Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.
This journal is © The Royal Society of Chemistry 2023

Supporting information

A Fluorescent Quaternary Phosphonium Main-Chain Type Polymer: An Opportunity to Fabricate Functional Materials with Excellent Antibacterial Activity and Bacterial Imaging Capability

Jiawei Lv,[a] Saicuo Wang,[b] Chunxuan Qi,[c] Muheman Li,[a] Yuqing Sun,[a] Yuan Yang,[a] Cheng Zeng,[a] Richao Shen,[a] Hengchang Ma*[a]

[a] Key Laboratory of Polymer Materials of Gansu Province, Key Laboratory of Eco-Environment-Related Polymer Materials Ministry of Education, College of Chemistry and Chemical Engineering, Northwest Normal University. Lanzhou 730070, P.R. China.

[b] China Agricultural Vet. Bio. Science and Technology Co., Ltd., Lanzhou 730046, P.R. China.

[c] AIE Research Center, Shaanxi Key Laboratory of Phytochemistry, College of Chemistry and Chemical Engineering, Baoji University of Arts and Sciences, Baoji 721013, P.R. China.

Table of Contents

1. ^{1}H and ^{13}C NMR Spectra of Compounds.

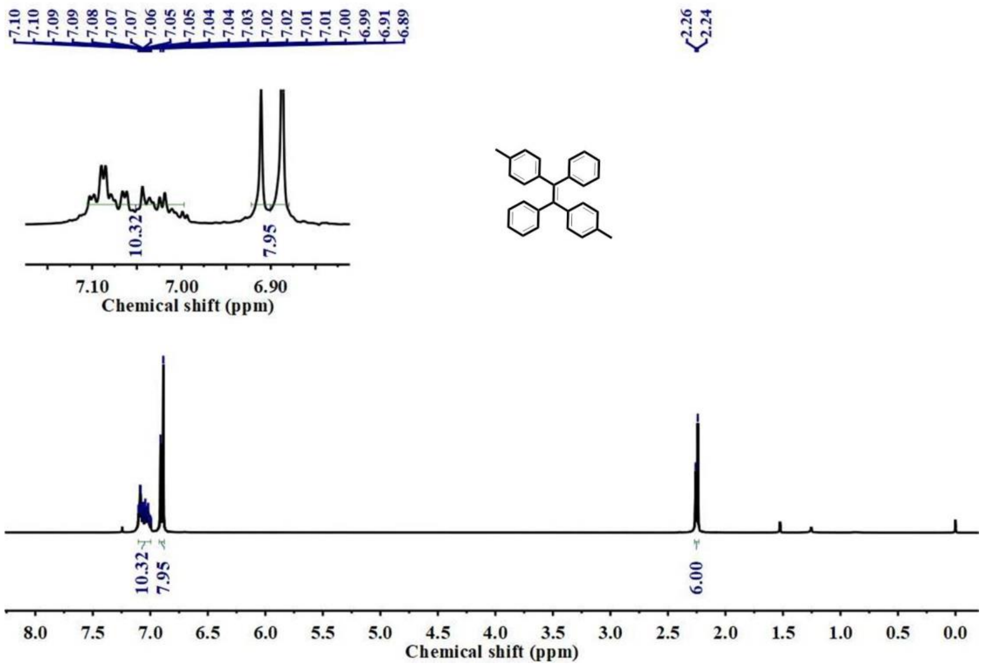


Figure S1. ^{1}H NMR spectrum of TPE-2CH_3 measured in $CDCl_3$ at room temperature.

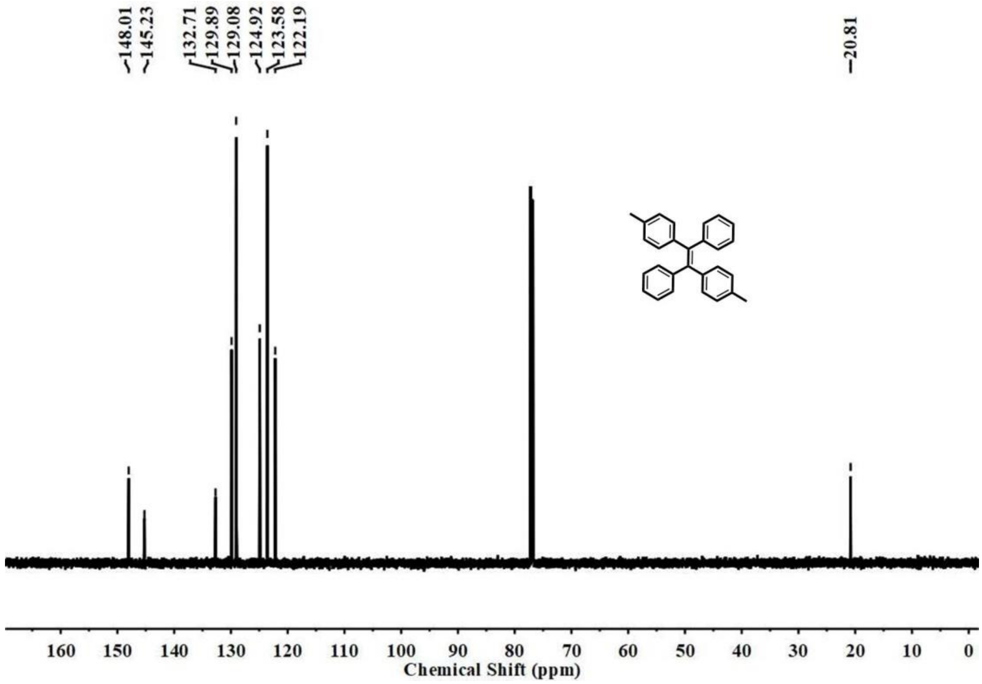


Figure S2. ^{13}C NMR spectrum of TPE-2CH_3 measured in $CDCl_3$ at room temperature.

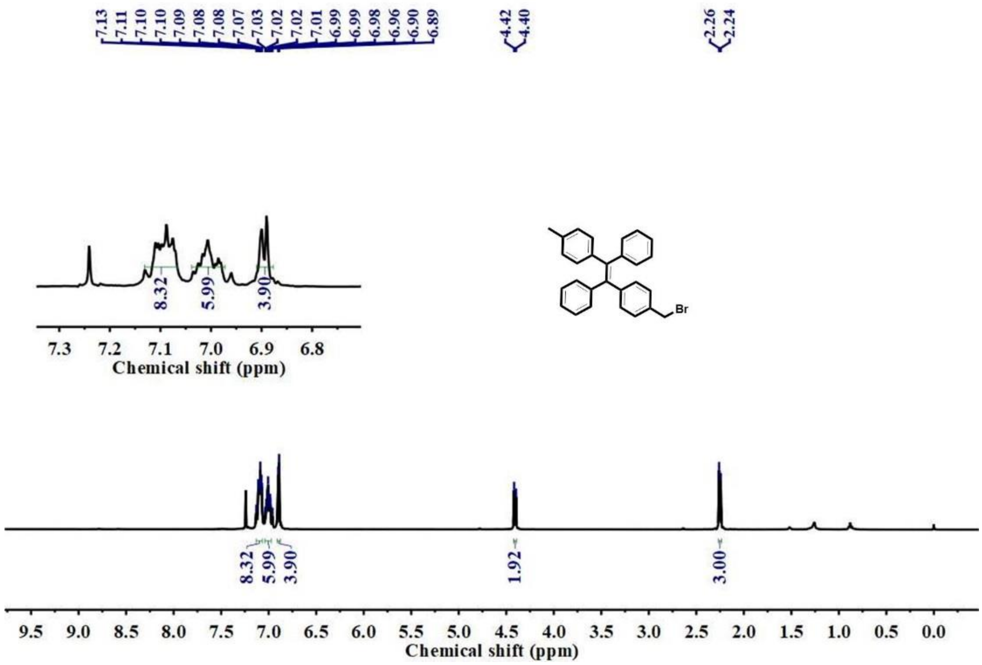


Figure S3. ^{1}H NMR spectrum of TPE-CH_2-Br measured in $CDCl_3$ at room temperature.

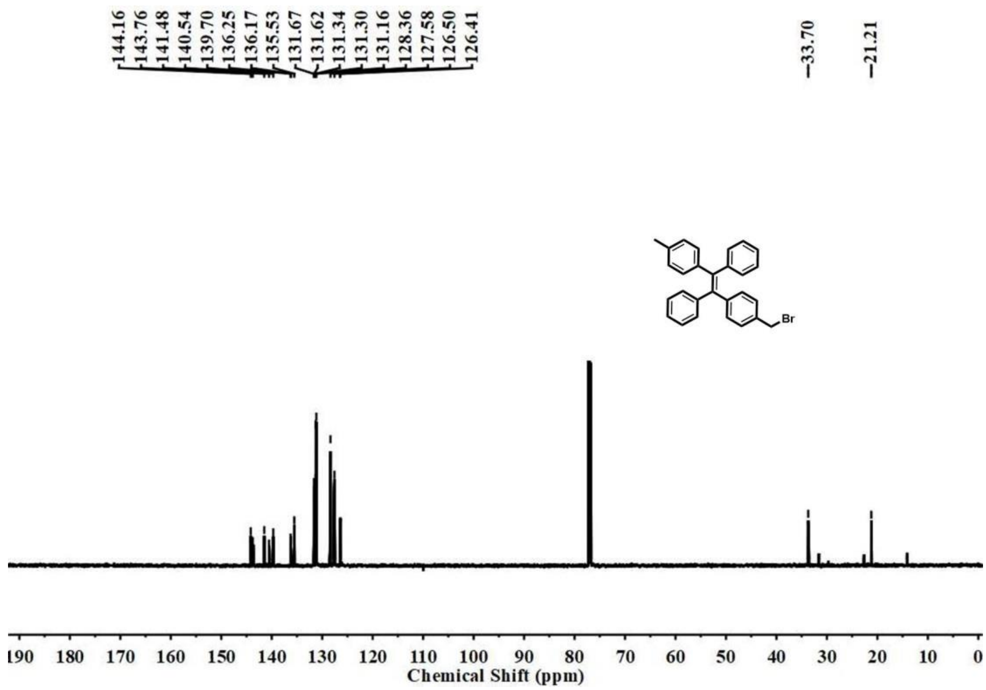


Figure S4. ^{13}C NMR spectrum of TPE-CH_2-Br measured in $CDCl_3$ at room temperature.

