Supporting Information

Intelligent antibacterial surface based on ionic liquid molecular brushes for bacteria killing and releasing

Lunqiang Jin,[a,b] Zhenqiang Shi,[a] Xiang Zhang,[a] Xiaoling Liu,[a] Huilin Li,[a] Jingxia Wang,[a] Feng Liang,[b,] Weifeng Zhao,[a,]* Changsheng Zhao[a,]**

[a] *College of Polymer Science and Engineering, the State Key Laboratory of Polymer Materials Engineering, Sichuan University , Chengdu, 610065, People's Republic of China.*

[b] *The State Key Laboratory of Refractories and Metallurgy, Coal Conversion and New Carbon Materials Hubei Key Laboratory, School of Chemistry & Chemical Engineering, Wuhan University of Science and Technology, Wuhan 430081, P. R. China.*

Corresponding author.

E-mail: feng_liang@whu.edu.cn (F. Liang*); Tel: +86-27-68862107

zhaoscukth@163.com (W-F. Zhao*); Tel:+86-28-85400453

zhaochsh70@163.com (C-S. Zhao*). Tel:+86-28-85400453

Synthesis 3-(12-mercaptododecyl)-1-methyl-1H-imidazol-3-ium bromide IL(Br)

The 3-(12-mercaptododecyl)-1-methyl-1H-imidazol-3-ium bromide IL(Br) was prepared by improvement of previous literature.[1] In the first step, 1-methylimidazole (25 mmol) and 1,12-dibromododecane (37 mmol) were dissolved in 25 mL methylene chloride (DCM) at room temperature. Then the reaction was refluxed for 16 h. After evaporation of the solvent, got the crude product 3-(12-bromododecyl)-1-methyl-1H-imidazol-3-ium bromide (yield = 95%) by column chromatography (CH_2Cl_2 : MeOH = 10 : 1).

In the second step, 3-(12-bromododecyl)-1-methyl-1H-imidazol-3-ium bromide (20mmol) and potassium thioacetate (30 mmol) were dissolved in 30 mL tetrahydrofuran (THF) at room temperature, Then the reaction was refluxed for 6 h. After filtration the solids, then evaporation of the solvent, got the crude product 3-(12-(acetylthio)dodecyl)-1-methyl-1H-imidazol-3-ium bromide (yield = 85%) by column chromatography (CH_2Cl_2 : MeOH = 8 : 1).

In the third step, 3-(12-(acetylthio)dodecyl)-1-methyl-1H-imidazol-3-ium bromide (10 mmol) was dissolved in EtOH (25 mL). Slowly added solutions of NaOH (15 mmol) in H_2O (20 mL) at 0 ℃. The reaction was stirred at the same temperature for 1 h, and then acidified with 2 N HBr. When the pH was 2, stop acidifying. Subsequently extracted the reaction with DCM, evaporated to obtain the product 3-(12-mercaptododecyl)-1-methyl-1H-imidazol-3-ium bromide (yield = 93%).

The antibacterial performance of modified and unmodified membranes

In this work, *Staphylococcus aureus* (*S. aureus*) (Gram positive) and *Escherichia coli* (*E. coli*) (Gram negative) were acted as model bacteria.[2] Bacterial solution of *S. aureus* and *E. coli* were diluted to 10^6 CFU mL^{-1} with normal saline. The antibacterial activities of the modified and unmodified membranes were investigated by agar plate counting and live/dead two color fluorescene methods. For the agar plate counting, 2 mL solution of the bacterial (10^6 CFU mL^{-1}) were added to centrifuge tubes , then the membranes (pristine PES, PDA@PES and IL(Br)/PDA@PES) were immersed into the solution above. After incubation at 37 ℃ for 6 h, the membranes were washed with normal saline for 3 times. Then the membranes were ultrasound with normal saline for 30 s, then 100 μL of diluted bacterial solutions were added to solid medium for spreading. The solid medium were incubated at 37 ℃ for 12 h used for calculating the killing efficiencies of bacteria for samples. For the live/dead two color fluorescene method, 2 mL bacterial solution (10^6 CFU mL^{-1}) were added to centrifuge tubes, pristine PES, PDA@PES and IL(Br)/PDA@PES were immersed into the solutions. After incubation at 37 ℃ for 6 h, the membranes were washed with normal saline for 3 times. After stained with diluted solutions of a Live/Dead Bacteria Staining Kit for 20 min, the membranes were observed under a fluorescent microscopy.

