

Supporting Information

Molecular Alignment and Ion Transport in Rigid Rod Polyelectrolyte Solutions

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Contents of supporting information

S.1 Chemical structure of poly-L-glutamic acid (PLGA)

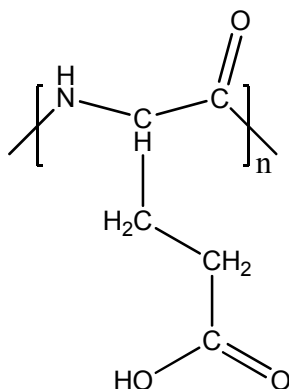


Figure 1. This is the chemical structure of PLGA. 1N NaOH aqueous solution was used to transform H⁺ form PLGA into Na⁺ form PLGA.

S.2 ^{23}Na spectra for PBDT, NaCl, NaTriflate, and PLGA aqueous solutions

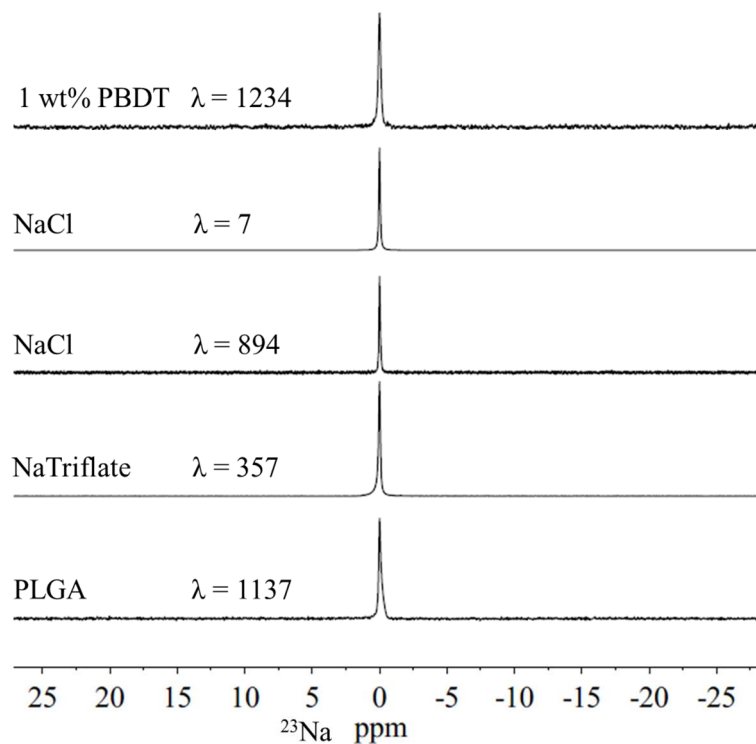


Figure 2. ^{23}Na 1D spectra for aqueous solutions of PBDT, NaCl, NaTriflate, and PLGA

with varying water uptake (λ). λ is defined as the mole ratio of ($\text{H}_2\text{O}+\text{D}_2\text{O}$) and Na^+ .

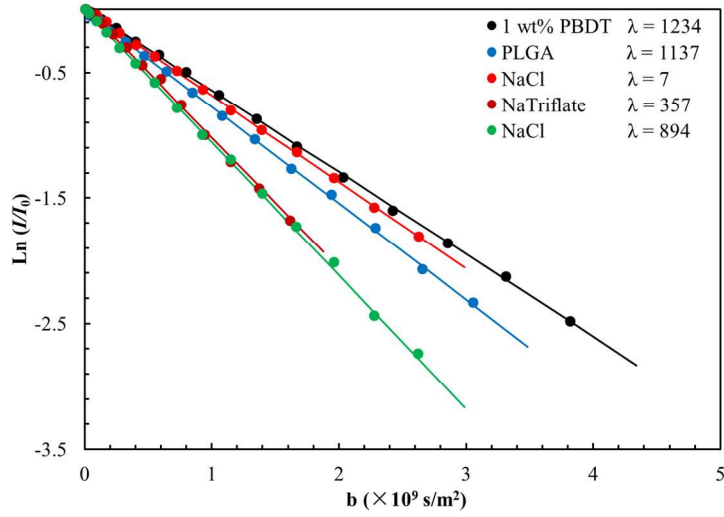


Figure 3. Normalized signal amplitudes (I/I_0) of stimulated echo decays vs Stejskal-Tanner parameter b for aqueous solutions of PBDT, PLGA, NaCl, and NaTriflate with different water uptake λ . Solid symbols indicate the experimental signal decay. The solid lines are linear least squares one-component fits for the experimental data.

$I = I_0 e^{-D\gamma^2 g^2 \delta^2 \left(\Delta - \frac{\delta}{3}\right)}$, $b = \gamma^2 g^2 \delta^2 \left(\Delta - \frac{\delta}{3}\right)$, I and I_0 refer to the spin-echo signal intensity and zero gradient spin-echo signal intensity, respectively. γ is the gyromagnetic ratio of the nucleus. g is the gradient strength. δ is the pulse duration time. Δ is the diffusion time.

Solutions	λ	$D \cdot 10^{-10} \text{ (m}^2\text{/s)}$
PBDT	1234	6.55
PLGA	1137	7.70
NaCl	7	6.92
NaTriflate	357	10.56
NaCl	894	10.60

Table 1. The fitting results are listed in the table. The maximum diffusion rate for Na^+ is around 10.60×10^{-10} , which is 30% larger than Na^+ ions diffuse in aqueous solutions of PBDT and PLGA with similar water uptake λ .

S.3 Negative intercept in the linear fit in Figure 5b

Curiously, we notice a small negative (-20 Hz) y-intercept in the Figure 5b plot. This suggests a small and constant reduction in average ordering of the D₂O over this linearly varying range of concentrations. Since our model for D₂O ordering (which would predict a zero intercept) essentially assumes infinitely long rods, this intercept might correspond to the small D₂O population interacting with the ends of each rod. In other words, D₂O interacting near the ends of the rods is not inheriting orientation relative to the LC phase. Further investigation is required to uncover the exact nature of this intercept.

S.4 Relative linewidths and areas of the peaks and corresponding dynamics relating to Figure 6c

² H Polymer Concentration (wt%)	Linewidth for left peak (Hz)	Linewidth for middle peak (Hz)	Linewidth for right peak (Hz)	Relative area for left peak	Relative area for middle peak	Relative area for right peak
1.9%	N/A	551	N/A	N/A	290428	N/A
3.0%	2602	268	2777	32425	8066	34873
4.1%	2212	283	2299	31190	11927	30254
5.2%	2279	181	2298	43909	9280	43586

The doublets associated with the polymer chain ²H labels possess broader lines (\approx 2500 Hz or $T_2 \approx$ 0.13 ms) due to the slower dynamics of the polymer chains in the LC phase as compared to chains in the isotropic phase, which in this case exhibit singlets with linewidths of 180-550 Hz. Future work can utilize the relative peak intensities and linewidths to further probe polymer dynamics and phase behavior.

Note that we did not strictly control the relative overlaps of the isotropic phase (singlet) and oriented phase (doublet) fractions in the sample tube relative to the rf coil. Thus, intensities gleaned from these spectra (table S.4) are not representative of the absolute phase quantities in the whole sample tube. One may use the relative areas of the middle peak with respect to the doublet peaks to quantify the amount of isotropic and anisotropic phase, but only if the total sample length is shorter than the rf coil and when using sufficiently enough relaxation delay time (D_1) to allow both signals to relax during signal averaging.