Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supporting information

Synthesis of Quantum Dot-Based Polymer Nanocomposites: Assessment of Their Thermoelectric Performances

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Mobility and charge carrier concentration calculation:

The dielectric properties of the TQDGO/PEDOT: PSS pellets in the low frequency region is shown in figure 1. These properties were analyzed using the Uemura model by using[1–3]:

$$\varepsilon'(f) = A.f^{3/2} + B$$

$$\varepsilon''(f) = C.f^{-1}$$

Where $A = \dfrac{2\,n\,q^2 D^{3/2}}{\varepsilon_0 \sqrt{\pi}\, d\, k_B T}$, B = ε_∞ , and $C = \dfrac{2\,n\,q^2 D}{\varepsilon_0\, k_B\, T}$

Dividing the coefficient A by C, we can calculate the diffusion constant, D, by:

$$D = \left(\frac{A}{C}\right)^2 \pi\, d^2$$

The charge carrier concentration, n, is calculated by:

$$n = \frac{C\,\varepsilon_0\, k_B\, T}{2q^2\, D}$$

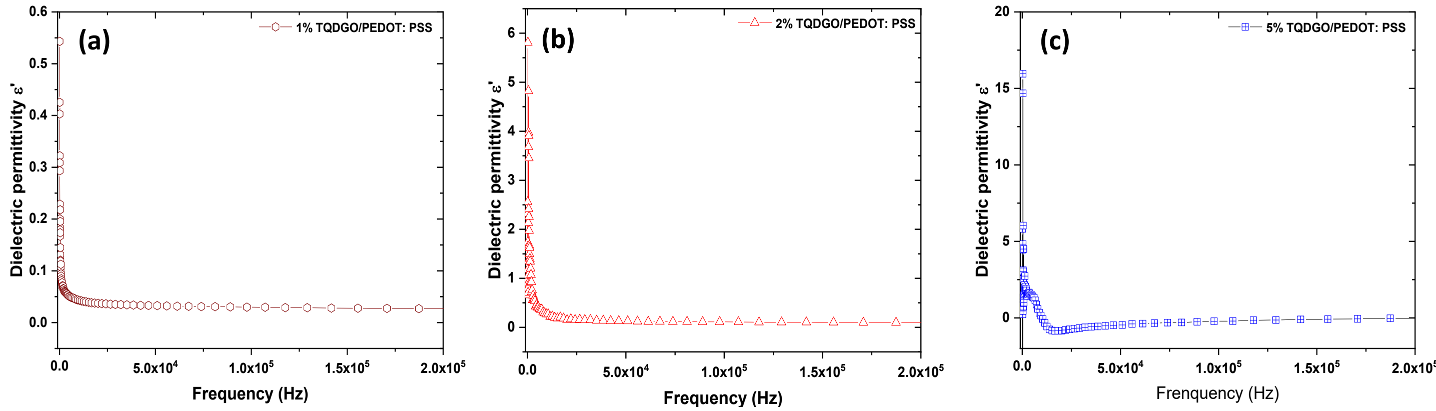
And finally the mobility, μ, was calculated from $\mu = \dfrac{\sigma}{n\,q}$

Where, f is the frequency, q is the electronic charge, k_B is the Boltzmann constant, ε_0 is the permittivity of free space, T is the absolute temperature, d is the sample thickness. The values of the constant A, B, C and the diffusion constant, D, charge carrier concentration, n, and mobility, μ, are given in the table 1.