The relationship between molecular grafting quantity and antibacterial efficiency

We chose 5 different concentrations (1, 0.2, 0.04, 0.008 and 0.0015 mg/mL) of IL(Br) to investigate the grafting density of the polymer on PES-based surface. As shown in **Fig. S7a** and **Table S1** the grafting ratio of the IL molecules increased from bottom to up, which was calculated by XPS (The XPS spectrum of N^+ was contributed by the molecule of IL(Br)). Compared with PDA@PES, the corresponding grafting ratios of the IL(Br)/PDA@PES membranes were 0.88, 0.55, 0.34, 0.22 and 0.09, respectively (from top to bottom). Subsequently, the loading densities of the IL molecules were 221, 132, 82, 53 and 22 μg/cm^2, which were calculated by comparing the loading density of the PDA on the membrane surface of PES. When the grafting density of the IL molecules got to 132 μg/cm^2, the antibacterial efficiency reached maximum (99%), which also proved that the antibacterial surface had remarkable bactericidal performance. Meanwhile, the distance between grafting sites was calculated by the the loading density of the IL molecules (The loading density of the IL molecules was 221 μg/cm^2 in this work.).

In addition, the gyration radius (Rg) of the molecules in the membrane of IL(Br)/PDA@PES was calculated by the following equation:

$R_g = \sqrt{\frac{\sum_i m_i (r_i - r_{cm})^2}{M}}$ (M is the total mass of the chain, m_i is the mass of atom i, r_i is the position of atom i, and r_{cm} is the position of the centre of mass of the polymer chain.). [3] In this study, the distance between grafting sites was smaller than R_g of the IL molecules, which proved that the grafted molecules on the surface was in brush state. [4] Therefore the grafted molecules on the surface can be considered as the molecule brush.

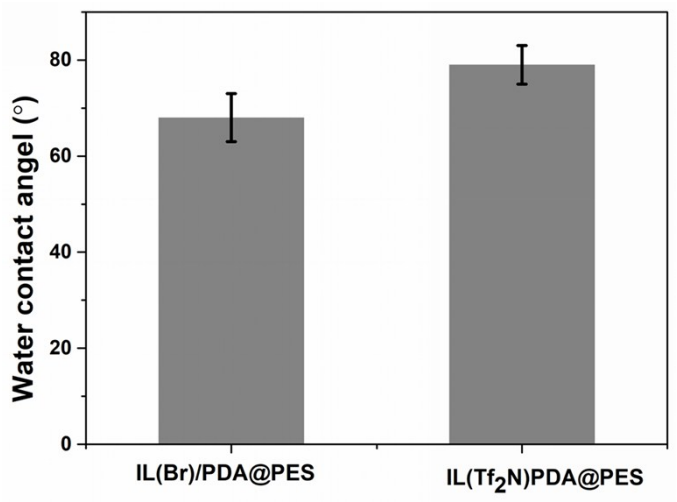

Fig. S1 The WCA for the membranes of IL(Br)/PDA@PES and IL(Tf_2N)/PDA@PES.

