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Review

Corannulene derivatives for organic electronics: From molecular engineering to applications

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ABSTRACT

This paper intends to provide an overview for using corannulene derivatives in organic electronics such as organic field-effect transistors (OFETs), organic solar cells (OSCs), and organic light-emitting diodes (OLEDs). We highlight the rational design strategies, tuning molecular orbital energy levels and arrangement in single crystals of corannulenes. The topological structure and properties of corannulene make it a unique candidate for organic electronics.

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1. Introduction

Corannulene, a bowl-shape fragment of C_{60} , was first synthesized in 1966 [1]; owing to the efforts of Siegel et al., it can be produced in kilogram scale now [2]. Over the past several decades, chemists have been fascinated by its unique topological structure, and endeavor to its functionalization and properties [3–6]. These derivatives have been applied in the fields of supramolecular chemistry [7–10], liquid crystals [11,12], chiroptical activity [7,13,14], bottom-up synthesis of carbon nanotubes [15], radicals [16–20] and lithium-ion cells [21]. Although its semiconducting properties are also interesting and have attracted considerable attention on the synthesis and basic characterization, the device performance based on corannulene derivatives has not been demonstrated until recently [22–27].

Unlike planar polycyclic aromatic hydrocarbons (PAHs), corannulene has a dipole moment as high as 2.1 Debye, resulting from the different electron densities on its concave and convex surfaces [28,29]. The dipole moment, the size of the bowl surface and bowl depth will significantly influence their packing in single crystals [5,26]. For corannulene, $CH\cdots\pi$ interactions instead of $\pi\cdots\pi$

interactions [30] dominate in single crystal, thus prohibiting intermolecular charge carrier transport. Molecular orbital energy decides the injection barrier of hole or electron to electrode. Pristine corannulene exhibits high electron affinity (–2.65 eV) and low ionization potential (–6.30 eV) [24,31]. Both values are far from the work functions of common metal electrodes (Au: 5.2 eV, Ag: 4.2 eV, Al: 4.2 eV) [32], indicating high injection barrier for both holes and electrons. Hence, modulating the packing and molecular orbital energy of corannulene derivatives are critical for their applications in organic electronics. Fortunately, the rich chemistry of corannulene allows such on-demand rational design of different corannulene molecules. We and Pei et al. have developed a series of corannulene derivatives and used them as p-channel [22], n-channel [23] and ambipolar materials [26]. In addition, we also used corannulene derivatives as non-fullerene acceptors in organic solar cells [24]. In this review, we intend to provide an overview of the past, present of and future of the application of corannulene derivatives in organic electronics. We first summarize the functionalization to extend the π -conjugated framework of corannulene or incorporation of heteroatom on the backbone of corannulene from 2007 to 2016 (for those before 2007, see reviews [3–5,33,34]), then present the applications and device characterization of corannulene derivatives in organic electronics, and finally we evaluate the prospective of using corannulenes in organic electronics and outlines the trends for their future development.

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2. Extended π -conjugated or nitrogen-doped corannulene derivatives

Extension of π -surface of the π -conjugated molecules both increases their intermolecular π - π interactions and effectively modulates their molecular optical and electrochemical properties [35,36]. As aforementioned, the dominating presence of CH... π interactions in pristine corannulene single crystals will prohibit intermolecular charge carrier transport [30]. To improve corannulene derivatives' intermolecular π - π interactions (electronic couplings) in the solid state, increasing the corannulene π -conjugated surface is effective [5,33]. Lash et al. prepared corannulenoporphyrins **2-1** (Fig. 1) from nitrocorannulene in five steps [37]. Corannulenoporphyrins **2-1** exhibited significantly red-shifted absorption with onset absorption wavelength at about 680 nm. Later, Osuka et al. fused porphyrins into dibenzo[*a,g*]corannulene in just two steps by coupling porphyrins at different positions with dibenzo[*a,g*]corannulene, and then oxidatively fusing to give 5- or 6-membered rings linked dibenzo[*a,g*]corannulene-porphyrin **2-2** and **2-3** [38]. The HOMO level of **2-2b** is 5.14 eV and that of **2-3b** is 5.28 eV, both match the work function of gold (5.2 eV), indicating their potential applications as p-channel materials. Wu et al. used the straightforward palladium-catalyzed cyclization to construct the highly curved bulkybowls **2-4** and **2-5** [39,40]. Both compounds showed 2D columnar stacking with large π -orbitals overlap, thus facilitating the intermolecular charge carrier transport. Siegel et al. fused graphene fragment into corannulene with the key step of activation of a C(Ar)-F bond to give compounds **2-6** [41]. Because of the steric hindrance, a *meso* pair of 5-helicenes existed in single crystals. And calculation revealed that the HOMOs mainly localized on graphenic region and the LUMOs on corannulene core, confirming that curvature changed the orbital levels and bandgap

compared to a planar graphenic form [42,43]. Scott et al. proved that highly distorted conjugated molecules, with curvatures surpassing that of C₆₀, can be synthesized by solution phase synthetic approach instead of extreme conditions like high-temperature flash vacuum pyrolysis method [39]. They synthesized a series of multiindenocorannulenes (compounds **2-7** to **2-13**) and investigated their optical properties, providing the basic ideas to extend corannulene π -system by Pd-catalyzed coupling reactions.

