



Design and synthesis of high performance π -conjugated materials through antiaromaticity and quinoid strategy for organic field-effect transistors



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ABSTRACT

Organic field-effect transistors (OFETs) have received significant interest due to potential applications from low-cost active circuit to wearable health care devices. Organic semiconductors as one of the key components in OFETs have drawn great attentions during last decades. Among them, antiaromatic and quinoidal materials have become the most intensively studied semiconductors. Therefore, this review describes the chemical structures and efficiency characteristics of π -conjugated materials through antiaromaticity and quinoid strategy for OFETs. In addition, rational designs and synthetic methods for these materials will be summarized, and a practical guideline for accelerating the development of high-performance semiconducting materials and devices will be provided.

1. Introduction

Thanks to many advantages for organic semiconductors (OSCs), such as lightweight, mechanical flexibility, low power consumption and solution-processable, a great deal of applications including radio-frequency identification tags [1], electronic paper [2], electronic skin [3], and biosensors [4] have attracted many scientists' great attention. Meanwhile, rapid development in materials design and synthesis methods with a continuous augment in foundational understanding has established and boomed the development of organic field-effect transistors (OFETs). The performances of organic semiconductors in OFETs have improved rapidly over the last decade. Many classic aromatic materials for OSCs like diketopyrrolopyrrole (DPP), isoindigo (IID), naphthalenediimide (NDI), and other electron-deficient acceptors are widely exploited [5–7].

In all of the reports so far, most high-performance p-channel OSCs show the hole mobilities (μ_h) over $10 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ with good processability [8]. In contrast, the stability and performance of n-channel and ambipolar OSCs are far less than the p-channel devices [9–11]. In recent years, antiaromatic and quinoidal materials were widely studied in many fields as they have moderate highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy levels, narrow band gaps and relative short bond length alternation in π -conjugated system [12–15]. In this review, we focused our attention on the latest developments of π -conjugated materials through

antiaromaticity and quinoid strategy for OFETs. The first part will describe the antiaromatic materials including indacenes, pentalenes and other representative structures. Then, the second part will deal with the quinoidal materials, like small molecules and polymers. Non-polycyclic and fused ring for molecules, thienoquinoids and others for polymers will also be included. Finally, we outline the main achievements, challenges and prospects for high-performance antiaromatic and quinoidal materials-based OFETs.

2. Antiaromatic materials in OFETs

Antiaromaticity, first proposed by Hückel in the 1930s, is defined as conjugated cyclic systems containing $4n$ π -electrons [16]. Antiaromatic compounds are appealing candidates for organic electronic applications on account of three characters: (1) small band gaps with respect to analogous aromatic systems, which could broaden the absorption spectrum [13]; (2) high polarizability, which could improve intermolecular interactions; (3) paratropic ^1H NMR chemical shift and large positive nucleus independent chemical shift (NICS) values, which the value of polycyclic aromatic hydrocarbons (PAHs) is negative [17]. Indeno [1,2-b] fluorene (IF) and pentalenes analogue whereas replacing two of the traditional six-membered rings by five-membered rings are two kinds of profile $4n$ π -electrons system compounds. The changes of both the physical and chemical properties by introduction of cyclopentadiene rings to PAHs prompted chemists to go into the potential

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Table 1
Summary of OFET device data for anti-aromatic materials.

Comp.	Deposition Process	HOMO/LUMO (eV)	Max μ_h ($\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$)	Max μ_e ($\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$)	$I_{\text{on}}/I_{\text{off}}$	Device structures	Ref.
C1	Single crystal	-6.17/-4.00	7.0×10^{-4}	3.0×10^{-3}	$10^4/10^5$	BGTC (N ₂)	[20]
C2	Evaporation	-5.71/-3.74	1.6×10^{-5}	–	60	BGBC (vacuum)	[21]
C3	Evaporation	-5.92/-3.86	1.9×10^{-5}	8.2×10^{-6}	10/10	BGBC (vacuum)	[21]
C4	Evaporation	-5.81/-3.69	1.1×10^{-5}	1.6×10^{-6}	$10^2/30$	BGBC (vacuum)	[21]
C5	Evaporation	-5.27/-3.82	2.0×10^{-3}	4.0×10^{-3}	$10^4/10^4$	BGTC (vacuum)	[22]
C6	Spin coating	-5.61/-4.18	0.44	–	10^2	TGBC (air)	[23]
C7	Single crystal	-5.46/-4.27	0.64	0.34	$10^2/10^2$	BGTC (air)	[24]
C8	Single crystal	-5.52/-3.61	5.0×10^{-3}	–	10^3	BGTC (N ₂)	[25]
C9	Evaporation	-5.44/-3.18	1.8×10^{-3}	–	10^5	BGTC (air)	[34]
C10	Single crystal	-5.50/-2.99	0.52	–	10^4	BGTC (air)	[35]
C11	Single crystal	-5.26/-2.91	6.55	–	10^4	BGTC (air)	[35]
C12	Spin coating	-5.03/-2.96	1.0×10^{-3}	–	10^4	BGTC (N ₂)	[36]
C13	Spin coating	-5.03/-3.02	0.65	–	10^5	BGTC (N ₂)	[36]
C14	Spin coating	-4.91/-3.58	1.6×10^{-2}	–	10^6	BGTC (N ₂)	[33]
C15	Spin coating	-4.79/-3.64	3.6×10^{-2}	–	10^4	BGTC (N ₂)	[33]
C16	Spin coating	-4.61/-3.62	1.0×10^{-2}	–	10^4	BGTC (N ₂)	[33]
C17	Spin coating	-5.84/-3.76	–	6.0×10^{-2}	10^6	BGTC (N ₂)	[37]
C18	Spin coating	-5.72/-3.45	–	3.4×10^{-2}	10^6	BGTC (N ₂)	[37]
C19	Evaporation	-4.79/-3.57	1.7×10^{-4}	–	10^5	BGTC (air)	[38]
C20	Evaporation	-4.87/-3.61	2.3×10^{-3}	–	10^5	BGTC (air)	[38]
C21	Evaporation	-4.92/-3.63	4.0×10^{-4}	–	10^3	BGTC (air)	[38]
C22	Evaporation	-4.94/-3.64	5.4×10^{-4}	–	10^5	BGTC (air)	[38]
C23	Evaporation	-5.07/-3.74	3.2×10^{-4}	5.8×10^{-5}	$10^3/10^4$	BGTC (argon)	[38]
C24	Spin coating	-4.95/-3.62	6.0×10^{-3}	–	10^5	BGTC (N ₂)	[39]
C25	Spin coating	-4.69/-3.75	1.7×10^{-3}	–	10^3	BGTC (N ₂)	[39]
C26	Spin coating	–	0.15	–	10^4	BGTC (air)	[40]
C27	Spin coating	-5.10/-3.40	2.4×10^{-2}	–	10^3	BGTC (air)	[40]
C28	Spin coating	–	0.19	–	10^4	BGTC (air)	[40]
C29	Spin coating	-5.00/-3.30	0.15	–	10^4	BGTC (air)	[40]
C30	Spin coating	-4.91/-2.70	2.7×10^{-2}	–	10^2	BGTC (N ₂)	[44]
C31	Spin coating	-4.88/-2.65	2.4×10^{-3}	–	10^2	BGTC (N ₂)	[44]
C32	Spin coating	-4.74/-2.35	1.8×10^{-3}	–	10^2	BGTC (N ₂)	[44]
C33	Single crystal	-5.20/-2.59	4.5×10^{-3}	–	10^5	BGTC (vacuum)	[45]
C34	Single crystal	-5.42/-3.52	0.4	0.18	10/10	BGTC (vacuum)	[45]

