

Free-Standing thermoelectric nanocomposite based on PEDOT:PSS, $\text{Cu}_{12+x}\text{Sb}_4\text{S}_{13}$, and MWCNTs

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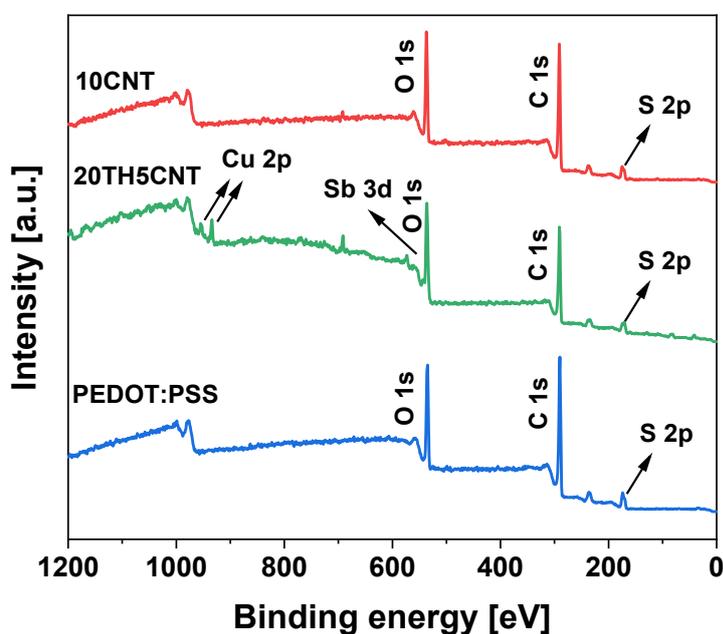


Figure S1. Survey scan of XPS spectra of samples PEDOT:PSS, 20TH5CNT, 10CNT.

The O 1s spectra for PEDOT:PSS and selected composite samples are presented in Figure S2. The observed peaks for PEDOT:PSS sample indicate the presence of an O atom within the PEDOT chain (C-O), localized within a higher binding energy at 532.5 eV [1,2]. In contrast, oxygen atoms within the PSS chain exhibit a lower binding energy peak at approximately 530.9 eV, assigned to C=O bonds [2,3]. Additional references have shown that peaks around 531 and 533 eV belongs to O-S and C-O-C of PSS and PEDOT, respectively [4,5]. A third peak appearing at approximately 533.9 eV is commonly associated with C-OH groups [3,6]. The presence of C-OH groups may result from residuals left after surfactant treatment (EG, DMSO).

The respective peaks have appeared with high energy shifts (531.1, 532.4, 533.1) and (531.3, 532.8 and 534.7) eV for 20TH5CNT and 10CNT. These shifts suggest changes in the chemical environment of oxygen atoms.

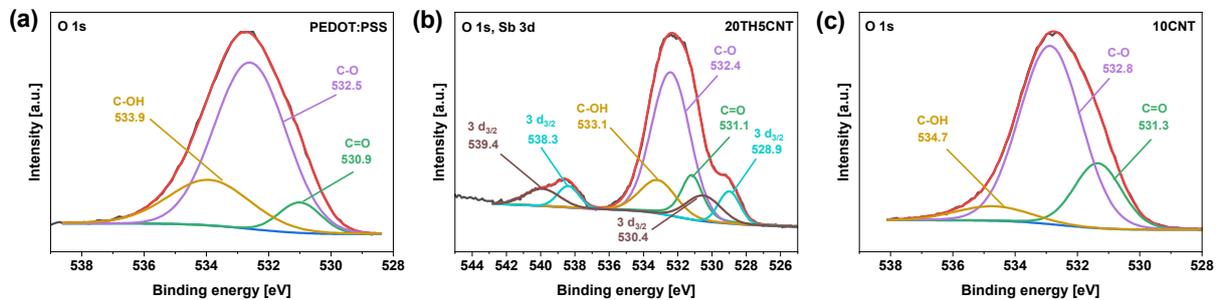


Figure S2. Deconvoluted O 1s core level spectra of PEDOT:PSS, 20TH5CNT, and 10CNT samples.

Figure S3 shows SEM images of samples with the addition of 20% MWCNT (Figure 7a,b) and samples with 20% TH and 20% MWCNT (Figure 6c,d). PEDOT:PSS combined with 20 % amount of MWCNTs forms a granular surface, probably due to the agglomeration of carbon nanotubes. MWCNT have low dispersion ability, high inter-tube van der Waals interaction energy of 500 eV/ μm , and also high aspect ratio, what makes the MWCNT to be intertwined and bundled [7]. Although PEDOT:PSS is considered to be a good dispersant for multi-walled carbon nanotubes (MWCNTs) and this hybrid is widely used [8,9], the phenomenon of mixing occurs at higher additive contents. This was confirmed by Cai-Wan Chang-Jian et al, who indicated that the highest concentration of MWCNTs they could use to prevent this was 10 wt% [10].