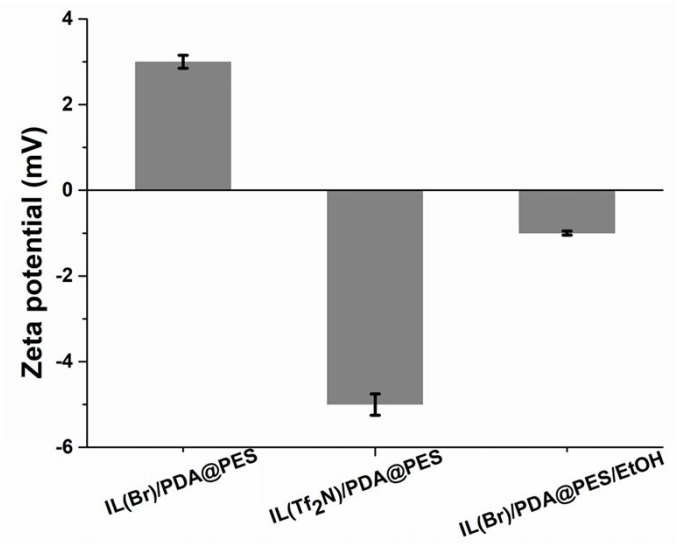

Fig. S2 The zeta potentials of the membranes (pH = 7).

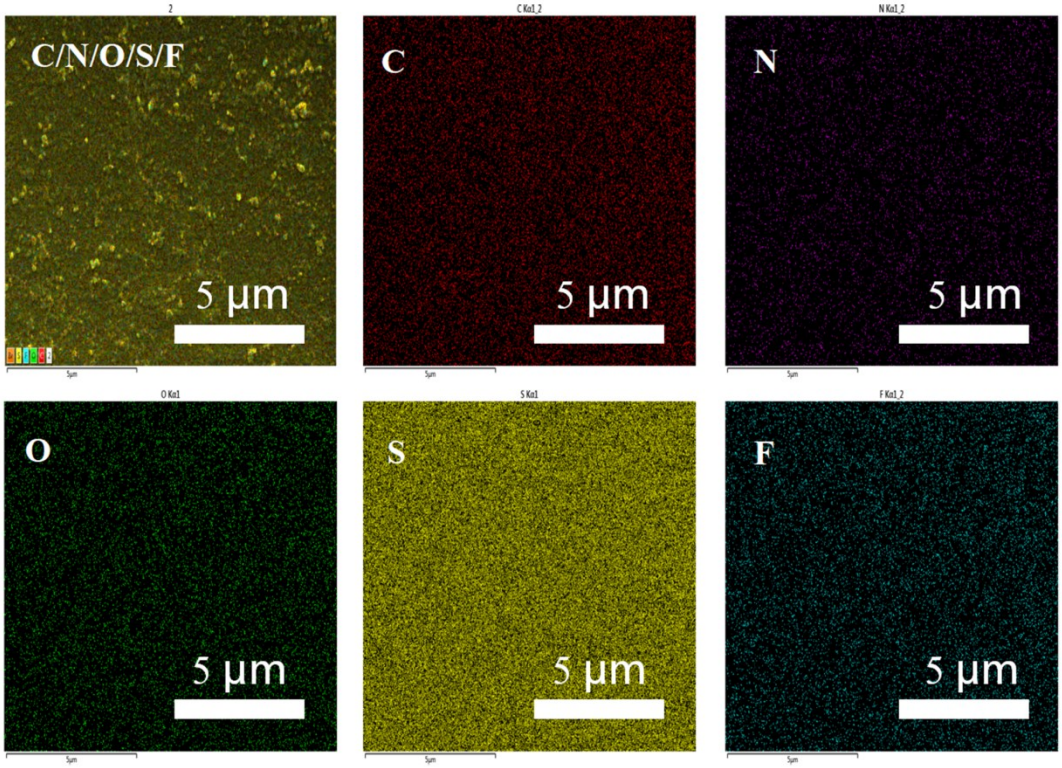

Fig. S3 The EDS mapping images of IL(Tf_2N)/PDA@PES.

