Herein, we synthesized a small series of novel biscarbazoles bridged emitters in organic light-emitting diodes (OLEDs). It is a conjugation between the Si σ orbital and the aryl π orbital. In the target molecules BCzSi_n, n = 2–4, the efficient σ–π conjugation elevated the highest occupied molecular orbital energy level with no influence on the lowest unoccupied molecular orbital. In the solid state, the emission full width at half-maximum (fwhm) of all the compounds narrowed significantly, while the emission efficiency increased and the emission color of carbazole was retained. This research provided a very simple and general way of subtly manipulating the electronic properties of organic materials to construct an emissive color-retaining system for multifunctional applications.

**INTRODUCTION**

The development of organic materials based on group 14 elements has attracted growing attention in recent years. Introducing silicon bridges in π-conjugated systems has been proven to be a promising way to modulate the electronic properties. This can allow functionality to be fine-tuned through the orbital interaction between the σ-orbital of silicon and the π-orbital of π-electron systems. Besides, the highly flexible nature of the Si–Si chain makes the molecule more soluble in common organic solvents and less possible to stack under concentrated conditions, which is beneficial for their practical application and the improvement of emission efficiency in the solid state. Oligosilanyl derivatives have been utilized as novel electronic and optical molecular materials, such as nonlinear optic materials, hole-transporting materials, and emitters in organic light-emitting diodes (OLEDs). It is a remarkable fact that the oligosilane-containing materials exhibit superior performance to some extent compared with the π-brided system.

Carbazole-based compounds have attracted considerable attention as hole-transporting and light-emitting materials in scientific and industrial fields. Carbazole derivatives are usually employed as an electronic donor group and they exhibit good absorption and fluorescence. Until now, research on carbazole derivatives focuses on π–π orbital interaction, and so far, only one study on carbazoyl–arysilane connected by the N–Si bond has been reported for OLEDs and its structure/property relationships have not been fully explored. Moreover, no conjugated molecules containing a carbazolyl group and Si bridged by the C–Si bond have ever been reported before. Understanding the effect of the smallest electronic building blocks represents a crucial step toward the development of new functionalized materials. Herein, we demonstrated the manipulation of photophysical properties of biscarbazole molecules through the adjustment of incorporated oligosilanyl bridges.

Permethyalted oligosilanyl units (−[Si(CH₃)₂]n−, n = 1–4) are the simplest alkyl-substituted oligosilane building blocks, which are stable and easy to prepare. We introduce the permethylated oligosilanyl bridges with the silicon number from one to four to evaluate the impact of the silicon chain length on the photophysical properties of carbazole systematically. We choose the 3-position of carbazole to connect with the silyl group considering that its reaction is relatively easier to achieve, and the postfunctionalization at this position retains the electron-donating properties of carbazole. The newly fabricated π−σ−π hybrids are highly thermally stable and exhibit a σ–π conjugation-induced spectral bathochromic shift. Interestingly, the full width at half-maximum (fwhm) of the solid-state emission decreased dramatically, while the emission efficiency increased and the emission color of parent carbazole retained. The relationship of the structure and properties was investigated in detail combined with quantum chemical calculations.
RESULTS AND DISCUSSION

