

Microphase Separation in Oriented Polymeric Chains at the Surface of Nanomaterials During Nanofibers Formation

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Data sheets-TPU & PAN

Typical Properties* For Natural Resin	ASTM Test Method (Other)	Units		Texin SUN-3006	
		U.S. Conventional	SI Metric	U.S. Conventional	SI Metric
General					
Specific Gravity	D 792 (ISO 1183)			1.08	
Shore Hardness	D 2240 (ISO 868)	A Scale		90	
Mold Shrinkage at 100-mil Thickness:	D 955 (ISO 2577)				
Flow Direction		in/in (mm/mm)		0.008	
Cross-Flow Direction		in/in (mm/mm)		0.008	
Water Absorption	D 570 (ISO 62)		%	1.3	
Light Transmission (350-1050 nm)	D 1003 (ISO 3538)		%	92.8	
Refractive Index	D 542 (ISO 489)			1.503	
Mechanical					
Tensile Strength	D 882	lb/in ²	MPa	4,100	28.3
Ultimate Elongation	D 882		%	370	
Tear Strength, Die "C"	D 1004	lbf/in	kN/m	440	95
Thermal					
Glass Transition Temperature (Tg)	(DMA) ^a	°F	°C	-40	-40
Softening Temperature	(TMA) ^b	°F	°C	228	109

*These values are provided as general information only. They are approximate values and are not part of the product specifications.
^a Dynamic Mechanical Analysis
^b Thermal Mechanical Analysis

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Product Specification

Product Name: Polyacrylonitrile - average M_w 150,000 (Typical)

Product Number: 181315
 CAS Number: 25014-41-9
 MDL: MFCD00084395
 Formula: C₃H₃N

TEST	Specification
Appearance (Color)	White to Yellow
Appearance (Form)	Conforms to Requirements
Powder and Chunks	
Infrared spectrum	Conforms to Structure

Fig S1: The data sheet of Texin SUN 3006 polyurethane (upper) and polyacrylonitrile (lower) provided by Covestro, India and Sigma Aldrich respectively. The molecular weight of the Texin Sun 3006 grade TPU was obtained from the reference paper, B. Adak, M. Joshi, B. Singh Butola, J. Appl. Polym. Sci. 2018, **135**, 46422-46426.

