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Conjugated silane-based arylenes as luminescent materials

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ABSTRACT

Symetric (**4a,b**) and asymmetric (**7b,c**) silane-containing conjugated compounds comprising electron rich benzofurazane, 10-hexylphenothiazine and ethylenedioxytiophene moiety were designed and successfully synthesized by the palladium-catalyzed Suzuki coupling. These compounds have a relatively small band gaps and show strong absorption in the region 300–340 nm. Furthermore, compounds **7b** and **7c** show light emission in almost the entire visible light (from blue to red region) when symetric compounds emit blue and green light. of synthesized structures The electrochemical study revealed the onset of the oxidation wave was found at rather low potentials. The optical band gap (1.8 eV - 3.39 eV) makes the structures potentially useful as an hosting material for emitters. The lowest electrochemical and optical band gap characterizes asymmetric structure containing silane unit, the largest - structure with benzofurazane moiety. The electrochemical behavior of tetraphenylsilane derivatives was also confirmed by EPR as well as theoretical (density functional theory (DFT)), and time dependent density DFT techniques. The calculations rationalize the difference between electrochemical and optical experimentally measured energy gaps.

1. Introduction

Tetrahedral silicon-centered organic structures have attracted comprehensive interest in regard to their potential application in sensor technologies and organic light emitting diodes (OLEDs) [1–5]. The utilization of phosphorescent emitter elements is one of the most efficient pathways to improve the quantum efficiency of OLEDs. As hole- and electron-transport materials may be used in all groups of PHOLEDs, these systems should possess higher triplet energy and energy levels for the hole or electron blocking than the phosphorescent emitters [6,7]. Tetraphenylsilane, as the stem of unit of high-triplet-energy materials, represents the convenient electron-transfer polymers [8–10]. In this context, silicon disconnects the conjugation between various building blocks, therefore polymer eludes the intramolecular charge transport from a donor to an acceptor parts [11,12]. Additionally, luminescent materials based on these kind of compounds may be curious due to well-defined structures and high color purity as classified by narrow emissions in solution and solid films [13–16]. Regarding high glass-transition temperature and high thermal stability, conjugation blocking for a wide band gap and fine film-forming properties, tetraphenylsilane derivatives can be applied to investigate non-aggregating amorphous electroluminescent tools [17]. Furthermore, Davies et al. [18] and M. Rose et al. [19] claimed that the tetrahedral shaped silane compounds can be used as promising building blocks to construct 3D porous metalorganic frameworks.

Achieving high performance blue, green and red electroluminescence through a simple material system with the aim to reduce the production cost of materials and simplify the manufacturing process is an important issue for i.e. OLED applications. Liu et al. [20] presented an efficient blue fluorescent and green and red phosphorescent material built of tetraphenylsilane-phenantroimidazole. Also the new host and blue emitting materials (4,4′-bis (triphenylsilyl)-biphenyl) were designed and synthesized by Fan et al. The design strategy enhanced their HOMO levels and glass transition temperatures. Moreover, new molecules retained the high triplet energies as the bis(triphenylsilyl)-biphenyl molecule because the perpendicular spiro-conformation effectively prevented the extension of π-conjugation [21].

A high triplet energy host material (also blue emitter) based on a tetraphenylsilane core - 4-((4-(9*H*-carbazol-9-yl) phenyl) diphenylsilyl)phenyl)diphenylphosphine oxide was synthesized as the bipolar host material for blue phosphorescent organic

