Supporting Information for

"Impact of bromination of carbazole-based D-π-A organic dyes on their photoelectrochemical properties and visible light-driven hydrogen evolution"

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1. Influence of bromination on the chemical shift of -*N*-CH_2-

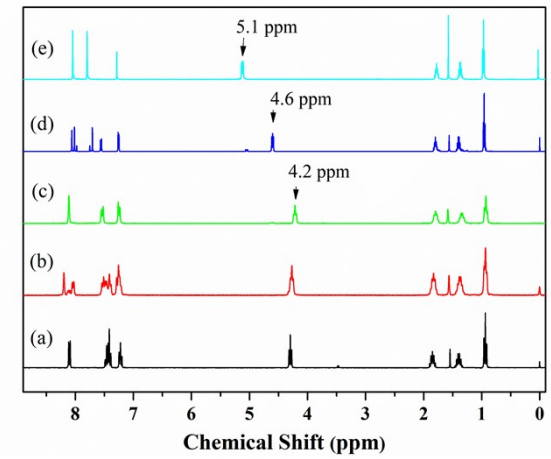

Fig.S1 ^{1}H NMR spectra of (a) *N*-butylcarbazole; (b) 3-Br-*N*-butylcarbazole; (c)3,6-di-Br-*N*-butylcarbazole;(d)1,3,6-tri-Br-*N*-butylcarbazole; (e) 1,3,6,8-tetra-Br-*N*-butylcarbazlole)

