Electronic Supplementary Material (ESI) for RSC Advances

Two-Component Gel of D-π-A-π-D Carbazole Donor and Fullerene Acceptor

Pengchong Xue,*[ab] Qiuxia Xu,[a] Peng Gong,[a] Chong Qian,[a] Zhenqi Zhang,[a] Junhui Jia,[a] Xin Zhao, [a] Ran Lu,*[a] Aimin Ren,[b] Tierui Zhang[c]

[a] State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, Changchun, PR China

[b] State Key Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, Changchun, PR China

[c] Key Laboratory of Photochemical Conversion and Optoelectronic Materials, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing, PR China

Email: xuepengchong@jlu.edu.cn luran@mail.jlu.edu.cn

Table S1. The photophysical properties of **PCQ**.

Compound	λ_{abs} [a] (nm)	ε_{max} [b]	λ_{em} [a] (nm)	Φ_F [c]	$E_{0\text{-}0}$ [d] (V)	E_{HOMO} [e] (eV)	E_{LUMO} [f] (eV)	E_{HOMO} [g] (eV)	E_{LUMO} [g] (eV)
PCQ	469	3.45	577	0.60	2.29	–4.80	–2.51	–4.71	–2.17

[a] Measured in THF (1×10^{-5} M). [b] ε ($\times10^{-4}$ $M^{-1}cm^{-1}$). [c] Measured in THF using Rhodamine 6G as reference (Φ_F = 0.75 in water), λ_{ex} = 488 nm. [d] $E_{0\text{-}0}$ was determined from the edge of the absorption spectrum. [e] E_{HOMO} was defined as the ground station potential (first oxidation peak) of the dyes was measured in THF with ferrocene/ferrocenium (Fc/Fc^+) as an internal reference, and the energy level of Fc/Fc^+ was assumed at –4.8 eV to vacuum. [f] E_{LUMO}= E_{HOMO} –$E_{0\text{-}0}$. [g] Energy levels of HOMO and LUMO versus vacuum were given after geometrical optimization.

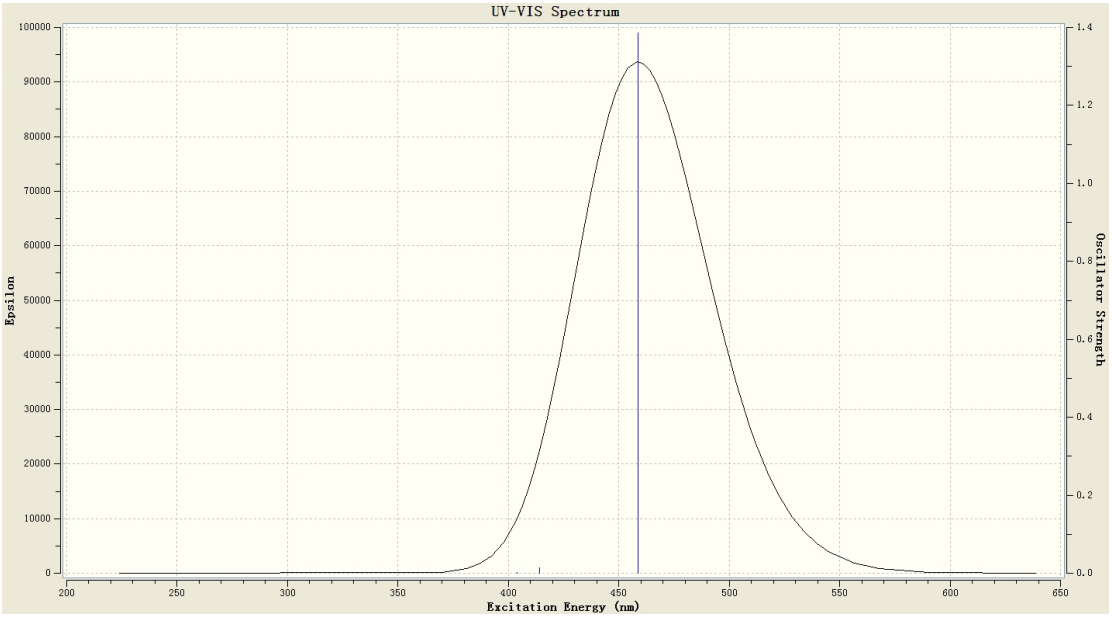

Fig. S1 Simulated UV-vis absorption spectrum of **PCQ**.