Synthesis. The oligosilanyl-bridged bisscarbazoles can be easily achieved by lithium salt-elimination reactions between 3-lithium-9-methyl-9H-carbazole (Cz-Li) and symmetric halogen- or triflate group (OTf)-substituted oligosilanes (Scheme 1). N-methyl substitution was installed to carbazole to prevent the NH proton from the side reaction in the following procedures. Cz-Li as a key intermediate is obtained through lithium–halogen exchange reaction between n-BuLi and 3-bromo-9-methyl-9H-carbazole, which further reacts with commercially available dichlorodimethylsilane and dichlorotramethyldisilane to give BCzSi1 and BCzSi2 in the yields of 48 and 71%, respectively. α,ω-Diphenyl trisilane and tetrasilane 2a and 2b are subjected to the reaction with trifluoromethanesulfonic acid (TfOH) to give OTf group-terminated silane 3a and 3b, which react with Cz-Li to produce BCzSi3 and BCzSi4 in moderate yields (49 and 55%, respectively). These oligosilanyl-bridged compounds are air-stable solids and can be stored under the ambient conditions for at least 10 months. 1H NMR, 13C NMR, X-ray single-crystal analysis, and high-resolution mass spectrometry (HR-MS) conformed the structures and their high purity. These compounds exhibit high thermostability with 5% weight loss ranging from 322 to 342 °C (Figure S1). The solubility of these compounds in common hydrocarbon and aromatic and chlorinated solvents is almost the same, and the absorption band appearing around 260 nm can be assigned to the π−π* transition of the silicon backbone in aggregation. In the solid state (powder), BCzSi4 exhibited a reduced fwhm from 28 to 56 nm, namely, 44–89% of Cz. Especially for BCzSi3, the fwhm is less than half of that of Cz, indicating its pure deep blue emission (Figure 2c,d). The Si-containing compounds, except BCzSi3, possessed enhanced solid-state emission quantum yields up to 33% (BCzSi2). The fluorescence lifetimes of BCzSi1, BCzSi2, and BCzSi4 exceeded 6 ns, whereas those of Cz and BCzSi3 were 5.80 and 5.65 ns, respectively (Table 1 and Figure S3). Upon carefully checking the knr and k∗ values, it is clear that the incorporation of Si suppressed the nonradiative decay path, thus improving the radiative decay.

X-ray Structure Determination. Single crystals of BCzSi1, BCzSi2, and BCzSi4 suitable for X-ray diffraction analysis were obtained by slow evaporation of n-hexane into their dichloromethane solution at room temperature. Both compounds BCzSi1 and BCzSi2 crystallized in the same chiral space group (P1). In BCzSi1, the geometry around the bridging Si atom is tetrahedral, with C–Si–C bond angles ranging from 107.8(1) to 110.3(7)°. BCzSi2 and BCzSi4 adopt extended, all-trans conformation with two terminal carbazole units parallel to each other. The torsion angles between the Si–Si σ bond and the carbazole plane for BCzSi2 and BCzSi4 are 77.5 and 79.9°, respectively (Figure 3d,f), which are close to the ideal angle for the maximum π−π* conjugation. The torsion angle of C(Cz)−Si−Si−C(Cz) in BCzSi2 is 180°, demonstrating its all-
and anti. For basis sets to investigate the electronic properties, TD-DFT calculations were performed using the B3LYP functional with the 6-31G(d) and 6-311+G(2d,2p) basis sets. The angular nodal patterns are shown at an isosurface value of 0.02 au. The HOMO−LUMO gap values are plotted against a secondary axis with green triangles.

Figure 3. X-ray single-crystal structures of (a) BCzSi1, (b) BCzSi2, and (c) BCzSi4. (d−g) Side and top views of BCzSi2 and BCzSi4, respectively. Ellipsoids are set at the 50% probability. H atoms are omitted for clarity. Si is shown in red, and N in blue.

The electronic energy than the anti conformation (Figure S5). Selected Frontier orbital diagrams and energies for all compounds are plotted in Figure 4. The σ−π mixing is not always observed in aryl-capped linear silanes; it is significantly dependent on the electronic nature of the end groups. The electron-rich and electron-poor aromatic systems have very different interactions with oligosilanyl bridges. In the electron-accepting group-capped oligosilanes, the highest occupied molecular orbital (HOMO) on the aromatic system, giving rise to charge-transfer characteristics.9,24

Table 1. Spectroscopic Data of Cz and BCzSi1−BCzSi4 in Solution and Solids

| compd. | UV−vis | PL |
|--------|--------|----|
|        | λ_{abs}^{a}/nm | λ_{em}^{a}/nm | Φ_{f}^{b} | λ_{em}^{c}/nm | fwhm^{a}/nm | QYc | (τ)_{f} | k_{nr}^{-1}(10^{8}s^{-1}) | k_{r}^{-1}(10^{8}s^{-1}) |
| Cz     | 263, 293, 331, 345 | 351, 367 | 0.09 | 395, 414 | 63 | 0.25 | 5.80 | 0.43 | 1.29 |
| BCzSi1 | 269, 297, 331, 346 | 352, 368 | 0.12 | 383, 394 | 44 | 0.29 | 6.68 | 0.43 | 1.06 |
| BCzSi2 | 271, 299, 334, 348 | 355, 372 | 0.10 | 396, 415 | 56 | 0.33 | 7.20 | 0.46 | 0.93 |
| BCzSi3 | 271, 299, 334, 348 | 356, 372 | 0.06 | 383 | 28 | 0.20 | 5.65 | 0.35 | 1.42 |
| BCzSi4 | 271, 299, 334, 348 | 355, 373 | 0.11 | 399 | 52 | 0.31 | 7.43 | 0.42 | 0.93 |