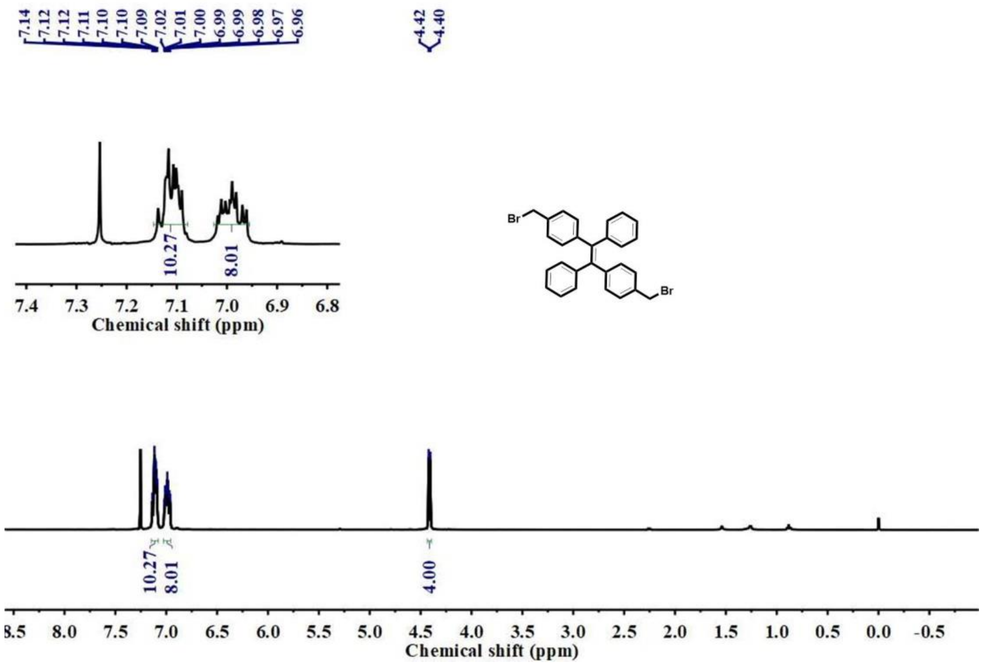


Figure S5. ^{1}H NMR spectrum of TPE-2CH_2Br measured in $CDCl_3$ at room temperature.

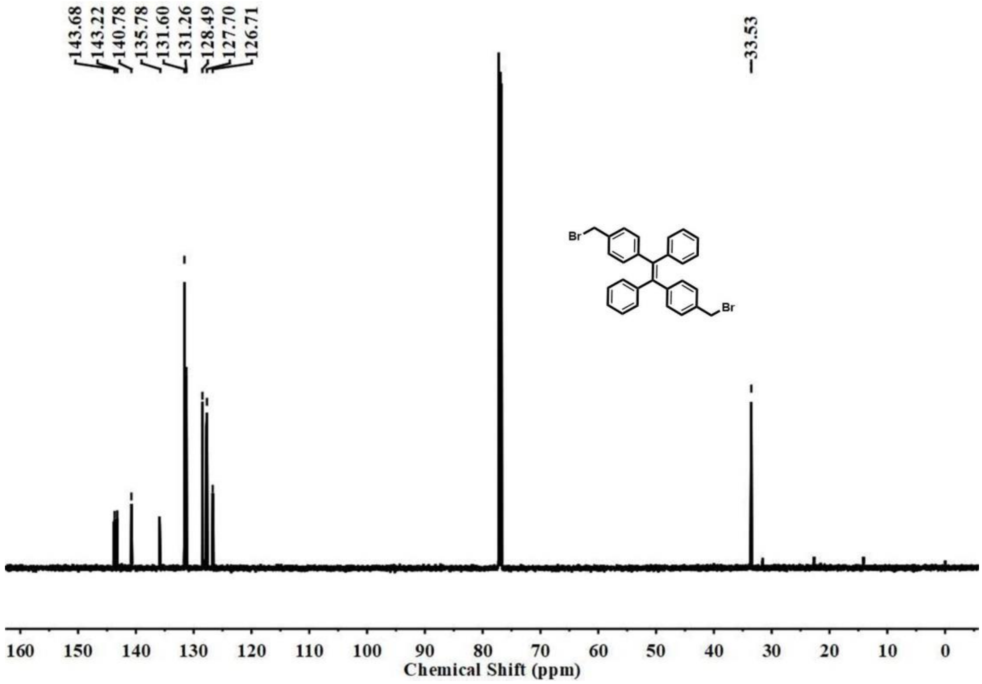


Figure S6. ^{13}C NMR spectrum of TPE-2CH_2Br measured in $CDCl_3$ at room temperature.

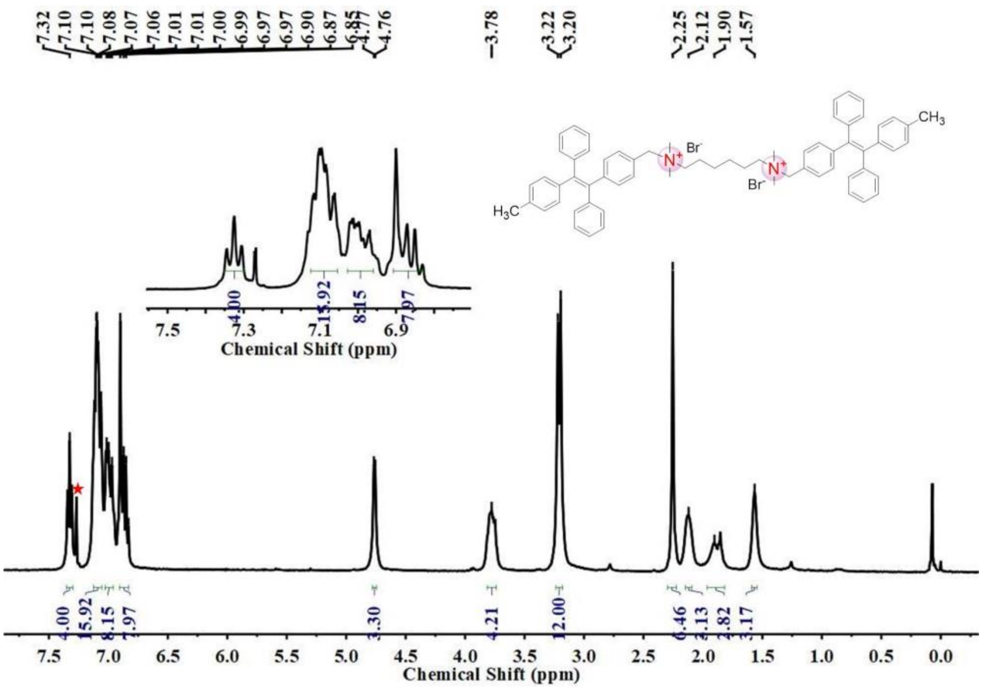


Figure S7. ^1H NMR spectrum of TPE-$2N^+$ measured in $CDCl_3$ at room temperature.

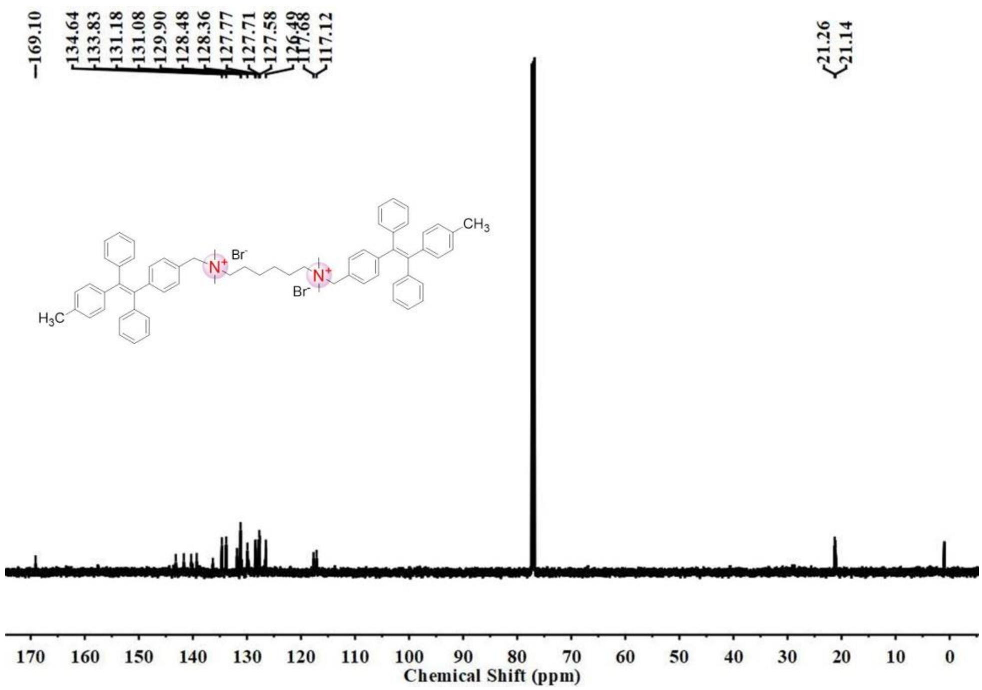


Figure S8. ^{13}C NMR spectrum of TPE-2N$^+$ measured in $CDCl_3$ at room temperature.