Schematics of low dimensional functional carbon based nanomaterials

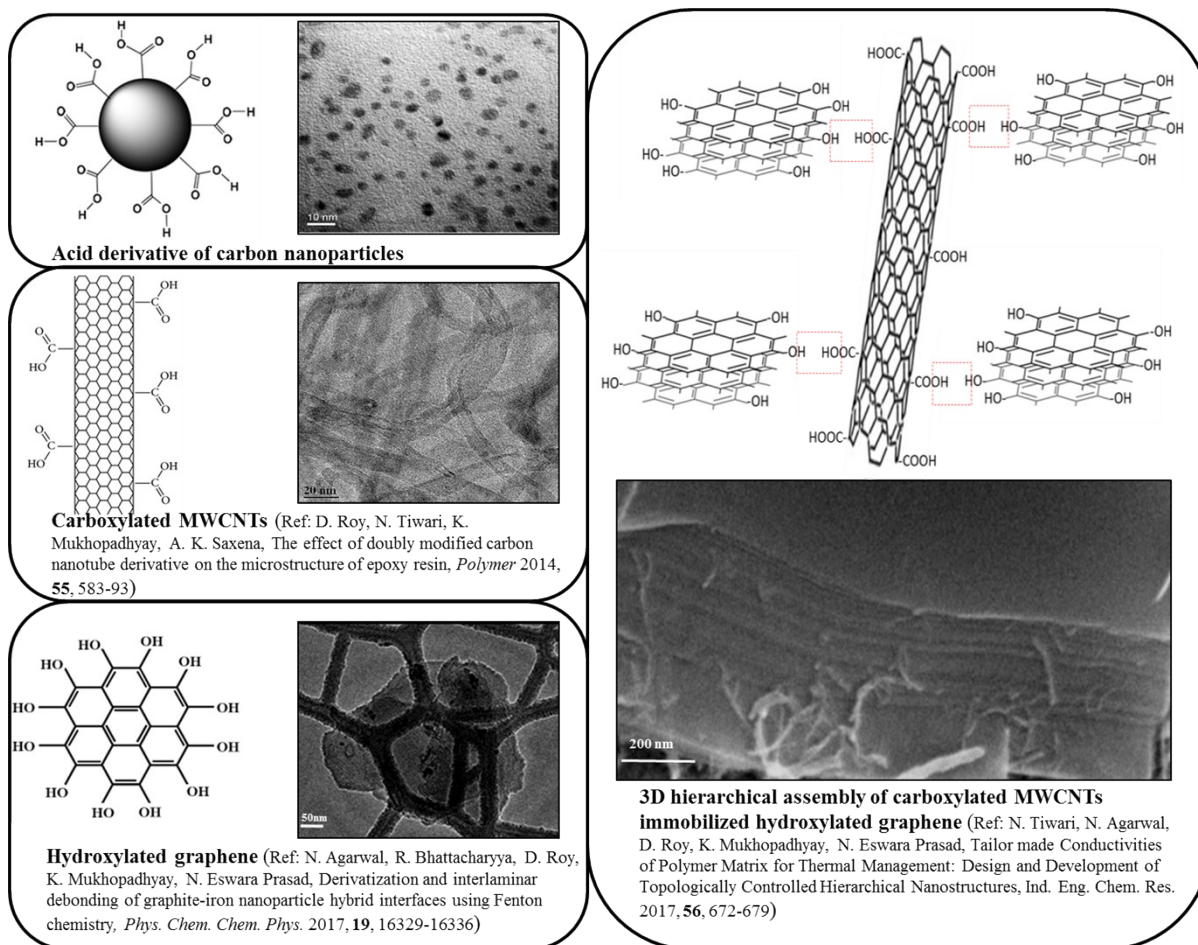


Fig S2: Schematic representation of different low dimensional functional carbon based nanomaterials selected in this study.

Materials and Method for carbon nanoparticles

The synthesis of carbon nanoparticles was carried out from graphene oxide (Fig S3A and Fig S3B), prepared from modified Hammer's method where the concentration of 70% HNO₃ was maintained at 1mg/ml. The 10 mg GO powder dispersed in HNO₃ solution was sonicated at 60 KHz frequency for 5 hrs in a sealed glass tube. The glass tube is broke open and the sonicated mixture was poured into the DI water of 50 times volume. The whole solution is centrifuge at 5000 rpm and the carbon nanoparticles which were attached on the walls of centrifuge tube was further washed by DI water to ensure the complete removal of HNO₃. The carbon nanoparticles pellet was again redispersed in 100 ml DI water and sonicated for 30 minutes followed by centrifugation to collect the carbon nanoparticles as pellet. The pellet was dried at 50°C under vacuum at over night and the dried pellet (Fig S3C) was sonicated in DMF at 1 mg/ml concentration for 3 hours. The highly dispersed DMF solution was centrifuge at 1500 rpm and the carbon nanoparticles of 5-10 nm diameter was collected by evaporation of DMF at reduced pressure (Fig S3D). The yield of the typical reaction is 15-20% depending upon the size of the nanoparticles.