Table S2 Electronic transition data obtained by the TD/DFT-B3LYP/6-31G calculation for **PCQ**

Electronic transition	λ_{abs} (nm)	E (eV)	Oscillator strength	Transition assignment
1	458.74	2.7027	1.3859	HOMO→ LUMO

Table S2. The gelation ability of three compounds in various solvents.[a]

solvent	**PCQ**	solvent	**PCQ**
Benzene	I	Cyclohexane	I
Toluene	I	THF	S
o-Dichlorobenzene	G (0.09)	DMF	S
Bromobenzene	G (0.06)	DMSO	G (1.0)
Ethanol	I	Acetophenone	G (0.1)
Ethyl acetate	I	Benzyl alcohol	G (0.5)
Hexane	I	Aniline	G (0.2)

[a] G – gel; P – precipitate; S – soluble. [b] The minimum gelation concentration (CGC), wt/vol%.

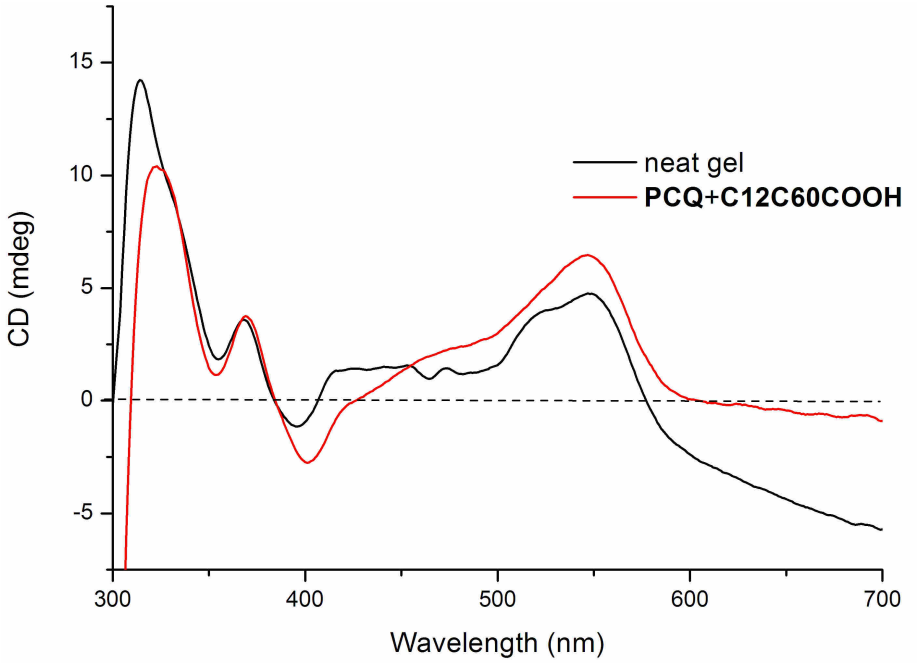

Fig. S2 CD spectra of **PCQ** gel (a) and two-component of **PCQ** and C12C60COOH (molar ratio = 1:1) in ODCB.