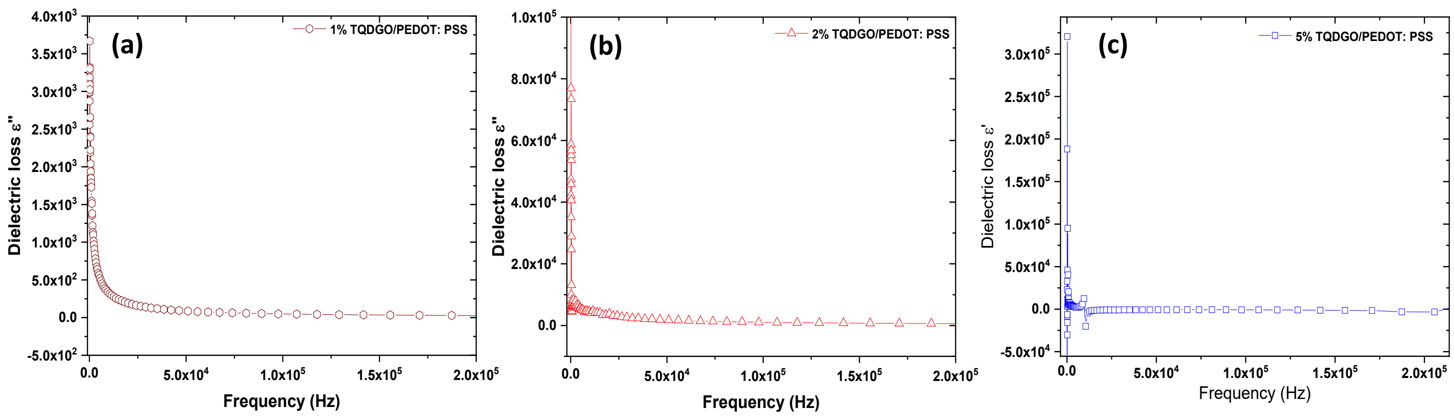
SI Table 1: The calculated values of the constants A, B, C, dielectric constant (D), carrier concentration (n), and mobility (μ) of the TQDGO/PEDOT: PSS pellets.

TQDGO wt. %	A	B	C	D ($m^2.s$)	n (m^{-3})	μ ($m^2.V^{-1}.s^{-1}$)
0%	3.96 e^4	0.0015	1.73 e^5	7.14 e^{-9}	1.74 e^{19}	6.101 e^{-5}
1%	1.79 e^5	0.02	3.37 e^6	2.02 e^{-9}	1.19 e^{21}	3.04 e^{-4}
2%	1.09 e^6	0.132	6.07 e^7	1.6 e^{-10}	6.18 e^{22}	3.71 e^{-4}