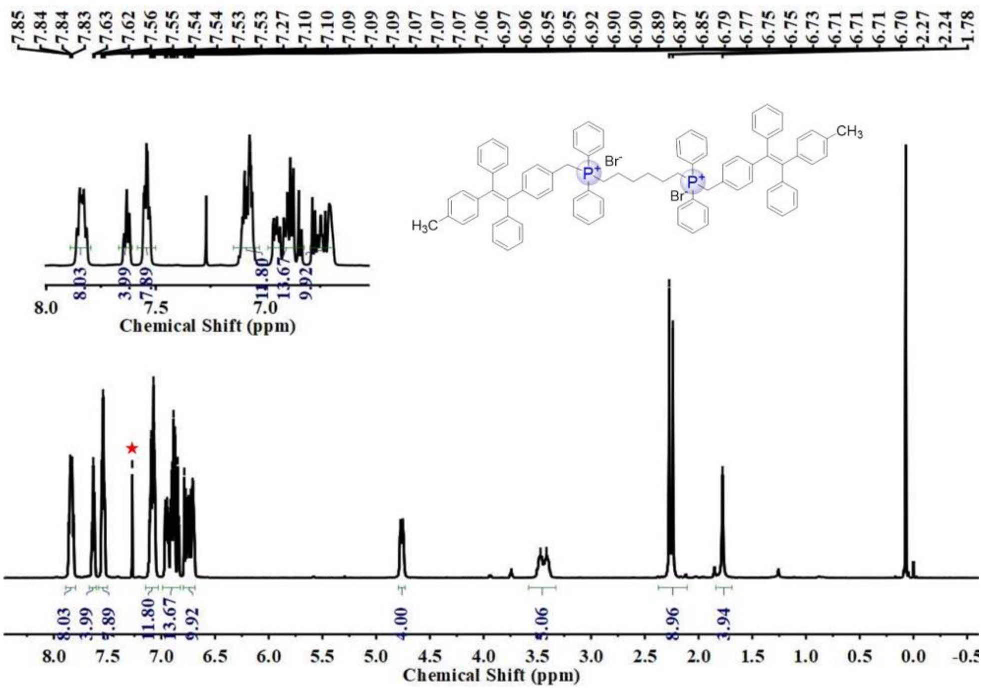


Figure S9. ^{1}H NMR spectrum of TPE-2P^{+} measured in $CDCl_3$ at room temperature.

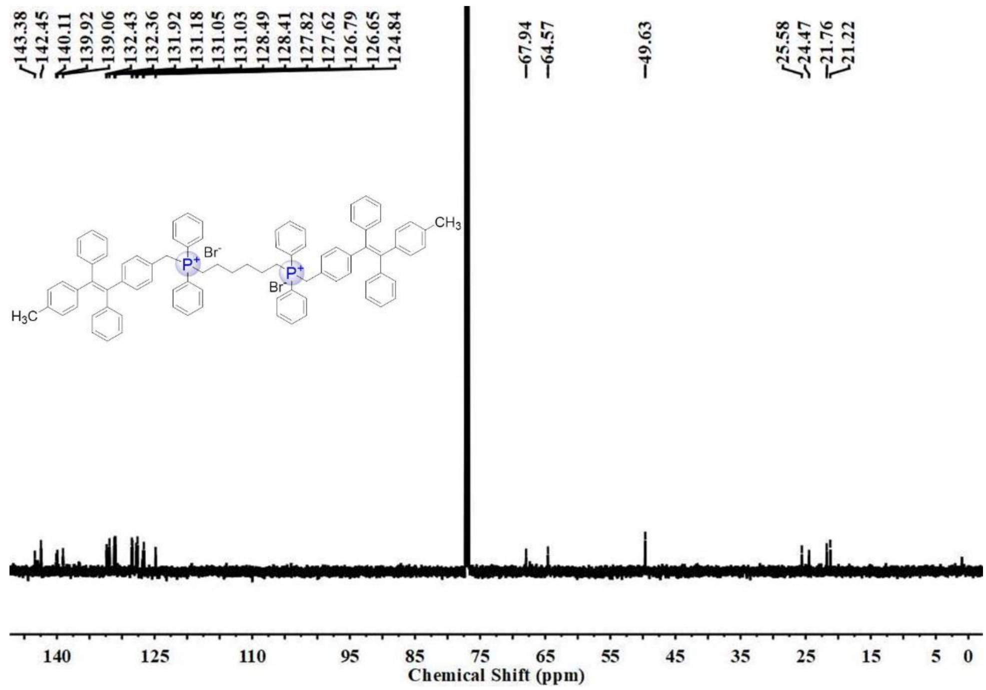


Figure S10. ^{13}C NMR spectrum of TPE-2P^{+} measured in $CDCl_3$ at room temperature.

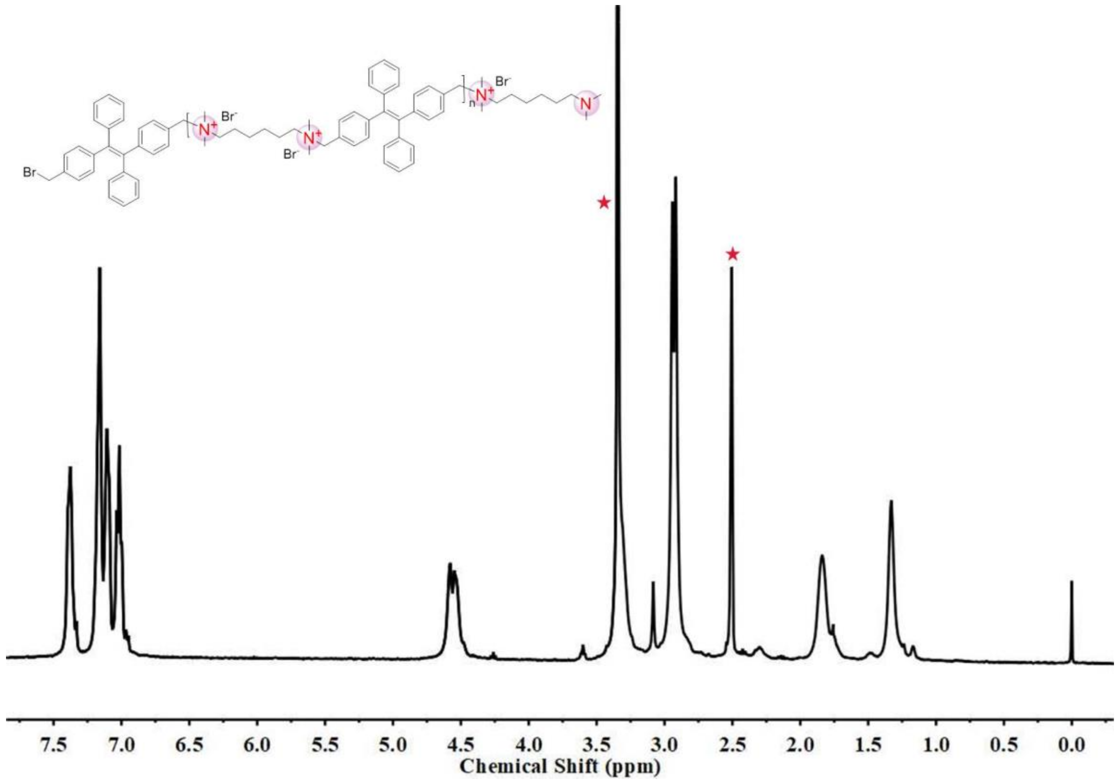


Figure S11. [1]H NMR spectrum of TPE-Ammonium polymer measured in DMSO-d_6 at room temperature.

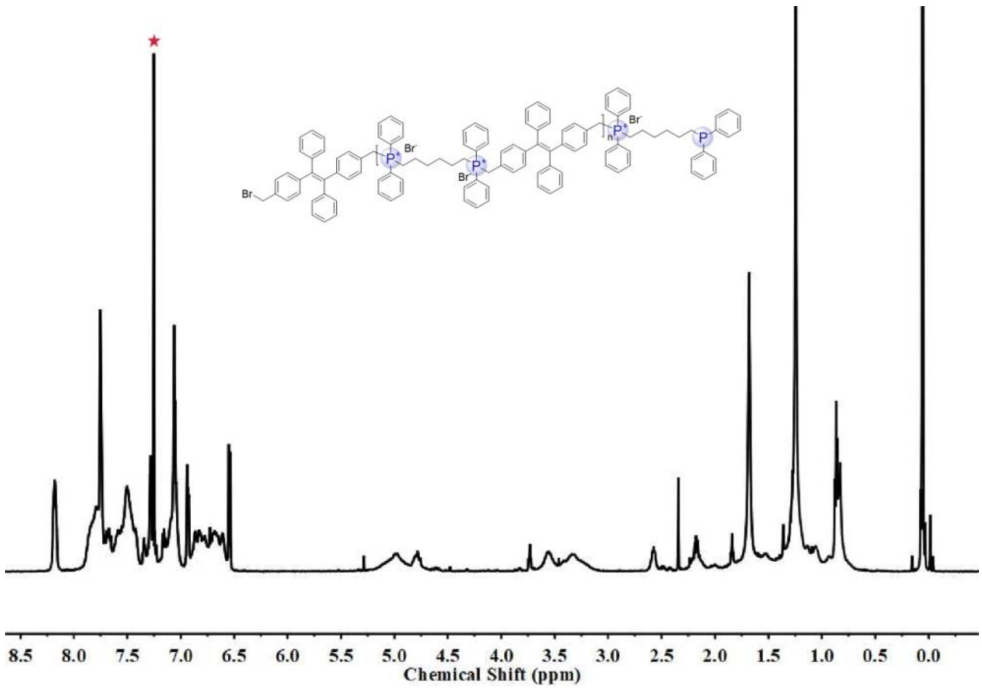


Figure S12. ^1H NMR spectrum of TPE-Phosphonium polymer measured in $CDCl_3$ at room temperature.

