design of efficient organic electroactive compounds.

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TRIAZOLO FRAGMENTUS TURINTYS ELEKTROAKTYVŪS JUNGINIAI ORGANINIAMS ŠVIESOS DIODAMS: APŽVALGA

S a n t r a u k a

Organiniai šviesos diodai (OLED) yra viena sparčiausiai besivystančių optoelektroninių technologijų, plačiai taikomų ekranų ir apšvietimo srityse. Jų veikimo efektyvumas ir stabilumas labai priklauso nuo tinkamų organinių medžiagų, pasižyminčių gera krūvininkų pernaša, efektyviu eksitonų panaudojimu bei dideliu terminiu ir cheminiu stabilumu, sukūrimo. Azoto atomą turintys heterocikliniai junginiai, ypač triazolai, sulaukia didelio dėmesio dėl gerų elektronų pernašos savybių. Struktūriškai jie skirstomi į 1,2,3- ir 1,2,4-triazolus, kurių savybės gali būti tikslingai modifikuojamos parenkant pakaitus heterociklinio žiedo struktūroje. Tokia struktūrinė įvairovė leidžia reguliuoti jų elektronines ir fotofizines charakteristikas. Dėl šių savybių triazolo dariniai yra perspektyvūs optoelektroninių prietaisų komponentai. Jie gali būti naudojami kaip krūvininkų pernašos arba šviesą spinduliuojančios medžiagos OLED įrenginiuose, taip pat taikomi fotovoltinėse sistemose ir jutikliuose. Šioje apžvalgoje aptariami triazolo darinių struktūriniai ypatumai ir jų vaidmuo elektronų pernašos ir šviesos emisinėse sistemose, pabrėžiant jų potencialą naujos kartos optoelektroniniuose prietaisuose.