# Understanding Fluorometric Interactions in Ion-Responsive Sustainable Polymer

### **Nanocomposite Scaffolds**

Shriram Janghela<sup>a,b</sup>, Sudeepa Devi<sup>a</sup>, Neelu Kambo<sup>b</sup>, Debmalya Roy<sup>a\*</sup>, N. Eswara Prasad<sup>c</sup>

<sup>a.</sup> Directorate of Nanomaterials and Technologies, DMSRDE, GT Road, Kanpur, India-13 <sup>b.</sup> DMSRDE, GT Road, Kanpur, India-208013.

Typical Properties*	AOTM	Uni	ts	Texin SU	N-3006
For Natural Resin	Test Method	U.S.	SI	U.S.	SI Metric
General	(other)	Conventional	metric	conventional	metric
Specific Gravity	D 792 (ISO 1183)			10	08
Shore Hardness	D 2240 (ISO 868)	AS	l cale	9	0
Mold Shrinkage at 100-mil Thick	kness: D 955 (ISO 2577)			Ĭ	
Flow Direction		in/in (mr	n/mm)	0.0	08
Cross-Elow Direction		in/in (mr	n/mm)	0.0	08
Water Absorption	D 570 (ISO 62)	0/	5	1	3
Light Transmission (350-1050 n	D 1003 (ISO 3538)	0/		92	8
Refractive Index	D 542 (ISO 489)	Î		1.503	
Mechanical					
Tensile Strength	D 882	lb/in <sup>2</sup>	MPa	4,100	28.3
Ultimate Elongation	D 882	0	6	37	0
Tear Strength Die "C"	D 1004	lbf/in	kN/m	440	95
Thermal	0 1004				00
Glass Transition Temperature (	Ta) (DMA)a	°F	°C	_40	-40
Softening Temperature	(TMA)b	°E	°C	228	109
SIGMA-AL	.DAICH®		3050 S	pruce Street, Saint Lou	sigma-aldrich iis,MO 63103,U
				Website: www	w.sigmaaldrich.c
	Produc	t Specific	ation	Website: www Email USA: Outside USA: eur	w.sigmaaldrich.o techserv@sial.o rtechserv@sial.o
Product Name: ?olyacrylonitrile - average N∞ :	Produc 150,000 (Typical)	t Specific	ation	Website: www Email USA: Outside USA: eur	w.sigmaaldrich.o techserv@sial.o rtechserv@sial.o
Product Name: Polyacrylonitrile – average Nrv ( Product Number:	Produc 150,000 (Typical) 181315	t Specific	ation	Website: www Email USA: Outside USA: eur	w.sigmaaldrich.o techserv@sial.o rtechserv@sial.o
Product Name: Yalyacrylonitrile - average N <sub>M</sub> : Product Number: CAS Number:	Produc 150,000 (Typical) 181315 25014-41-9	t Specific	ation	Website: www Email USA: Outside USA: eur	w. sigmaaldrich. o techserv@sial. o rtechserv@sial. o
Product Name: Yolyacrylonitrile – average N <sub>W</sub> : Product Number: CAS Number: WDL:	Produc 150,000 (Typical) 181315 25014-41-9 MFCD00084395	t Specific	ation	Website: www Email USA: Outside USA: eur	w.sigmaaldrich.o techserv@sial.o rtechserv@sial.o
Product Name: Yolyacrylonitrile – average Nw 3 Product Number: CAS Number: MDL: Formula:	Produc 150,000 (Typical) 181315 25014-41-9 MFCD00084395 C3H3N	t Specific	ation	Website: www Email USA: Outside USA: eur	w. sigmaaldrich. o techserv@sial. o rtechserv@sial. o
Product Name: Yolyacrylonitrile – average Nw 3 Product Number: CAS Number: MDL: Formula:	Produc 150,000 (Typical) 181315 25014-41-9 MFCD00084395 C3H3N	t Specific	ation	Website: www Email USA: Outside USA: eur	v. sigmaaldrich. o techserv@sial. o rtechserv@sial. o
Product Name: Yolyacrylonitrile – average Nrv 1 Product Number: CAS Number: MDL: Formula:	Produc 150,000 (Typical) 181315 25014-41-9 MFCD00084395 C3H3N	t Specific	ation	CN	w.sigmaaldrich.o techserv@sial.o rtechserv@sial.o
Product Name: Yolyacrylonitrile – average Nm 1 Product Number: DAS Number: MDL: Formula:	Produc 150,000 (Typical) 181315 25014-41-9 MFCD00084395 C3H3N	t Specific		CN	₩. sigmaaldrich. o techserv@sial. o rtechserv@sial. o
Product Name: Polyacrylonitrile – average Nw 3 Product Number: CAS Number: MDL: Formula:	Produc 150,000 (Typical) 181315 25014-41-9 MFCD00084395 C3H3N	t Specific		Website: www Email USA: Outside USA: eur	w.sigmaaldrich.o techserv@sial.o rtechserv@sial.o
Product Name: Yolyacrylonitrile – average Nw 3 Product Number: CAS Number: MDL: Formula: Formula:	Produc 150,000 (Typical) 181315 25014-41-9 MFCD00084395 C3H3N	t Specific		Website: www Email USA: Outside USA: eur	w.sigmaaldrich.o techserv@sial.o rtechserv@sial.o
Product Name: Yolyacrylonitrile – average Nw 3 Product Number: CAS Number: MDL: Formula: Formula:	Produc 150,000 (Typical) 181315 25014-41-9 MFCD00084395 C3H3N	t Specific	cation	Website: www Email USA: Outside USA: eur	w.sigmaaldrich.c techserv@sial.c rtechserv@sial.c
Product Name: Yolyacrylonitrile – average Nw 3 Product Number: CAS Number: MDL: Formula: FEST Papearance (Color) Nopearance (Form)	Produc 150,000 (Typical) 181315 25014-41-9 MFCD00084395 C3H3N	t Specific Speci White Confor	cation	Website: www Email USA: Outside USA: eur	w.sigmaaldrich.o techserv@sial.o rtechserv@sial.o
Product Name: 'olyacrylonitrile - average Nw ' Product Number: 2AS Number: MDL: Formula: FEST Spearance (Color) Spearance (Form) Powder and Chunks	Produc 150,000 (Typical) 181315 25014-41-9 MFCD00084395 C3H3N	t Specific Speci White Confor	fication	Website: www Email USA: Outside USA: eur	w.sigmaldrich.o techserv@sial.o rtechserv@sial.o