2.^{1}H NMR and MALDI-TOF MS spectra

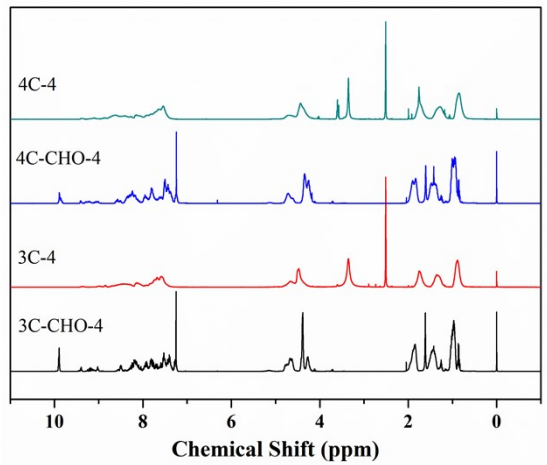

Fig.S2 ^{1}H NMR spectra of 3C-CHO-4, 3C-4、4C-CHO-4 and 4C-4

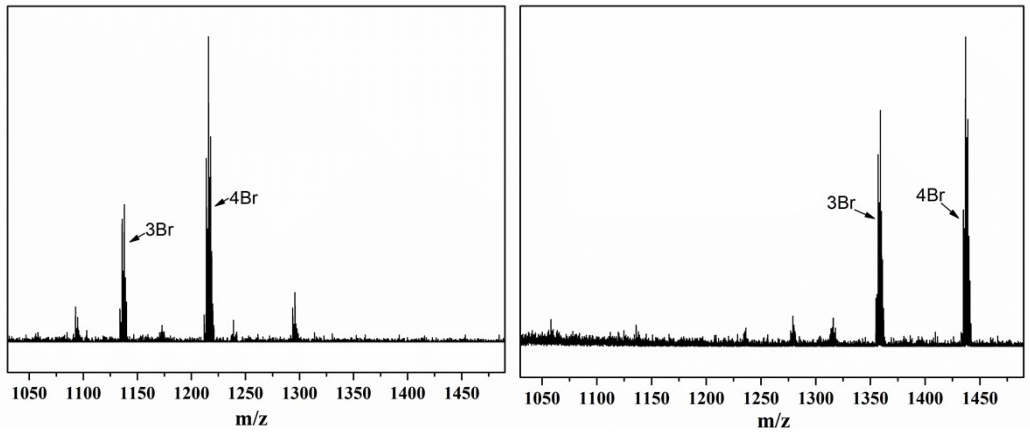

Fig.S3 MALDI-TOF MS spectra of 3C-4（left）and 4C-4（right）

3.Theoretical calculation

3.1 Dihedral angles

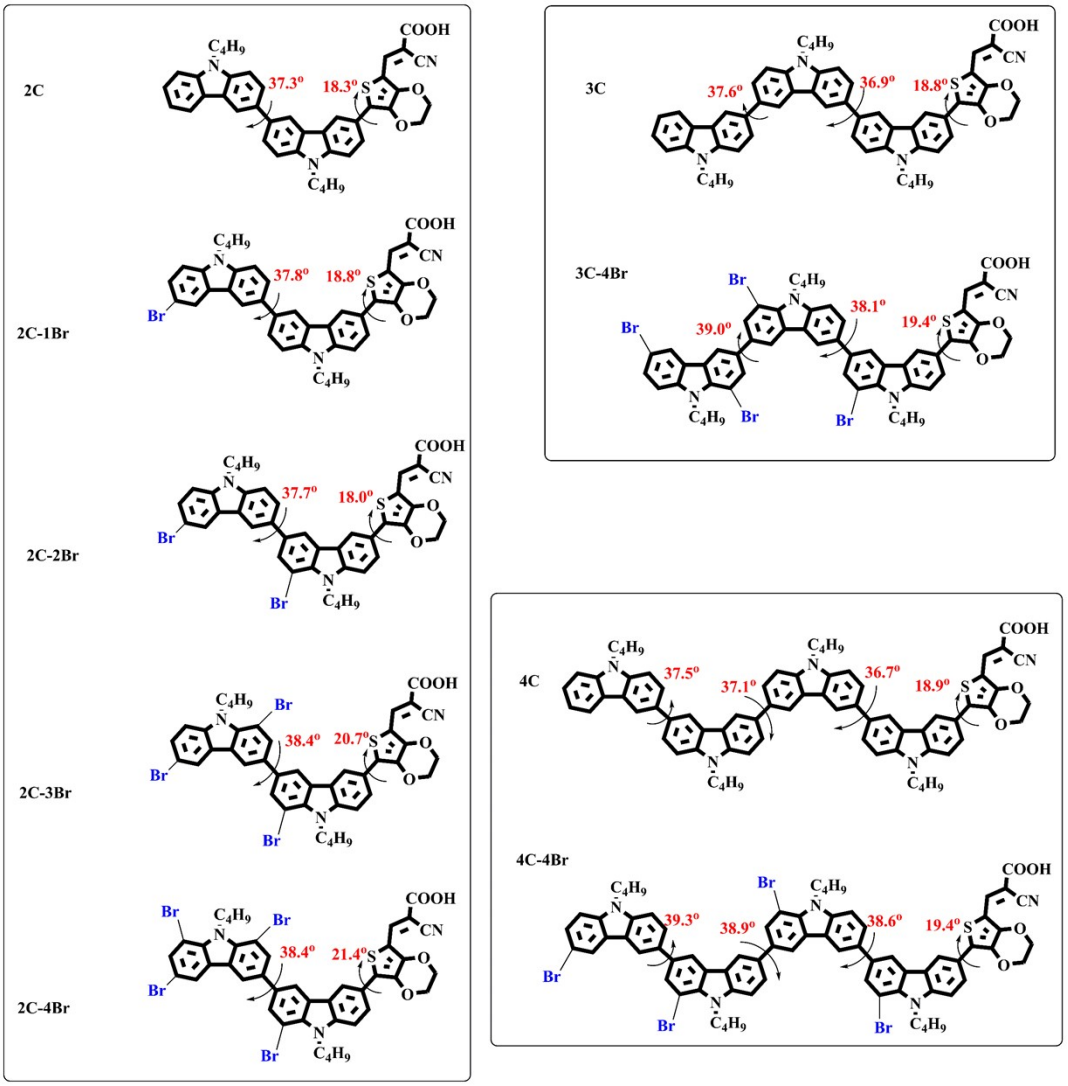

Fig.S4 Dihedral angles between heteroaromatic cycles in brominated dyes

3.2 HOMO and LUMO levels

Table S1 Calculated HOMO and LUMO levels of dyes

Dye	HOMO (eV)	LUMO (eV)	$E_{0\text{-}0}$ (eV)
2C	-2.42	-5.00	2.58
2C-1Br	-2.46	-5.12	2.67
2C-2Br	-2.53	-5.23	2.70
2C-3Br	-2.54	-5.34	2.80
2C-4Br	-2.57	-5.42	2.85
3C	-2.41	-4.82	2.41
3C-4Br	-2.53	-5.18	2.64
4C	-2.41	-4.74	2.32
4C-4Br	-2.53	-5.03	2.50