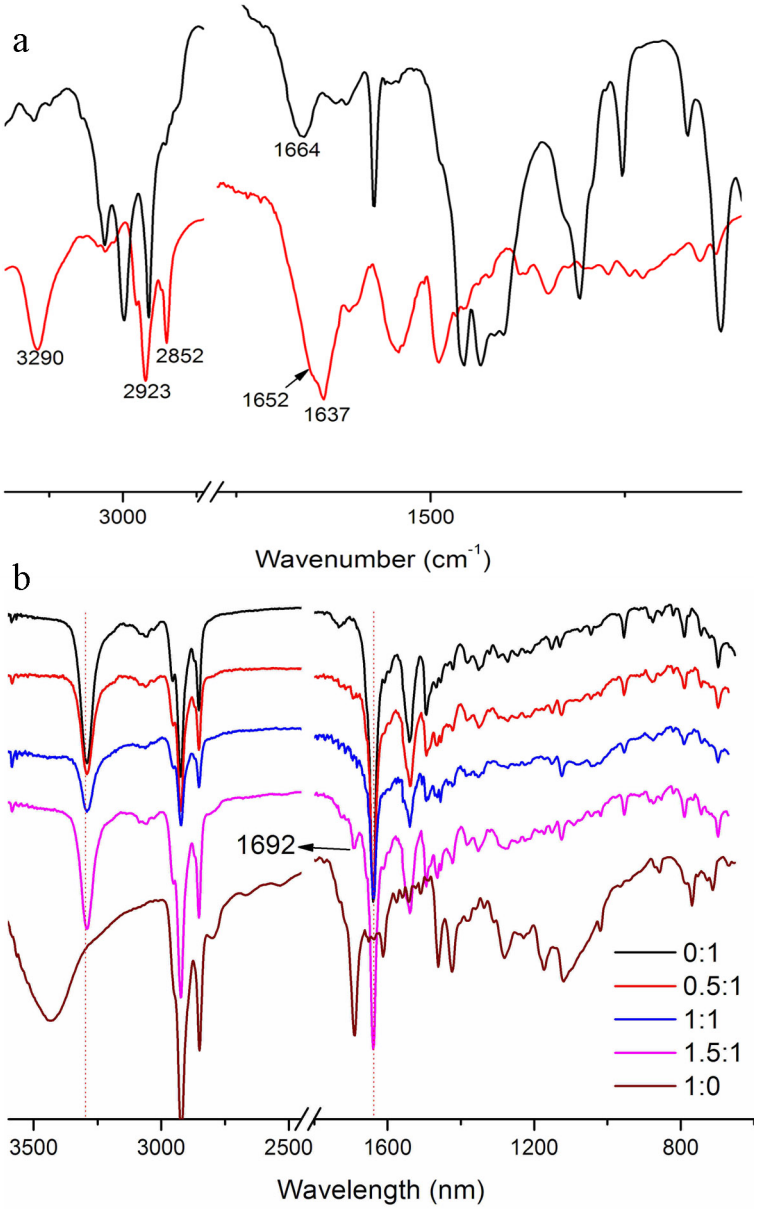

Fig. S3 FT-IR spectra of (a) **PCQ** xerogel (red) and solution (black) in ODCB/DMSO (v:v = 1:1), and (b) two-component gel of C12C60COOH and **PCQ** with different molar ratio.

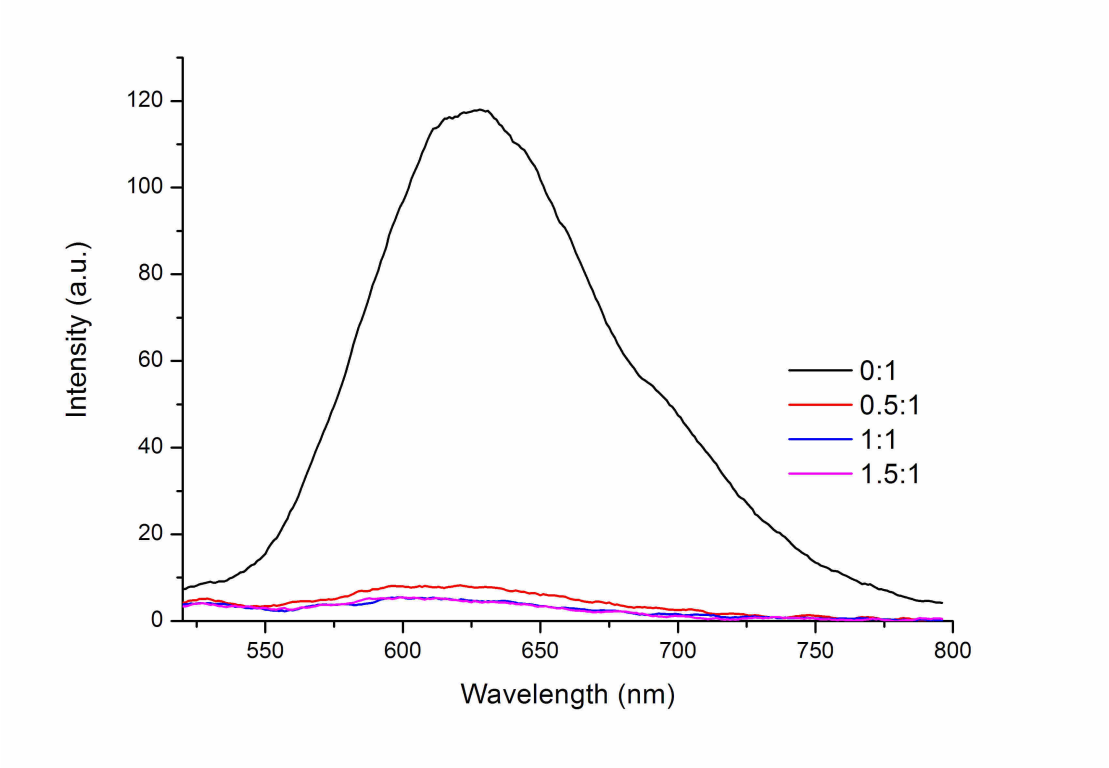

Fig. S4 Fluorescence spectra of xerogel films of C12C60COOH and **PCQ** with different ratio; the concentration of PCQ in all samples is 0.1 wt/vol. Films were prepared by dropping the corresponding hot solutions of 20 μL on the silicon plate and evaporating solvent naturally. λ_{ex} = 480 nm.