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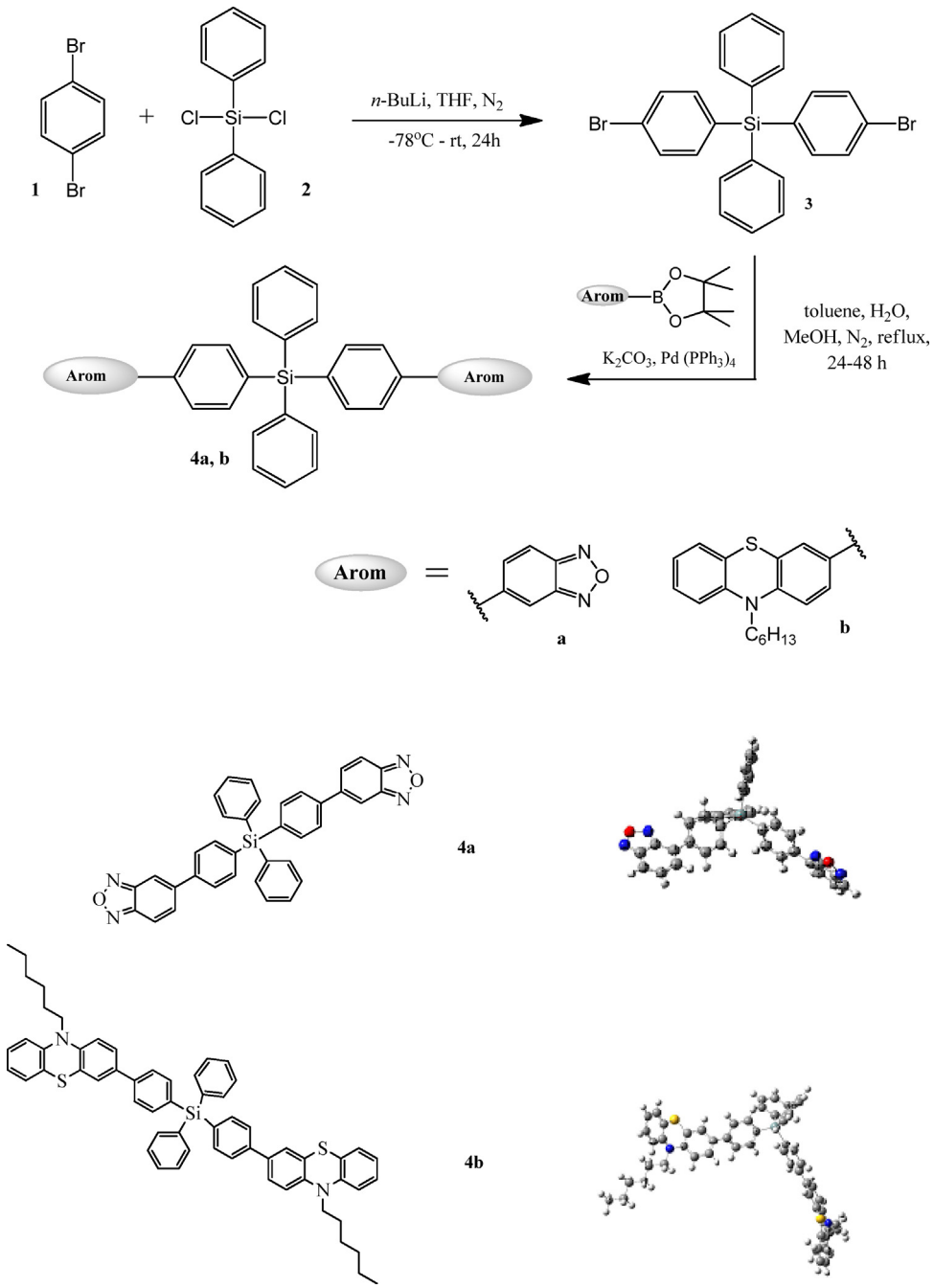
light-emitting diodes by Cho and Lee [22]. A diphenylphosphine oxide group and a carbazole group were attached to the tetraphenylsilane core to improve the hole and electron transport properties while keeping the high triplet energy of the core structure.

Given these, several efficient multi-color emitting materials, based on a universal host, have been achieved in the literature [13–16,20–22]. However, the design and synthesis of an organic molecule that can be employed as a host to realize the efficient OLED devices with a relatively long-wavelength light is still a considerable challenge.

In the present work, we report the design and synthesis of multi-redox systems of functionalized arylenes. The tetraphenylsilane derivatives seem to be a good example of charge transporting optical materials. The group of structures provides a basis for an understanding of effects of the backbone ring, heteroatom, and fused rings on the geometric and electronic properties of model compounds. The work reports also electrochemical and spectroscopic properties of obtained macrostructures. Moreover, to gain the deeper insight into the electronic structures of the new silanes, theoretical studies are performed within by the density function theory. The effects of the acceptor



Scheme 1. The synthetic route of the symetric resulting (**4a**,**b**) silane-based molecules and optimized structure for **4a**,**b**.