*aUV−vis absorption peaks measured in the THF solution. bFluorescence measured in the THF solution; fluorescence quantum yields were calculated using quinine sulfate (Φ = 0.52) in 0.05 M H_{2}SO_{4} solution as the reference. The standard errors are less than 5% from three independent measurements. cMeasured in solids. dFluorescence quantum yields measured in solids. eThe average fluorescence lifetimes fitted by the double-exponential function. fThe radiative decay rate in solids, k_r = QY/τ. gThe nonradiative decay rate constant in solids, k_{nr} = 1/τ − k_r.
However, in the electron-donating group (4-thiomethyl)phenyl-capped oligosilanes, the $\sigma$–$\pi$ mixing is seen in the HOMO between the aromatic end group and the oligosilanyl chain. In our carbazole-capped systems, the electron density of the HOMOs was spread over the entire molecule across the oligosilanyl chain (Figure S6). The electron densities of LUMOs of BCzSi1 and BCzSi2 were mainly localized on two carbazole units, while for BCzSi3 and BCzSi4, those were only localized on one of the two carbazole units. The LUMO orbital of BCzSi2 and BCzSi4 is doubly degenerate in energy because of the C$_{3v}$ symmetry. The incorporation of the Si–Si chain into biscarbazole molecules increased the HOMO energy rather than the LUMO energy level. The LUMO energies of BCzSi2, BCzSi3, and BCzSi4 are almost the same, while their HOMO energy is elevated 0.13–0.16 eV higher than that of Cz, indicating the significant influence of $\sigma$–$\pi$ conjugation on the bonding orbitals. However, as for monosilyl-bridged BCzSi1, the electron-donating inductive effect and electron-withdrawing $\sigma^*(\text{Si–C})$–$\pi^*$ conjugation resulted in very slightly lifted HOMO and stabilized LUMO energy (0.03 eV). The HOMO–LUMO gaps decreased with the increase of the bridged Si number and became constant when more than two Si were employed in the molecules (Figures S6 and S7). These results account for the relatively larger bathochromic shift in UV–vis absorption of BCzSi2–BCzSi4 than that of BCzSi1. The isomer of 2-carbazole-substituted oligosilane compounds displays similar trends (Figures S8 and S9).

## CONCLUSIONS

In conclusion, we synthesized a series of symmetrically functionalized oligosilanyl-bridged compounds BCzSi$n$ ($n = 1–4$) with electron-donating carbazoles as end groups. The newly prepared molecules BCzSi$n$ are highly thermally stable. The bathochromic shift in the UV spectra and all-trans conformation in the crystal structures confirmed the existence of efficient $\sigma$–$\pi$ conjugation in BCzSi$2$–BCzSi$4$, which elevated the HOMO energy level with almost no influence on the LUMO. Through careful selection of the Si–Si chain length, the emission efficiency in the solid state could be enhanced, while the emission fwhm decreased dramatically. In addition, the incorporation of oligosilanyl linkages did not change the original emission color of the parent carbazole. This design strategy would give insights into the construction of novel $\sigma$–$\pi$ hybrids and provide a promising strategy for the rational design of stable and pure blue emission chromophores with an enhanced emission efficiency.

## EXPERIMENTAL SECTION

Reagents and solvents were purchased from commercial suppliers and used without further purification unless otherwise indicated. All air- and moisture-sensitive reactions were carried out under an argon atmosphere in an oven-dried glassware. The glassware was dried in an oven at 120 °C and cooled under a stream of inert gas before use. Tetrahydrofuran was distilled over sodium with benzophenone just before use. Acetone and THF were dried with sodium with benzophenone just before use. All reagents were used without further purification.