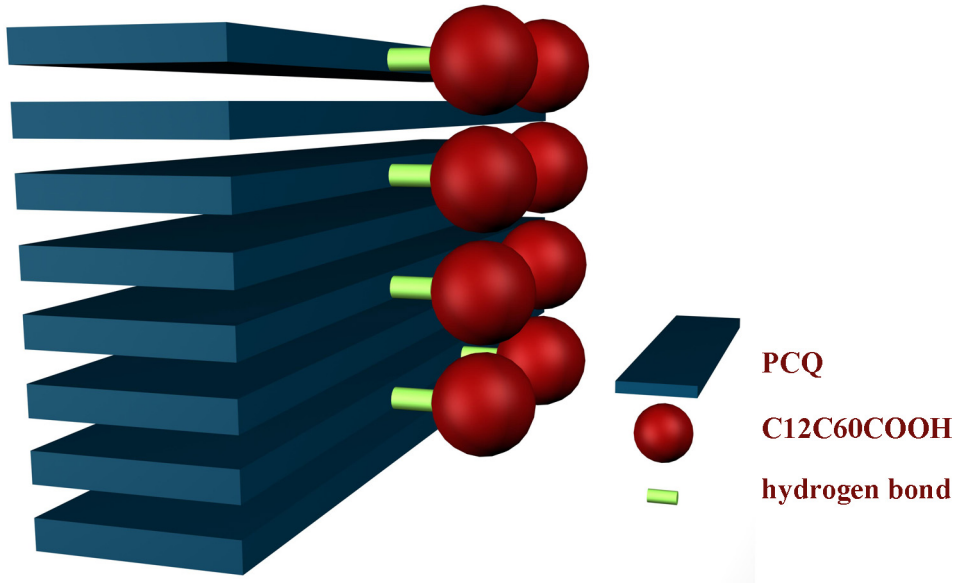

Fig. S5 Schematic representation of molecular packing model in two-component gel with **PCQ** and C12C60COOH.

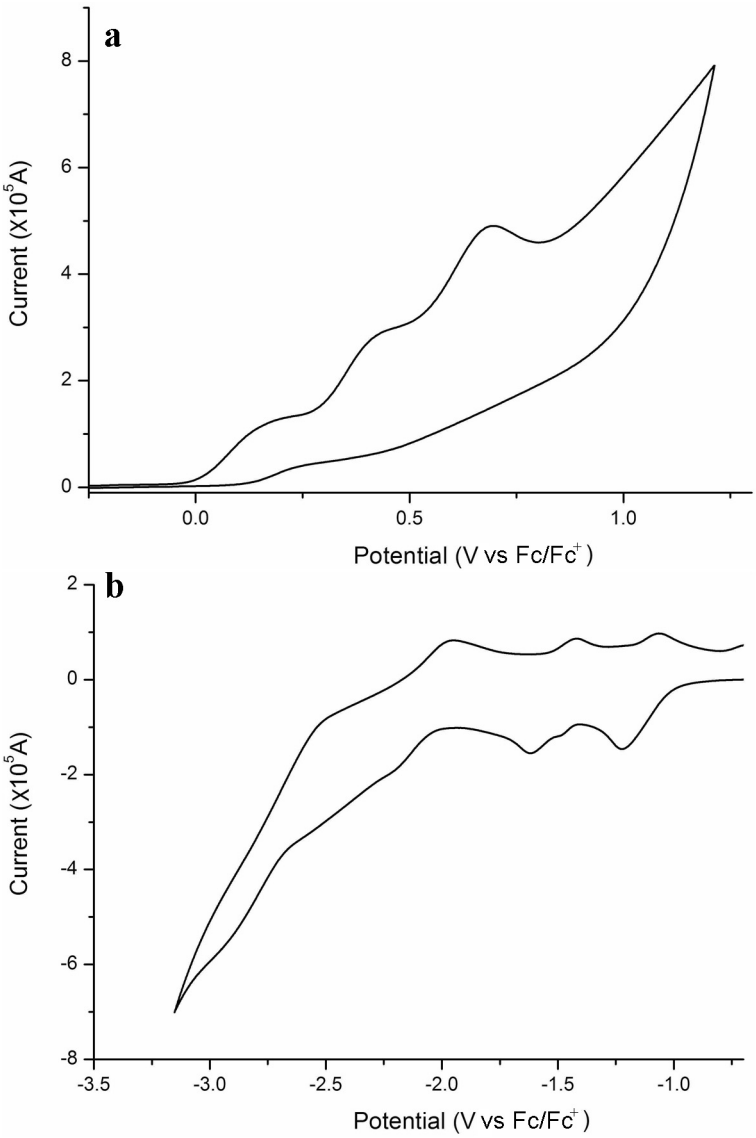

Fig. S6 Cyclic voltammogram of **PCQ** (a) and C12C60COOH in THF and ODCB, respectively.