Electronic supporting information

Bicarbazole-benzophenone Based Twisted D-A-D Derivatives as Blue Emitters for Highly Efficient Fluorescent OLEDs

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Synthesis of 9H,9′H-[3,3′]bicarbazole

9H,9′H-[3,3′]bicarbazole was obtained by chemical oxidation of 9H-carbazole in the presence of $FeCl_3$. Anhydrous $FeCl_3$ (20 g, 120 mmol) was added to a magnetically stirred solution of 9H-carbazole (5 g, 30 mmol) in 100 ml of chloroform. The mixture was stirred for 30 min and poured into methyl alcohol. The precipitated material was recovered by filtration and the crude product was purified by silica gel column chromatography using hexane/ ethylacetate (vol. ratio 1:1) as an eluent. The yield of the 9H,9′H-[3,3′]bicarbazole was 62 % (3.13 g). MS(APCI$^+$, 20 V), m/z(%): 334 ([M+H]$^+$, 95). ^{1}H NMR spectrum (DMSO, δ, ppm): 11.31 (s, 2H, NH), 8.55 (s, 2H), 8.27 (d, 2H, *J*=7.8 Hz), 7.84 (d, 2H, *J*=9 Hz), 7.62 (d, 2H, *J*=8.4 Hz), 7.55 (d, 2H, *J*=7.8 Hz), 7.46-7.4 (m, 2H), 7.25-7.18 (m, 2H). IR (KBr): 3419, 3048, 1604, 1491, 1468, 1456, 1241, 753. Elemental analysis for $C_{24}H_{16}N_2$: % Calc. N 8.43, C 86.72, H 4.85; % Found N 8.52, C 86.77, H 4.82.

Results of DFT Calculations of DB14 and DB29

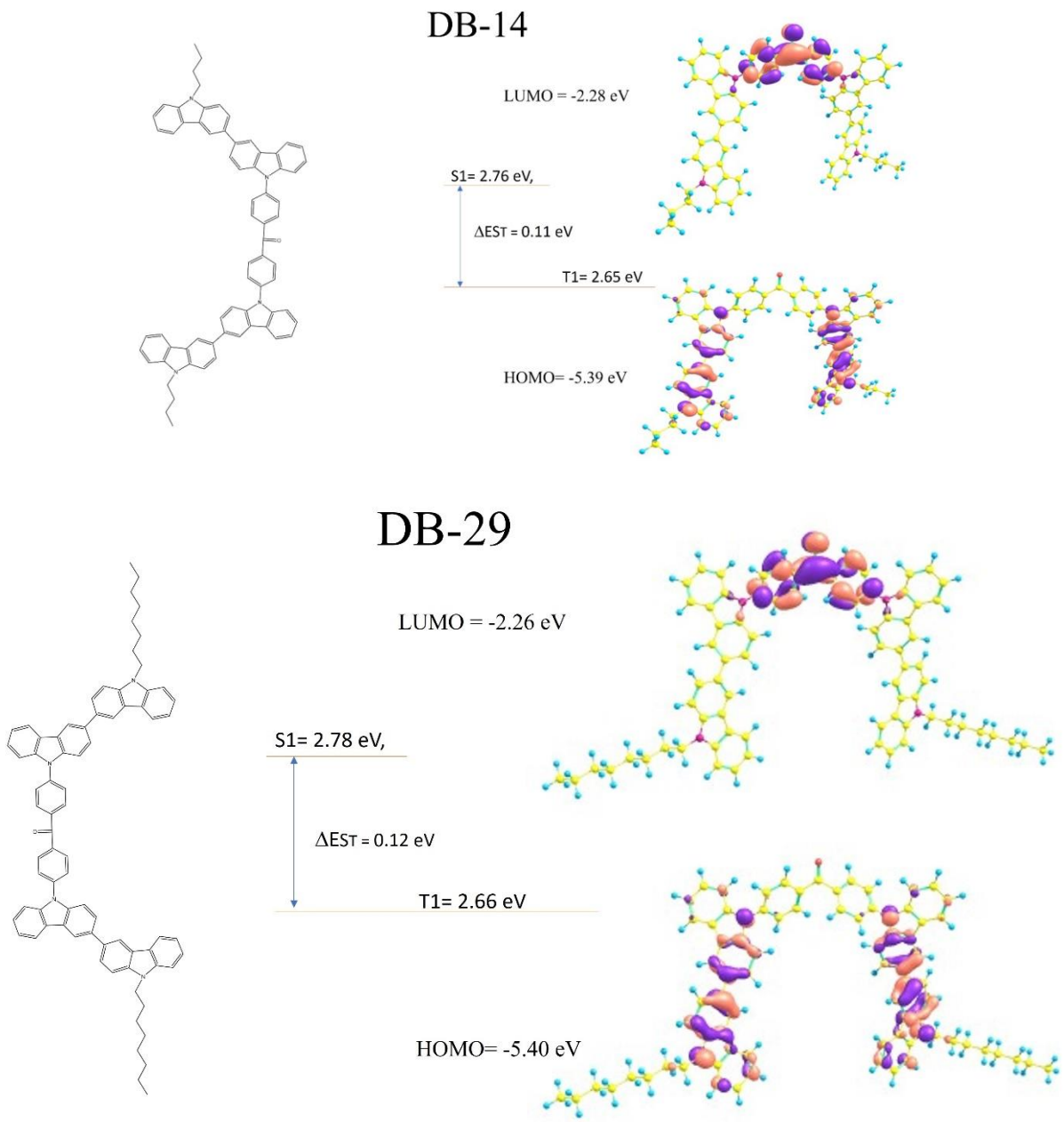

Figure S1. Electron density contours of FMO and HOMO, LUMO, singlet, triplet, and singlet-triplet energy gap electron distribution of the compounds **DB14** and **DB 29**.