**Synthesis of BCzSi1.** 1 (500 mg, 1.92 mmol) was dissolved in dry THF (15 mL) and stirred at ~78 °C for 0.5 h under argon in a 50 mL Schlenk flask. n-BuLi (1.32 mL, 2.11 mmol, 1:1 equiv, 1.6 M solution in n-hexane) was introduced dropwise to the flask. The reaction mixture was stirred for another 1 h at ~78 °C. Dichloro(dimethyl)silane (92.9 µL, 0.96 mmol, 0.5 equiv) was added dropwise, and the resulting mixture was stirred for another 1 h at the same temperature. The mixture was warmed slowly to room temperature over 2 h before being neutralized by aqueous NH₄Cl, extracted with CH₂Cl₂, and the organic layer was dried over Na₂SO₄. The crude product was purified by silica gel column chromatography (eluent: DCM/PE = 1/4). Compound BCzSi1 was obtained as a white powder in the yield of 48% (385 mg). $^1$H NMR (500 MHz, CDCl$_3$): δ 8.33 (s, 2H), 8.09 (d, $J = 7.8$ Hz, 2H), 7.68 (d, $J = 8.1$ Hz, 2H), 7.47 (t, $J = 7.6$ Hz, 2H), 7.41 (t, $J = 7.7$ Hz, 4H), 7.22 (t, $J = 7.4$ Hz, 2H), 3.86 (s, 6H), 0.74 (s, 6H). $^{13}$C NMR (101 MHz, DMSO-d$_6$): δ 141.3, 140.5, 131.2, 126.0, 125.7, 121.9, 121.8, 120.1, 118.8, 109.1, 108.6, 28.9, −1.4 ppm. HR-MS calcd for C$_7$H$_{24}$N$_2$NaSi [M + Na$^+$]: 441.1757; found, 441.1739.

**Synthesis of BCzSi2.** 1 (500 mg, 1.92 mmol) was dissolved in dry THF (15 mL) and stirred at ~78 °C for 0.5 h under argon protection in a 50 mL Schlenk flask. n-BuLi (1.32 mL, 2.11 mmol, 1 equiv, 1.6 M solution in n-hexane) was introduced dropwise to the flask. The reaction mixture was stirred for 1 h at ~78 °C. 1,2-Dichlorotetramethyldisilane (177 µL, 0.96 mmol, 0.5 equiv) was added dropwise at the same temperature. The mixture was warmed slowly to room temperature over 2 h before being quenched with NH$_4$Claq extracted with CH$_2$Cl$_2$, and the organic layer was dried over Na$_2$SO$_4$. The crude product was evaporated to dryness and purified by silica gel column chromatography (eluent: THF/PE = 1/24). Compound BCzSi2 was obtained as a white powder in 71% yield (649 mg). $^1$H NMR (500 MHz, CDCl$_3$): δ 8.12 (s, 2H), 7.99 (d, $J = 7.7$ Hz, 2H), 7.56 (t, $J = 10.5$, 8.2 Hz, 4H), 7.46 (d, $J = 8.1$, 1.0 Hz, 2H), 7.46–7.41 (m, 2H), 7.15–7.10 (m, 2H), 3.84 (s, 6H), 0.43 (s, 12H). $^{13}$C NMR (101 MHz, DMSO-d$_6$): δ 141.0, 140.4, 131.9, 130.9, 126.7, 125.6, 121.9, 121.7, 120.0, 118.7, 109.0, 108.8, 28.8, −3.1 ppm. HR-MS calcd for C$_7$H$_{24}$N$_2$NaSi$_2$ [M + Na$^+$]: 499.1996; found, 499.1995.