2. ^{31}P NMR Spectra of Compounds

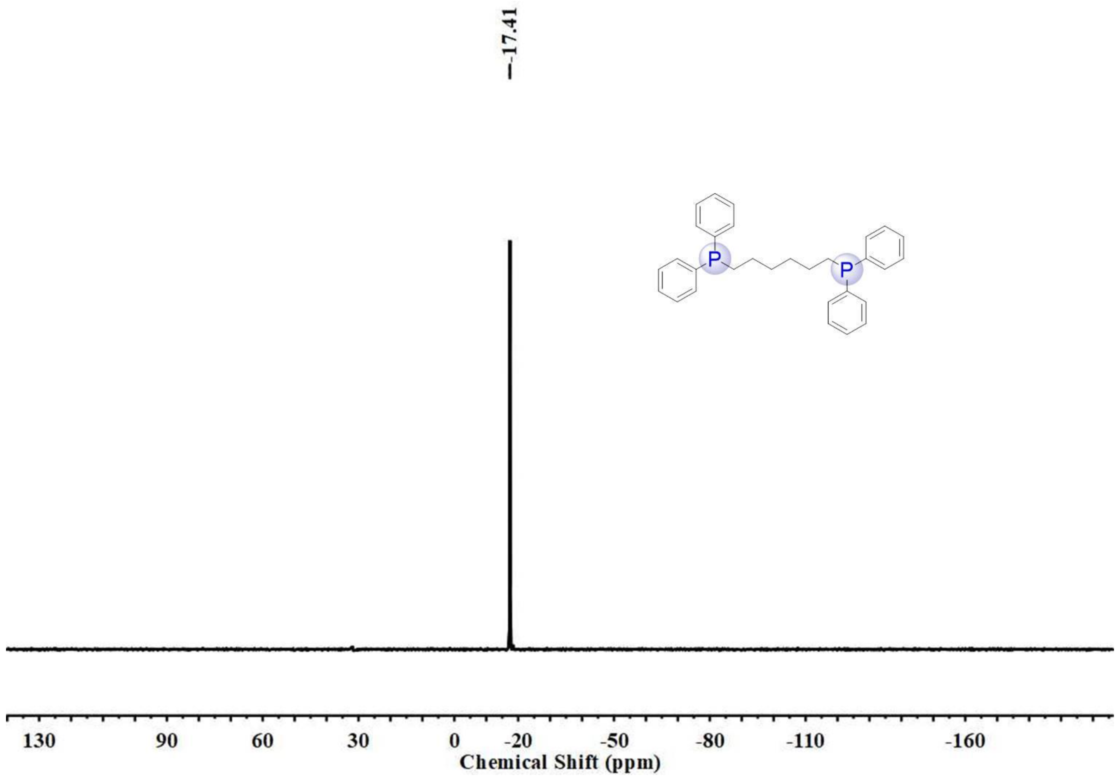


Figure S13. ^{31}P NMR spectrum of DPPH measured in $CDCl_3$ at room temperature.

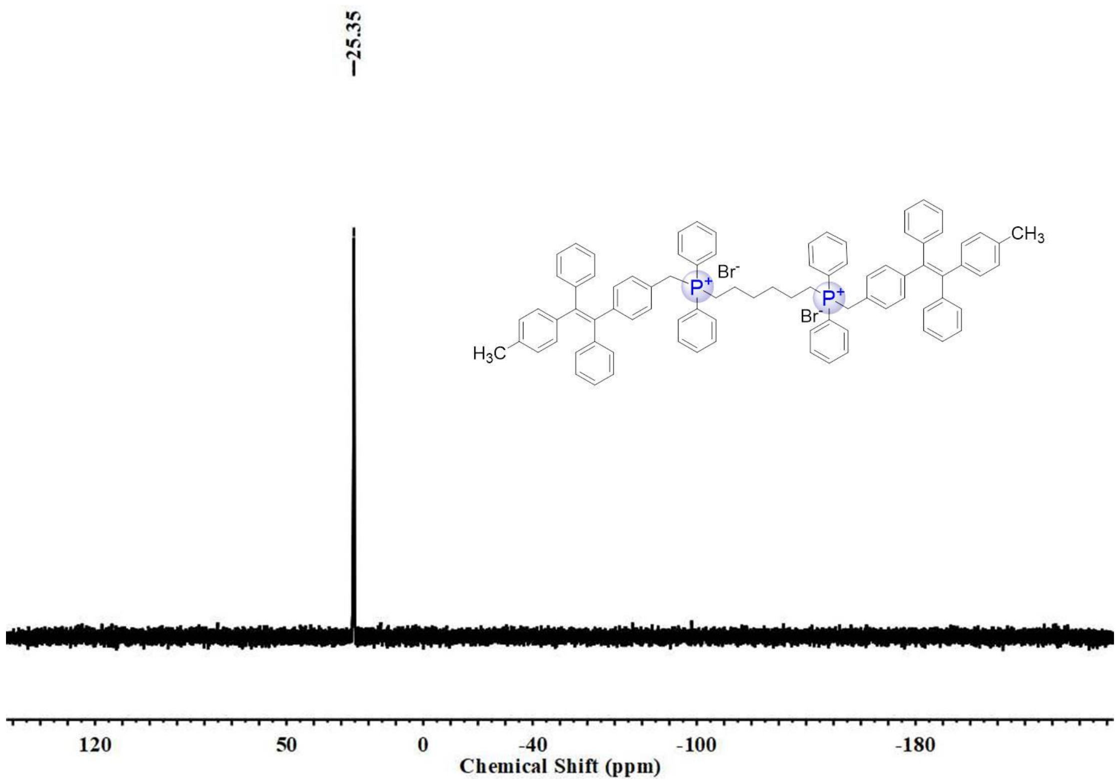


Figure S14. ^{31}P NMR spectrum of TPE-2P^{+} measured in $CDCl_3$ at room temperature.

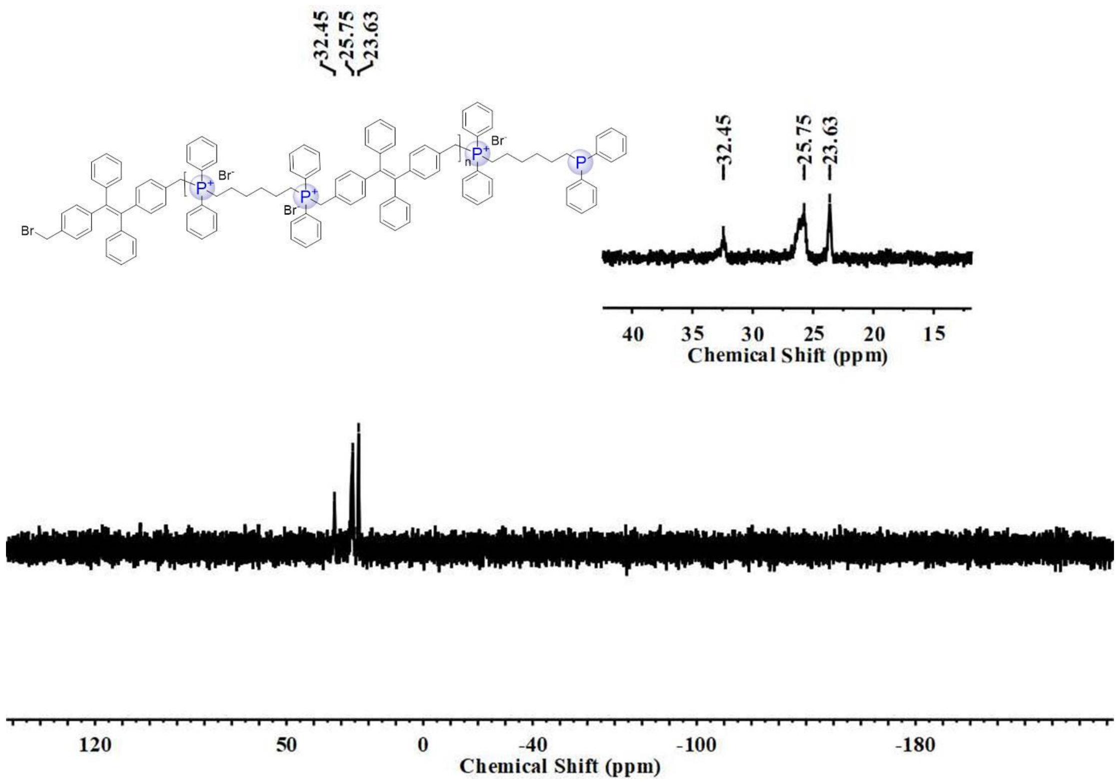


Figure S15. ^{31}P NMR spectrum of TPE-Phosphonium polymer measured in $CDCl_3$ at room temperature.

3. UV-*vis* and PL Spectra of Compounds

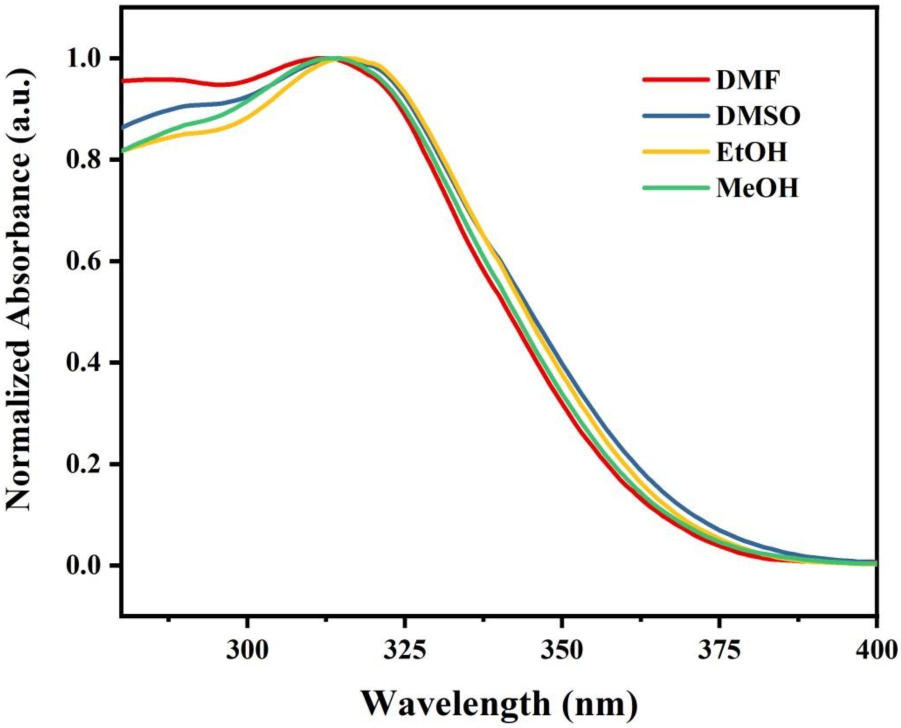


Figure S16. Normalized UV-*vis* absorption spectra of TPE-2N^{+} in DMF, DMSO, EtOH and MeOH.