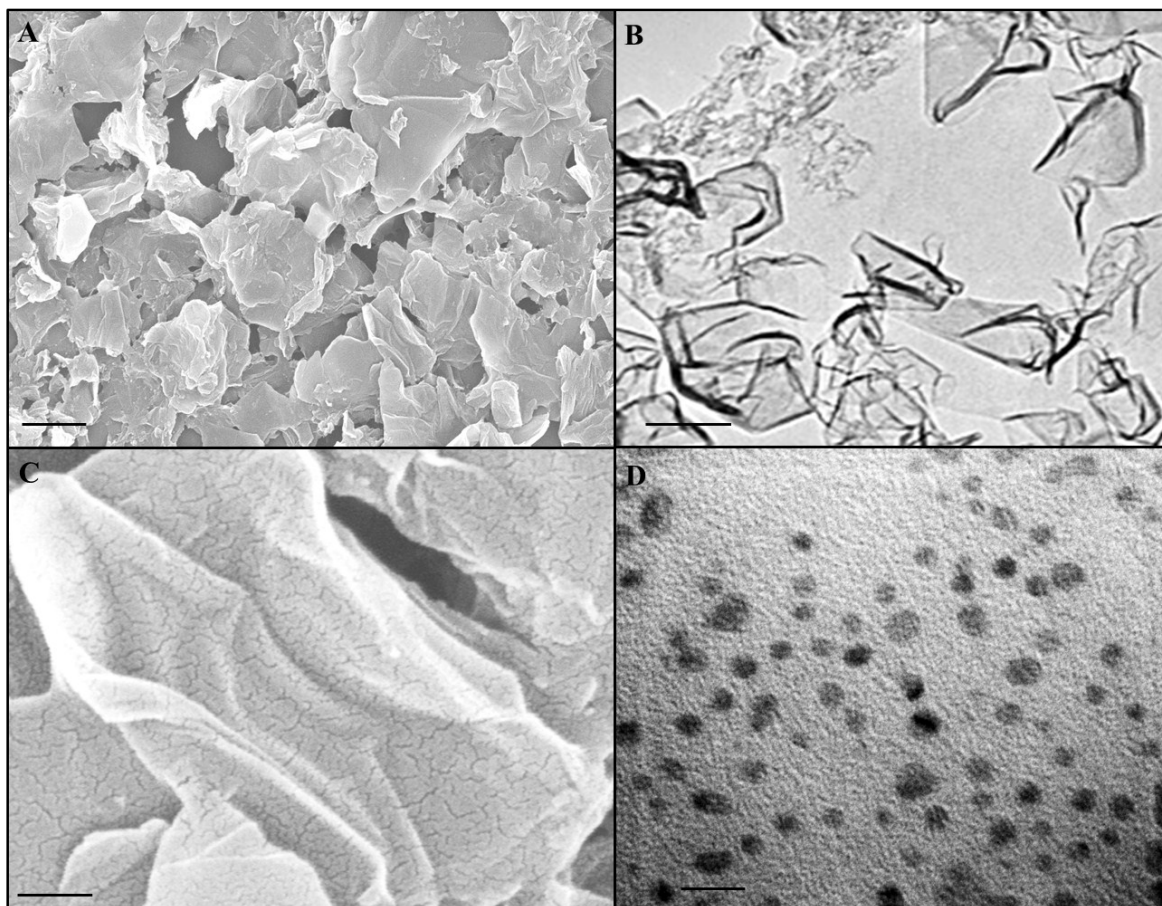


Fig S3: The synthesis of carbon nanoparticles by solution method and their corresponding SEM & TEM images. Figure A (SEM) & B (TEM) represent the graphene oxide by modified Hammer's method, Fig C illustrates the SEM images of the cleaved graphene sheet by acid refluxing and Fig D displays the TEM image of the carbon nanoparticles. The scale bars are 1 μ m, 100 nm, 300 nm, 10 nm for Fig A-D respectively.

Oswald Viscometric data of TPU, PAN and their corresponding composite solution

Composition in DMF	Conc. (mg/mL) w.r.t base matrix material (TPU/PAN)	Weight percentage of Nanofillers (wt. %)	Viscosity (centi stokes) at 25°C
TPU	20	0.0	2.8310
PAN	20	0.0	22.5920
TPU/3D Fillers	20	0.5	04.3726
TPU/3D Fillers	20	1.0	04.5962
TPU/3D Fillers	20	2.0	04.7931
PAN/3D Fillers	20	0.5	22.6579
PAN/3D Fillers	20	1.0	22.8973
PAN/3D Fillers	20	2.0	22.9321
TPU+1D Fillers	20	0.5	4.6520
TPU+1D Fillers	20	1.0	5.5779
TPU+1D Fillers	20	2.0	5.9703
TPU+2D Fillers	20	0.5	3.8842
TPU+2D Fillers	20	1.0	4.5969
TPU+2D Fillers	20	2.0	5.0173
TPU+0D Fillers	20	0.5	5.0374
TPU+0D Fillers	20	1.0	5.5219
TPU+0D Fillers	20	2.0	5.8582

Fig S4: Viscosity of the polymer nanocomposite solution was measured using Ostwald's Viscotube (C-55) make Cannon Instrument Company. The temperature of the unit was maintained at 25°C (298 K).

