Supplementary Information

Self-doped polyaniline derived from poly(2-methoxyaniline-5-phosphonic acid) and didodecyldimethylammonium salt

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Calculation of the composition

The structure of the obtained mixture in the experiment can be drawn as shown in Fig. S1.

Fig. S1. Structure of the mixture.

Here, \( W(\text{Atom or Molecule}) \) means the percentage of weight (wt\%) for “Atom or Molecule” in the above mixture. \( M_w(\text{Molecule}) \) and \( A_w(\text{Atom}) \) mean molecular weight and atomic weight for “Molecule” and “Atom”, respectively.

PMAP-DDDMA before washing

\[ W(P) = \frac{1.75 \times (20/1000)}{1.9068 \times 100} = 1.835 \text{ wt\%}, \]  
the value of ppm for phosphorus was obtained from the ICP-AES analysis [1.75 ppm (average number of the three experiments) in the concentrated nitric acid solution of the above mixture (1.9068 mg in 20 mL)].
W(Br) = 8.76 wt%, the value was obtained from the ion-chromatography.
W(O) = 100-{W(C)+W(H)+W(N)+W(Br)+W(P)} = 8.68 wt%, the values for W(C), W(H) and W(N) were obtained from the elementary analysis {W(C), W(H) and W(N) = 65.58, 11.88 and 3.70 wt%, respectively}.

\[ m = \frac{W(\text{DDDMABr})}{W(P)} = 1.85, \text{where } W(\text{DDDMABr})= W(\text{Br}) \times \frac{M_w(\text{DDDMABr})}{A_w(\text{Br})} \]

\[ M_w(\text{all}) = M_w(\text{monomer}) + (1+x)M_w(\text{DDDMA}^+) + (0.5-x)A_w(H^+) + mM_w(\text{DDDMABr}) + nM_w(H_2O) \]

\[ W(O) = 100 \times \left[ 4A_w(O) + nA_w(O) \right] / M_w(\text{all}), \text{because oxygen is included in the components for monomer and } H_2O \text{ in the above mixture.} \]
\[ W(P) = 100A_w(P) / M_w(\text{all}) \]

From the above two equations concerning the percentage of weight for oxygen and phosphorous, \( x \) and \( n \) were calculated.

i.e. \( M_w(\text{all}) = 100A_w(P) / W(P) \)

\[ n = \frac{W(O)*M_w(\text{all}) - 100*4A_w(O)}{(100A_w(O))} = \frac{W(O)*100A_w(P)/W(P) - 100*4A_w(O)}{(100A_w(O))} = 4.70 \]

\[ x = \frac{M_w(\text{all}) - M_w(\text{monomer}) - M_w(\text{DDDMA}^+) - 0.5A_w(H^+) - nM_w(H_2O)}{M_w(\text{DDDMA}^+) - A_w(H^+)} = \frac{100A_w(P)/W(P) - M_w(\text{monomer}) - M_w(\text{DDDMA}^+) - 0.5A_w(H^+)}{M_w(\text{DDDMA}^+) - A_w(H^+)} = 0.431 \]

Therefore, molecular formula of the above mixture is described as shown below.

C_{92.32}H_{199.22}N_{4.28}O_{8.70}P_{1.00}Br_{1.85}

The percentage of weight for each element is described as shown below (elementary analysis).

C, 65.71; H, 11.90; N, 3.55

Cf. the experimental values: C, 65.58; H, 11.88; N, 3.70.

**PMAP-DDDMA after washing**

W(P) = [3.50*(20/1000)]/2.1865*100 = 3.20 wt%, the value of ppm for phosphorus was obtained from the ICP-AES analysis [3.50 ppm (average number of the three experiments) in the concentrated nitric acid solution of the above mixture (2.1865 mg in 20 mL)].

W(Br) = 5.43 wt%, the value was obtained from the ion-chromatography.
\[ W(O) = 100 - (W(C) + W(H) + W(N) + W(Br) + W(P)) = 11.74 \text{ wt\%}, \] the values for W(C), W(H) and W(N) were obtained from the elementary analysis \{W(C), W(H), and W(N) = 64.38, 11.16 and 4.09 wt\%, respectively\}.

The values for \( m, n \) and \( x \) were calculated in the same way as PMAP-DDDMA before washing.

\[ m = 0.66, \quad n = 3.10 \quad \text{and} \quad x = 0.0660 \]

Therefore, molecular formula of the above mixture is described as shown below.

\[ \text{C}_{51.87} \text{H}_{109.14} \text{N}_{2.72} \text{O}_{7.10} \text{P}_{1.06} \text{Br}_{0.66} \]

The percentage of weight for each element is described as shown below (elementary analysis).

C, 64.32; H, 11.37; N, 3.94

Cf. the experimental values: C, 64.38; H, 11.16; N, 4.09.

\[ \text{Fig. S2} \] Pictures of PMAP-DDDMA (a) before and (b) after washing in various solvents (from left to right, diethyl ether, ethyl acetate, DMSO, CH\textsubscript{2}Cl\textsubscript{2}, ethanol, 2-propanol, acetone, hexane, toluene and THF ).
Fig. S3 Photos of spin-coated film of PMAP-DDDMA before (left) and after (right) washing on glass substrates.