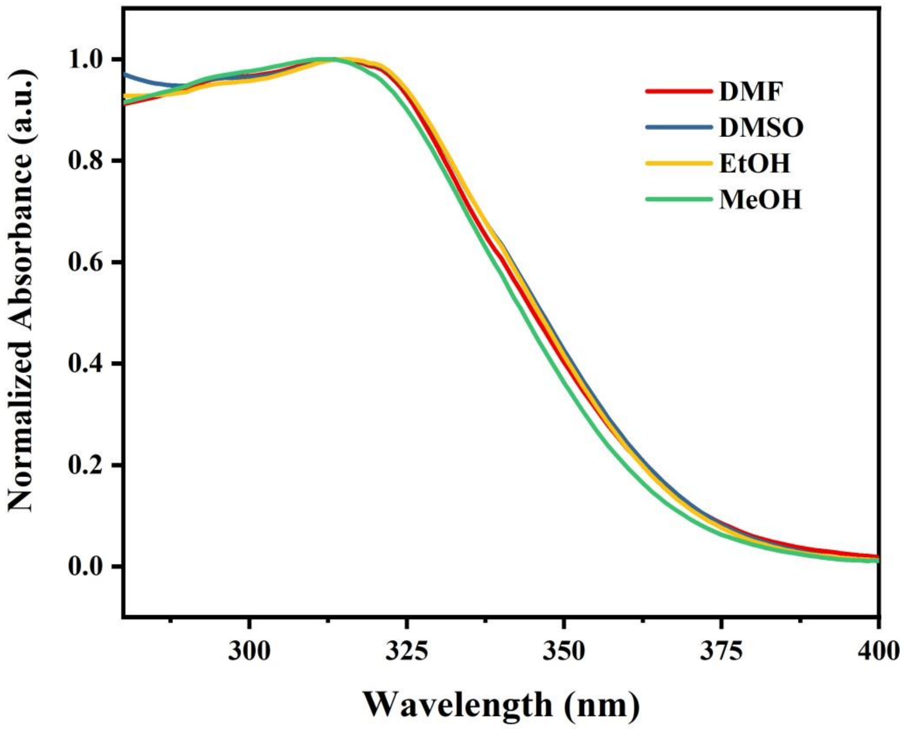


Figure S17. Normalized UV-*vis* absorption spectra of TPE-2P^{+} in DMF, DMSO, EtOH and MeOH.

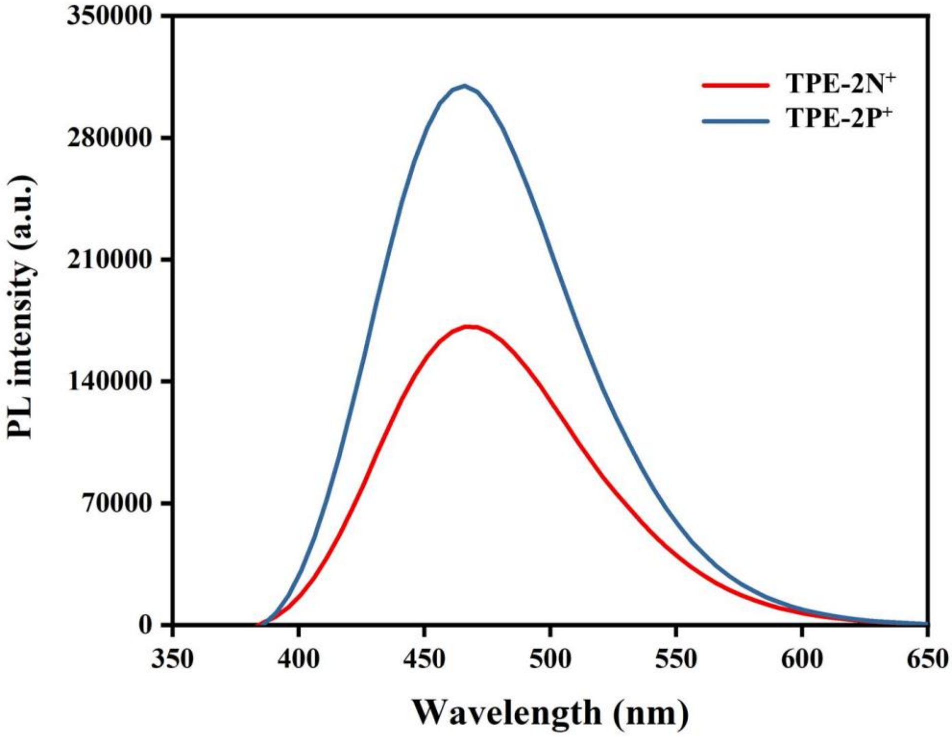


Figure S18. Photoluminescence spectra of TPE-2N$^+$ and TPE-2P$^+$ in solid state. (λ_{ex} = 316 nm).

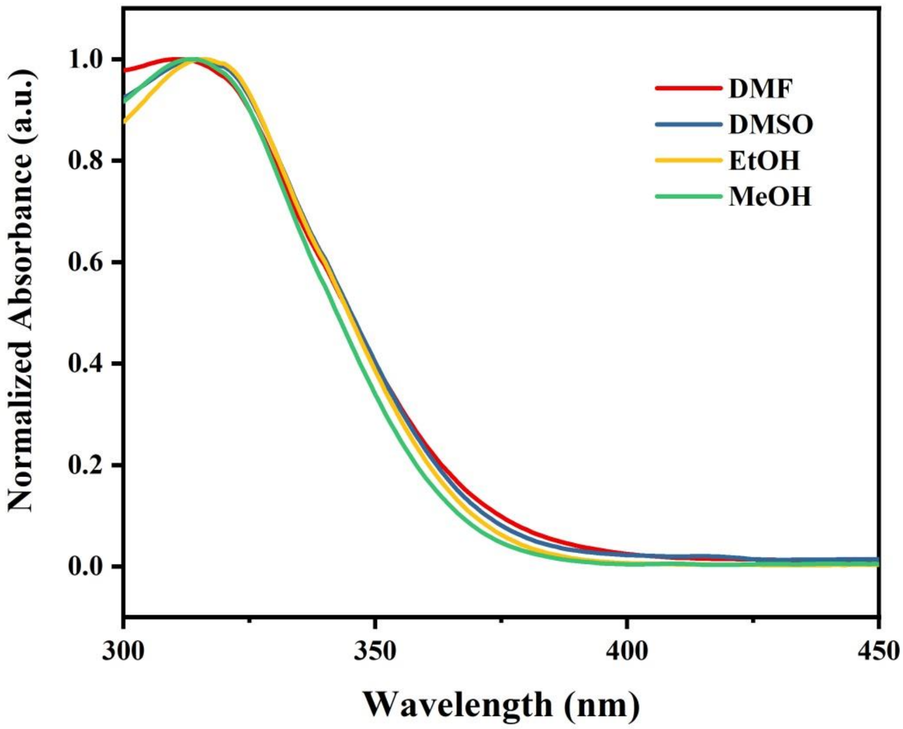


Figure S19. Normalized UV-*vis* absorption spectra of TPE-Ammonium polymer in DMF, DMSO, EtOH and MeOH.

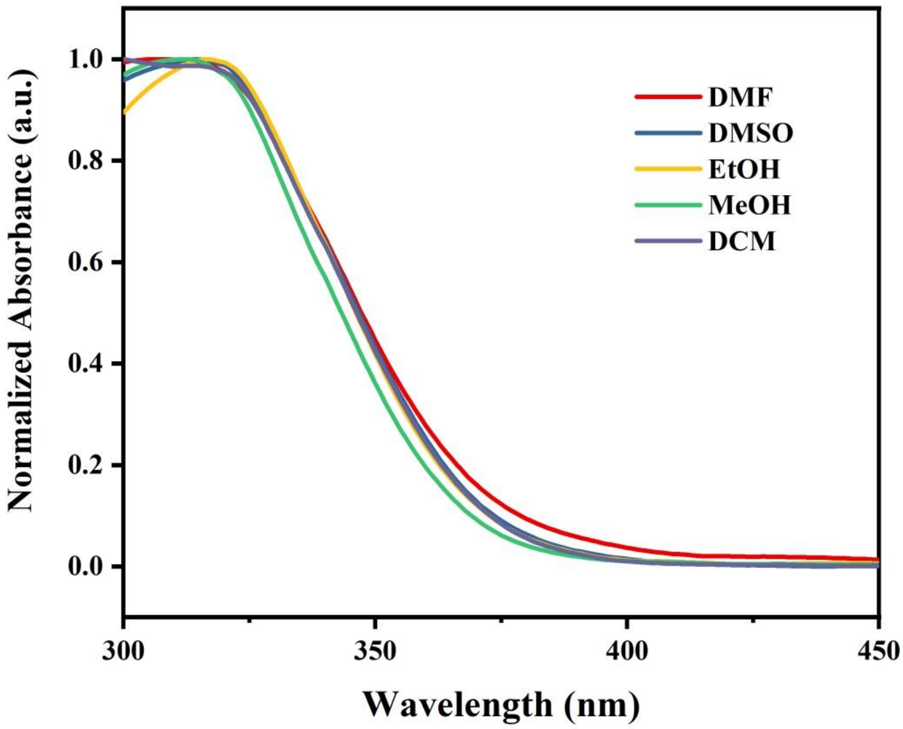


Figure S20. Normalized UV-*vis* absorption spectra of TPE-Phosphonium polymer in DMF, DMSO, EtOH, MeOH and DCM.

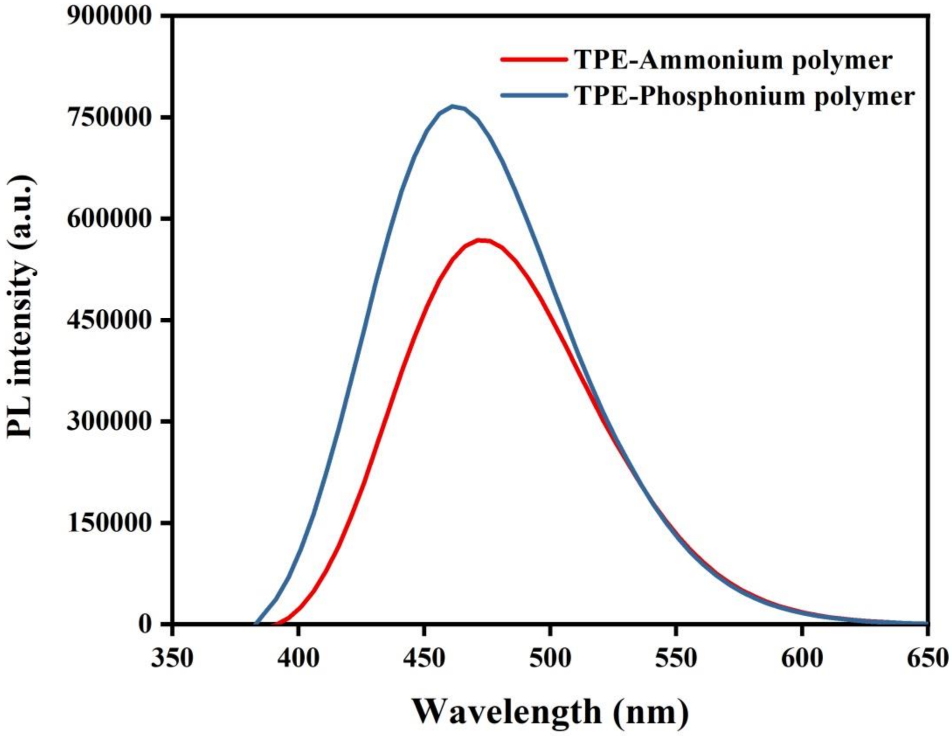


Figure S21. Photoluminescence spectra of TPE-Ammonium polymer and TPE-Phosphonium polymer in solid state. (λ_{ex} = 316 nm).