5%	$9.7\ e^{5}$	0.043	$4.84\ \ e^{7}$	$5.9\ e^{-9}$	$5.8\ e^{21}$	$1.0\ e^{-2}$

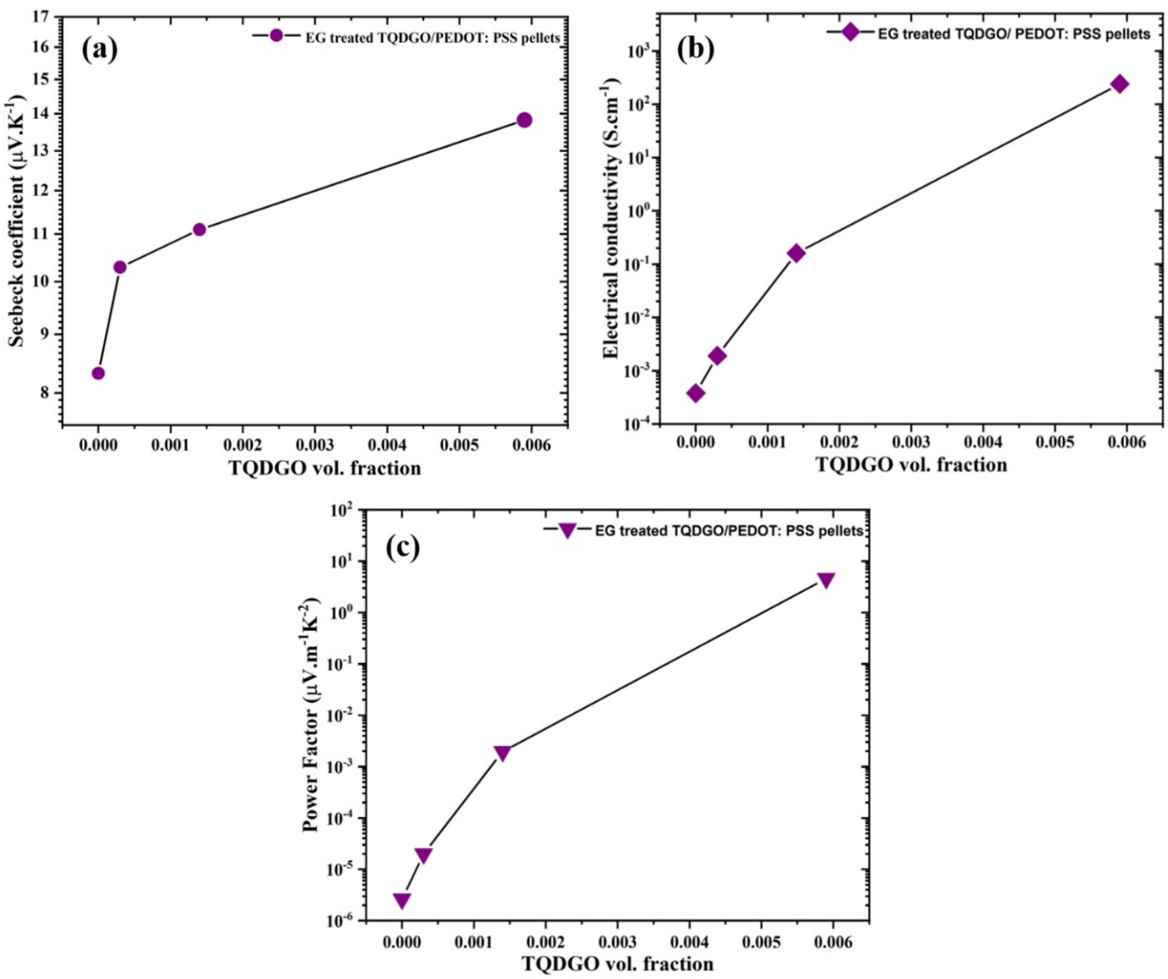


SI Figure 1: Dielectric permittivity as a function of frequency for (a) 1%, (b) 2%, and (c) 5% TQDGO/PEDOT: PSS pellets.



SI Figure 2: Dielectric loss as a function of frequency for (a) 1%, (b) 2%, and (c) 5% TQDGO/PEDOT: PSS pellets.