TEM images of MWCNTS reinforced TPU nanofibers

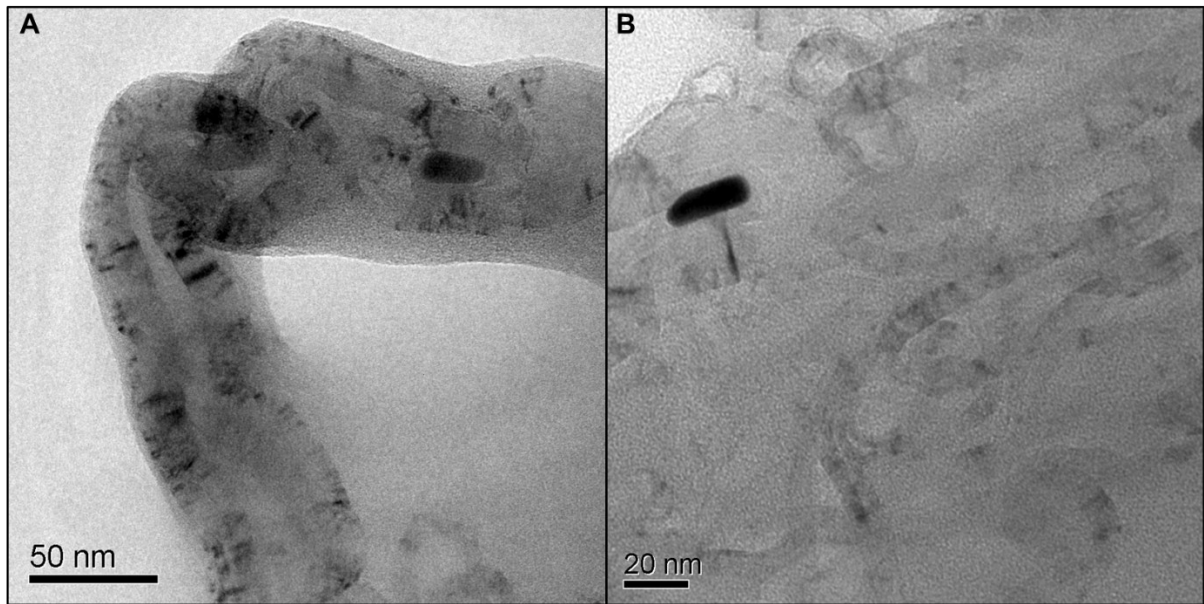


Fig S5: The TEM images of (A) 1 & (B) 2 weight percentage carboxylated MWCNTS reinforced TPU nanofibers.