## Data sheets-PU & PAN

Fig S1: The data sheet of Texin SUN 3006 polyurethane (upper) and polyacrylonitrile (lower) provided by Covestro, India and Sigma Aldrich respectively.

# Schematic and representative images of different low dimensional carbonaceous nanomaterials



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

#### Fluorescence images of before and after dichromate treatment of pristine and nanocomposite of polyurethane and polyacrylonitrile



Fig S3: Fluorescence images of before (A, C & E, H') and after (B, D & F, H) metal ions treatment in pristine TPU (C, D), nanocomposite TPU (A, B), pristine PAN (G, H) and nanocomposite PAN (E, F) respectively. The samples were dried and fixed on a glass slide with a drop of epoxy glue and viewed under a epi-fluorescence microscope by excitation at 488 nm where the scale bar is 50  $\mu$ m.

Dynamic Mechanical Analysis studies of PU and PU nanocomposite of 01 weight percentage of hybrid nanofillers



Fig S4: Dynamic Mechanical Analysis (DMA) studies of storage modulus (A) and glass transition temperature (B) of polyurethane matrix (blue dashed line) by addition of 01 weight percentage of hybrid nanofillers (red solid line) from -50 to 100<sup>o</sup>C in tension mode with an oscillatory frequency of 1 Hz at a heating rate of 05<sup>o</sup>C/min.

Transmission Electron Microscopy (TEM) images of pristine Polyurethane



Fig S5: TEM images of ultramicrotome TPU sample where the scale bar is 50 nm.

XRD and FT-IR spectra of the pristine and nanocomposite PU after treatment with enzyme



Fig S6: Figures a & b represent the XRD and FT-IR spectra of the starting PU (A) and after treatment with enzyme for 48 hrs. of PU (B), PU with 1 wt% reinforced CNP (C), CNT (D), graphene (E) and 3D hierarchical geometries (F) respectively.





Fig S7: The comparative  $N_2$  adsorption and desorption isotherm for TPU pristine gel (blue stars and blue circles respectively) and nanocomposite TPU gel with 1 wt% addition of hybrid nanofillers (red stars and blue circles respectively) are represented.



Zeta potentials for isoelectric points of functionalized nanomaterials

Fig S8: The point of zero charge of acid functionalized MWCNTs (black diamonds), hydroxylated graphenes (blue triangles) and f-MWCNTs embedded in to graphene flakes (1:1) (red circles) were measured by zeta potentials as a function of pH.



Fluorescence intensities with time at low concentration of different metal ions

Fig S9: Fluorescence images of TPU nanocomposite gel before (A) and after treatment of 0.1 ppm chromium ions for 06 hrs (B), 12hrs (D) and 18hrs (C). The treatment of 0.1 ppm iron (E) and lead (F) ions on TPU nanocomposite gels for 12hrs are represented. The samples were dried and fixed on a glass slide with a drop of epoxy glue and viewed under an epi-fluorescence microscope by excitation at 488 nm where the scale bar is 50  $\mu$ m.



UV-VIS intensities with wavelengths of different functionalized carbon nanomaterials

Fig S10: UV-VIS absorbance of acid functionalized MWCNTs (black line), hydroxylated graphenes (blue line) and f-MWCNTs embedded in to graphene flakes (1:1) (red line) were measured as a function of wavelength at 0.01 mg/ml concentration in DI water.