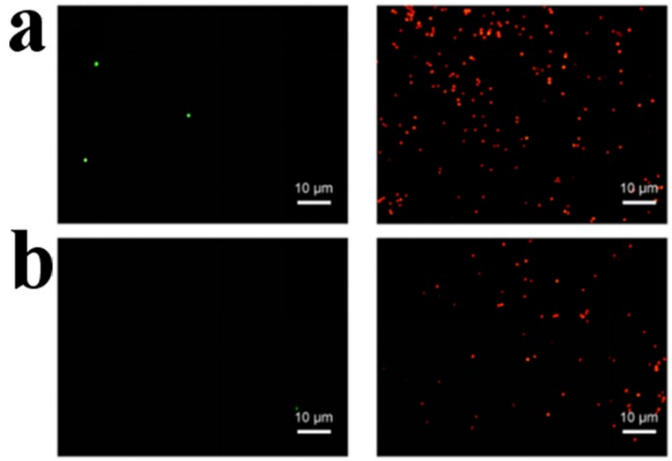

Fig. S4 Fluorescence microscopy images of *S. aureus* attached on the membrane surfaces of IL(Tf_2N)/PDA@PES (a) and (b) before and after washing with 0.1 M $LiTf_2N$ solution (Green staining and red staining represent live bacteria and dead bacteria, respectively.).

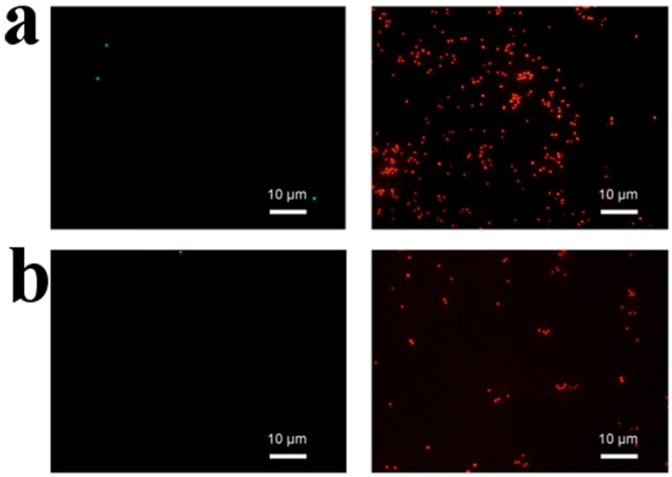

Fig. S5 Fluorescence microscopy images of *S. aureus* attached on the membrane surfaces of IL(Br)/PDA@PES (a) before and (b) after washing with ethanol (Green staining and red staining represent live bacteria and dead bacteria, respectively.).

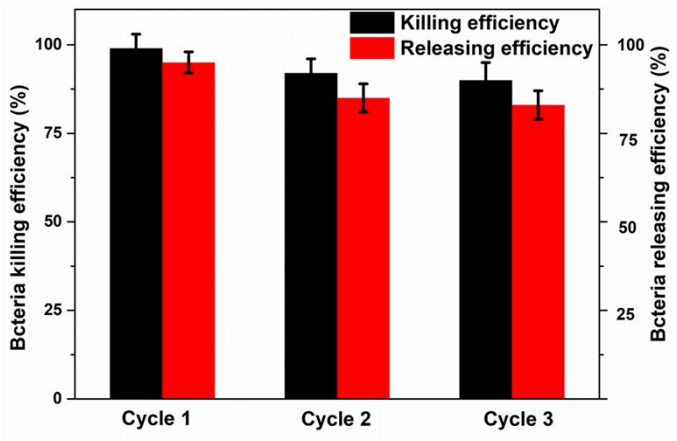

Fig. S6 The bacterial killing and releasing efficiencies of the IL(Br)/PDA@PES for the cycle utilization.