C-K, O-K and N-K elemental mapping using TEM EDAX

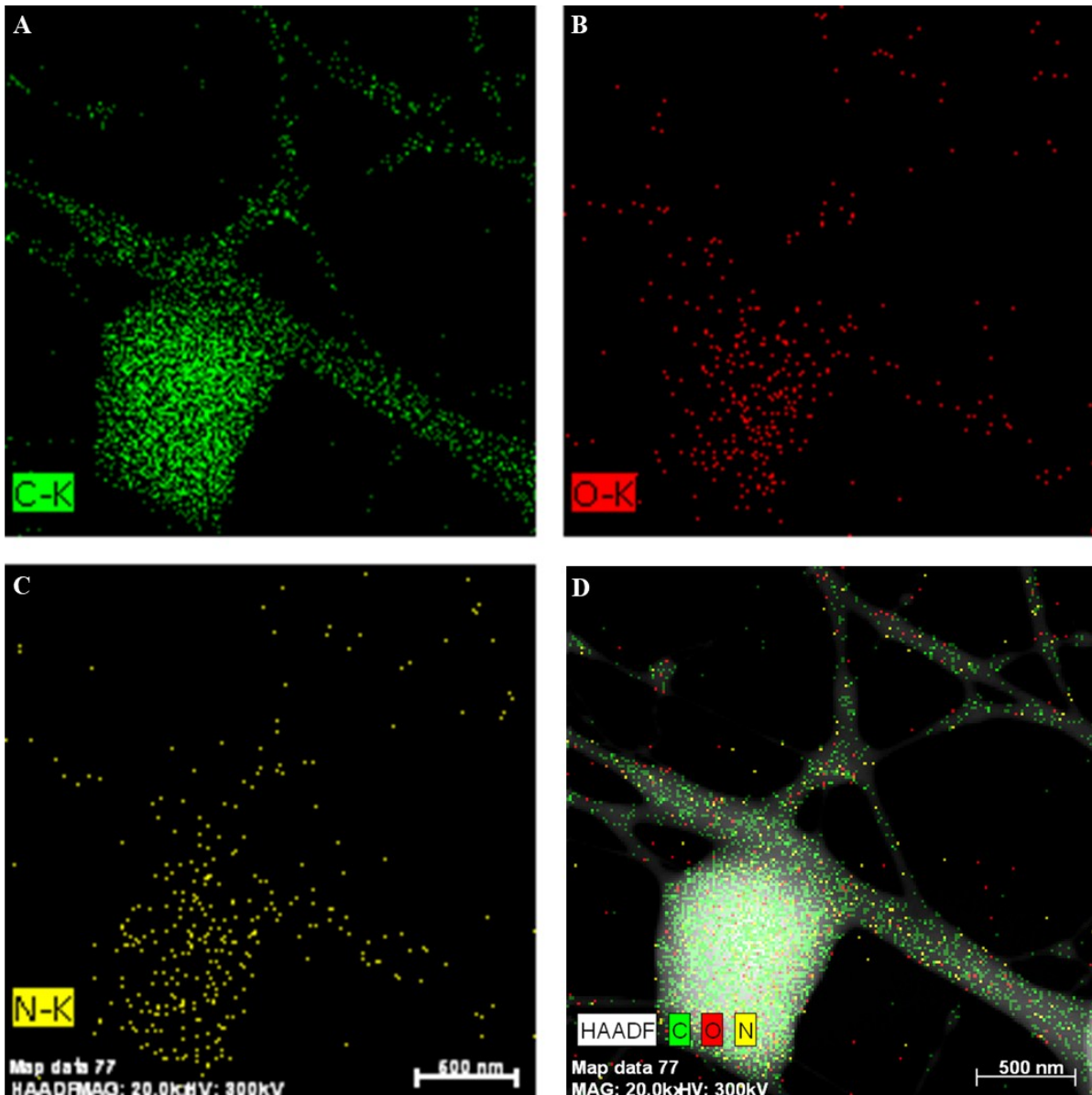


Fig S6: The (A) carbon, (B) oxygen, (C) nitrogen and (D) C-O-N overlapped elemental mapping of the 0.5 weight percentages of carbon nanoparticles reinforced composite nanofiber. As both the polyurethane and functionalized carbon nanoparticles contain, carbon and oxygen, so in the elemental mapping the interface of carbon nanoparticles and polymer fiber matrix is not very clear and the boundaries of carbon nanoparticles were not distinctly visible in TEM-EDX mapping.

TEM images of carbon nanoparticles reinforced TPU nanofibers

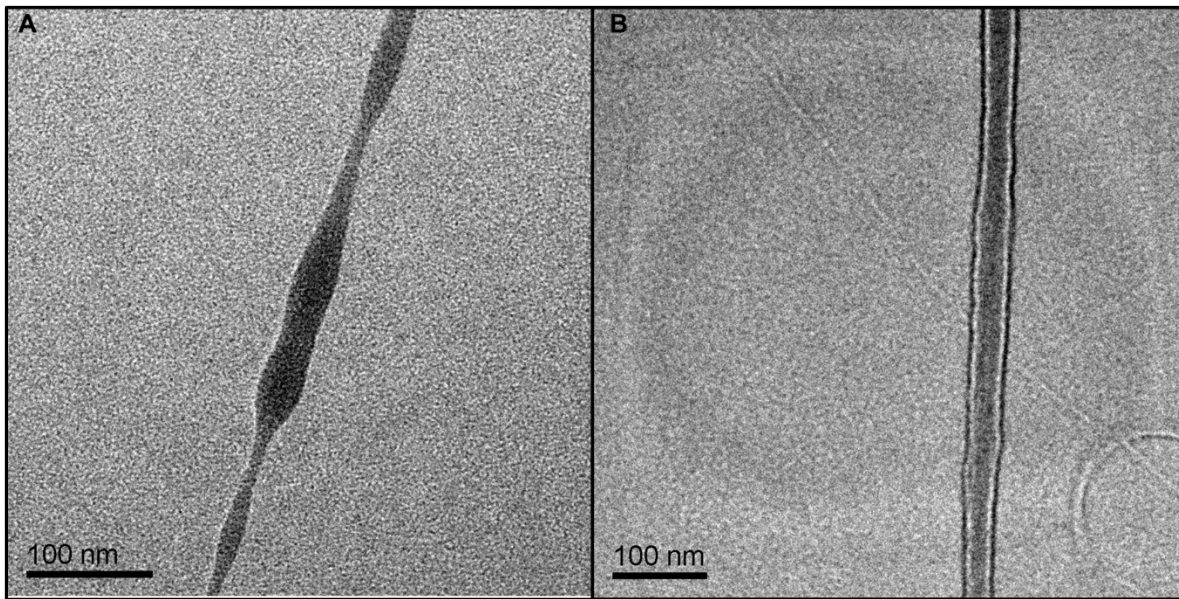


Fig S7: The TEM images of (A) 1 & (B) 2 weight percentage carboxylated carbon nanoparticles reinforced TPU nanofibers.

