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Dielectric properties and charge transport mechanism of π -conjugated segments decorated with intrinsic conducting polymer

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Supporting Information

The accelerating nature of the frequency dependent conductivity approximately follows universal power law, represented by equation [1]:

$$\sigma'_{ac}(\omega) = A(T)\omega^{S}$$

Where A(T) is dispersion parameter, ω is frequency and S ($0 \le S \le 1$) is dimensionless exponent of frequency. Values of A and S are calculated using power law least square fitting equation all measured temperature are tabulated in table 2 and table 3 for PVA/PVP and PVA/PVP/PANI(20weight%). The variation in the value of S with respect to temperature is further used to verify conduction mechanism in PVA/PVP and PVA/PVP/PANI.

Ac conductivity at (10MHz), low frequency conductivity (DC conductivity) (0.1Hz) and dielectric at 1KHz as well as at 10MHz is shown in table 2 and table 3 for both PVA/PVP and PVA/PVP/PANI (20weight%) respectively for various range of temperature (0°C to 100°C).

Table 1. Dielectric constant and ac conductivity at different frequency and fitting parameter A and frequency exponent S (equation 4) at various temperatures for PVA/PVP films.

PVA/PVP						
Temp.	σ_{DC} (s/cm)	σ _{ac} (s/cm)	A	S	ε' at	ε' at
(°C)	at 0.1Hz	at 10MHz			1KHz	10MHz
0	1.39x10 ⁻¹³	1.67x10 ⁻⁶	8.35x10 ⁻¹⁴	0.95	6.45	5.07
10	1.84x10 ⁻¹³	1.94 x10 ⁻⁶	1.72x10 ⁻¹³	0.92	6.86	5.42
20	3.71x10- ¹³	2.35 x10 ⁻⁶	5.00x10 ⁻¹²	0.72	7.31	5.47
30	8.21x10 ⁻¹²	2.86 x10 ⁻⁶	3.99 x10 ⁻¹⁰	0.25	7.80	5.74
40	3.05x10 ⁻¹²	3.53 x10 ⁻⁶	2.34 x10 ⁻⁹	0.19	8.51	6.11

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50	2.41x10 ⁻¹¹	4.51 x10 ⁻⁶	1.33 x10 ⁻⁸	0.06	9.79	6.63
60	2.85x10 ⁻¹⁰	6.01 x10 ⁻⁶	1.37 x10 ⁻⁸	0.24	12.3	7.36
70	1.71x10 ⁻⁹	7.90 x10 ⁻⁶	6.66 x10 ⁻⁹	0.50	16.2	8.29
80	6.75x10 ⁻⁹	9.99 x10 ⁻⁶	3.20 x10 ⁻⁹	0.74	21.9	9.36
90	2.18x10 ⁻⁸	1.19 x10 ⁻⁵	1.54 x10 ⁻⁹	0.91	28.3	10.5
100	5.32x10 ⁻⁸	1.36 x10 ⁻⁵	7.74 x10 ⁻¹⁰	0.97	31.1	11.7

Table 2. Dielectric constant and ac conductivity at different frequency and fitting parameter A and frequency exponent S (equation 4) at various temperatures for PVA/PVP/PANI (20wt%).

PVA/PVP/PANI (20 weight%)						
Temp.	σ_{DC} (s/cm)	σ_{ac} (s/cm)	A	S	ε' at	ε' at
(°C)	at 0.1Hz	at 10MHz			1KHz	10MHz
0	4.05x10 ⁻⁷	2.36 x10 ⁻⁵	3.64x10 ⁻⁶	0.19	52.3	2.2
10	5.21 x10 ⁻⁷	1.98 x10 ⁻⁵	2.39 x10 ⁻⁷	0.18	64.9	2.97
20	8.76 x10 ⁻⁷	2.19 x10 ⁻⁵	4.65 x10 ⁻⁷	0.16	87.8	3.03
30	1.62 x10 ⁻⁶	5.19 x10 ⁻⁵	9.77 x10 ⁻⁷	0.14	1.31x10 ²	11.9
40	2.98 x10 ⁻⁶	6.64 x10 ⁻⁵	2.08 x10 ⁻⁶	0.11	2.2×10^2	14.2
50	5.03 x10 ⁻⁶	7.88 x10 ⁻⁵	3.95 x10 ⁻⁶	0.096	6 x10 ²	15.9
60	7.56 x10 ⁻⁶	9.15 x10 ⁻⁵	6.43 x10 ⁻⁶	0.084	6.5×10^2	16.5
70	1.03 x10 ⁻⁵	1.04 x10 ⁻⁴	9.26 x10 ⁻⁶	0.077	1.07×10^3	17.2
80	1.27 x10 ⁻⁵	1.13 x10 ⁻⁴	1.18 x10 ⁻⁵	0.073	$1.57x10^3$	20.6
90	1.43 x10 ⁻⁵	1.14 x10 ⁻⁴	1.39 x10 ⁻⁵	0.069	1.98 x10 ³	21.8
100	1.48 x10 ⁻⁵	1.17 x10 ⁻⁴	1.43 x10 ⁻⁵	0.068	$2.09x10^3$	22.8

Using CBH mechanism model, hopping distance (R_H) and maximum barrier width (W_m) is calculated for different concentration using equation $^{[2]}$:

$$R_{H} = \frac{e^{2}}{\pi \varepsilon \varepsilon_{0}} \left(\frac{1}{W_{m} + k_{B}T \ln(\omega \tau_{I})} \right)$$

$$S = 1 - \frac{6k_{B}T}{W_{m}}$$

Where ϵ is dielectric constant, ϵ_0 is permittivity of free space, W_m are maximum barrier height, K_B boltzmann constant and T is temperature. The calculated value of R_H and W_M is tabulate in table 4 along with the roughness value obtained for FSPC having different concentration of PANI.

Table 3: $W_{\rm M}$, $R_{\rm H}$ and Roughness of FSPC film for different weight% of PANI.

Weight%	W _M (ev)	R _H (A°)	Roughness (μm)	
5% PANI	0.210	16.10	1.20	
10% PANI	0.192	9.89	1.48	
15% PANI	0.187	8.48	1.90	
20% PANI	0.169	2.35	2.60	

Reference

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- 2. Gmati F, Fattoum A, Bohli N. and Mohamed AB, J. Phys. Condens. Matter., 2008, 20, 125221-125230.