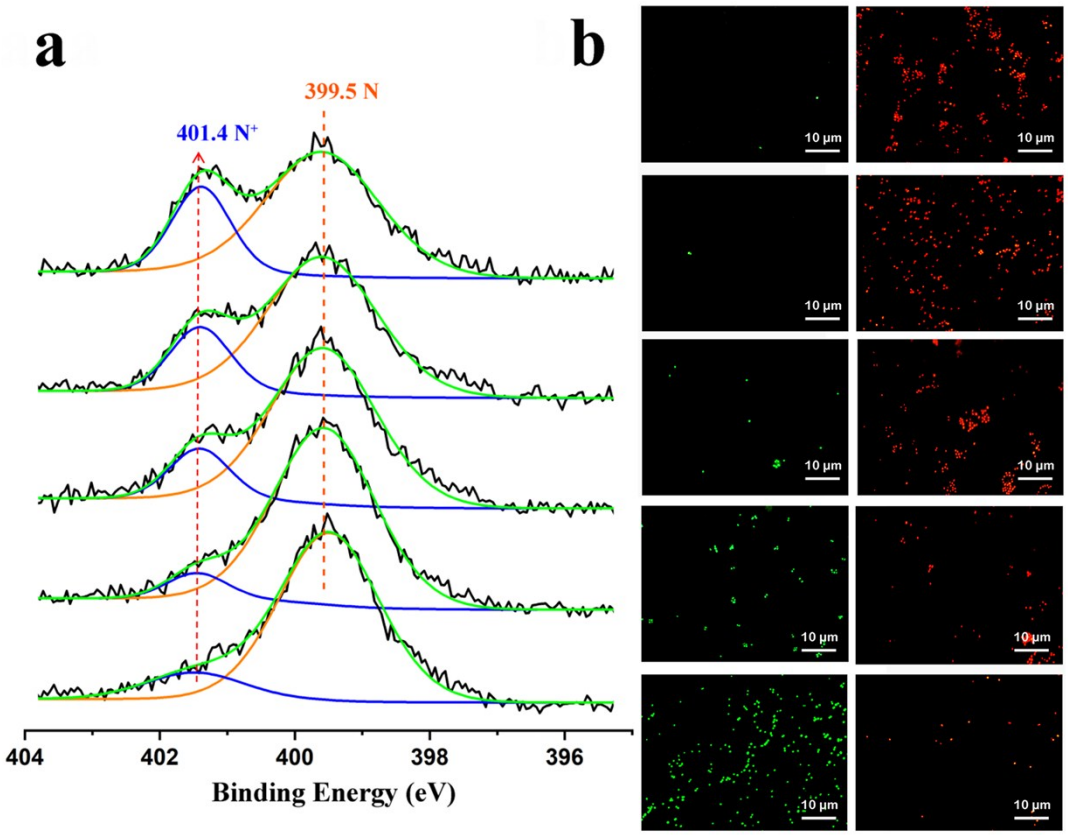

Fig. S7 (a) The XPS spectra of IL(Br)/PDA@PES for N^+ and N; (b) Fluorescence

microscopy images of *S. aureus* attached on IL(Br)/PDA@PES (Green staining and red staining represent live bacteria and dead bacteria, respectively.).

Table S1 The relationship of concentration, grafting ratio, loading density and antibacterial efficiency.

Concentration (mg/mL)	1	**0.2**	0.04	0.008	0.0016
Grafting ratio	0.88	**0.55**	0.34	0.22	0.09
Loading density (μg/cm^2)	221	**132**	82	53	22
Antibacterial efficiency (%）	99%	**99%**	83%	67%	24%

References

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3. S. J. Rukmani, G. Kupgan, D. M. Anstine, C. M. Colina, *Mol. Simul.*, 2018, **45**, 310–321.

4. L. Ionov, A. Sidorenko, M. Stamm, S. Minko, B. Zdyrko, V. Klep and I. Luzinov, *Macromolecules*, 2004, **37**, 7421–7423.