Device architectures, BGTC: bottom gate top contact; BGBC: bottom gate bottom contact; TGBC: top gate bottom contact.

applications in many fields, especially in OFETs [15]. In addition, some indacene-based small molecules display quinoidal properties dominantly with incorporation bulky substitutions to stabilize the indacene core. Some pentalene-based materials show small positive NICS(1)zz values with a small antiaromatic character, even small negative NICS(1)zz values with a small aromatic character. With these features, some antiaromatic materials show excellent charge transport behaviors due to quinoids and aromaticity which can stable electron delocalization in π -conjugated systems. The mobility, deposition process, and $I_{\text{on}}/I_{\text{off}}$ ratio as well as HOMO/LUMO energy levels and device structures with corresponding structures are depicted below (Table 1 and Fig. 1A).

2.1. Indacene-based materials

Among the polycyclic $4n \pi$ systems, the skeleton of IF, *s*-indacene is prominent 20π -electron, a fully conjugated analogue having 6–5–6–5–6 fused rings which was first reported by Swager's group in 1994 [18]. Due to its high reactivity (an unstable biradicaloid resonance contributor, see Fig. 2), the bulky substitution, π -extended both in lateral and longitudinal and introduction of fused benzene rings as effective means are adopted by many chemists to improve the stability. Wang and co-workers [19] proposed a new method to synthesize terphenyl easily by three-step pathway using Suzuki cross-coupling without any regioisomers which boosted the development of indacene-fluorene (IF) derivatives greatly (see Fig. 3). To our best knowledge, the first effectively IF-based compound for OFETs was reported by Haley and co-workers [20] in 2012 via substituted-pentafluorophenyl at the 6,12-position. Due to the strong electron-withdrawing property, it gave low HOMO (–6.17 eV) and LUMO (–4.00 eV)

energy levels. Thereby C1 showed an ambipolar semiconductor behavior with the hole and electron mobility of 7×10^{-4} and $3 \times 10^{-3} \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$, respectively. Almost simultaneously, Yamashita et al. [21] prepared C2–C4 with relatively low mobilities about $10^{-5} \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$. The bond lengths (red double bond, see Fig. 2) indicated quinoid structure to the indacene core by X-ray crystal-structure analysis. The low mobility may be ascribed to the relative high HOMO–LUMO energy levels, large dihedral angle (76.5°) and the less-ordered molecular arrangements in the thin films. C5 (DIAn), with fusion of an anthracene and introduction of bulky mesityl groups, gave ambipolar performances with quite balanced electron ($4.0 \times 10^{-3} \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$) and hole mobilities ($2.0 \times 10^{-3} \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$) [22]. The introduction of (triisopropylsilyl) ethynyl groups from the outset improved solubility and stability with resistance towards oxidation, leading to relative high electron mobility. Moreover, the third strategy was applied by fusion thiophene (C6) which made low LUMO energy levels and narrow band gap (1.43 eV). The introduction of rich-electron thiophene units in this molecule exhibited the highest hole mobility up to $0.44 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$ by spin-coating process [23]. Using this tactic, Zhu et al. [24] obtained an ambipolar semiconductor behavior of C7 with the p-channel up to $0.64 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$ and n-channel up to $0.34 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$, which to our best knowledge was one of the highest record in ambipolar OFETs for single crystal in anti-aromatic semiconductors. The bond lengths revealed the quinoidal property for the backbone by single crystal analysis. The backbone and TIPSA pendants jointly facilitated one-dimensional intermolecular π - π stacking with a short distance of 3.304 Å, which was smaller than that of TIPSA-pentacene (3.349 Å). The most optimized HOMO/LUMO energy levels (–5.46 eV for the HOMO and –4.27 eV for the LUMO) and ordered intermolecular π - π stacking with a

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