TEM images of graphene reinforced TPU nanofibers

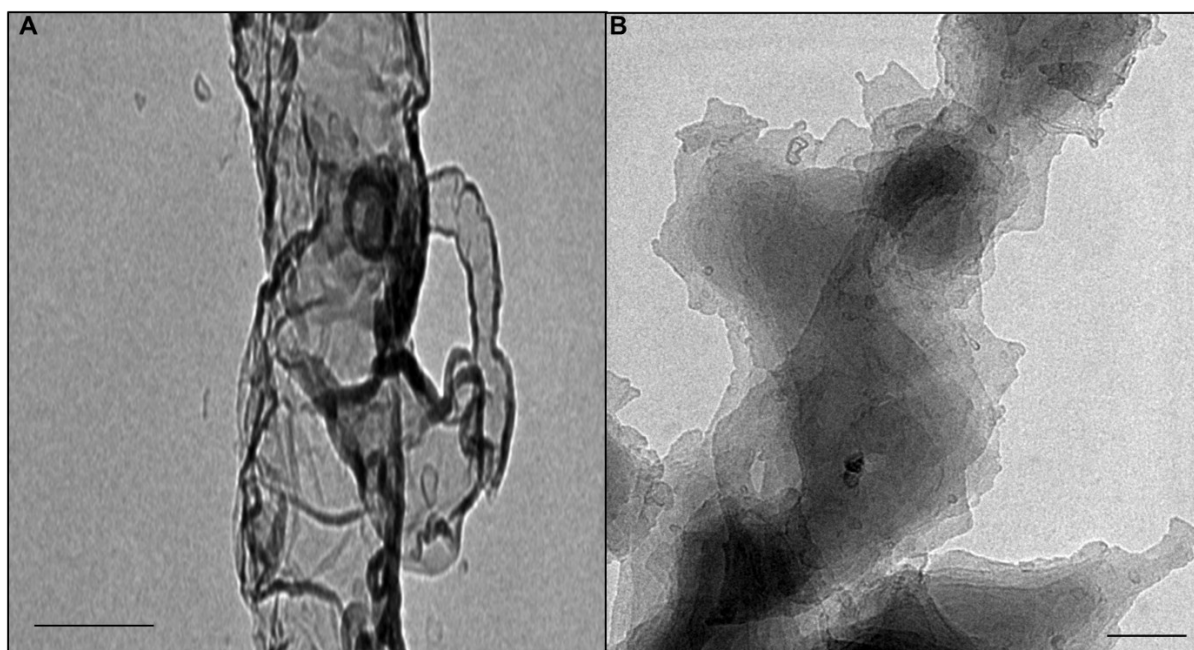


Fig S8: The TEM images of (A) 1 & (B) 2 weight percentage hydroxylated graphene reinforced TPU nanofibers. The scale bars of TEM images are 200 nm.