4. FT-IR spectrum of Compounds

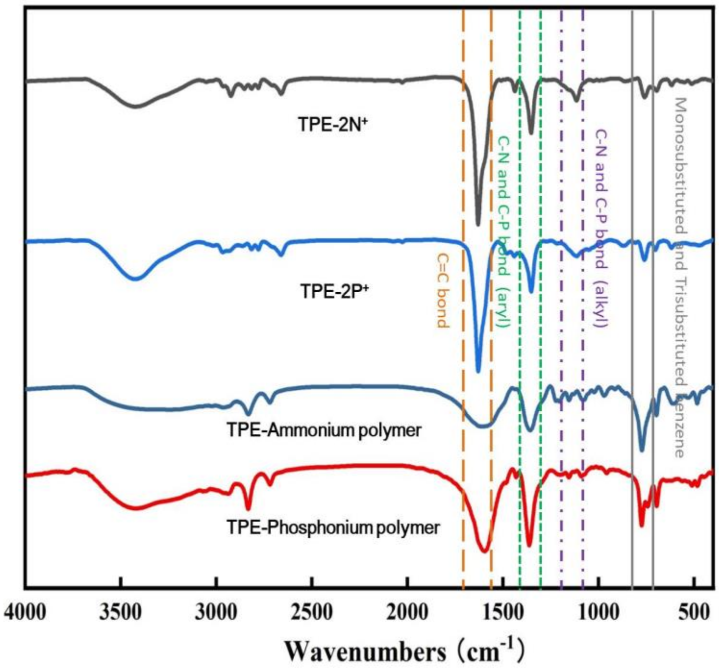


Figure S22. FT-IR spectra of TPE-2N^{+}, TPE-2P^{+} and polymers (KBr tablet).

5. AIE test of two polymers

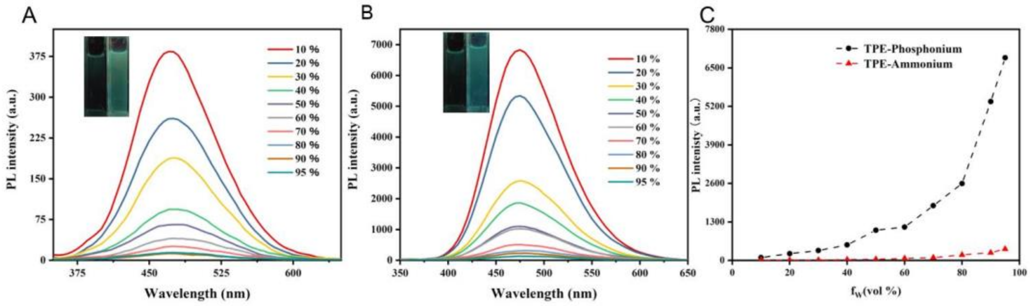


Figure S23. Photoluminescence spectra of (A) TPE-Ammonium polymer and (B) TPE-Phosphonium polymer at different ratios of water/ethanol. Inset: photographs of TPE-Ammonium polymer in ethanol and in water/ethanol mixtures when the addition of water was 95%, respectively, taken under illumination at 365 nm; (C) Plots of the maximum emission intensities of TPE-Phosphonium and TPE-Ammonium polymer with V_{water} : V_{EtOH} from 0 to 0.95. (Conc.：1 mg/mL).

6. Wettability test

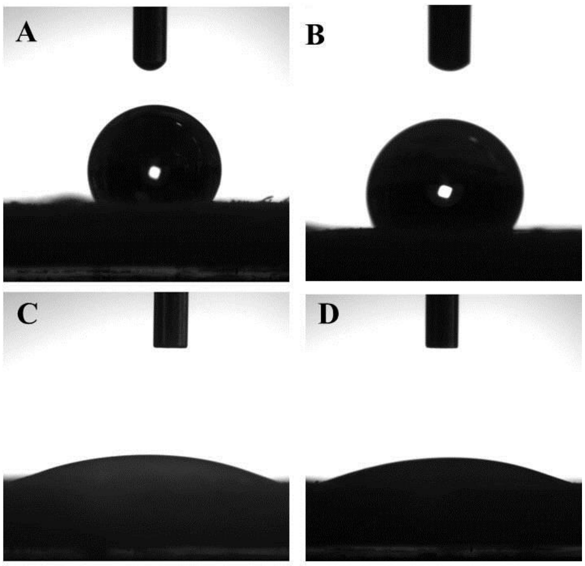


Figure S24. Contact angle of (A) TPE-2N$^+$, (B) TPE-2P$^+$, (C) TPE-Ammonium polymer and (D) TPE-Phosphonium polymer.

7. SEM images

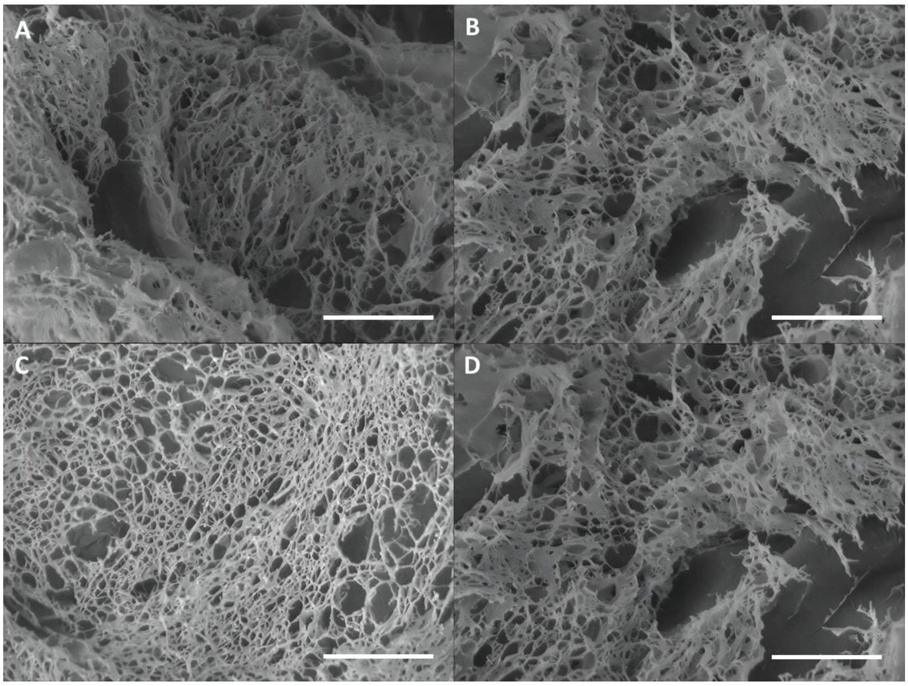


Figure S25. SEM images of the xerogel of TPE-Phosphonium polymer with CNCs. Scale bar: 2 μm.

8. EDS images

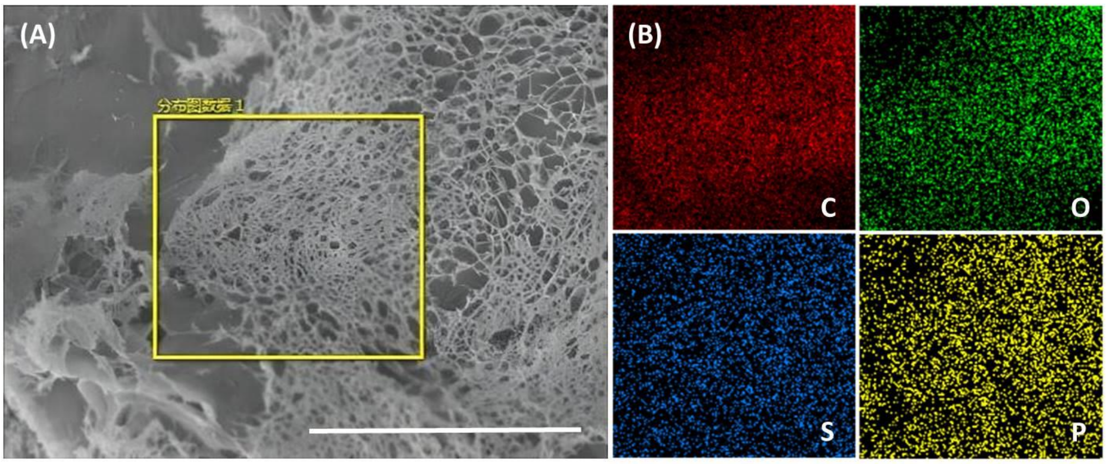


Figure S26. SEM images of the scanned area (A). Electron probe micro-analysis of xerogel tested by Energy Dispersive Spectrometer (EDS) (B). Scale bar: 5 μm.