4.Transient photocurrent responses

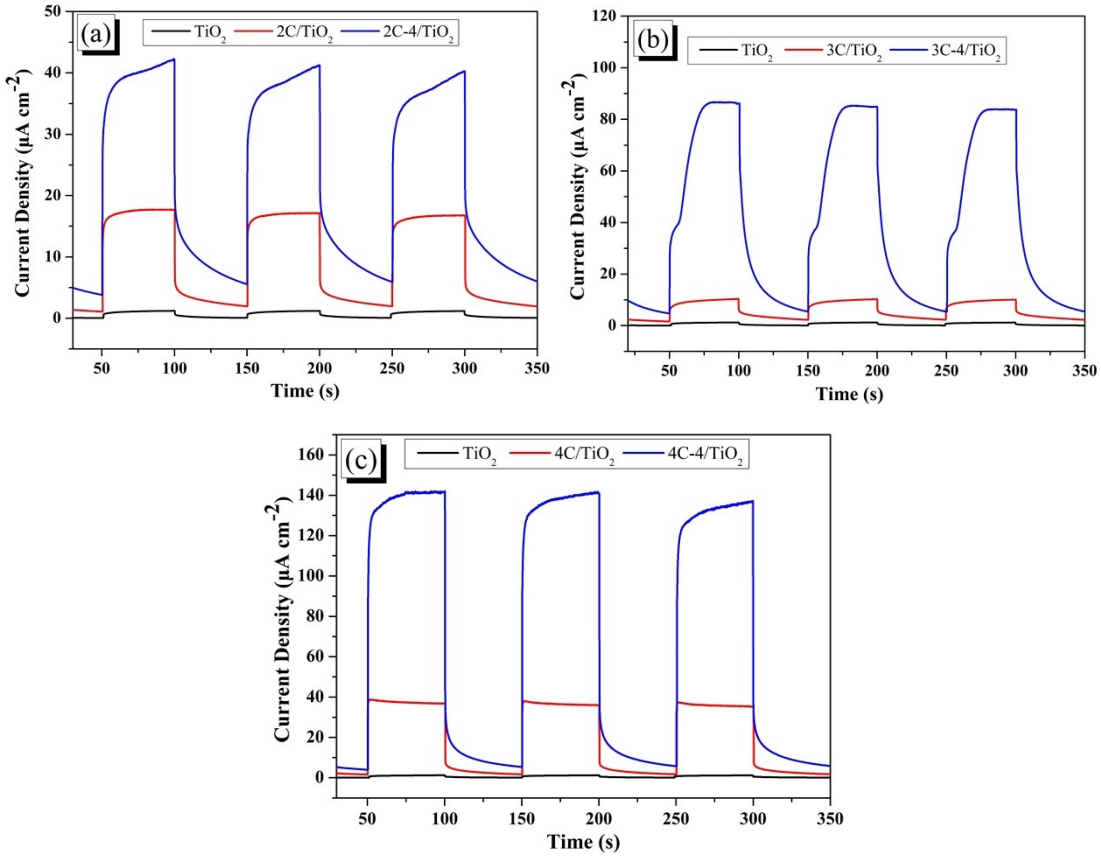

Fig.S5 Transient photocurrent densities of TiO_2 and dye-sensitized TiO_2 in 0.1 M Na_2SO_4 TEOA solution under visible light irradiation.

5. Apparent quantum yields (AQY) *

Table S2 Calculated AQY of 3C-4 under monochromatic light irradiation

Wavelength (nm)	Light intensity (mW/cm^{-2})	Amount of H_2 (μmol)	AQY
450	37	3.96	2.58
475	82	2.55	2.67
500	59	2.62	2.70

*AQY data were calculated according to the method from the literature (*J. Mater. Chem. C*, 2020,8, 14864-14872)