Thermoelectric properties of ethylene glycol treated TQDGO/PEDOT: PSS pellets

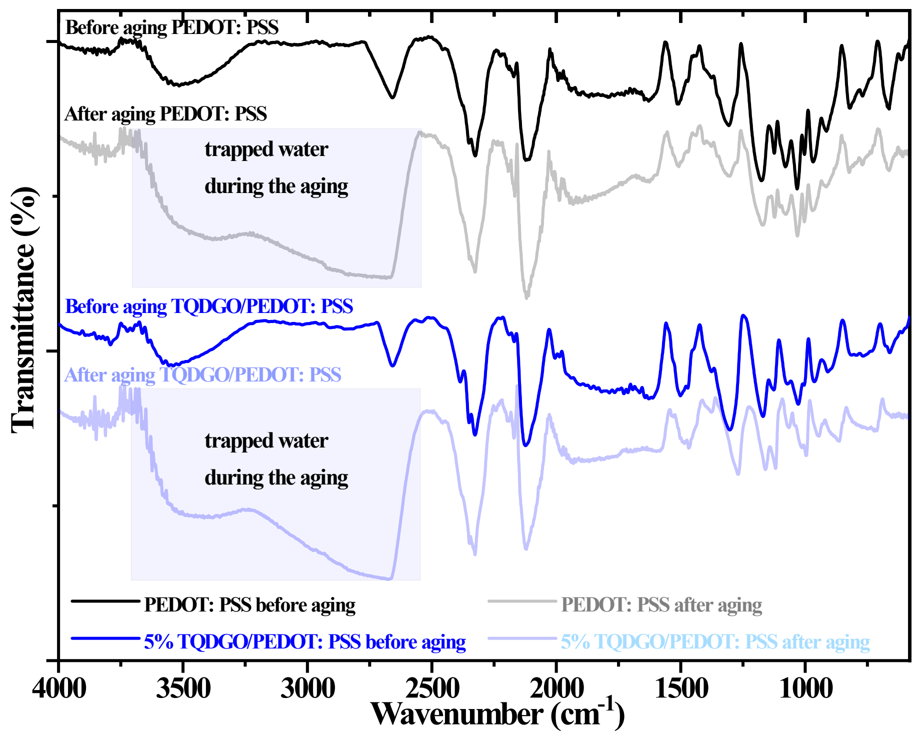


SI Figure 3: (a) Seebeck coefficient, (b) Electrical conductivity, and (c) Power factor of ethylene glycol treated TQDGO/PEDOT: PSS pellets as a function of TQDGO vol. fraction.

Effect of aging (1 year in ambient environment):

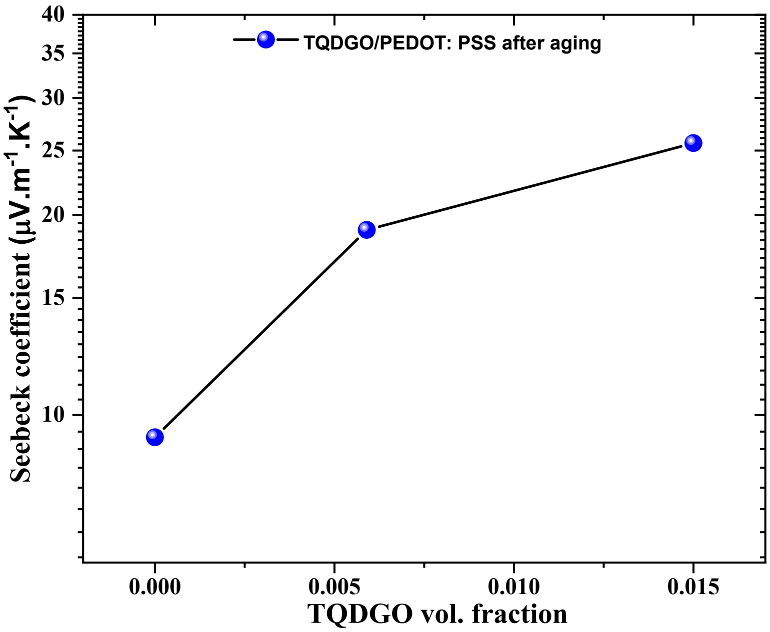
The FTIR and Seebeck coefficient measurements have been done to test the stability of the samples. The samples were kept in an ambient environment for 1 year for the aging process (in North Europe climate).

1. **FTIR:** The FTIR showed a broad hump corresponding to the OH group. This indicates that the samples have absorbed the environmental water due to the humidity.



SI Figure 4: FTIR of PEDOT: PSS and TQDGO/ PEDOT: PSS before and after aging in ambient environment.

2. **Seebeck coefficient measurements:** The Seebeck coefficient measurement shows that the performance of the 5% TQDGO/PEDOT: PSS has decreased from 37 to 27.67 µV/K (32.43 %). It may be due to the FTIR-observed trapped water.



SI Figure 5: Long term stability performance of TQDGO/PEDOT: PSS pellets Seebeck coefficient as a function of TQDGO vol. fraction.

References:

1. S. Uemura, *J. Polym. Sci. Part -2 Polym. Phys.*, 1972, **10**, 2155–2166.
2. S. Uemura, *J. Polym. Sci. Polym. Phys. Ed.*, 1974, **12**, 1177–1188.
3. B. P. Singh, S. Sikarwar, K. K. Pandey, R. Manohar, M. Depriester and D. P. Singh, *Electron. Mater.*, 2021, **2**, 466–481.