TEM images of hybrid CNT-graphene nanofillers reinforced TPU nanofibers

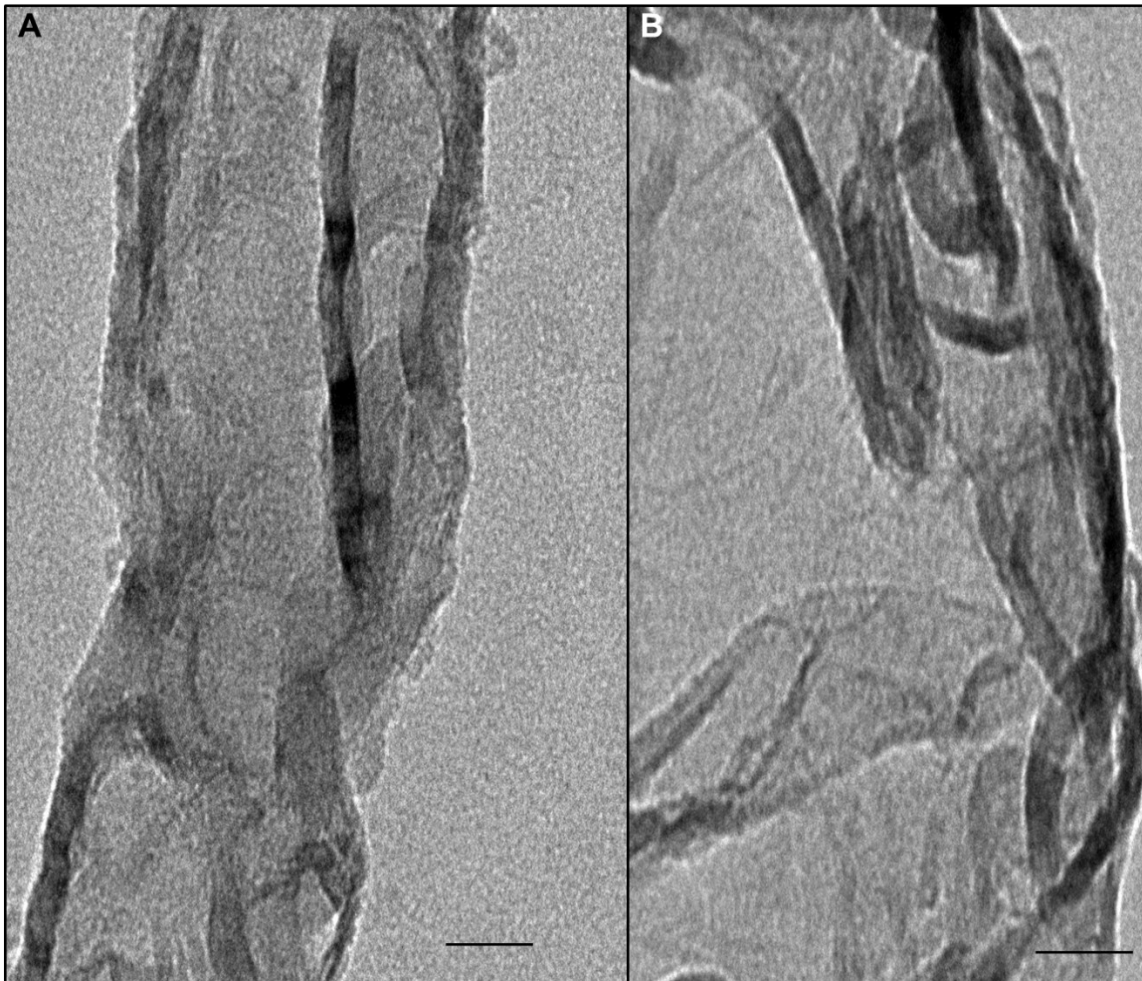


Fig S9: The TEM images of (A) 1 & (B) 2 weight percentage hybrid carboxylated CNT-hydroxylated graphene nanofillers reinforced TPU nanofibers. The scale bars of TEM images are 50 nm.