**Synthesis of BCzSi3.** To a solution of 1 (500 mg, 1.92 mmol) in THF (40 mL) at ~78 °C under argon was added n-BuLi (1.4 mL, 2.24 mmol, 1.6 M solution in n-hexane). The solution was stirred at this temperature for an hour and then temperature was increased to ~60 °C and stirred for another 30 min. To a solution of 1,1,2,3,3,3-hexamethyl-1,3-diphenylsilan-2a (328 mg, 1 mmol) in toluene (5 mL) at 0 °C was added trifluoromethanesulfonic acid (228 µL, 2.4 mmol). The solution was stirred for 20 min before being cooled to ~60 °C. The as-prepared mixture was added dropwise to the above carbazole lithium reagent solution at ~60 °C. The reaction temperature was maintained at ~60 °C for another hour before the solution was warmed to ~50 °C and stirred overnight. After that, the solution was warmed to room temperature. Saturated NH$_4$Cl solution (10 mL) was added, the mixture was extracted with DCM (3 × 10 mL), and the combined organic layers were dried over Na$_2$SO$_4$ and concentrated in vacuum. Purification of the residue by column chromatography (eluent: PE) gave product BCzSi3 as a white solid in 49% yield (502 mg). $^1$H NMR (500 MHz, CDCl$_3$): δ 8.09 (s, 2H), 8.04 (d, $J = 7.7$ Hz, 2H), 7.56 (d, $J = 8.2$ Hz, 2H), 7.49 (d, $J = 8.1$ Hz, 2H), 7.43 (m, 4H), 7.19–7.11 (m, 2H), 3.80 (m, 6H), 0.35 (s, 12H), 0.11 (s, 6H).
13C NMR (126 MHz, DMSO-d6): δ 141.01, 140.48, 130.78, 127.07, 125.66, 125.39, 121.92, 121.75, 120.05, 118.82, 108.78, 28.88, −2.42, −5.54 ppm. HR-MS calcld for C32H44N2Si4 [M + Na]+, 592.2582; found, 592.2560. C32H38N2NaSi3 [M + Na]+, 557.2235; found, 557.2250.

Synthesis of BCzSi4. To a solution of 1 (500 mg, 1.92 mmol) in THF (40 mL) at −78 °C under argon was added n-BuLi (1.4 mL, 2.24 mmol, 1.6 M solution in hexane). The mixture was stirred for 20 min before being cooled to 0 °C. The as-prepared mixture was added dropwise to the carbazole lithium reagent solution at −60 °C and stirred for another 30 min. To a solution of 1,1,2,2,3,3,4,4-octamethyl-1,3-diphenyl-disilane (386 mg, 1 mmol) in toluene (5 mL) at 0 °C was added trifluoromethanesulfonic acid (228 µL, 2.4 mmol). The solution was stirred for 20 min before being cooled to −60 °C. The as-prepared mixture was added dropwise to the carbazole lithium reagent solution at −60 °C. The reaction temperature was maintained at −60 °C for a further hour before the solution was warmed to −50 °C and stirred overnight. The solution was warmed to room temperature. Saturated NH4Cl solution (10 mL) was added, the mixture was extracted with DCM (3 × 10 mL), and the combined organic layers were dried over Na2SO4 and concentrated in vacuum. Purification of the residue by column chromatography (eluents: PE) gave product BCzSi4 as a white solid in 55% yield (626 mg). 1H NMR (400 MHz, DMSO-d6): δ 8.19–8.11 (m, 4H, 4H), 7.56 (m, 4H, 4H), 7.44 (d, J = 8.1 Hz, 4H), 7.19 (d, J = 7.4 Hz, 2H), 3.84 (s, 6H), 0.40 (s, 12H), 0.02 (s, 12H). 13C NMR (126 MHz, DMSO-d6): δ 141.01, 140.48, 130.78, 127.07, 125.66, 125.39, 121.92, 121.75, 120.05, 118.82, 109.07, 108.78, 28.88, −2.42, −5.54 ppm. HR-MS calcld for C34H44N2Si4 [M]+, 592.2582; found, 592.2560.

ASSOCIATED CONTENT

Supporting Information
The Supporting Information is available free of charge at https://pubs.acs.org/10.1021/acsomega.0c02559.

Accession Codes
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H.L. and Z.Z. contributed to the experimental design and writing of the manuscript. Z.Q. supervised the synthesis of target compounds and acquisition of crystal structures. S.F. carried out the synthesis, purification, and characterization of target compounds. X.X. contributed to the preparation of single crystals. H.F. contributed to the absorption and emission measurements.

Notes
The authors declare no competing financial interest.

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