In 2012, Scott et al. developed an elegant "dynamic covalent" [44-46] approach to 1,3,5,7,9-pentakis(Bpin)corannulene after 96 h through Ir-catalyzed C-H polyborylations [47]. The polyborylated corannulene is an important building block for a series of π -conjugated extended corannulene derivatives. Later, Siegel et al. optimized the procedures using microwave-assisted method to decrease the reaction time from 96 h to 4 h compared with the routine bench-top preparation [48]. The polyborylations of corannulene provide the multi positions for coupling reactions. 1,3,5,7,9-Pentakis(Bpin)corannulene coupled with 2-bromo-1,3-dichlorobenzene followed by flash vacuum pyrolysis to give isomerically pure [5,5]nanotube **2-14** [47]. Itami, Scott et al. also used 1,3,5,7,9-pentakis(Bpin)corannulene as a starting material to synthesize the defect nonplanar nanographene compound **2-15** with odd-membered rings [49,50].

Doping of heteroatoms into conjugated systems is an efficient method to alter their intrinsic properties such as orbital energy and optical properties [51-53], and thus to influence their semiconducting properties. It has been proved that nitrogen-doping can significantly increase the mobilities of conjugated molecules [54,55]. Several theoretical calculations on nitrogen-doped corannulenes have been reported [56,57] and revealed that the substitution of carbon atoms with nitrogen atoms in corannulene lowered the HOMO-LUMO gap. Nevertheless, it is

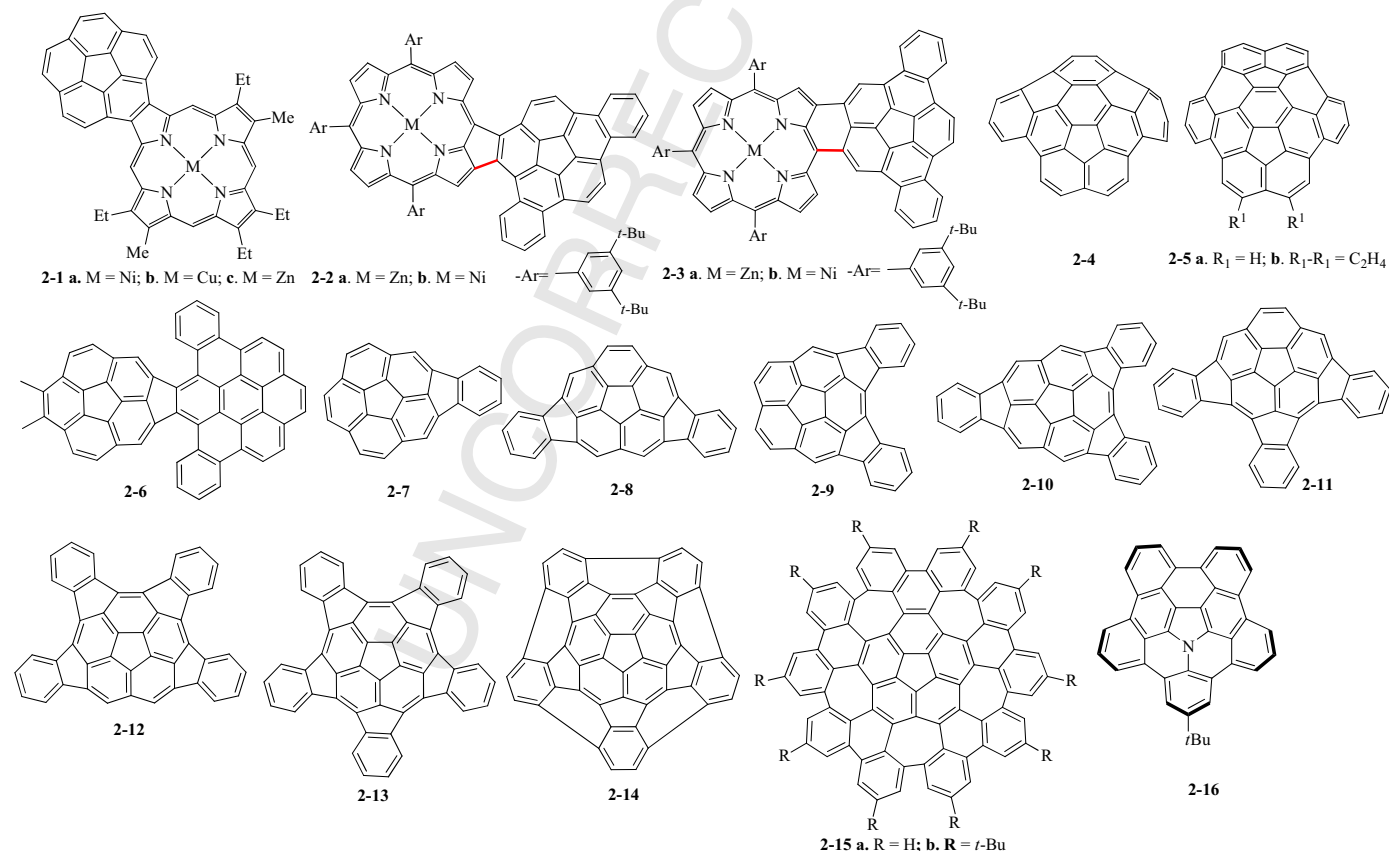


Fig. 1. π -surface extended corannulene derivatives.

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