Contact angle of nanomaterials and nanofibers

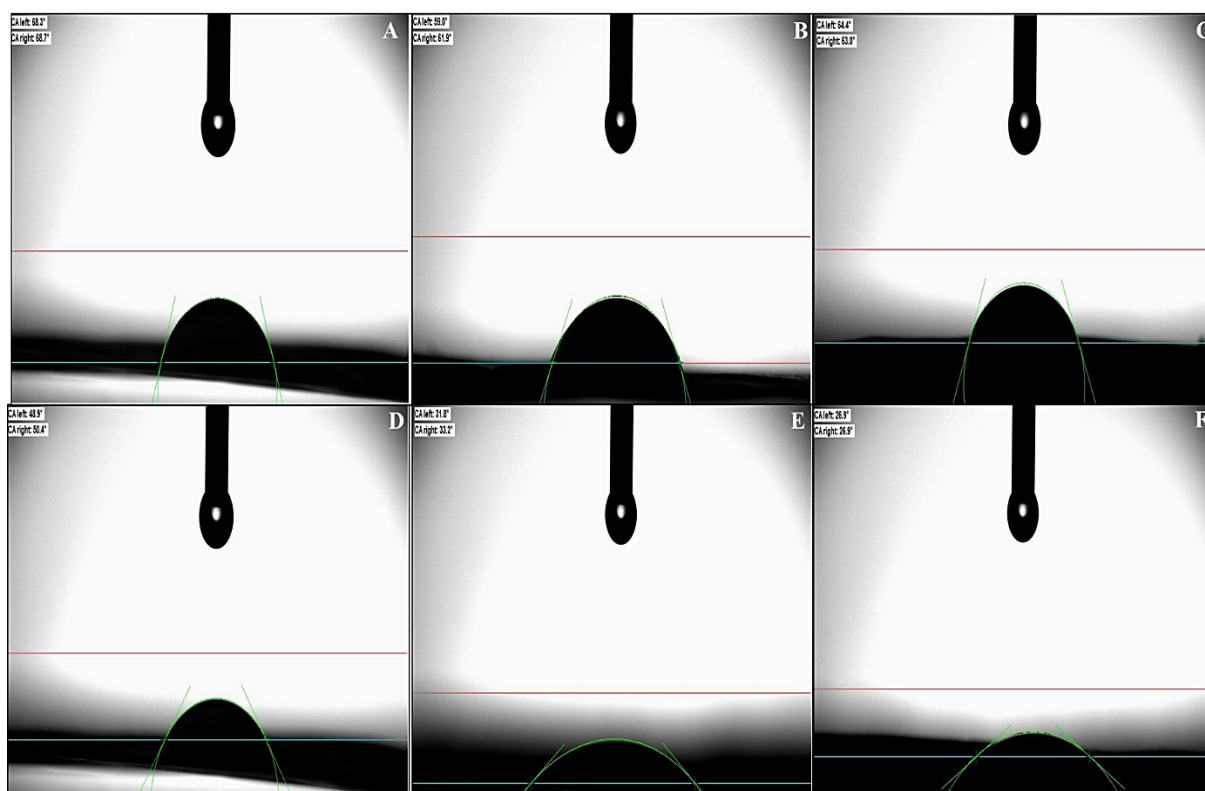


Fig S10: The contact angle images of (A) pristine, (B) 0.5 weight percentage reinforced CNT, (C) carbon nanoparticles, (D) graphene, (E) hybrid CNT-Graphene reinforced TPU free standing nanofibrous film and (F) pristine hybrid CNT-graphene pallet where the average contact angles are 68.5, 60.4, 63.7, 49.6, 32.5 and 26.9 respectively. The powder sample of hybrid CNT-graphene was put inside the palletizer used for FT-IR sample preparation and the 2 mm thick pallet was used for contact angle measurement, the sample thickness was kept at a higher side to ensure the better compactness of the pallet.

Helium pycnometric measurement

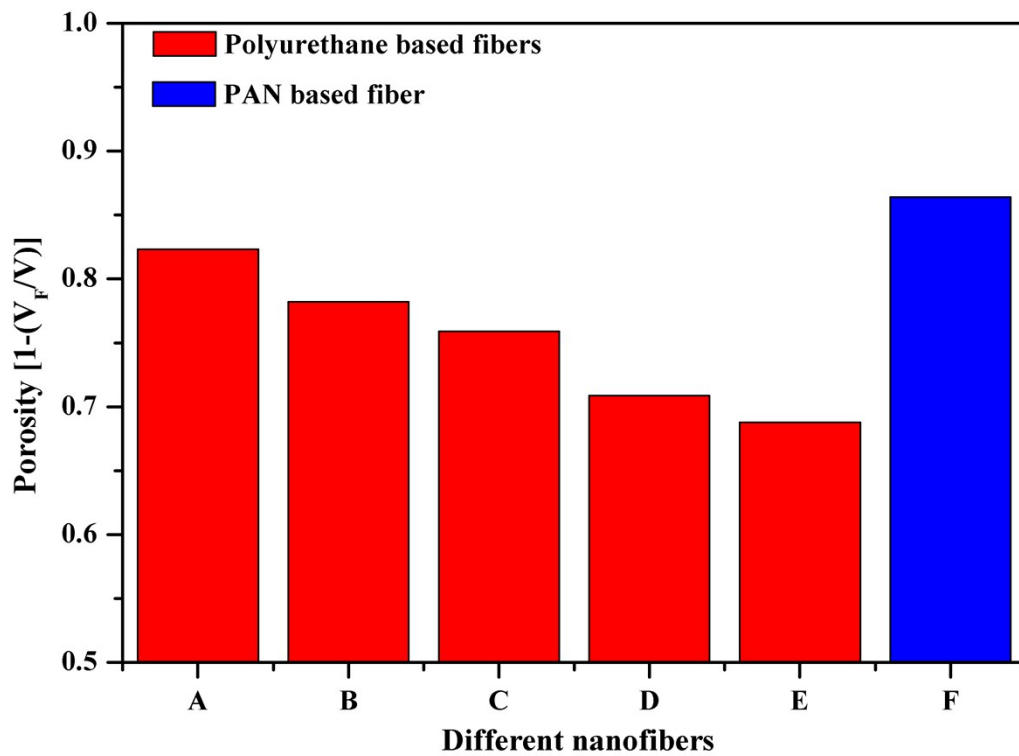


Fig S11: Helium pycnometric data of (A) pristine, (B) 05 weight percentage reinforced carbon nanoparticles, (C) CNT, (D) graphene, (E) hybrid CNT-Graphene reinforced TPU nanofibers and (F) pristine free-standing PAN nanofibrous film respectively. The porosity of nanofibers film was measured as per the procedure described earlier [S. S. Sreedhara, N. R. Tata, A Novel Method for Measurement of Porosity in Nanofiber Mat using Pycnometer in Filtration, *J. Eng. Fiber Fabr.* 2013, **8**, 32-137]. The porosity is calculated by the standard formula, porosity= 1- [volume of the nanofibrous film (V_F) using pycnometer-total volume of the film (V)].