9. Antibacterial activity test

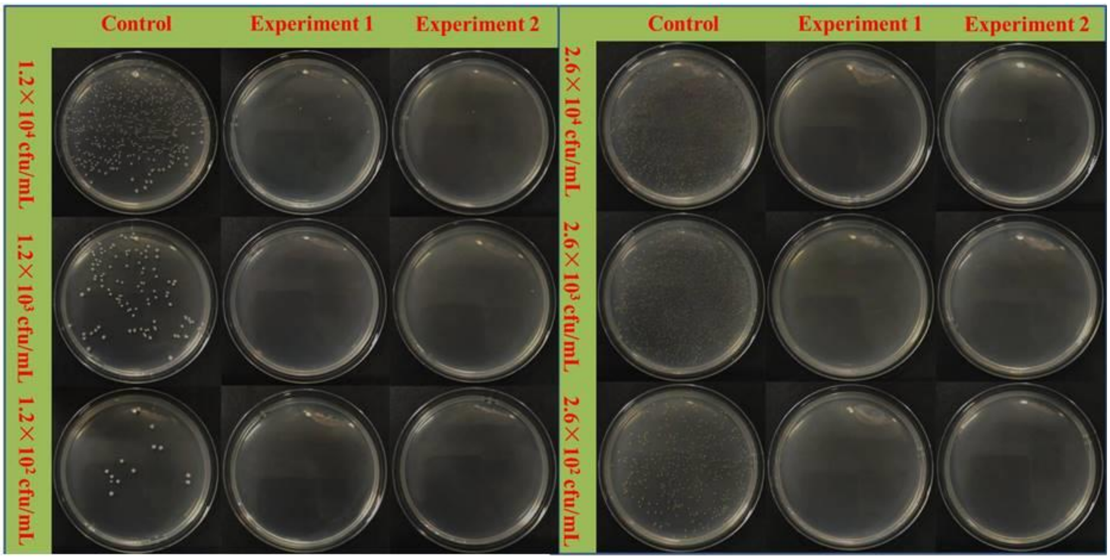


Figure S27. Antibacterial activities against *E. coli* (left) and *S. aureus* (right) of TPE-Phosphonium polymer (Conc.：0.02 mg/mL).

10. Bacterial imaging

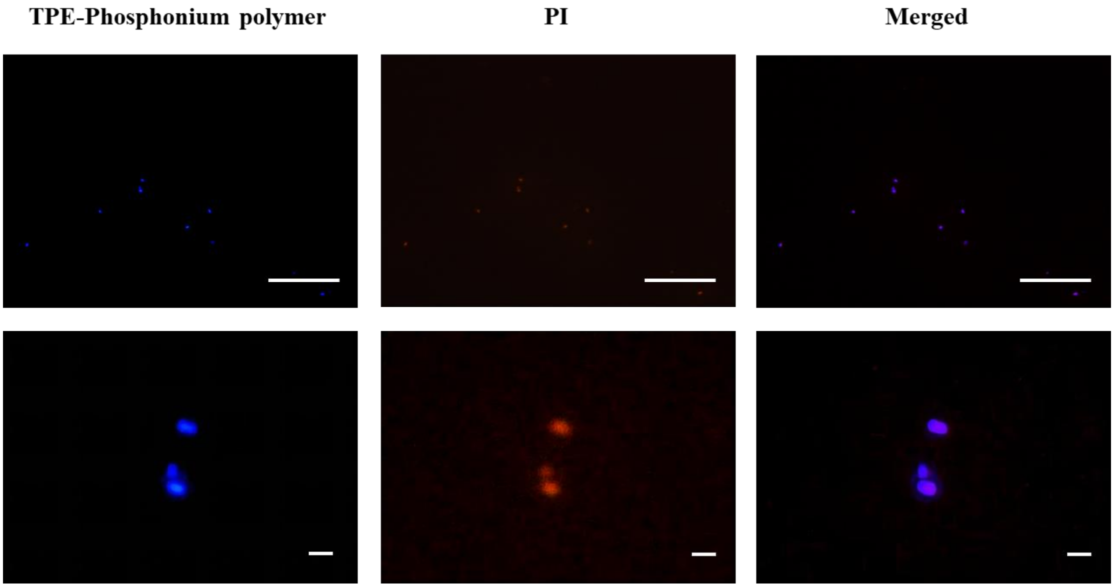


Figure S28. Fluorescence images of *E. coli* incubated with 0.2 mg/mL^{-1} of TPE-Phosphonium polymer for 12 h, PI for 12h and merged. The bottom images were enlarged. Excitation wavelengths: TPE-Phosphonium polymer for 300 - 400 nm and PI for 440 - 550 nm. (scale bar = 25 μm).

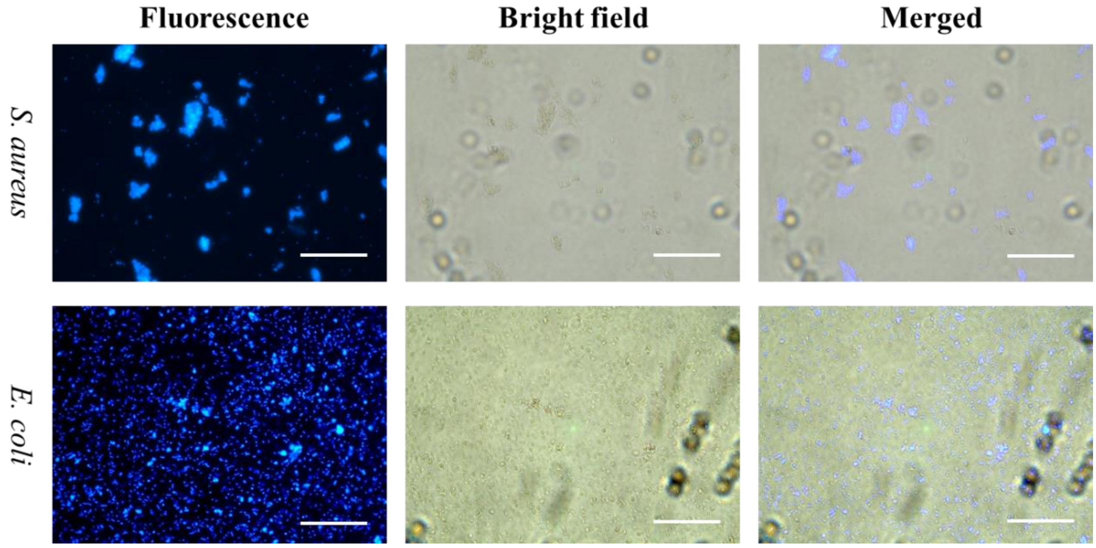


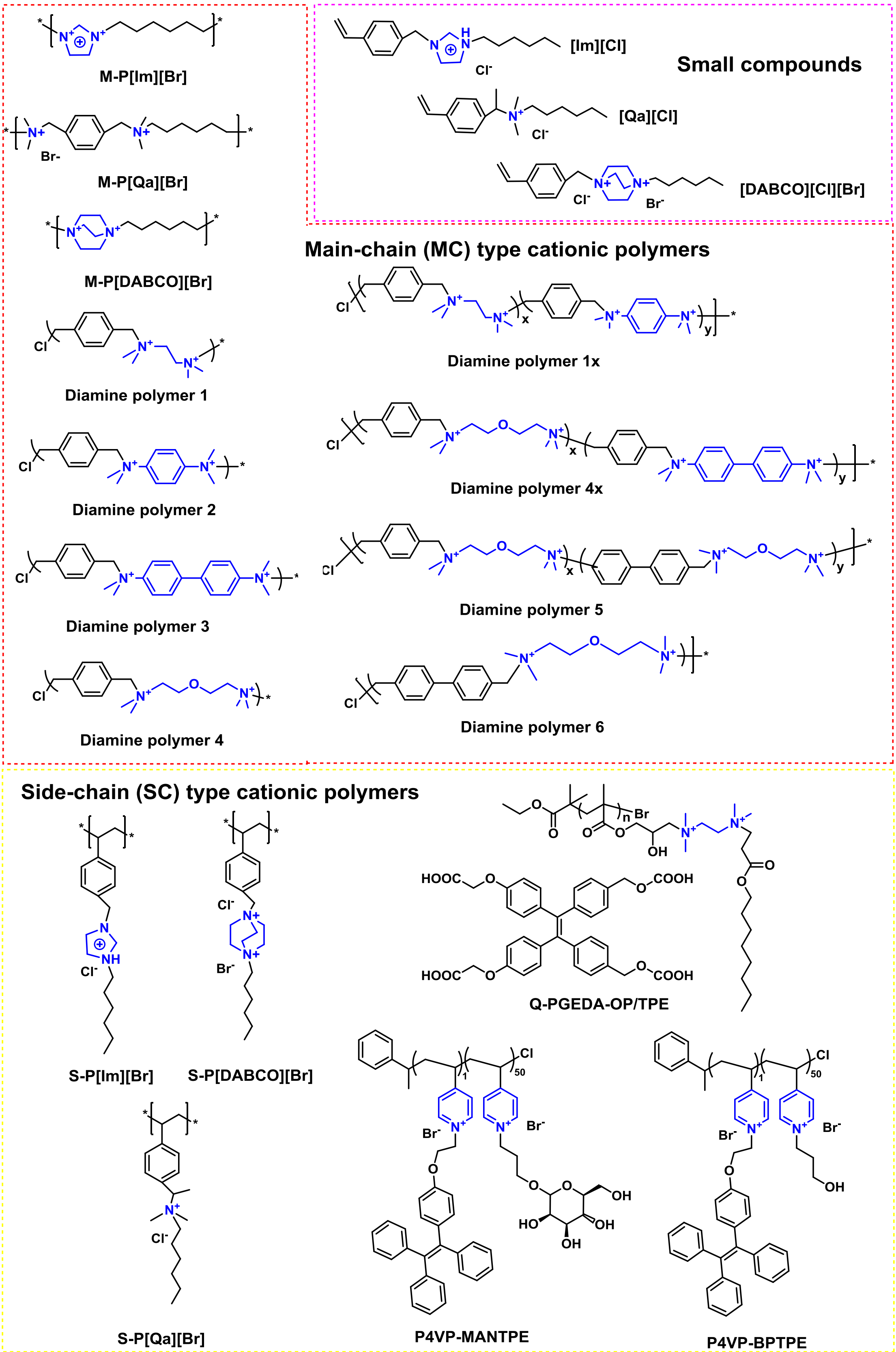
Figure S29. Fluorescence microscope images of *S. aureus* and *E. coli* incubated with TPE-Phosphonium polymer (0.2 mg/mL^{-1}) for 12 h. Excitation wavelengths: 300 - 400 nm. (scale bar = 25 μm).

11. MIC data and the chemical structures of representative antibacterial agents

Table S1 MIC data from previous works and our work.