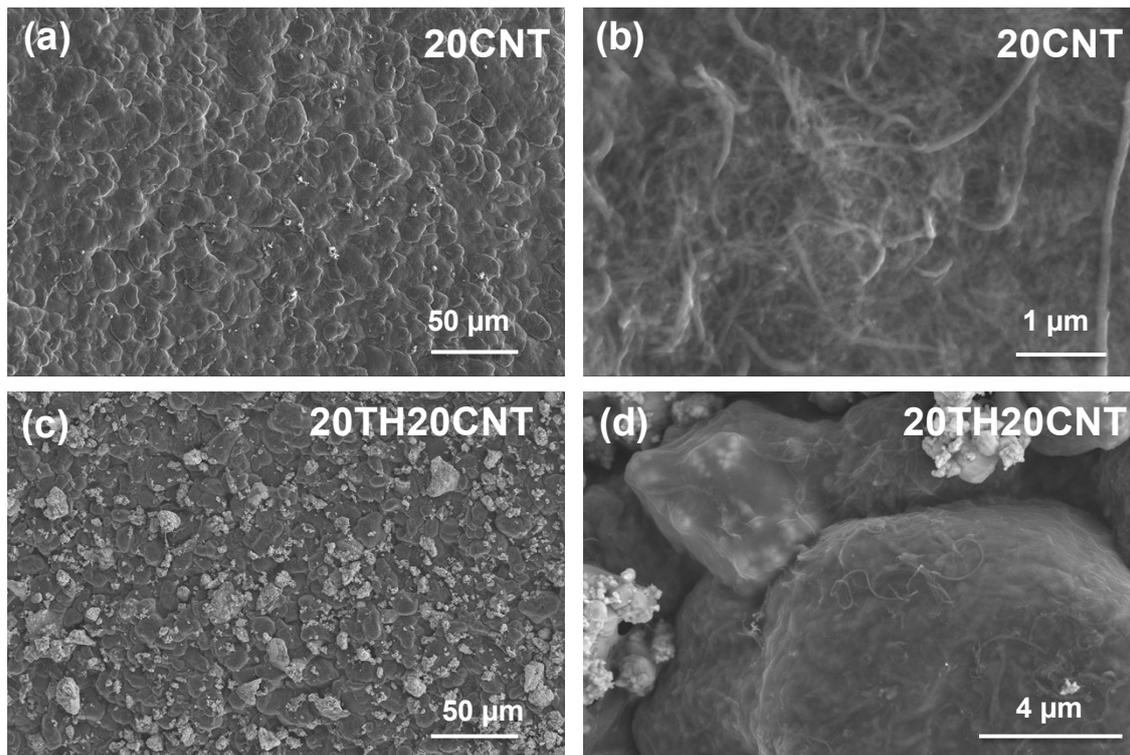


Figure S3. SEM images of the surface composite with 20% MWCNT (a,b); with 20 %TH and 20% MWCNT.

Table S1. Bending durability results for the 20TH5CNT composite film

Cycles	σ before	σ after	Retention σ (%)	S before	S after	Retention S (%)
100	762.6	759.5	99.6	24.84	24.85	100
500	759.5	757.2	99.3	24.85	24.73	99.6
1000	757.2	748.8	98.2	24.73	24.60	99.0

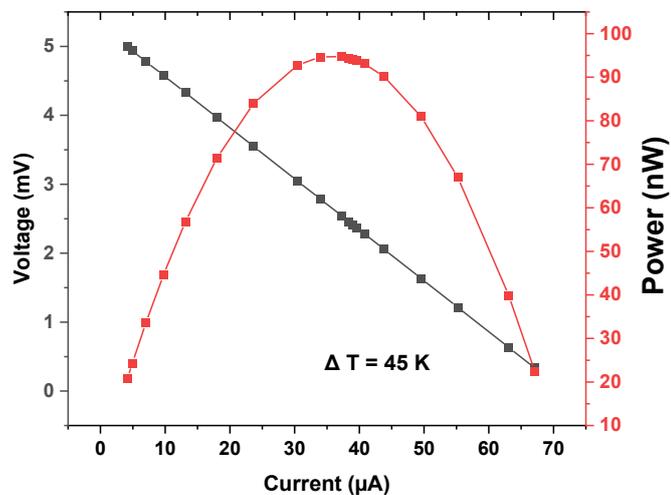


Figure S4. Output voltage (U) and output power (P) versus current (I) at ΔT of 45 K of prepared prototype generator.

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