Samples	MIC (μg/mL)	
	S. aureus	*E. coli*
[Im][C]*(*Polym. Chem-UK.* **2018**, *9*, 4611-4616)	460	440
[Qa][Cl]* (*Polym. Chem-UK.* **2018**, *9*, 4611-4616)	748	654
[DABCO][Cl][Br]*(*Polym. Chem-UK.* **2018**, *9*, 4611-4616)	2685	2350
S-P[Im][Cl]-L#(*Polym. Chem-UK.* **2018**, *9*, 4611-4616)	320	265
S-P[Im][Cl]#(*Polym. Chem-UK.* **2018**, *9*, 4611-4616)	275	235
S-P[Qa][Cl]-L# (*Polym. Chem-UK.* **2018**, *9*, 4611-4616)	365	285
S-P[Qa][Cl]# (*Polym. Chem-UK.* **2018**, *9*, 4611-4616)	257	220
S-P[DABCO][Cl][Br]-L# (*Polym. Chem-UK.* **2018**, *9*, 4611-4616)	887	787
S-P[DABCO][Cl][Br]#(*Polym. Chem-UK.* **2018**, *9*, 4611-4616)	550	497
Q-PGEDA-OP/TPE# (*Chem. Mater.* **2018**, *30*, 1782-1790)	15.5	125
Q-PGEDA-OA# (*Chem. Mater.* **2018**, *30*, 1782-1790)	31.5	500
P4VP-ManTPE# (*Biomacromolecules* **2021**, *22*, 2224-2232)	15.63	1000
P4VP-BPTPE# (*Biomacromolecules* **2021**, *22*, 2224-2232)	7.81	500
M-P[Im][Br]& (*Polym. Chem-UK.* **2018**, *9*, 4611-4616)	52	26
S-P[Qa][Cl]# (*Polym. Chem-UK.* **2018**, *9*, 4611-4616)	120	58
M-P[Qa][Br] & (*Polym. Chem-UK.* **2018**, *9*, 4611-4616)	200	180
Diamine polymer 1& (*Biomaterials* **2017**, *127*, 36-48.)	3.9	7.8
Diamine polymer 2& (*Biomaterials* **2017**, *127*, 36-48.)	7.8	31.3
Diamine polymer 4& (*Biomaterials* **2017**, *127*, 36-48.)	3.9	3.9
Diamine polymer 1a& (*Biomaterials* **2017**, *127*, 36-48.)	1.95	3.9
Diamine polymer 4a& (*Biomaterials* **2017**, *127*, 36-48.)	1.95	3.9
Diamine polymer 5& (*Biomaterials* **2017**, *127*, 36-48.)	3.9	3.9
Diamine polymer 6& (*Biomaterials* **2017**, *127*, 36-48.)	3.9	7.8
TPA-Ammonium polymer& (Our work)	**1.95**	**3.90**
TPE-Phosphonium polymer& (Our work)	**0.24**	**0.98**

*Small Cationic compound. #Side-chain polymer. &Main-chain polymer.



M-P[Im][Br]
M-P[Qa][Br]
M-P[DABCO][Br]
Diamine polymer 1
Diamine polymer 2
Diamine polymer 3
Diamine polymer 4
Small compounds
[Im][Cl]
[Qa][Cl]
[DABCO][Cl][Br]
Main-chain (MC) type cationic polymers
Diamine polymer 1x
Diamine polymer 4x
Diamine polymer 5
Diamine polymer 6
Side-chain (SC) type cationic polymers
S-P[Im][Br]
S-P[DABCO][Br]
S-P[Qa][Br]
Q-PGEDA-OP/TPE
P4VP-MANTPE
P4VP-BPTPE

12. Density functional theory (DFT) calculations

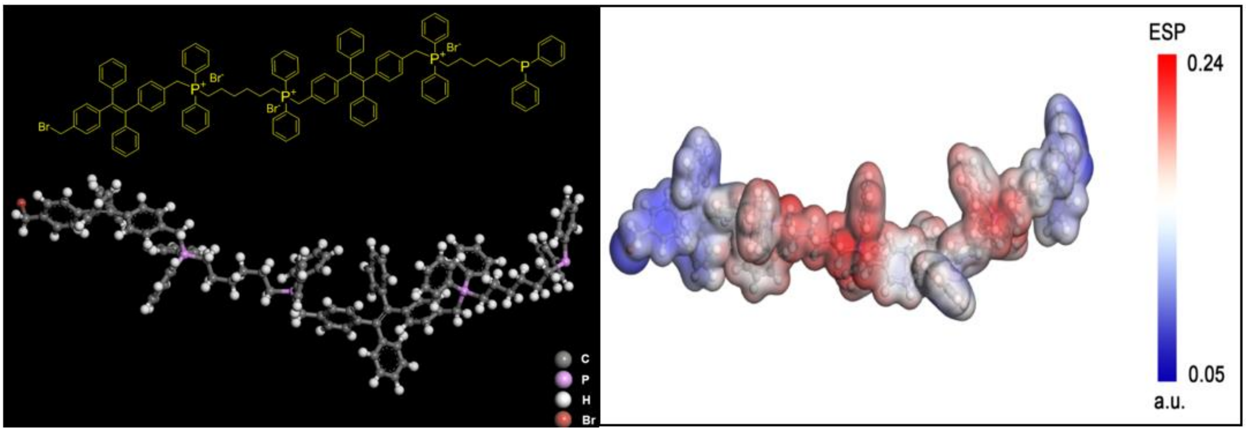


Figure **S30**. The chemical structure used for density functional theory (DFT) calculations (Upper left), and the optimized configuration (Lower left), The ESP diagram of TPE-Phosphonium polymer's molecular fragment (Right).

13. Cytotoxicity

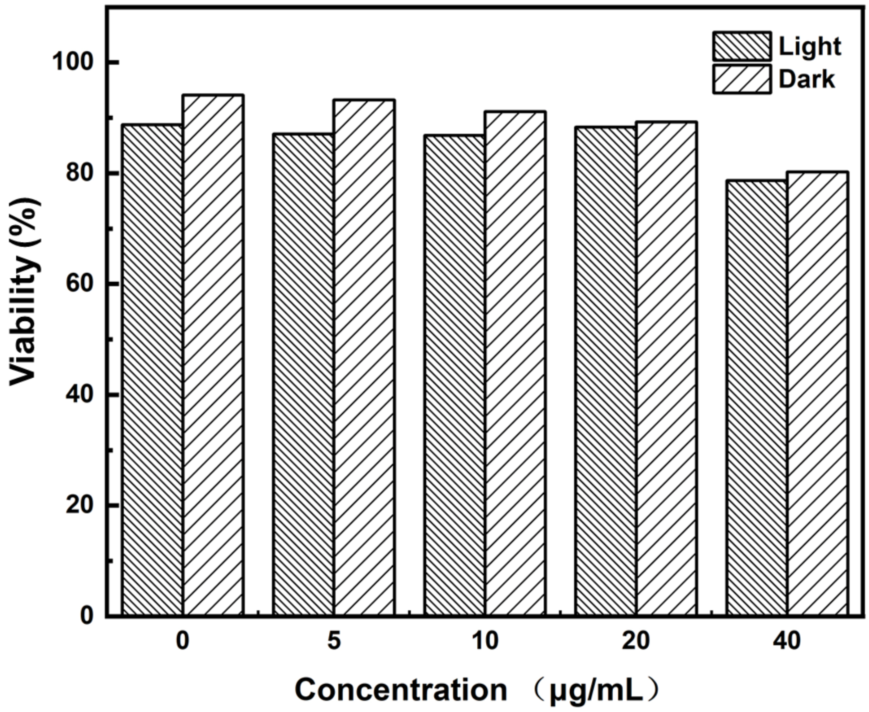


Figure S31. HeLa cells were incubated with TPE-Phosphonium polymer for 24h at different concentration: 0, 5, 10, 20 and 40 μg/mL.

14. Cell imaging

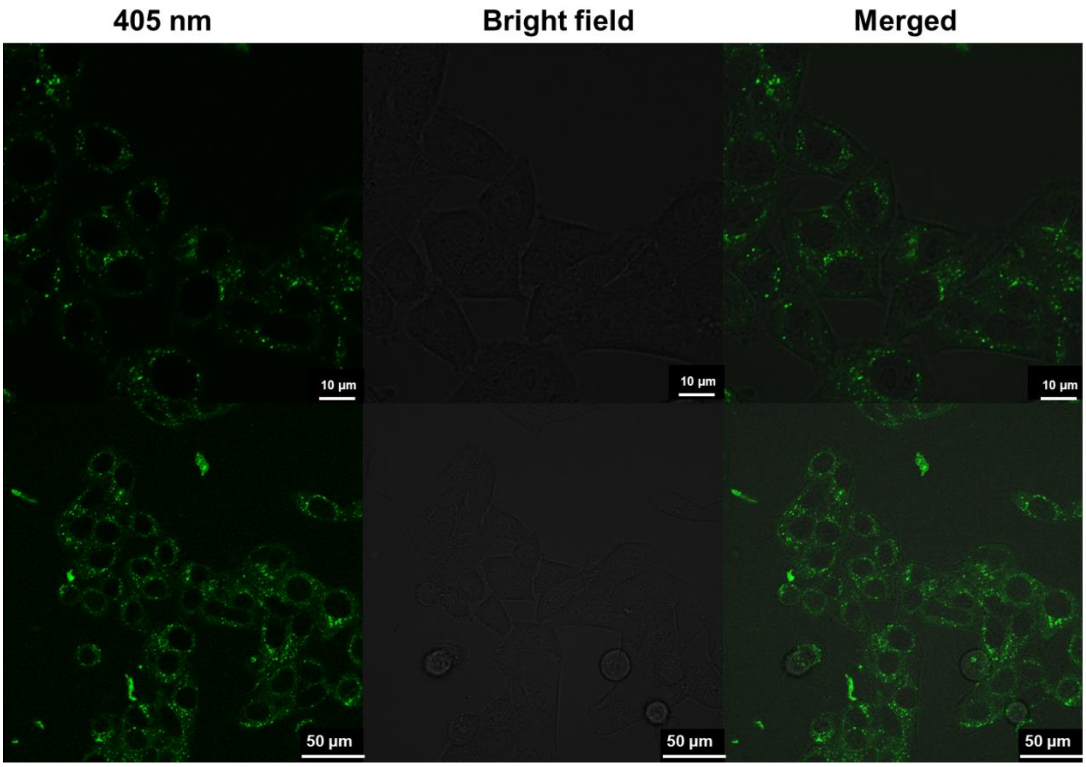


Figure S32. Fluorescence images of HeLa cells incubated with 20 μg/mL of TPE-Phosphonium polymer for 12 h (Excitation wavelength: 405 nm), the bright field images and the overlay images.